

Lagrangian Perspectives on Ocean Ventilation

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*A thesis submitted for the degree of
Doctor of Philosophy*

Trinity 2017

Abstract

Within the global climate system, the ocean operates as a vast store of important components such as heat and carbon dioxide that it exchanges with the atmosphere on timescales from days to millennia. Its facility to do so is in large part due to the process of ocean ventilation by which water is moved from the surface mixed layer, where it is in contact with the atmosphere, and transported through the subsurface. An understanding of ocean ventilation, therefore, is crucial in establishing the magnitudes and timescales of ocean-atmosphere exchange.

In this thesis, a predominantly Lagrangian approach is adopted, evaluating trajectories in an eddy-permitting numerical ocean circulation model to explore different aspects of the ventilation process. Following critical assessment of the fidelity of the trajectory analysis, a dynamical systems approach is applied to assess the role of ocean turbulence in the transport of ventilated water in the subsurface, with application to the subtropical gyre of the North Atlantic. The pathways of ventilation, represented by Lagrangian maps, are found to be highly chaotic and characterised by a non-dimensional filamentation number that compares the ventilation and filamentation timescales of the flow. Subsequently, the mechanisms and variability of ventilation of dense water masses in the high-latitude North Atlantic are considered, a crucial component in present-day oceanic uptake of heat and carbon dioxide. A Lagrangian approach allows us to link surface processes to their subsurface signature, and reveals that variations in annual re-entrainment establish substantial inter-annual variability in the water that enters the deep ocean. Furthermore, the results reveal that mechanisms of ventilation in the numerical simulation differ substantially from observations, with possible implications for the fidelity of future climate projections. Finally, the translation into the ocean interior of a biologically and chemically active tracer, such as carbon dioxide, is considered, and how this is dependent on the interaction between ventilation, circulation and biogeochemical processes. From observations in the Weddell Gyre, it is shown that biological export and the horizontal circulation are critical in sustaining regional uptake of carbon dioxide from the atmosphere.

Broadly, these various results serve to emphasise the complexity of the ventilation process and its associated role in the oceanic storage of climate-relevant components, from the chaotic nature of pathways, short timescales of variability, its difficulty of representation in numerical models, and its interaction with the biogeochemical system.

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Acknowledgements

Sincere thanks to my supervisors, Helen and David, for their support, academic and otherwise. Also to Camille Lique for much the same, and to Alberto Naveira Garabato for his ongoing support. Many thanks to my two supervisors at the Met Office, Laura Jackson and Richard Wood. Thank you to Matt Thomas, Pete Brown and Simon Josey for their help and guidance with many of the technical aspects of this work. Finally to family, friends, housemates, teammates, and colleagues. Thank you.

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Introduction

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Water in the well-mixed, unstratified layer at the ocean surface — the surface mixed layer — is in persistent contact with the atmosphere. As such, the hydrographic and chemical properties in this layer are strongly influenced by atmospheric conditions. When water moves out of the surface mixed layer and spreads in the ocean interior — a process called ‘ventilation’ — it carries with it the imprint of these atmospheric conditions, while at the same time becoming isolated from further influence. Ventilation is thus a fundamental mechanism by which the atmosphere communicates with and impacts the ocean, and by which properties are removed from the atmosphere and stored in the subsurface. That these properties include

high levels of oxygen relative to the ocean interior is the reason that the process is called ventilation — it is how the ocean ‘breathes’.

We use the term ventilation, here and throughout the thesis, in reference to the combination of processes that bring water, along with its properties, from the surface mixed layer into any region of the ocean interior. As such it includes a chain of events from water mass formation in the surface mixed layer, to subduction into and re-entrainment (or ‘obduction’) from the ocean interior, to spreading in the subsurface. For clarity, we consider ventilation as a purely physical process, involving the advection and diffusion of a conserved, passive tracer into and around the ocean interior. Further complexity arises when considering the transport of chemically or biologically active tracers, in which the interaction of physical and biogeochemical processes is fundamental. In this chapter, we introduce the physical process of ventilation, and how it relates to the establishment of the hydrographic properties of the ocean interior. We defer to the end a discussion of ventilation in relation to the transport of biogeochemical tracers.

1.1 The ventilation process

The temperature and salinity (and therefore density) of water in the surface mixed layer is established by air-sea fluxes (Speer and Tziperman, 1992), lateral mixing processes in the mixed layer (Nurser *et al.*, 1999) including non-linear thermodynamic effects (Thomas and Shakespeare, 2015), and entrainment from the ocean subsurface (Large *et al.*, 1994; Garrett and Tandon, 1997). Such surface processes are the primary means by which much of the hydrographic properties and stratification of the interior ocean is set (Speer, 1993; Nurser *et al.*, 1999; Groeskamp *et al.*, 2017), though interior mixing processes are important for certain water masses (Speer, 1997; Nurser *et al.*, 1999; Baringer and Price, 1999; Garton and Sanford, 2003), in specific regions (Naveira Garabato *et al.*, 2004; Waterhouse *et al.*, 2014) and on long timescales (Munk, 1966; Munk and Wunsch, 1998).

The translation of water with these properties from the mixed layer into the ocean subsurface is called subduction. The name, derived by analogy to the

subduction of tectonic plates and invoking a perspective of long time and large spatial scales, belies the complexity of the process, and the range of spatial and temporal scales involved. Cushman-Roisin (1987) laid out a framework for the processes contributing to subduction, through an equation for the instantaneous subduction rate per unit area, S :

$$S = -\frac{\partial h}{\partial t} - \mathbf{u}_b \cdot \nabla h - w_b \quad (1.1)$$

where h is the thickness of the mixed layer, $\mathbf{u}_b$ and w_b are the horizontal and vertical velocities at the base of the mixed layer, respectively, and t is time.

The first term on the right hand side of equation 1.1, $\partial h/\partial t$, corresponds to the temporal evolution of the mixed layer depth, which can either leave water in the subsurface as it shallows, or re-entrain it back to the mixed layer as its depth increases. Thus it is unique in equation 1.1 in that it does not correspond to a flow of water into or out of the mixed layer. Across the ocean, the depth of the mixed layer exhibits significant seasonality, being shallow in summer when the surface is warmed and deep in the winter by surface cooling and wind-driven vertical mixing. Such seasonality is particularly pronounced at high latitudes. Consequently, this term tends to dominate equation 1.1 on sub-annual timescales (Cushman-Roisin, 1987).

Rather than adding complexity, the seasonality of the mixed layer greatly simplifies understanding, modelling and measurement of the subduction process, as first noted by Stommel (1979). Following subduction into the subsurface, a water parcel must move to a region where it will escape the deepening mixed layer in the following winter. This is generally impossible for all water parcels except those subducted in late winter, that may subsequently be transported to a region of shallower winter mixed layer. Consequently, water subducted into the ocean interior is mediated by this so-called ‘demon’, such that only late winter mixed layer water remains in the subsurface on timescales longer than a year (Iselin, 1939; Marshall *et al.*, 1993; Williams *et al.*, 1995).

A consequence of Stommel’s demon is that the annual subduction rate can be derived from equation 1.1 by removal of the time-dependent term, $\partial h/\partial t$, and

calculation of the other terms at the base of the late-winter mixed layer (Marshall *et al.*, 1993). This is only valid, of course, on timescales over which the winter mixed layer depth can be assumed constant. On inter-annual timescales, the contribution from variations in the winter mixed layer depth could be large. In addition, eddying motions, discussed more below, can be important (Marshall, 1997; Kwon, 2013).

The second term in equation 1.1, $\mathbf{u}_b \cdot \nabla h$, corresponds to lateral flow across a sloping mixed layer base. As noted above, on timescales longer than one year, the mixed layer base in late winter can be adopted. The depth of the winter mixed layer varies substantially on the basin scale (Kara, 2003), such that large-scale horizontal flow will act to move water into and out of the mixed layer. This process, sometimes referred to as ‘lateral induction’, is considered to be important for the time-mean subduction rate in parts of the subtropical North Atlantic (Qiu and Huang, 1995) and the Southern Ocean (Sallée *et al.*, 2010).

Due to incompressibility, the vertical velocity at the base of the mixed layer, w_b , arises from horizontal convergence or divergence of the flow within the mixed layer. This can result from wind-driven Ekman fluxes or from the large-scale flow (Marshall *et al.*, 1993). Such processes are particularly important in the subtropical gyre, where the term is dominated by Ekman pumping (Marshall *et al.*, 1993; Qiu and Huang, 1995).

It should also be noted that time-dependent, eddying motions play a crucial role in subduction in certain regions (Marshall, 1997; Gebbie, 2007). Marshall (1997) showed that the time-average of equation 1.1 in a time-varying ocean includes a term associated with correlations between the outcrop area over which subduction occurs and the velocity and mixed layer depth. This eddy-subduction has been shown to be of leading order importance in regions of intense eddy energy, such as the Antarctic Circumpolar Current (Marshall, 1997; Kwon, 2013) and Gulf Stream (Hazeleger and Drijfhout, 2000), as well as the relatively quiescent ocean interior (Gebbie, 2007; Valdivieso Da Costa *et al.*, 2005).

Following subduction, waters spread in the ocean interior, translating properties from the surface mixed layer to remote regions of the subsurface. This spreading is

achieved by a combination of the large-scale advective flow and ‘diffusive’ processes — the down-gradient transfer of properties in the absence of time-mean flow. In the ocean, a substantial part of this diffusive spreading is achieved by eddying motions at the mesoscale (Mecking *et al.*, 2004; Smith and Ferrari, 2009; Kamenkovich *et al.*, 2017). Eddying motion acts to stir the properties of subsurface waters, reducing the lateral scale of gradients until smaller scale processes (such as internal wave motions) begin to dominate, eventually leading to irreversible mixing of properties by molecular diffusion (Smith and Ferrari, 2009).

In the generally low mixing environment of the ocean interior (Ledwell *et al.*, 1993; Waterhouse *et al.*, 2014), spreading is largely adiabatic such that water will conserve its locally referenced potential density. Consequently, water will spread approximately along neutral surfaces (McDougall, 1987a). Note, however, that the non-linear nature of the equation of state (which relates temperature and salinity of a parcel to its density at a given pressure) means that defining exactly neutral surfaces in the ocean is not possible (McDougall, 1987b; Tailleux, 2016).

For water masses formed in certain regions, diabatic processes are central to their spreading pathways below the mixed layer. Specifically, dense water formed in marginal seas such as the Mediterranean (Price *et al.*, 1993) and the Greenland-Iceland-Nordic seas (Girton and Sanford, 2003) as well as water formed around the Antarctic continental shelf (Orsi *et al.*, 1999). When these waters overflow into the open ocean, they mix vigorously with the ambient open-ocean fluid (Legg, 2012), a process that fundamentally changes their properties and ventilation pathways, as well as those of the water with which they mix. In addition, high levels of mixing (relative to observations in the open ocean thermocline; Ledwell *et al.*, 1993) are being observed over an increasingly wide expanse of the ocean subsurface (Waterhouse *et al.*, 2014), related to flow over rough topography and internal tide generation, with implications for the spreading pathways of ventilated water, particularly in the abyssal ocean.

1.2 The role of ventilation in ocean circulation and climate

As a primary means of communication between the atmosphere and ocean interior, ventilation plays a crucial role in the climate and earth system. In the first place, the formation and ventilation of water masses is important in establishing ocean stratification and therefore the baroclinic structure of the large-scale circulation (Luyten *et al.*, 1983). Secondly, and arguably its most important role, is the sequestration and storage of climatically important substances such as heat (Balmaseda *et al.*, 2013) and carbon dioxide (Williams and Follows, 2011; Gruber *et al.*, 2009), as well as a wider role in the biogeochemical cycles of many other elements (Sarmiento and Gruber, 2006).

The ocean interior is a vast reservoir of carbon and heat, which it exchanges with the overlying atmosphere (Gruber *et al.*, 2009; Abraham and Baringer, 2013). This exchange has become increasingly important in an era when the climate is being perturbed out of steady state by the anthropogenic emission of carbon dioxide (Rhein *et al.*, 2015). It has been estimated that the ocean has taken up 93% of the additional heat present in the earth system since 1955 (Levitus *et al.*, 2012), and around 25% of the additional carbon dioxide, due to fossil fuel burning and land use changes, since the pre-industrial era (Sabine *et al.*, 2004). Crucially, the ability of the ocean to store these substances is achieved not simply by exchange across the ocean surface, but by translation into the ocean interior.

The role of ventilation in the uptake and storage of heat and carbon, and its variability, is not straightforward. This is because uptake and storage of these components can vary as a result of both atmospheric concentration changes and ocean circulation changes (Banks and Gregory, 2006). If ventilation locations, rates and pathways are constant over time, the rate of uptake of heat or carbon will change as their atmospheric levels vary (Church *et al.*, 1991; Khatiwala *et al.*, 2009). On the other hand, variations in ocean circulation, and concurrent changes in ventilation, will redistribute these components in the ocean and affect the locations and timescales on which they are stored (Banks and Gregory, 2006). An insightful

example is ventilation of intermediate and deep waters in the high latitude North Atlantic, which are predominantly formed by heat loss to the atmosphere (Lazier *et al.*, 2001). In the event that this ventilation decreased, the ocean storage of heat would increase (Palter *et al.*, 2014). The relative contributions to the variability in the ocean storage of heat and carbon from ocean circulation variability and atmospheric concentration changes remains unclear (Banks and Gregory, 2006; Marshall and Zanna, 2014).

Beyond heat and carbon dioxide, ocean ventilation plays a critical role in the cycling of many biogeochemical elements through the earth system (Sarmiento and Gruber, 2006). Perhaps most immediately apparent is that of oxygen — the reason that ventilation gets its name. The oxygen content and distribution in the ocean exhibits control on the patterns of life in the ocean (Vaquer-Sunyer and Duarte, 2008), as well as exhibiting substantial control on the cycling of other elements in the ocean, including nitrogen and carbon (Meissner *et al.*, 2005). Following subduction, ocean waters are persistently depleted of oxygen through bacterial respiration of organic detritus in the water column. Consequently, dependent on the balance of oxygen supply from the surface ocean and consumption by bacterial respiration, regions of the subsurface will be oxygen rich or poor. Most striking in this respect is the presence of so-called oxygen minimum zones (OMZs) across large regions of the eastern tropics in the Atlantic and Pacific basins, at depths between 100 and 1000 *m* (Karstensen *et al.*, 2008). The oxygen content and distribution in the ocean has undergone substantial changes over recent decades (Emerson *et al.*, 2004; Tanhua and Keeling, 2012; Hahn *et al.*, 2017) and is expected to change further under the effects of climate change (Matear *et al.*, 2000; Bopp *et al.*, 2002; Keeling *et al.*, 2010), with changes in ventilation consistently implicated as a major driver of these changes (Deutsch, 2005; Bopp *et al.*, 2002; Matear *et al.*, 2000).

1.3 Measuring and understanding ventilation

Over the last three decades, substantial effort has been devoted to establishing the mechanisms, locations, timescales and variability associated with ocean ventilation.

These efforts have only increased with the growing appreciation of the ocean's role in mediating anthropogenic climate change and the crucial part of this played by ventilation (Khatiwala *et al.*, 2009; Levitus *et al.*, 2012). In addition, many of the processes inherent in ventilation stand to be affected in unknown ways by the warming of the planet and associated changes in atmospheric circulation and surface ocean forcing (Matear *et al.*, 2000).

Following the formulation of Cushman-Roisin (1987) (equation 1.1), there proceeded many attempts to measure subduction into the main ocean thermocline, below the region that is seasonally re-entrained by Stommel's demon. Much of this work followed the Eulerian framework, evaluating the transport of water across the late winter mixed layer from climatological observations (Marshall *et al.*, 1993) as well as numerical simulations (Williams *et al.*, 1995). Coincident with this, efforts were made to evaluate the role of ventilation in establishing the stratification (by means of the potential vorticity structure) of the ocean thermocline (Williams, 1991; Marshall and Nurser, 1992). While early application of this Eulerian approach was to the subtropical gyres, particularly that of the North Atlantic, it has since been applied to the Southern Ocean thermocline (Sallée *et al.*, 2010; Kwon, 2013).

An alternative approach to evaluating subduction into the main thermocline adopts a Lagrangian perspective, whereby one can follow the water column as it moves to a region of shallower winter mixed layer (Nurser and Marshall, 1991; Qiu and Huang, 1995). This has been applied in observations and models to establish both the time-mean rate of subduction (*e.g.* Qiu and Huang, 1995; Trossman *et al.*, 2009), as well as its variability (*e.g.* Qu and Chen, 2009; Liu and Huang, 2012) across much of the ocean.

Deviating from the kinematic approach above, Walin (1982) showed that the formation and destruction of water masses can be diagnosed in a thermodynamic framework. Balancing the budgets of volume and buoyancy (or any conserved quantity Viúdez, 2000), volume transport across a density surface can be related to the divergence of buoyancy fluxes at the ocean surface and in the ocean interior (Walin, 1982; Nurser *et al.*, 1999). In the absence of buoyancy fluxes in the mixed

layer, therefore, subduction rates can be inferred from surface heat and freshwater fluxes (*e.g.* Speer and Tziperman, 1992). However, model results suggest that subduction rates for certain density classes are substantially influenced by buoyancy fluxes within the mixed layer (Nurser *et al.*, 1999; Marshall *et al.*, 1999). Indeed, comparison of volume transports and surface fluxes can be used to diagnose mixing in the surface mixed layer and ocean interior, and has been done in both observations (Speer, 1997) and numerical simulations (Lee *et al.*, 2001).

With regard to pathways of ventilation, much of the early understanding was established on theoretical grounds. Luyten *et al.* (1983) showed that in a layered, steady-state ocean, assuming linear vorticity balance, fluid parcels subducted into the main thermocline follow the path of the gyre circulation, established by the curl of the wind-stress. Conservation of potential vorticity then dictates that layers deepen toward the corner of the gyre that is furthest from the ventilation region *e.g.* the north west corner for the subtropical North Atlantic, consistent with observations (McDowell *et al.*, 1982). Furthermore, this ‘ventilated thermocline theory’, predicts a pool of stagnant, unventilated water in the south eastern corner (for the North Atlantic example) of the domain. These so-called ‘shadow zones’ closely corresponds to regions of low oxygen concentration (alluded to in Section 1.2) in observations, supporting the expectation that they are poorly ventilated (Karstensen *et al.*, 2008).

Deep ocean pathways have also been considered in the steady state ocean. Stommel and Arons (1959) showed that uniform upwelling from a constant density, flat-bottomed deep ocean, would lead to weak, poleward flow of water, again based on a linear vorticity balance. If the source of deep ocean water were at high-latitudes therefore, as is the case in the ocean, this would mean waters moving towards the source. Consequently, mass balance and vorticity constraints requires that a relatively rapid, equatorward flow persists on the western side of the basin, in which the linear vorticity balance breaks down. While assumption of a flat-bottomed basin and uniform upwelling are violated in the ocean, the presence of a Deep Western Boundary Current (DWBC) from the high-latitude North Atlantic is well established (Lozier, 2012; Toole *et al.*, 2017). In a deep ocean of variable

topography, the linear vorticity balance can be extended to show that interior pathways should follow contours of large-scale (and constant density) potential vorticity (f/h ; where f is the Coriolis parameter, and h is the ocean depth) in the absence of forcing (Stephens and Marshall, 2000).

Central in understanding ventilation is the concept of the ocean’s ‘age’ — the time since water was last within the surface mixed layer. The advent of transient tracers — tracers for which the atmospheric history and/or the radioactive decay rate is known — enabled for the first time this age to be estimated from observations. Consequently, a much more detailed picture of ventilation pathways and timescales could be derived (*e.g.* Weiss *et al.*, 1985; Jenkins, 1988; Sarmiento, 1983; Fine *et al.*, 2002; Rhein *et al.*, 2002). Transient tracers include chlorofluorocarbons (CFCs) and sulfurhexafluoride (SF₆), as well as radioactive elements including tritium (³H), its decay product 3-helium (³He), and bomb radiocarbon (¹⁴C). These elements have well-measured atmospheric histories and are easily detected in ocean water at low concentration and with high accuracy, making them ideal candidates as tracers of the ocean circulation from surface to interior (Fine, 2011). The age of water is then established from the ratio of two tracers, and knowledge of their atmospheric history. This tracer-derived age has large uncertainties, however, due to the fact that it is not conserved under the effects of mixing between water masses with different tracer concentrations (Thiele and Sarmiento, 1990; Khatiwala *et al.*, 2001).

In the ocean (as in any turbulent geophysical flow) the time taken for water to arrive at a certain location is not a single value but rather a distribution (Khatiwala *et al.*, 2001). As such, the age of the ocean interior was recast as a transit time distribution (Hall and Haine, 2002; Deleersnijder *et al.*, 2001; Primeau, 2005). Efforts to determine the transit time distribution in the ocean interior were advanced by its description as a ‘Green’s function’, the solution for which is mathematically analogous to that of the three-dimensional advection-diffusion equation. Consequently, the transit time distribution (as well as the distribution of subduction locations) is described by the evolution of a tracer in a numerical simulation (Holzer and Hall, 2000). Most importantly, the Green’s function, and

therefore the transit time distribution, can be derived from tracer observations in the ocean (Waugh *et al.*, 2004; Hall *et al.*, 2007).

In addition to the measurement of tracers, experiments with autonomous subsurface floats have been carried out to establish ocean ventilation pathways and timescales (Lavender *et al.*, 2000; O'Dwyer *et al.*, 2000; Bower *et al.*, 2009). There has been a particular focus on the pathways of so-called Labrador Sea Water, formed by convective processes in the high-latitude North Atlantic, and its southward export (or not) along the western boundary of the Atlantic domain (Lavender *et al.*, 2000; Bower *et al.*, 2009). Float trajectories revealed a much more complex circulation than had previously been inferred from the theoretical arguments outlined above. In addition to floats launched with the express purpose of following a particular water mass (*e.g.* Bower *et al.*, 2009), much has been learnt about the mid-depth circulation, including export pathways from ventilation regions, from subsurface displacements of free-drifting profiling floats such as the Argo array (Palter *et al.*, 2008; Colin de Verdière and Ollitrault, 2016; Sévellec *et al.*, 2017).

Finally, we note that despite their more comprehensive data, assessing ventilation in numerical ocean circulation models can be almost as challenging as in the ocean. This results from the fact that ventilation is an inherently Lagrangian process, while most numerical models are established on a fixed, Eulerian grid (Griffies *et al.*, 2000a). Consequently, a common approach is to simulate artificial tracers or floats and observe their transport through the model, just as one would in the ocean (*e.g.* Speich *et al.*, 2001; Booth and Kamenkovich, 2008; Sallée *et al.*, 2010; Gary *et al.*, 2012; Jones *et al.*, 2016).

1.4 Some outstanding issues

Over the course of this thesis, we address some outstanding issues related to ocean ventilation. An outline of the research questions are given below, with a more detailed background provided in the introduction of each individual chapter.

1.4.1 Lagrangian analysis of ocean ventilation in numerical circulation models

The extent to which water flows along or across density surfaces in the ocean interior, is central to our understanding of the rates and pathways of ventilation. As mentioned above, it is thought that isopycnal flow dominates, and that diapycnal fluxes are important only in certain regions and on long timescales. In numerical simulations, (particularly those whose vertical coordinate is depth, rather than density) it is notoriously difficult to avoid spurious diapycnal fluxes arising from explicit parameterisations and numerical errors (Roberts and Marshall, 1998; Griffies *et al.*, 2000b; Hill *et al.*, 2012). This can have a substantial effect on the properties of subsurface watermasses (Lee *et al.*, 2001), causing them to deviate substantially from those in the ocean. Given the role of ventilation in decadal to centennial climate change, this poses a substantial challenge to the fidelity of climate projections.

As noted previously, assessing ventilation is not straightforward, even in numerical simulations. Often, research relies on the simulation of artificial tracers or Lagrangian trajectories to assess the mechanisms and variability of subduction and spreading. The calculation of Lagrangian trajectories — the pathways of zero-mass particles passively advected by the model velocity field — are a commonplace tool for kinematically assessing the output of numerical simulations (*e.g.* Speich *et al.*, 2001; van Sebille *et al.*, 2011; Thomas *et al.*, 2015). Such calculations, however, require assumptions and truncations that can lead to errors in the trajectories. Furthermore, analysis is often done ‘offline’, *i.e.* using time-averaged output of the simulated velocity fields, possibly leading to further errors (Chenillat *et al.*, 2015).

Thus, in both numerical simulation and calculation of Lagrangian trajectories, there is potential for error in the fidelity of ventilation pathways, specifically in their diapycnal nature. To our knowledge, this has not been critically assessed for trajectories in a complex ocean simulation, despite a wealth of studies adopting such analysis. We undertake a critical analysis of this in Chapter 2.

1.4.2 The role of mesoscale eddies in subtropical thermocline ventilation

The spreading of watermass properties in the ocean interior is a combination of advective and diffusive processes. Of particular relevance is the role played by mesoscale (50 to 100 *km* horizontal scale) eddies — ubiquitous in the ocean — in stirring the background gradient of tracers, invoking a cascade of variance down to increasingly small scales, a process commonly referred to as eddy diffusion. There is good evidence that eddy diffusion plays an important role in ventilation (Abernathy and Ferreira, 2015; Kamenkovich *et al.*, 2017), particularly in specific regions (Robbins *et al.*, 2000).

The stirring of tracers by mesoscale eddies falls under the category of ‘chaotic advection’ (Wiggins, 2005), a topic that borrows heavily from work on dynamical systems. There is a wealth of research on the cascade of variance under chaotic advection (Pierrehumbert, 1994; Neufeld *et al.*, 2000), along with efforts to apply this understanding to evaluate stirring in the surface ocean (Abraham and Bowen, 2002; Waugh and Abraham, 2008; Keating *et al.*, 2011). Nevertheless, such an approach has not previously been applied to investigate the role of eddy diffusion in ventilation, which we undertake in Chapter 3. Of particular interest in the case of ventilation is the occurrence of a distinct timescale over which stirring takes place — the time since subduction — which results in the faculty to characterise the amount of stirring that has taken place.

1.4.3 Variability in the ventilation of North Atlantic Deep Water

The subpolar North Atlantic ocean has played a disproportionate role (relative to surface area) in the recent oceanic uptake of heat (Levitus *et al.*, 2012; Abraham and Baringer, 2013) and carbon dioxide (Sabine *et al.*, 2004; Khatiwala *et al.*, 2009). Its importance in the climate system is thought to be entangled in the regional ventilation of the intermediate and deep water masses of the North Atlantic ocean (Gebbie and Huybers, 2010; Khatiwala *et al.*, 2012). Several decades of

oceanographic observations in the region have revealed substantial variability in ventilation on inter-annual to decadal timescales (Rhein *et al.*, 2015; Yashayaev and Loder, 2016). Particular attention has been paid to this variability due to its possible link to changes in the Atlantic Meridional Overturning Circulation (Curry *et al.*, 1998; Lozier, 2012), with consequentially broader climate impacts (Zhang and Delworth, 2006; Sutton and Dong, 2012). More recent efforts have focussed on possible impacts on the variability in heat (Robson *et al.*, 2012; Williams *et al.*, 2015b; Häkkinen *et al.*, 2016) and carbon (Levine *et al.*, 2011; Keller *et al.*, 2012; Tanhua and Keeling, 2012) uptake and storage, with the necessity to elucidate long-term, forced trends from oscillatory changes and intrinsic variability.

Variability in the subpolar North Atlantic ocean ventilation tends to be characterised in terms of variability in processes local to the dense water formation site, such as surface forcing or mixed layer depth (*e.g.* Lazier *et al.*, 2002; Marsh *et al.*, 2000), or by subsurface hydrographic and chemical changes in remote regions (*e.g.* Curry *et al.*, 1998; Stramma *et al.*, 2004; Rhein *et al.*, 2011). A major goal of the research community has been to establish the nature of the link between the two (Rhein *et al.*, 2011; Lozier, 2012). While such a link has been forthcoming locally within the subpolar gyre (Rhein *et al.*, 2011) and, to some extent, further south (Schott *et al.*, 2004), variability is substantially modified and detailed understanding remains obscure. Recently, it has become clear that the connection between surface forcing variability and its signature in the subsurface is eroded in the ocean in part due to the varied and diffuse nature of ventilation pathways in the deep North Atlantic (Bower *et al.*, 2009; Gary *et al.*, 2012; Zou and Lozier, 2016).

In Chapter 4 we investigate the processes establishing the inter-annual to decadal variability of ventilation in the subpolar North Atlantic by explicitly linking water in the deep North Atlantic to the location and time of subduction through backward-in-time, entirely advective Lagrangian trajectories in a numerical ocean circulation model. This allows us to establish how ventilation is achieved in this simulation, how and why ventilation varies over time, and the manner in which the signature of this variability is retained in the subsurface.

1.4.4 The role of ventilation in polar Southern Ocean carbon uptake

Alluded to at the start of the introduction, an understanding of the physical process of ventilation is insufficient to describe the translation of chemically or biologically active tracers into the ocean interior (Sarmiento and Gruber, 2006; Williams and Follows, 2011). An example of this is in the polar Southern Ocean, south of the Antarctic Circumpolar Current, where a complex interaction between ocean circulation and biogeochemical processes is critical to the operation of the local carbon cycle. Regional upwelling of carbon-rich deep waters toward the ocean surface, and the formation and ventilation of abyssal ocean water, each have the capacity to strongly affect whether carbon is outgassed to, or taken up from, the atmosphere. Consequently, the region is thought to be of critical importance for millennial timescale climate dynamics, including transitions between glacial and inter-glacial states (Sigman *et al.*, 2010).

In Chapter 5, we use observations around the boundary of the Weddell Gyre, an important region of the polar Southern Ocean, to explore the present day operation of the regional carbon cycle. We decompose the transport of carbon into components associated with the vertical overturning circulation and the horizontal circulation, and further into transports associated with different physical and biogeochemical processes. In so doing, we investigate whether a two-dimensional perspective of the regional carbon cycle, as has traditionally been adopted, gives undue weight to the role of the overturning circulation and deep ocean ventilation at the expense of other processes.

The results of Chapter 3 have been published in MacGilchrist *et al.*, 2017, Characterising the Chaotic Nature of Ocean Ventilation, *Journal of Geophysical Research: Oceans*, 122. Related ideas were contributed to van Sebille *et al.*, 2018, Lagrangian Ocean Analysis: Fundamentals and practices, *Ocean Modelling*, 121:49–75.

Preliminary results from Chapter 5 were included in Naveira Garabato *et al.*, 2017, High-latitude Ocean Ventilation and its Role in the Earth's Climate Transitions, *Philosophical Transactions of the Royal Society A*, 375(2102).

Results from Chapters 4 and 5 are in preparation for submission.

2

Diapycnal nature of Lagrangian trajectories in an ocean circulation model

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2.1 Introduction

Mixing and surface buoyancy and momentum forcing play a central role in establishing the properties of water masses in the surface ocean mixed layer (Large *et al.*, 1994; Garrett and Tandon, 1997). Following subduction, however, levels of mixing and forcing are thought to be low, except in certain localised regions (Waterhouse *et al.*, 2014). In the complete absence of mixing, fluid parcels will flow in the direction that conserves their locally referenced potential density (McDougall, 1987a). Surfaces tangent to this direction are called neutral surfaces. Consequently,

ventilation pathways in the subsurface are thought to be predominantly along rather than across neutral surfaces.

Mixing is notoriously difficult to handle in numerical models (Griffies *et al.*, 2000b). In the first place, the magnitude and spatial distribution of subsurface mixing is poorly known in the ocean (Waterhouse *et al.*, 2014). Small magnitudes have been measured across much of the ocean interior (Ledwell *et al.*, 1993), and set as such in numerical simulations (MacKinnon *et al.*, 2017). However, a host of processes, including wave generation and breaking in areas of rough topography (Ledwell *et al.*, 2000; Watson *et al.*, 2014) and dense water overflows (Price *et al.*, 1993; Garton and Sanford, 2003), are known to lead to levels of mixing orders of magnitude greater than this background level. Due to the small-scale nature of these processes, they are heavily parameterised in most numerical ocean circulation models, often in a crude manner (Legg *et al.*, 2009; MacKinnon *et al.*, 2017).

In addition to the difficulties in implementing appropriate levels of *explicit* mixing, circulation models also suffer from spuriously high levels of *implicit* mixing associated with numerical errors (Griffies *et al.*, 2000b; Lee and Williams, 2000). This is particularly true of models that employ depth as their vertical coordinate (as opposed to another branch of models that employ density as the vertical coordinate, so-called isopycnal models). Early issues associated with horizontal mixing across sloping density surfaces (Veronis, 1966) have been largely resolved (Griffies *et al.*, 1998). However, difficulties persist in simulating adiabatic transport of tracers (Griffies *et al.*, 2000b; Getzlaff *et al.*, 2010, 2012; Hill *et al.*, 2012) and momentum (Ilicak *et al.*, 2012).

Lagrangian analysis of numerical ocean circulation models is commonplace in attempts to understand the kinematics of ocean circulation (e.g. Speich *et al.*, 2001; van Sebille *et al.*, 2011; Thomas *et al.*, 2015). The trajectory calculation attempts to replicate the pathways of water (or, if diffusive parameterisations are applied, tracers) through the model. However, such calculations rely on a host of choices and/or assumptions, such as the advection scheme employed or the use of time-average velocity fields, that may erode their accuracy (van Sebille *et al.*, in review).

Consequently, it may be the case that the water pathways resolved by Lagrangian analysis have a larger diapycnal component than the model velocity field itself.

In this chapter, we set out to establish (a) the extent to which trajectories in a subsurface of a global $1/4^\circ$ ocean circulation model move along or across neutral surfaces, and (b) whether the ‘across neutral surface’ movement is due to mixing in the numerical simulation, or errors in the Lagrangian trajectory calculations. We start the chapter by outlining the details of the numerical ocean circulation models used in this and subsequent chapters. After that, we provide details of the trajectory calculation tool, highlighting its inherent choices and assumptions. In the final section, we address the aims outlined above.

2.2 Numerical simulations

The primary simulation used in this thesis is a global implementation of the Nucleus for European Modelling of the Ocean (NEMO) model (Madec, 2008). The simulation was carried out as part of the Drakkar project (Barnier *et al.*, 2006). The ORCA025 configuration is used, which has a grid resolution is $1/4^\circ$ ($\sim 27.75\text{ km}$ at the equator, refined at high latitudes) and 75 uneven vertical levels. The model is within the so-called ‘eddy-permitting’ regime of ocean models. This means that, in most regions of the ocean, mesoscale features with length scales on the order of 50 to 100 km will be captured by 2 or 3 grid points (Hallberg, 2013). As such, nonlinear behaviour in the circulation emerges, but the full extent of ocean turbulence does not develop (Barnier *et al.*, 2006). The grid is ‘tripolar’, meaning that it converges at two points over land in the northern pole, thus avoiding convergence in the Arctic Ocean. The ocean model is coupled to a thermodynamic sea-ice model, LIM2 (Bouillon *et al.*, 2009). Comparison of the model configuration with observations can be found in Grégorio *et al.* (2015) and Barrier *et al.* (2015).

The simulation runs from 1958 to 2015, and is forced with historical atmospheric reanalysis. The reanalysis used is the ‘Drakkar Forcing Set 5’, which is an updated version of the fields described in Brodeau *et al.* (2010). This forcing set is an adjusted version of the ERA40 reanalysis (Dee *et al.*, 2011), with modifications

applied to ensure approximate global near-balance of heat and freshwater, such that it can be used to drive inter-annual numerical ocean simulations. The simulation is initialised from rest with temperature and salinity from the Levitus climatological hydrography (Levitus *et al.*, 1998), augmented with the Polar Science Center Hydrographic Climatology for the Arctic regions. With no spin-up, the model fields undergo significant adjustment in the first 10-15 years, and results from these years should be treated with caution. Velocity, variable parameter (*e.g.* vertical diffusivity), and hydrographic fields are output as 5-day means.

Advection of active tracers, potential temperature and salinity, is achieved using a ‘Total Variance Dissipation’ (TVD) scheme. The TVD scheme is equivalent to a centred-difference scheme, but acts to damp tracer variance when advection produces local tracer extrema (Madec, 2008). The coefficient and mixing length scales for vertical diffusion of tracers are determined via a turbulent kinetic energy (TKE) closure, which depends on velocity shear, stratification, diffusion and dissipation (Blanke and Delecluse, 1993). Values of the vertical diffusion coefficient are increased above a background value of $1.2 \times 10^{-5} m^2 s^{-1}$, and can become as large as $1 m^2 s^{-1}$ in regions of convection. Laplacian lateral tracer diffusion is implemented along isopycnal slopes (Griffies *et al.*, 1998). The slope is defined such that the diffusion of locally referenced, potential density (as evaluated by the EOS80 equation of state) is zero. The simulation does not include parameterised eddy-induced advection (Gent and McWilliams, 1990).

The simulation described above is the only one used in Chapters 3 and 4 of this thesis. In this chapter, we also use a regional setup of ORCA025, which extends from approximately $27^\circ N$ to Bering Strait on the far side of the Arctic. In its resolution, parameterisations and atmospheric forcing, the simulation is identical to that outlined above. For this simulation, velocity, variable parameter and hydrographic fields are saved at every model timestep (720 seconds), for a subdomain centred around the Gulf Stream region of the North Atlantic. Throughout the chapter, we refer to this as the Arctic-Atlantic model, while the other model is referred to as the ‘primary’ model or simulation.

2.3 Lagrangian trajectory calculation

To evaluate trajectories in the numerical simulation, we use the Lagrangian analysis tool, Ariane (Blanke and Raynaud, 1997). The tool was developed to compute the advective component of volume transports in an ocean model, and was established with the intention of use with the NEMO model. For a steady velocity field, and under the assumption that volume transports vary linearly between grid cell faces, an analytical expression for the streamlines between grid cell faces can be defined. Due to volume conservation, particles conserve their infinitesimal transport along trajectories and, for a sufficient number particles, volume transports between sections can be established (*e.g.* Speich *et al.*, 2001; Blanke *et al.*, 2001; Thomas *et al.*, 2015). The benefit of the analytical approach is that particles do not have to be explicitly evolved forwards in time (*i.e.* with a time-stepping scheme), but rather their future position can be evaluated directly from the streamline calculation. This makes the calculation of large numbers of trajectories extremely efficient.

Trajectories can be evaluated both forwards and backwards in time. Tracers, such as temperature, salinity and density, along trajectories are evaluated via trilinear (linear in the x, y and z directions) interpolation from the closest surrounding model grid points at which the variable is defined. Since Ariane is designed to evaluate advective volume transports in the model, no attempt is made to parameterise sub-grid scale physics through the addition of stochastic noise as is done in other Lagrangian codes (*e.g.* Koszalka *et al.*, 2013).

The analytical streamline calculation applies only for a stationary velocity field. To evaluate trajectories through a time-varying velocity field, we must assume that the field is piece-wise stationary. That is, that the velocity field changes in a discrete fashion at each timestep. In the case of our primary simulation, this means a discrete change in the velocity field at 5-day intervals.

Ariane has been well established as a tool to diagnose volume transports in numerical ocean models (Speich *et al.*, 2001; Blanke *et al.*, 2001; Thomas *et al.*, 2015). The volume-conservation basis of Ariane is identical to that of another tool, TRACMASS (Döös, 1995), the utility of which in diagnosing volume transports has

also been considered (*e.g.* De Vries and Döös, 2001; Döös *et al.*, 2004; Berglund *et al.*, 2017). Broadly speaking, however, these analyses focus on net transports between sections (*e.g.* Lique *et al.*, 2010; Desbruyères *et al.*, 2013; Thomas *et al.*, 2015), and pay less attention to diabatic changes occurring therein.

In Chapters 3 and 4 of this thesis, Lagrangian trajectories are calculated as a means of determining the pathways and timescales of ventilation. For the most part, this is done by initialising particles (within a volume or on a density surface) below the surface ocean mixed layer, and evaluating trajectories backwards in time until the mixed layer is intercepted. As noted in the introduction to this chapter (and in Chapter 1), spreading pathways of ventilated water in the ocean are approximately adiabatic such that, in our backwards-in-time experiments, particles are expected to have broadly the same density when they move into the mixed layer as when they were initialised.

We are thus motivated by the findings of an experiment in which particles were initialised throughout the entire North Atlantic domain of the primary simulation described above. Figure 2.1 shows a two-dimensional volumetric histogram (where each particle is assigned a volume based on the size of the grid cell in which it is initialised) of the density of particles when they were initialised in March 2012 (close to the end of the simulation) and when they were subducted. Note that the colour scale is logarithmic. If spreading pathways, as evaluated by these trajectories, were adiabatic the entire volume would fall on the 1:1 line. It is clear that this is not the case for a substantial number of particles, in both the upper and deep ocean. We return to this figure in more detail in Section 2.4.1, using it here simply as motivation. Depending on the absolute magnitude and causes of this diapycnal motion, it could represent a problem for the fidelity of ventilation pathways either in the model itself, or in their diagnosis via Lagrangian trajectory calculation. Thus, in the following section, we seek a deeper understanding of the processes contributing to Figure 2.1, and its implications.

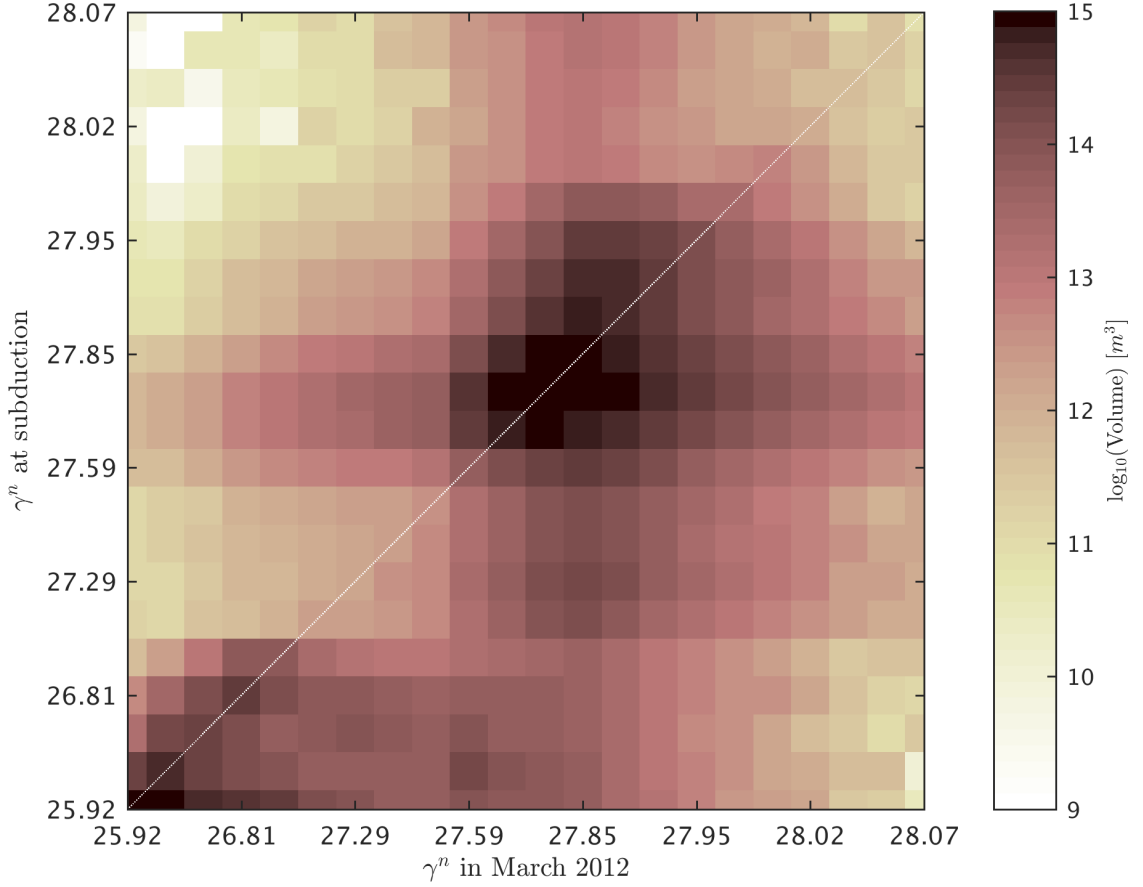


Figure 2.1: Volumetric histogram of subduction density (y -axis) against density in March 2012 (x -axis) for water ventilated during a 54-year hindcast simulation, derived from Lagrangian analysis. The bin spacing of the histogram is adopted to account for the exponential stratification, such that deeper density classes have smaller bin widths. Note, therefore, that the x and y axes are non-linear. The colour scale is logarithmic. The white dotted line shows the 1:1 line.

2.4 Diapycnal Lagrangian motion

Before embarking on a discussion of density changes along trajectories in our simulation, it is important to establish precisely what such an occurrence means, and identify potential sources of error around which we can frame the subsequent discussion. In particular, we wish to make a distinction between *local* and *global* diapycnal motion diagnosed from trajectories.

Consider a numerical ocean circulation model, in steady-state, that is completely adiabatic beneath the surface mixed layer. Furthermore, for simplicity, consider that density is entirely defined by potential temperature, with no contribution from

salinity. In the model, velocity and temperature are defined at discrete points in space. Advection of temperature is done by way of an advection scheme, combining velocity and temperature values from these discrete grid locations in such a way that $D\theta/Dt = \nabla \cdot \mathbf{u}\theta = 0$ (where we have used incompressibility, $\nabla \cdot \mathbf{u} = 0$, to write this in ‘flux form’ as is common for numerical simulations). That is to say, the flow of water in the Eulerian frame induces no change in potential temperature.

From the same discrete grid locations, a (purely advective) Lagrangian trajectory calculation attempts to represent this flow of water precisely. Unlike the model, however, the velocity and temperature of the Lagrangian trajectory are defined continuously throughout space, not simply at discrete points. In the case of Ariane, the velocity is defined through an analytic expression for the streamlines between velocity points, and temperature is defined through linear interpolation from tracer points. The change of temperature along the Lagrangian trajectory is the result of advection across the temperature gradient: $\partial\theta/\partial s = \mathbf{u}_L \cdot \nabla\theta_L$, where s is the line element tangent to the trajectory and the subscript L establishes the Lagrangian velocity and temperature as distinct from that on the Eulerian grid.

At any point along the trajectory, $\partial\theta/\partial s$ may be non-zero due to the pathway, defined by $\mathbf{u}_L$, or the temperature gradient, defined by θ_L . Importantly, the former indicates that the Lagrangian scheme is fundamentally diabatic, and the trajectory is therefore not consistent with advection of water in the model. The latter on the other hand, is due to inaccuracy in the interpolation of temperature onto the trajectory location. Since the temperature has no dynamical effect on the trajectory, but rather is evaluated passively along its path, this is a local effect. In other words, even a trajectory that accurately represent the adiabatic flow of water in the model can be locally diabatic due the temperature interpolation.

As will be seen in the following section, particles are seen to change their density in a consistent manner over long timescales, which we call ‘global’ diapycnal motion. If this is due to a Lagrangian scheme that is more diabatic than the numerical simulation, it must be the case that local diapycnal motion, as described above, accumulates over time. Such an accumulation is not possible from diapycnal

motion associated with the temperature gradient discrepancies, and must be due to pathway divergence. However, in attempting to assess the origins of such global diapycnal motion, it is necessary to consider the spatial structure of local diapycnal motion. This is done with the caveat, therefore, that a component of the observed diapycnal motion may be local and not cumulative, therefore not contributing to global changes.

We can get a sense for the magnitude of local diapycnal motion by comparing the temperature change experienced along a trajectory initially at a tracer point to the temperature advection tendency over one timestep of the Arctic-Atlantic model (720 seconds). In this way, we can evaluate both $\mathbf{u}_L \cdot \nabla \theta_L$ and $\nabla \cdot \mathbf{u} \theta$ directly. Since we evolve the trajectory for only one timestep, and stop it before the temperature field updates, these two terms should be equal for a Lagrangian calculation that accurately represents the volume flux *and* temperature gradient in the model. We perform this experiment across a Gulf Stream-centred domain of the Arctic-Atlantic model described in Section 2.2, with particles initialised on each tracer point. The temperature advection tendency is shown in Figure 2.2, and the difference between this and the rate of change of temperature of the Lagrangian particle is shown in Figure 2.3.

The difference between the advective tendency and the change of particle temperature is, in some regions, the same order of magnitude as the tendency itself. The largest discrepancies are seen in the thermocline, in particular within the Gulf Stream and extension. In this region, discrepancies exhibit a large-scale pattern related to isotherm slopes, with maximum values where the slope is steepest. Positive differences ($\mathbf{u}_L \cdot \nabla \theta_L > \nabla \cdot \mathbf{u} \theta$) are seen on the warm side of sloping isotherms, while the opposite is true on the cold side. This is true even in the narrow boundary near bathymetry, seen in the longitudinal section. In the offshore thermocline, away from energetic regions, discrepancies are smaller and with a broad pattern that switches from positive to negative at around 800 *m*.

It is not possible to directly establish whether these discrepancies are due to the velocity or the temperature gradient at the particle location. However,

given the manner in which the particle velocity is established, being intentionally consistent with volume advection in the model, it is unlikely that large errors would appear over such a short timescale. Furthermore, the spatial pattern of differences, particularly having the largest values where the temperature gradient is largest, is highly suggestive of errors associated with the interpolation of the temperature field onto the particle location. Thus, we surmise that errors associated with the inferred temperature (later density) gradient can dominate changes along trajectories on short timescales, particularly in energetic regions.

When the velocity field evolves in time, there are two further potential sources of erroneous diapycnal motion in the Lagrangian trajectory calculation, beyond those associated with spatial interpolation outlined above. Firstly, the analytical calculation of streamlines, that is built on volume conservation, applies only for a stationary velocity field. This is dealt with in the trajectory calculation by assuming that the velocity field is piece-wise stationary. Doös *et al.* (2017) assessed the effect of different timestep assumptions on evaluated trajectories for the TRACMASS code. They considered the effect of subsampling averaged velocity fields (*i.e.* shortening the time over which stationarity is assumed) as well as an extension of the analytical calculation to include linear interpolation in time as well as space. They found that individual trajectories could show large discrepancies, but that the large-scale statistics and transports were broadly unaffected.

Perhaps a more substantial source of error in the Lagrangian calculation is the use of time-average velocity fields. Implicit in this assumption is that variations in the velocity field at time scales below the averaging timescale are uncorrelated in time and space. Consider two particles that are initially at the same location and subsequently evolved forward in time, one with the full velocity field and the other with the time-average field. A local difference between the velocity fields can cause the particle locations to deviate temporarily. If velocities in the particles' new positions cause further deviations, the difference will grow. If not, they will remain close over long timescales. For example, if the full velocity field was oscillatory in nature with constant period and amplitude, and the time-averaging was done

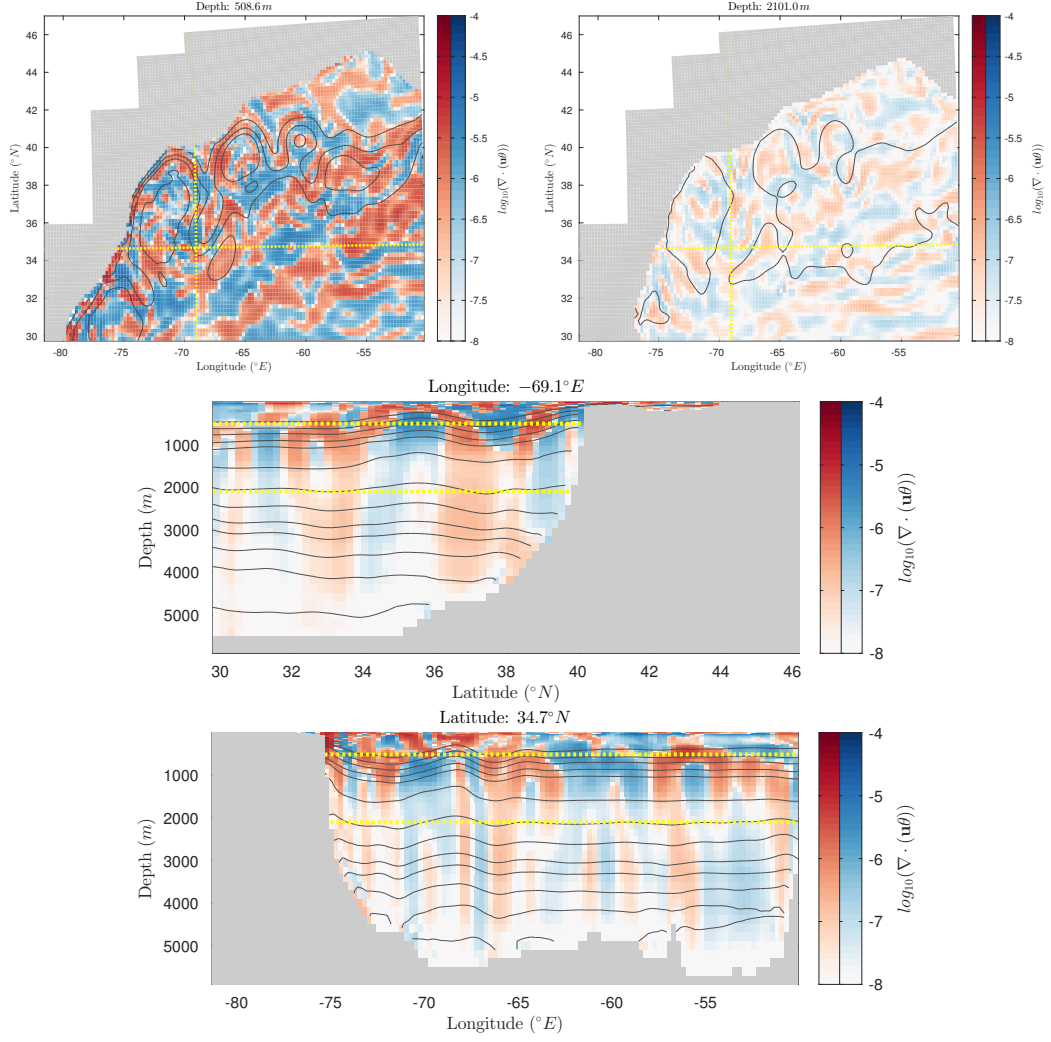


Figure 2.2: Advective tendency of temperature, $\nabla \cdot \mathbf{u}\theta$, over one model timestep in the Gulf Stream domain of the Arctic-Atlantic model, detailed in Section 2.2. Values are shown at each tracer point on two depth levels (top panels), at 510 m and 2100 m, and along a meridional (middle panel) and zonal (bottom panel) section. The colour scale is logarithmic for both positive (blue) and negative (red) tendencies. Contours of potential density referenced to the surface over the same model timestep are shown in black. Contour spacing is derived from the mean stratification, taking values every 200 m in the upper 1000 m and every 500 m below that. Yellow dotted lines show the locations of each intersecting section.

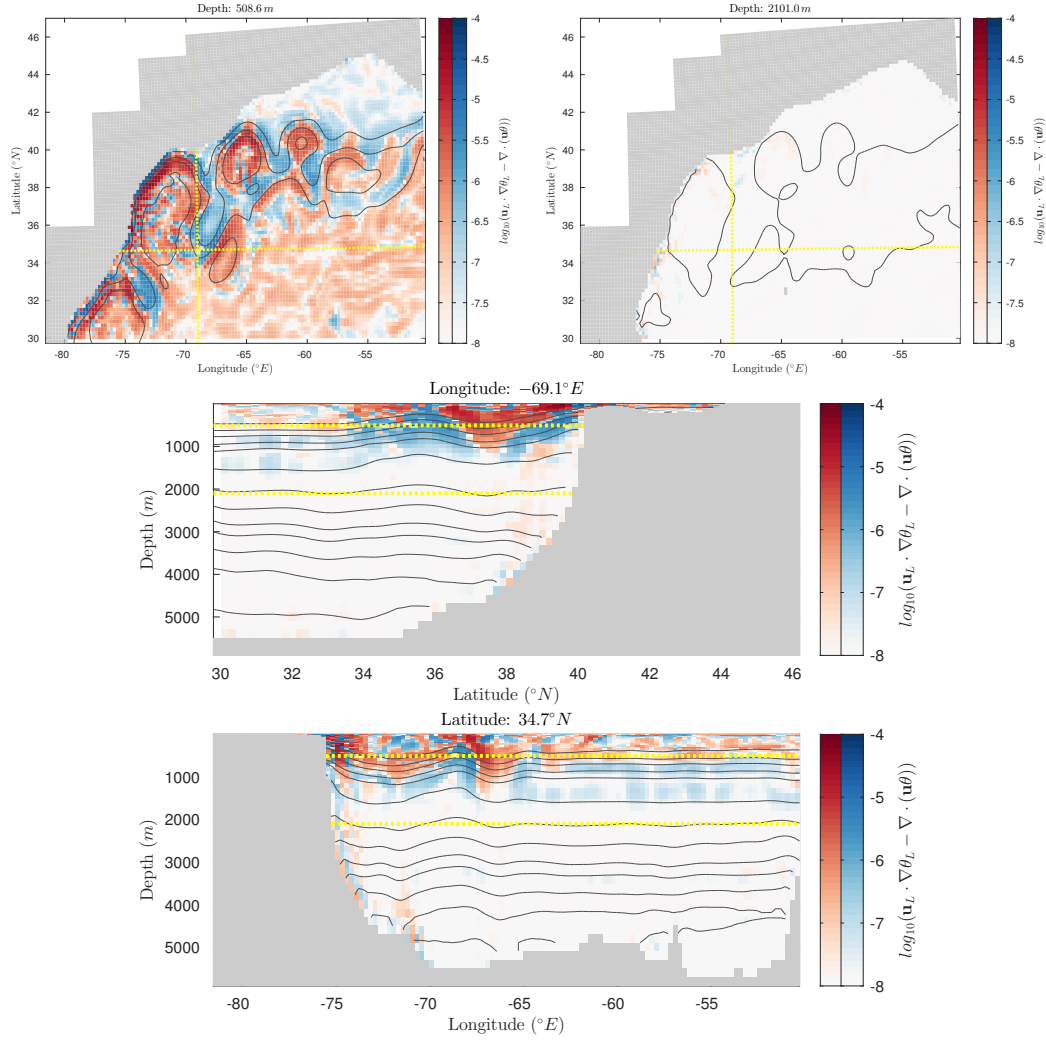


Figure 2.3: Difference between the change in temperature along the path of particles initialised at each tracer point, $\mathbf{u}_L \cdot \nabla \theta_L$, evolved for one timestep, and the advective tendency of temperature, $\nabla \cdot \mathbf{u} \theta$, at the same tracer point. Evaluated in the Gulf Stream domain of the Arctic-Atlantic model, detailed in Section 2.2. Values are shown at each tracer point on two depth levels (top panels) and along a meridional (middle panel) and zonal (bottom panel) section. The colour scale is logarithmic for both positive (blue) and negative (red) tendencies. Contours of potential density (referenced to the surface) over the same model timestep are shown in black. Contour spacing is derived from the mean stratification, taking values every 200 m in the upper 1000 m and every 500 m below that. Yellow dotted lines show the locations of each intersecting section.

over one period, then the difference in particle position could be locally large, but would not accumulate in time. On the other hand, if the oscillatory behaviour was coupled to a vertical velocity shear, a particle evolved with the full field would sample different parts of the shear at different times, and its position would diverge over time from that of the particle evolved with the time-average field. Thus, when moving through a background density field, time-averaging could lead to either local or global diapycnal motion.

In reality, numerical ocean circulation models are not adiabatic, even away from the surface mixed layer. Explicit mixing is applied in an attempt to reproduce realistic levels of diapycnal motion from processes known to occur in the subsurface. More troublesome, perhaps, is the widespread occurrence of *implicit* or numerical mixing (Griffies *et al.*, 2000b). Even if a model were set up to be adiabatic, diabatic motion could occur as a result of truncation errors in the advection scheme, momentum transport scheme and even time-stepping scheme.

In the presence of model mixing, the density will change along trajectories even if the Lagrangian calculation perfectly reflects the advective flow of volume through the model. While such mixing can be local in space and time, it irreversibly changes the density structure in the subsurface, which feeds back onto the velocity field. Consequently, both explicit and implicit model mixing will induce global diapycnal motion. However its relative magnitude compared to the sources of global diapycnal motion coming from the trajectory calculation is what remains uncertain.

While it is possible to locally establish the neutral tangent plane along which a particle will move, defining a neutral surface across the entire ocean subsurface is not possible (McDougall, 1987a; Tailleux, 2016). The problem is one of non-zero *helicity*, itself related to the fact that the density of ocean water is established by both its temperature and salinity. As such, when considering large areas of the ocean, it is common to make an approximation of neutral surfaces. This can be done through the calculation of potential density, ρ_θ , at a specific reference pressure or patched across multiple discrete pressures, or through an approximation of so-called ‘neutral density’, γ^n (Jackett and McDougall, 1997). In this thesis, we use either potential

density referenced to the surface and calculated using the EOS80 equation of state, or an empirical form of neutral density developed by McDougall and Jackett (2005). The general difficulty in defining an exact neutral surface means that at any location, the slope of the approximated neutral surface may deviate from the actual direction of the neutral tangent plane. Consequently, adiabatic motion of trajectories may appear diabatic due to the inadequate definition of the neutral surface. This could result in the erroneous diagnosis of both local and global diapycnal motion.

In summary, there are several potential sources of density changes along Lagrangian trajectories. Some of these, such as in relation to the interpolation of density onto particle location, are entirely local, and will not accumulate over time. Others, including model mixing and errors in particle pathways, have the capacity to result in global diapycnal motion — that is, consistent changes that accumulate over time. In the following sections, we assess the extent to which global diapycnal motion is present in the model, and attempt to establish possible contributing mechanisms.

2.4.1 Evidence for diapycnal motion

We wish to consider the extent to which Lagrangian trajectories move along or across isopycnal surfaces. Moreover, we wish to establish whether this is in keeping with our expectations. We consider a simple scaling to establish the magnitude of density changes that we would expect from known processes, against which we can compare the density changes observed along trajectories.

The rate of change of density for a stationary water mass in the presence of vertical diffusion is given by:

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial z} \left(k_z \frac{\partial \rho}{\partial z} \right), \quad (2.1)$$

from which we can derive the scaling:

$$\frac{\Delta \rho}{\Delta t} \sim k_z \frac{\Delta \rho_s}{\Delta z_s^2}, \quad (2.2)$$

where k_z is the vertical diffusivity, and $\Delta \rho_s$ and Δz_s are a typical density variation and depth scale in the local stratification.

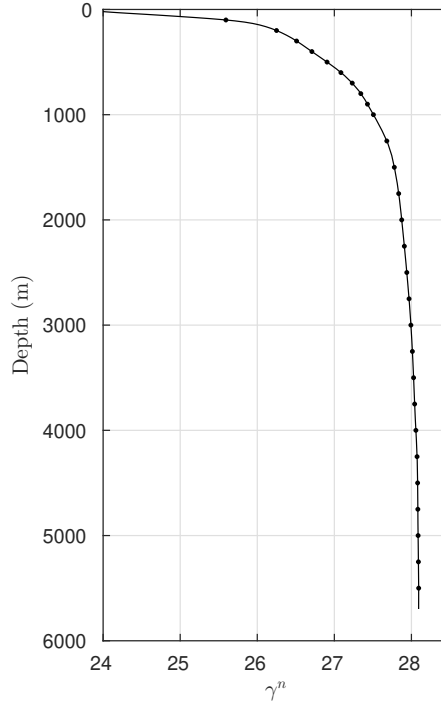


Figure 2.4: Zonal and meridional mean neutral density, γ^n , in the subtropics of the hindcast simulation at the end of June, 2012. Dots indicate the bin spacings used in subsequent histogram analysis.

The background diapycnal (approximately vertical) mixing diffusivity is small, estimated at around $k_z \sim 10^{-5} m^2 s^{-1}$, for most of the quiescent ocean interior (Ledwell *et al.*, 1993). In regions of relatively fast flow over rough topography or areas where there are substantial internal tides, it can reach $k_z \sim 10^{-3} m^2 s^{-1}$ and greater at a considerable height above the bathymetry. Consequently, if we consider the density change along a trajectory as diffusive, we may expect an average k_z on the order of $10^{-4} m^2 s^{-1}$. Indeed, the ocean is thought to require $k_z \sim 10^{-4} m^2 s^{-1}$ to maintain the observed stratification (Munk, 1966).

Figure 2.4 shows the zonally and meridionally averaged density in the subtropical gyre at the end of March 2012 in our simulation. From this we can see that in the thermocline, density varies by around $1 kg m^{-3}$ over $500 m$, while in the deep it varies by around $0.1 kg m^{-3}$ over $1000 m$. So, a value of $k_z = 10^{-4} m^2 s^{-1}$, gives a rate of change of density of $4 \times 10^{-10} kg m^{-3} s^{-1}$ in the thermocline and around $1 \times 10^{-11} kg m^{-3} s^{-1}$ in the abyss. Over 50 years, this translates to a density change of $\sim 0.6 kg m^{-3}$ in the thermocline and $\sim 0.015 kg m^{-3}$ in the abyssal ocean.

We start by considering broad density changes across the North Atlantic basin. At each tracer point in the North Atlantic domain of the primary simulation, we initialise a particle at the end of March, 2012, and evaluate their trajectory backwards in time until they intercept the mixed layer. The mixed layer is defined to be when the particle density is within 0.01 kgm^{-3} of the density at 10 m , following (Thomas *et al.*, 2015). We explore the sensitivity of the analysis to this choice of mixed layer depth in the following section. Results from this experiment (Figure 2.1) were shown in Section 2.3 as motivation for the present work, and are discussed in more detail here.

Figure 2.1 shows a two-dimensional volumetric histogram of the initial and final density of the trajectories in this experiment. In other words, their density in March 2012 and their density when they left the mixed layer, respectively. We adopt a bin width for the histogram to account for the exponential nature of the stratification. To derive this, we take the zonally and meridionally averaged density in the subtropical gyre at the end of March 2012 (Figure 2.4), and interpolate this onto evenly spaced depth surfaces every 100 m . Note therefore, that the x and y axes reflect this exponential binning. We exclude particles that were initialised within or close to the mixed layer, so as to only include particles that have moved around substantially in the subsurface. The volume falling on the 1:1 line has moved isopycnally since leaving the mixed layer (or at least has ended up on the same isopycnal onto which it was subducted). Volume above the 1:1 line has become lighter since subduction, while the volume below the line has become more dense over time.

The volume is spread across the histogram, implying a substantial level of diapycnal motion in the subsurface. In density classes corresponding to the permanent thermocline (γ^n between 26 and 27.5 kgm^{-3}) water appears to have become generally more dense since subduction. It appears that a substantial fraction of the water ventilated in the upper thermocline moves into the deeper parts of the thermocline and indeed deeper still into the ocean abyss. The pattern of density changes in the ocean abyss appears to be more evenly spread, with water moving to/coming from both lighter and denser classes.

The density changes seen in Figure 2.1 are associated with all ventilated particles and so may have emerged over a range of timescales. In Figure 2.5, we separate the volumetric histogram based on particle age (time since subduction) and present the results for four discrete age ranges, which gives an impression of the timescale over which the pattern in Figure 2.1 emerges. The youngest water (panel a) predominantly falls along the one-to-one line, implying little or no diapycnal motion over this timescale. Some water within the lower thermocline (γ^n between 27.1 and 27.7 kgm^{-3}) as well as in the deep ocean shows evidence of more substantial diapycnal motion. Over the subsequent 4 years (panel b), densification within the permanent thermocline emerges, as does the two-way diapycnal motion in the deep ocean, whereby water between $\gamma^n = 27.7$ and 27.9 kgm^{-3} is transported upward into and downward from the lower thermocline. A broadly similar pattern is evident in water aged between 10 and 15 years (panel c). For water aged between 30 and 40 years, the predominant pattern is one of densification within the permanent thermocline and in the deep ocean. In summary, Figure 2.5 implies that the diapycnal motion apparent in Figure 2.1 emerges progressively over time, with the distribution of volume becoming increasingly spread across densities as we consider older water.

We can derive a more complete picture of the movement of water between density classes by considering the fraction in each class that comes from, or moves to, the others. This is displayed in Figure 2.6, in which we cumulatively sum up the columns (left panel) and rows (right panel) of Figure 2.1 and divide by the total volume in that row or column. Consequently, the columns in the left panel of Figure 2.6 correspond to cumulative distribution functions of subduction densities for each density class in March 2012, while the rows in the right panel correspond to cumulative distribution functions of densities in the subsurface for each subduction density class. Solid contours correspond to fractions of 0.1 and 0.9, and the dashed contour corresponds to a fraction of 0.5.

As noted also in Figure 2.1, water present in the thermocline (γ^n between 26 and 27.5 kgm^{-3}) in March 2012 has become more dense over time. As much as 90% of the water in these density classes in March 2012 has come from lighter

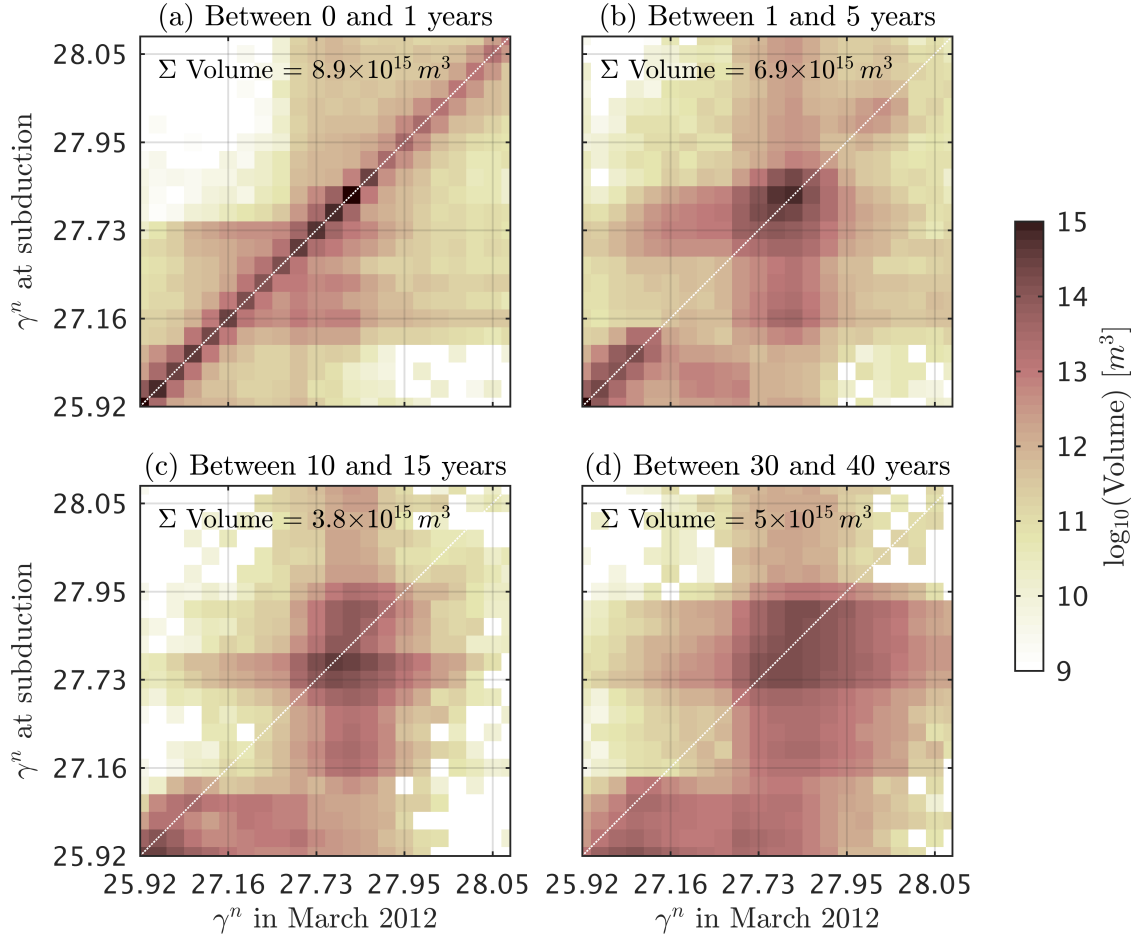


Figure 2.5: Volumetric histogram of subduction density (y -axis) against density in March 2012 (x -axis), as in Figure 2.1, but now with the volume separated based on time since the water subducted. Separation is by ventilation age between (a) 0 and 1 year, (b) 1 and 5 years, (c) 10 and 15 years, and (d) 30 and 40 years. The bin spacing of the histogram is adopted to account for the exponential stratification, such that deeper density classes have smaller bin widths. Note, therefore, that the x and y axes are non-linear. The colour scale is logarithmic. The white dotted line shows the 1:1 line. The total volume associated with the particles in each age class is shown.

classes, and around 50% of this motion is from classes more than $0.5 kgm^{-3}$ lighter. Water subducted into thermocline density classes on the whole moves to denser classes, although 50% stays close to or lighter than its subduction density. The water made more dense is spread over a wide range.

In the deep ocean in March 2012, around $\gamma^n = 27.85 kgm^{-3}$, the distribution of water present that has become lighter or denser over time is reasonably evenly spread, with a slight majority having become more dense. Deeper still, almost all of the water present in March 2012 has come from lighter classes, with more

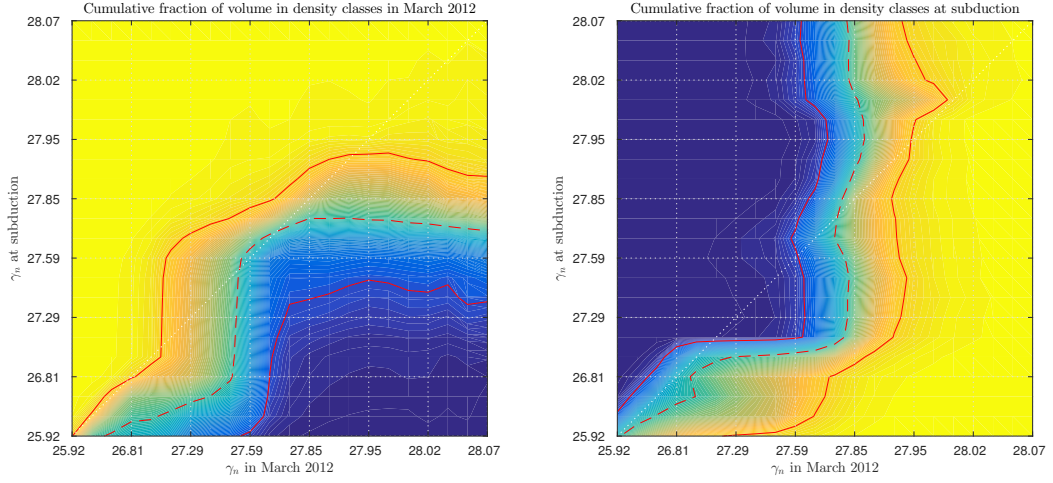


Figure 2.6: Cumulative fractions of water in a particular density class in March 2012 (left panel) or at the time of subduction (right panel) that came from or moves to different density classes. In the left panel, each column is the volumetric cumulative distribution function for the columns in Figure 2.1, and in the right panel, it is the same but for the rows. The colour scale goes from 0 (blue) to 1 (yellow). Contours in red are for the 0.1 and 0.9 levels (solid lines) and the 0.5 levels (dashed line).

than 50% subducting at densities lighter than $\gamma^n = 27.85 \text{ kgm}^{-3}$ and more than 90% from densities lighter than $\gamma^n = 27.9 \text{ kgm}^{-3}$. Considering the movement of water from densities in which they are subducted (right panel) reveals a pattern that pivots around $\gamma^n = 27.85 \text{ kgm}^{-3}$. Water subducted at densities both lighter and denser than this move in their entirety to densities in the range between $\gamma^n = 27.6$ and 27.95 kgm^{-3}

With water of a variety of ages contributing to the picture in Figure 2.1, it is not easy to establish whether the observed density changes are within the range of our expectations, since they occur over different lengths of time. We establish an estimate of the density change rate for each particle in the experiment by dividing the density change by the time since that particle left the mixed layer. This represents a broad average rate of change for each particle, that may or may not be indicative of the density change experienced by the particle at any moment in time. In Figure 2.7, we show the fraction of each density class that has become lighter (red) and denser (blue) over time (panels a and c; note these are equivalent to summing the contributions on either side of the 1:1 lines in the left and right panels of Figure 2.6), as well as the volume-weighted mean density change rate for particles

in that density class (panels b and d). In the upper two panels, the density classes are defined by the particle's density in March 2012 and in the bottom two panel they are defined by the density at subduction. The total mean density change rate (black dashed line in panels b and d) could obscure the signal of large changes of opposing signs, such that we also separate the averages into those of positive (blue) and negative (red) density change rates. The blue and red envelopes correspond to plus and minus the volume-weighted standard deviation, that has been cut off at the origin of the y-axis for clarity. The grey envelope in the background shows the limits of the scaling analysis presented above, taking $k_z = 10^{-4}$ and estimating $\Delta\rho_s/\Delta z_s$ from the subtropical stratification (Figure 2.4).

Figure 2.7 immediately shows a rich structure of diapycnal motion of ventilated water in the ocean subsurface. Considering first the waters present in March 2012, the majority of water in the main thermocline ($\gamma^n = 25.89$ to around 27.5 kgm^{-3}) has become more dense since subduction (panel a). In the upper thermocline ($\gamma^n < 27.17 \text{ kgm}^{-3}$), these changes occur at rates that are within the range of our scaling analysis, but exceed it in the lower thermocline (panel b). At the base of the thermocline and into deeper water (from around $\gamma^n = 27.5$ to 27.8 kgm^{-3}) there is a shift in the origin of the water mass such that the majority (up to 75%) has come become lighter over time, arriving from denser classes (panel a). In the denser classes of this range, the rate of lightening falls close to the upper bound of the scaling analysis (panel b). Denser still ($\gamma^n > 27.81 \text{ kgm}^{-3}$), there returns a dominance of waters that have become denser since subduction, at rates exceeding the bounds of the scaling analysis. At densities greater than $\gamma^n = 27.96$, around 95% of water has been subducted at lighter densities and become more dense over time.

The bottom two panels of Figure 2.7 show the fate of water subducted into each density class. There is an overall structure, centred around $\gamma^n \approx 27.83$, with water subducted lighter than this mostly becoming more dense over time and water subducted denser than this mostly becoming more dense over time. In the upper thermocline, lighter than $\gamma^n \approx 26.5$, the rates of density changes are within the limits implied by our scaling analysis, but exceed them elsewhere. Notably, water

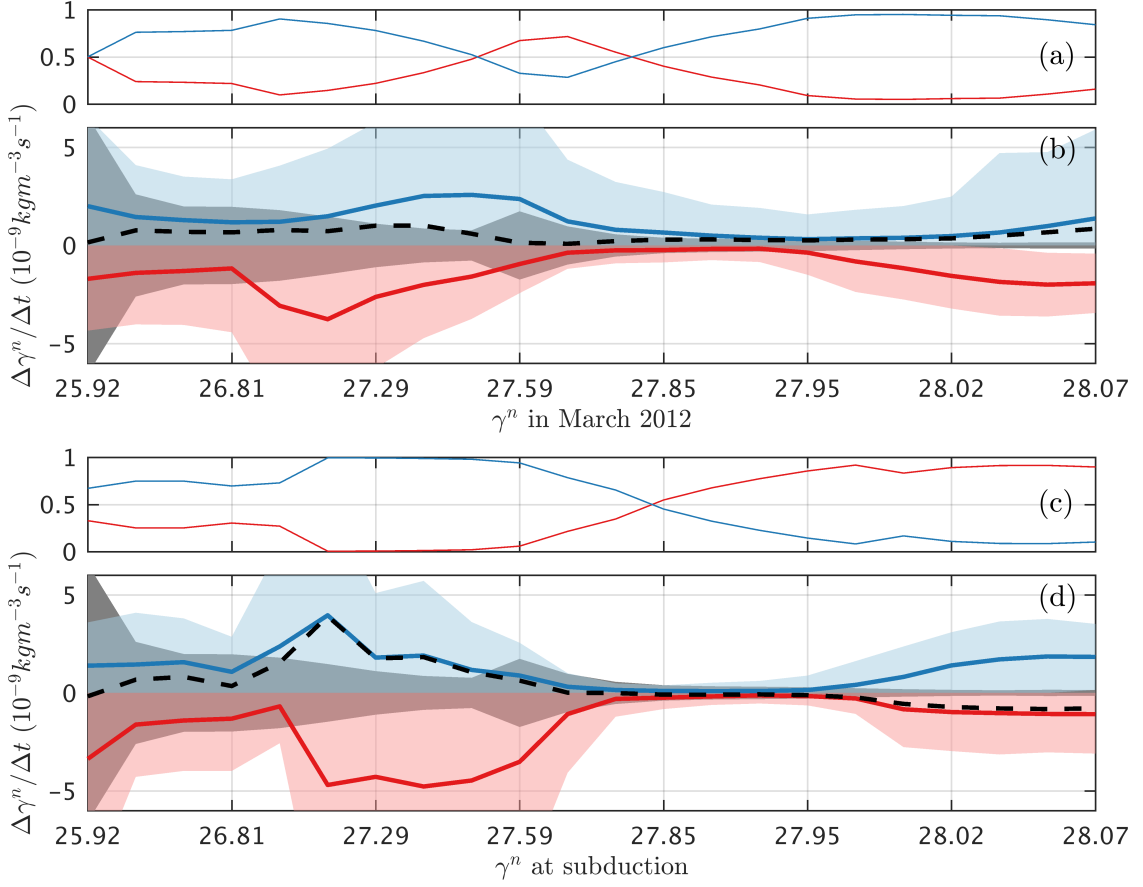


Figure 2.7: (a and c) The fraction of particles in each neutral density class that became less dense (red) or more dense (blue) since subduction into the subsurface. (b and d) The average rate of change of neutral density of particles (evaluated as the density at the end of March 2012 minus the density at subduction, divided by the particle age) in each density class. The black dashed line corresponds to the average for all particles. The blue and red lines correspond to the average for positive (blue) and negative (red) density changes, with transparent envelopes corresponding to ± 1 standard deviation (limited to not cross the origin of the y -axis for clarity). The grey envelope corresponds to the limits of the scaling analysis detailed in Section 2.4.1 utilising the stratification in Figure 2.4. In the upper two panels, particles were categorised based on their density in March 2012. In the bottom two panels, particles were categorised based on their density at subduction.

subducted in the deep ocean density classes, $\gamma^n \approx 27.7$ to 27.96 kg m^{-3} , experience density change rates that fall within or close to expected bounds.

To summarise the findings of this experiment, we find that water in the ocean subsurface experiences substantial diapycnal motion, with the direction of this motion showing some large-scale structure. Water in the upper thermocline and the deep and abyssal ocean has generally subducted in lighter classes and been made more dense over time. In the lower thermocline and intermediate density classes,

the opposite is true, with water arriving from denser classes. Considering things from the perspective of subducted watermasses, we find that those ventilated into the thermocline and intermediate water generally become more dense over time, while those subducted into the deep and abyssal ocean become lighter. Rates of density change generally exceed the bounds of a simple scaling analysis for the rates that would be expected from long term background diffusion, except in the upper thermocline as well as for the lightening of water in the deep ocean and for the changes associated with the water subducted into the deep ocean density classes.

We wish to establish the locations where the density changes, evident from the broad ventilation analysis presented above, take place. To do this, we initialise particles in regions of the subtropical and subpolar gyre throughout the water column in June, 1982, and run them forwards in time for 30 years, evaluating their location and density every 5 days. Particles are again stopped when they enter the mixed layer (same definition as above). The locations of these initialisations, along with maps of the pathway probability for particles that are initially in two density ranges (corresponding to regions of the thermocline and deep ocean), can be seen in Figure 2.8. Pathway probabilities are calculated by counting the number of crossing of particles across each grid cell and dividing by the total number of crossings. We see that particles released in the thermocline spread westward from the ocean interior and are advected northward in Gulf Stream and North Atlantic Current. For the deep ocean density class, particles initialised in the subtropics again move westward to the edge of the basin where they are advected southward in the Deep Western Boundary Current. Particles initialised in the subpolar region spread throughout the subpolar gyre and are exported southward by a broad range of pathways. Relatively few trajectories are observed in the Labrador Sea, since particles entering this region are often re-entrained to the surface mixed layer.

First, we consider whether particles in these experiments do indeed experience diapycnal motion akin to that of the previous analysis. Figure 2.9 shows the mean and standard deviation of density over time, for particles initially within particular density ranges. We show the two density ranges considered above, as well as two

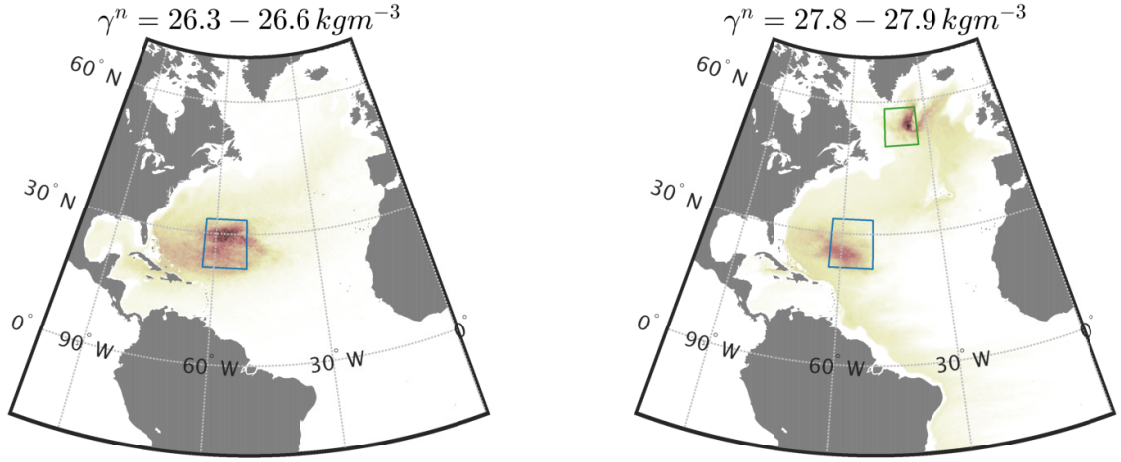


Figure 2.8: Pathway probabilities (number of particles crossing each grid cell divided by the total number of crossings) for particles initialised in two neutral density volumes in the subtropical and subpolar gyres on 30th June, 1985. The neutral density range is shown above the figure. The initialisation locations are shown by the blue (subtropical) and green (subpolar) boxes. The lighter neutral density volume is not present in the subpolar gyre.

other ranges in the thermocline and deep ocean. In the thermocline, after the first few years of relatively little change, the mean density starts to increase, coincident with an increase in the standard deviation. The increase in mean density is initially more rapid in the lighter density class, but rates of increase converge at long times. The mean density continues to decrease throughout the thirty years of the experiment, while the increase in the standard deviation stops after around 5 years in the upper thermocline, and between 15 and 20 years in the lower thermocline.

For the deep ocean density classes, we separated the particles into those released in the subtropical and subpolar regions. Overall, the changes in mean density are more marked for particle released in the subpolar gyre. In the lighter classes, the mean density stays roughly constant for several years before increasing. On the deeper surface, a change in mean density is occurs from the start of the simulation and is of the opposite sign, with particles becoming lighter on average. For particles initialised in the subtropics, the mean density barely changes in the lighter density class, but the standard deviation increases notably. In the denser class, the sign of changes is the same as that of the subpolar initialisation, with density decreasing over time.

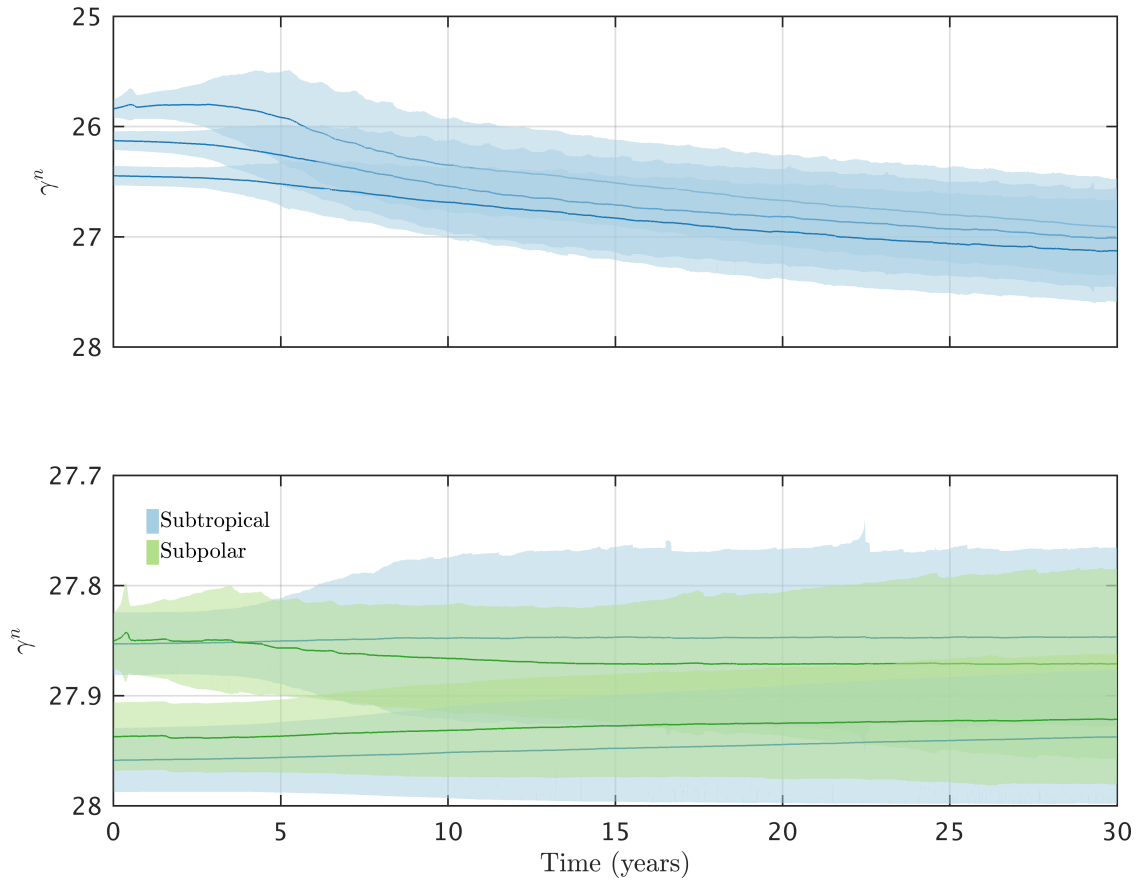


Figure 2.9: Evolution over 30 years of the mean density of particles that are initially within a certain density range. In the top panel are densities corresponding to the upper ocean and thermocline. In the bottom panel are densities for the deep ocean. For the deep ocean density classes we separate particles into those initialised in the subtropical (blue) and subpolar (green) regions. Transparent envelopes in both panels correspond to ± 1 standard deviation around the mean.

To establish where density changes are taking place, we calculate the mean rate of change of density ($\partial\gamma^n/\partial t$) of the particles crossing each grid cell (Figure 2.10). The approach is not comprehensive, since a different number of particles will have passed through each box, and there is an inherent time sampling bias due to the fact that particles are initialised at a specific moment. However, it provides a qualitative perspective on where density changes occur. Note that a component of this spatial pattern is likely to be associated with local density changes, as discussed in the previous section, and therefore not a contribution to the global diapycnal motion seen in the previous figures. We address this issue below. Note that Figure 2.10 displays both positive (blue) and negative (red) rates of change on a logarithmic scale.

For particles initialised in the thermocline, the Gulf Stream immediately stands out as a region of relatively large density changes, of order $10^{-6} \text{ kg m}^{-3} \text{ s}^{-1}$. Furthermore, there is a strong spatial structure, with particles becoming lighter on the shoreward flank, and denser on the oceanward flank. Following separation from the coast, substantial changes of both sign persist, but regions of densification (blue) are more widespread, particularly off the Canadian coast at around 45°N . The dominance of negative density changes persists into the subpolar gyre. Everywhere, the ocean boundaries stand out as regions of substantial and structured diapycnal motion, particularly around the Gulf of Mexico and the Strait of Gibraltar. The region off the coast of Africa, around 15°N , although frequented by only a limited number of particles, shows a broad pattern of lightening.

For the deep ocean particles, rates of density changes are lower, as would be expected. Nevertheless, there is a pattern that highlights the dominance of ocean bathymetry in diapycnal motion. Notably, the mid-Atlantic Ridge emerges in this figure as a region of marginally elevated diapycnal motion. In the Labrador Sea, particles becoming lighter in the central region could be suggestive of an imperfect mixed layer definition that allows particles to be affected by convective events. Around the boundary, the largest rates occur in the north, with particles becoming more dense in the very inshore region, lighter within the core of the current and denser further offshore. In the eastern subpolar region, diapycnal motion is relatively high just to the south of the Greenland-Scotland ridge, and appears positive in sign close the ridge bathymetry itself and negative to the south and west. Further south, in the Deep Western Boundary Current, particles on the whole become lighter in the inshore areas, although the pattern is highly variable and confined to a width of only one or two grid cells. The region around the Gulf Stream, north of 30°N again stands out as one of relatively large rates of diapycnal motion.

Widespread lightening of water close to topography is consistent with the perspective that most ocean upwelling, particularly from the deep ocean, occurs close to boundaries (Garrett *et al.*, 1993; Ferrari *et al.*, 2016). This upwelling is the result of mixing-derived buoyancy forcing in the presence of a sloping boundary

(Armi, 1978; Garrett, 1990). Furthermore, nearby offshore downwelling, evident in the densification of particles that can be seen across much of the thermocline and deep ocean, is also consistent with this perspective (McDougall and Ferrari, 2017)

To examine the extent to which the magnitude and pattern of density changes in Figure 2.10 is due to local diapycnal motion, we repeat the analysis for density changes observed over 20 days (Figure 2.11). Under the assumption that the imprint of non-cumulative local diapycnal motion will decrease with averaging time, persistence of patterns supports the role of these features in longer timescale diapycnal motion. Since particles move further over 20 days, the spatial information will be somewhat eroded. In the thermocline, the magnitude of density changes within and north of the western boundary are marginally reduced. On the other hand, the prominence of density increases (blue colours) is more widespread in the Loop Current of the Gulf of Mexico, along the Gulf Stream and off the coast of the Grand Banks and into the subpolar gyre. In the deeper volume, notable differences are apparent in the Labrador and Irminger Sea where density changes do not persist when considered over 20 days. Furthermore, on the western boundary, a previously noisy pattern becomes well defined, with persistent regions where particles become lighter or denser.

It is not evident from any of the previous analysis whether the density changes experienced along trajectories accumulate over a long period of time, or whether they are sudden. The magnitude of the rate of change of density in Figures 2.10 and 2.11 implies that the latter is true in certain localised regions. In Figure 2.12, we show the progression of density for a random subset of particles that are initially within the thermocline (top panel) and the deep ocean (bottom panel). This provides a qualitative impression of the timescales over which density changes occur. What is perhaps most informative about this figure is that there is no one single manner in which these density changes occur. Some particles change density in discrete jumps of as short as one timestep (5 days) but often longer, others exhibit substantial changes over periods of a few years, while others accumulate smaller

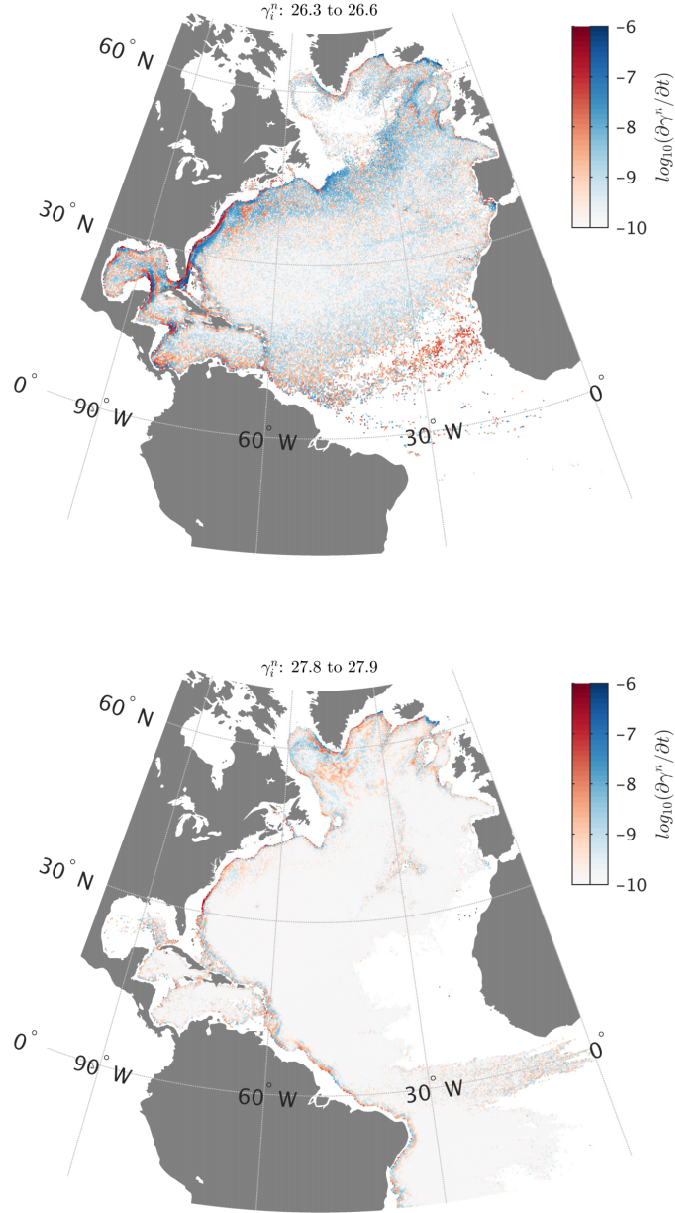


Figure 2.10: Average rate of change of density, $\partial\gamma^n/\partial t$, for particles crossing each grid cell. The rate of change of density is derived from the difference in density every 5 days along the Lagrangian trajectory. The location of the density change is attributed to occur at the mean latitude and longitude along that 5 day path. Only information for grid cells with more than 10 crossings are shown. The colour scale is logarithmic for both positive (blue) and negative (red) density changes. The two neutral density volumes correspond to those in Figure 2.8 and are representative of patterns in the thermocline (upper panel) and deep ocean (lower panel).

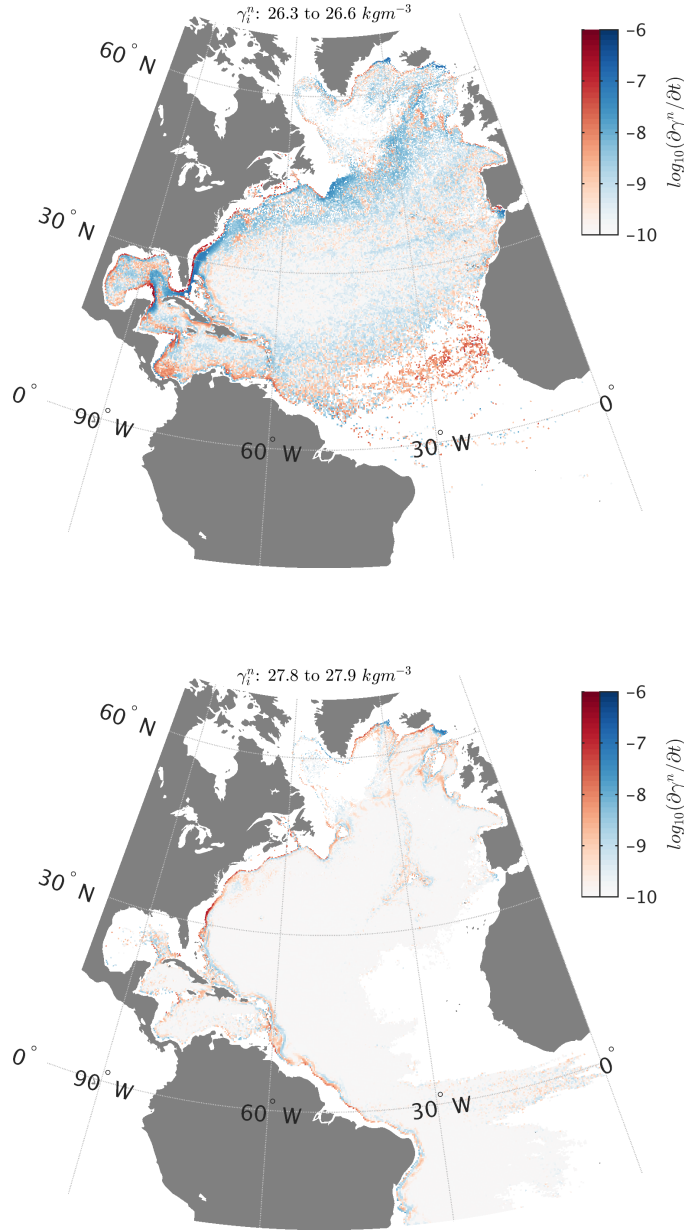


Figure 2.11: As for Figure 2.10, but evaluating changes over a 20 day period. Average rate of change of density, $\partial\gamma^n/\partial t$, for particles crossing each grid cell. The rate of change of density is derived from the difference in density every 20 days along the Lagrangian trajectory. The location of the density change is attributed to occur at the latitude and longitude of the trajectory at 10 day mark. Only information for grid cells with more than 10 crossings are shown. The colour scale is logarithmic for both positive (blue) and negative (red) density changes. The two neutral density volumes correspond to those in Figure 2.8 and are representative of patterns in the thermocline (upper panel) and deep ocean (lower panel).

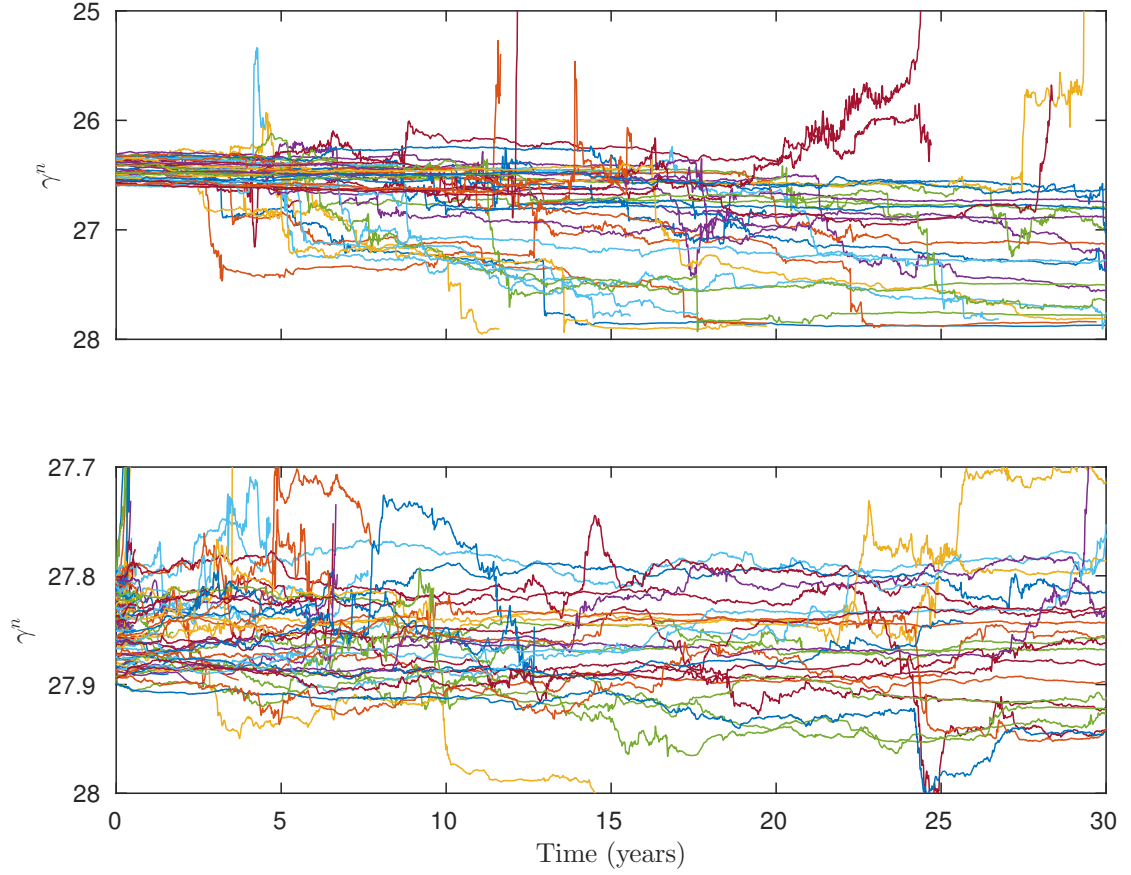


Figure 2.12: The change in density over time for a random sample of trajectories in (top panel) the subtropical thermocline and (bottom panel) the deep ocean in the subpolar region. Colours are random.

density changes over decadal timescales. Furthermore, there is no clear distinction in the manner of these changes between the thermocline and the deep ocean.

2.4.2 Exploring sources of diapycnal motion

The qualitative results of these experiments suggest that particles experience subsurface density changes that are large relative to what we would expect in an ocean with realistic levels of vertical diffusion in the subsurface. Furthermore, these density changes appear to have a systematic spatial structure on a basin and local scale. We explore possible explanations for the root cause of these density changes. We focus particularly on the mixed layer definition and use of time-average velocity fields in the trajectory calculation, as well as making some observations of the levels of explicit mixing in the model subsurface.

In our Lagrangian calculation, we attempt to define the subsurface as the depth below which water does not experience the explicit forcing that characterises the surface mixed layer. There are a number of possible ways to define the surface mixed layer (de Boyer Montégut *et al.*, 2004), based on stratification and mixing criteria. We choose to define the depth of the mixed layer as being where the density is within 0.01 kgm^{-3} of the density at 10 m . It is possible that this definition is insufficient to capture the depth down to which mixing takes place in the model. Furthermore, deriving the mixed layer depth from 5-day average density field means that temporal variations in the depth of mixing could be missed. Consequently, particles that are in the subsurface according to our definition, may in fact still be moving through regions of elevated mixing associated with surface ocean forcing.

Evidence of this potential is provided in Figures 2.13 and 2.14 in which we show the vertical mixing coefficient (k_z ; elevated in regions of substantial mixing to homogenise the properties of the water column, replicating convection) at the end of March and the end of June, respectively, in 2012. In the upper panel of each figure, we show the value of k_z two grid points below a mixed layer based on our definition. In the middle and bottom panels we show a zonal and meridional section of the upper $\sim 500 \text{ m}$ of the water column. These sections are overlain with white lines corresponding to different mixed layer definitions. Our standard definition is the solid line and a broader density difference criteria of 0.1 kgm^{-3} is shown as a dashed line. A third mixed layer depth is defined from elevated levels (greater than $k_z = 10^{-4} \text{ m}^2 \text{ s}^{-1}$) of the vertical diffusivity coefficient itself (also output from the simulation as a 5-day average). Since this coefficient can be elevated close to bathymetry (discussed in more detail later), we set a broad density criteria (within 0.4 kgm^{-3} of the density at 10 m) to ensure that we capture upper ocean vertical mixing. Black contours correspond to surfaces of neutral density at 0.25 kgm^{-3} intervals.

Focussing on the late March picture initially, it is clear that the standard definition of the mixed layer depth does not capture the full depth down to which mixing occurs. This is particularly evident from the plan view, where there are

vast regions of elevated mixing (values as large as $k_z = 1 \text{ m}^2 \text{ s}^{-1}$) in what we define as the subsurface, most notably across the subtropical gyre. Similarly in the zonal section, we see that the region of elevated vertical mixing extends up to 100 m below this depth. Broadening the definition of the mixed layer captures the majority of this elevated mixing, with levels below being closer to the background level of $k_z = 1.2 \times 10^{-5} \text{ m}^2 \text{ s}^{-1}$

In summer, there remain large regions of elevated k_z below our standard mixed layer definition, albeit smaller in magnitude and extent than was the case in winter. Focussing on the zonal and meridional sections, elevated mixing (on the order of $k_z \sim 10^{-4} \text{ m}^2 \text{ s}^{-1}$) persists over large regions of the well stratified seasonal thermocline, as much as 100 m below the surface. Even broadening the mixed layer density difference criteria to 0.4 kg m^{-3} does not capture all of this region. Thus it appears to be a subsurface signature, removed from surface forcing. Its spatial pattern, consistent with the depth of the late winter mixed layer depth, suggests that it is a remnant of the mixing associated with the previous winter.

We examine the sensitivity of the density changes observed in the experiments above to the definition of the mixed layer. In Figure 2.15, we reproduce the result in Figure 2.7, but now with the broader definitions of the mixed layer introduced above. Despite the seemingly large impact of changing the mixed layer depth on the isolation of regions of elevated vertical mixing, changing the mixed layer definition appears to have little effect on the patterns and magnitude of mean rates of change of density in the experiment.

The use of time-averaged fields is commonplace in offline studies of tracer and particle evolution in numerical models. The implicit assumption is that correlations in volume, temperature and salinity transports on timescales less than the averaging timescale are unimportant. This of course, depends inherently on the model dynamics (a high resolution model will have more short timescale variability than a low resolution model), while the assessment of what qualifies as important or not depends on the research question being addressed. Studies adopting Lagrangian trajectories will often assess the sensitivity of their results to the use of time-average

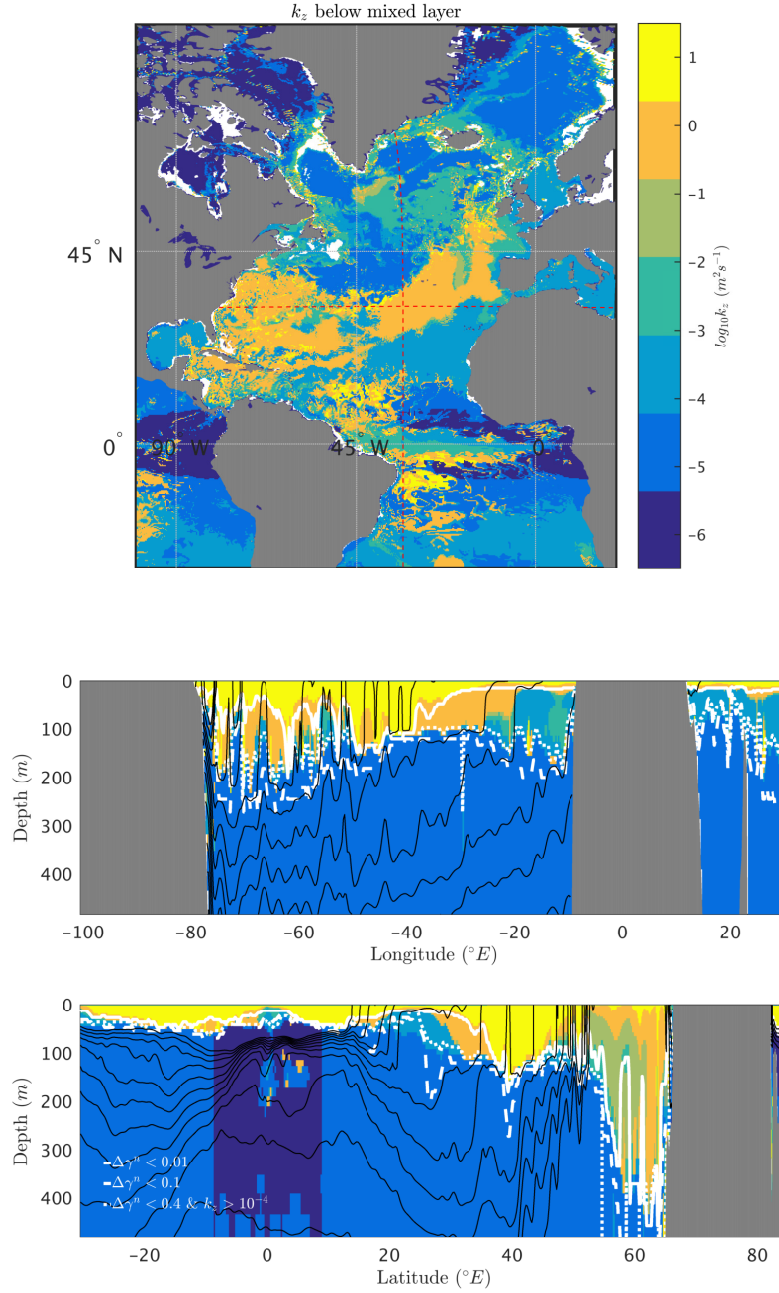


Figure 2.13: Coefficient of vertical diffusion, k_z , from the Eulerian model output at the end of March 2012. (top panel) k_z two vertical velocity grid points below the mixed layer depth, as defined by a density difference criteria of 0.01 kgm^{-3} . (middle panel) Zonal section of k_z . (bottom panel) Meridional section of k_z . The colour scale for all plots is logarithmic. On the middle and bottom panels, white lines correspond to mixed layers as determined by different criteria: (solid line) density difference criteria of 0.01 kgm^{-3} ; (dashed line) density difference criteria of 0.1 kgm^{-3} ; (dotted line) joint vertical diffusivity coefficient and density difference criteria. Black contours correspond to density intervals of 0.25 kgm^{-3} between $\gamma^n = 25$ and 27.5 kgm^{-3} . The location of the zonal and meridional section are shown by the red dotted line in the top panel.

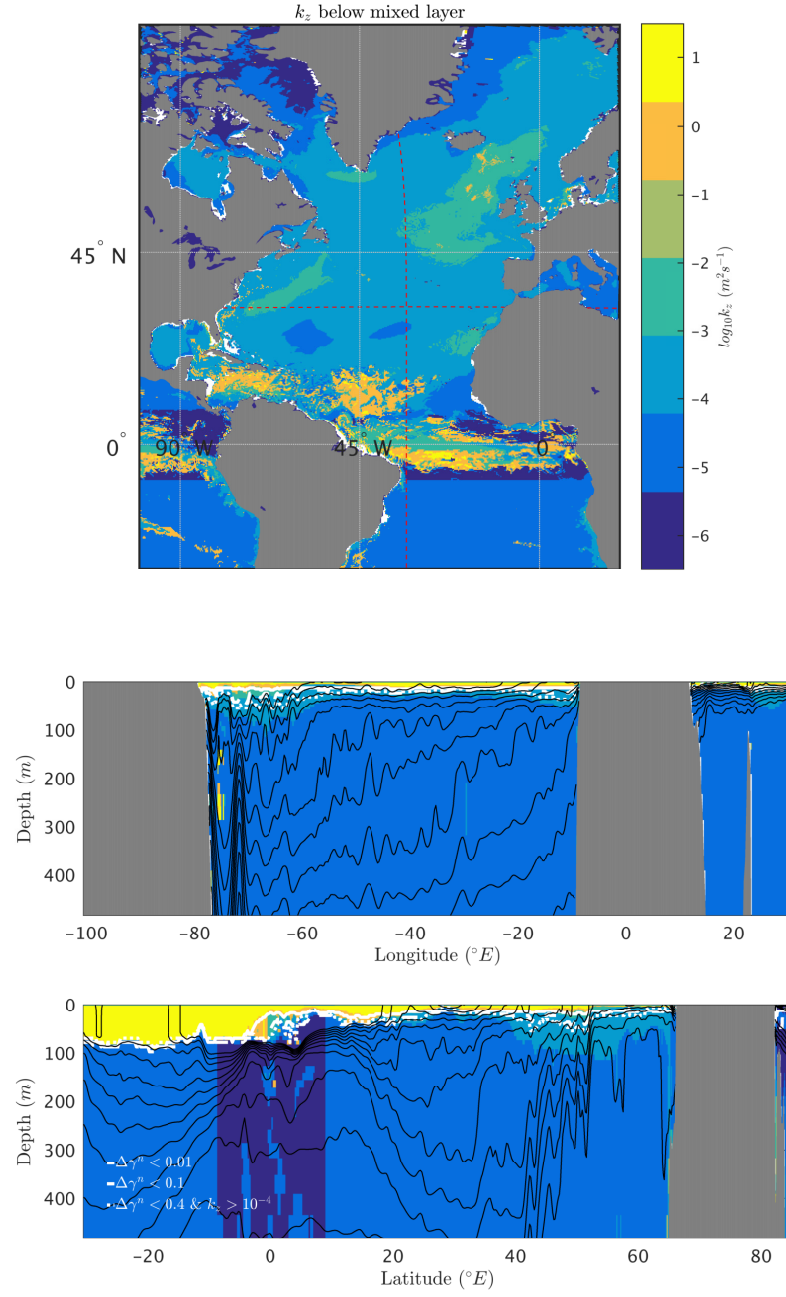


Figure 2.14: As for Figure but at the end of June, 2012.

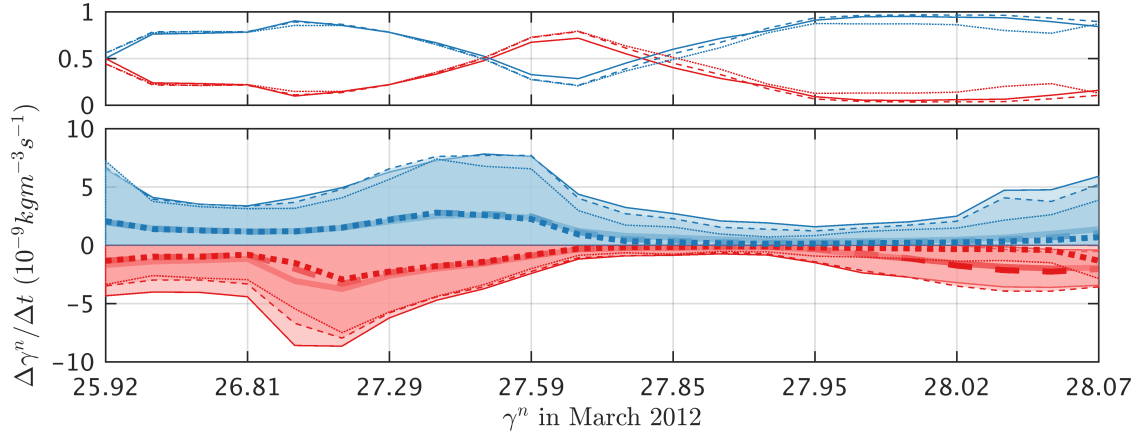


Figure 2.15: As for the upper two panels in Figure 2.7, now showing results corresponding to experiments using different mixed layer definitions: (solid line) density difference criteria of 0.01 kg m^{-3} ; (dashed line) density difference criteria of 0.1 kg m^{-3} ; (dotted line) joint vertical diffusivity coefficient and density difference criteria. (upper panel) The fraction of particles in each neutral density class that became more dense (red) or less dense (blue) since subduction into the subsurface. (lower panel) The average rate of change of neutral density of particles in each density class (evaluated as the density at the end of March 2012 minus the density at subduction, divided by the particle age). Blue and red lines correspond to the average for positive (blue) and negative (red) density changes, with transparent envelopes corresponding to ± 1 standard deviation (limited to not cross the origin of the y -axis for clarity). Density class bin widths are defined based on the stratification in Figure 2.4, such that the x -axis is non-linear.

velocity fields (*e.g.* Chenillat *et al.*, 2015). However, there has been no systematic study of the impact of using time-average fields on the diapycnal motion of particles and inferred water mass transformations.

We perform a series of experiments to assess the impact of time-averaging on the diapycnal transport of trajectories. For this purpose, we use the Gulf Stream-centred subdomain of the Arctic-Atlantic sector model described in Section 2.2, for which we have velocity fields and potential density at the model timestep (720 seconds) and subsampled to 5 day means. We initialise particles on tracer points throughout the domain at five day intervals during June, 2006, and evolve them forwards in time for five days. To avoid the complicating factor of local diapycnal motion, we do not assess differences in density changes directly. Instead we focus on discrepancies in the pathways of particles evolved using 5-day average velocities fields and those using timestep velocity fields.

Figure 2.16 shows the difference in the vertical position of particles after 5 days,

gridded on the initial location of the particle. We are showing here the difference for particles initialised at 00:00 on the 5th June. Isopycnals of the 5-day mean density field are overlain. Immediately apparent is the presence of large discrepancies in the thermocline, along the path of the Gulf Stream as it flows along the North American coast. Differences in the depth of particles are greater than 150 *m* in places, with particles evolved with 5-day means ending up both shallower and deeper than timestep-evolved particles. Large differences are apparent for particles initialised within detached eddies (apparent from the closed isopycnal contours in the constant-depth sections), with this signature extending almost to the seafloor. There is an indication of consistent structure of the depth differences within these eddies, with particles initialised in the core of the eddy ending up shallower when evolved with 5-day mean velocities, and those on the outside ending up deeper.

The large differences in depth observed in Figure 2.16 indicate that the use of time-average velocity fields has a significant impact on particle pathways. We wish to establish if such errors are cumulative, or if opposing vertical excursions cancel out over time. To do so, we evolve particles forward from 00:00 on the 1st June, for one month, outputting the vertical location of the particle every 2 days. The mean and standard deviation of the depth difference between 5-day particles and timestep particles is shown in Figure 2.17, where we have plotted positive and negative differences separately. We plot averages in different density classes separately, but not that the broad results are consistent across all classes. The mean difference increases over time for both positive and negative differences. After one month, particles are an average of ~ 20 *m* apart, with a broad standard deviation. Looking at individual particles reveals that some trajectories can end up as much as 1000 *m* apart in depth after a month.

While the cumulative differences in depth indicate a substantial contribution toward diapycnal motion from the use of time-average velocity fields, both the domain and timescale of this simulation are limited. Storing output at the model timestep over a larger domain or for long times is not practical. Thus, we explore further the impacts of velocity field time-averaging by subsampling the North

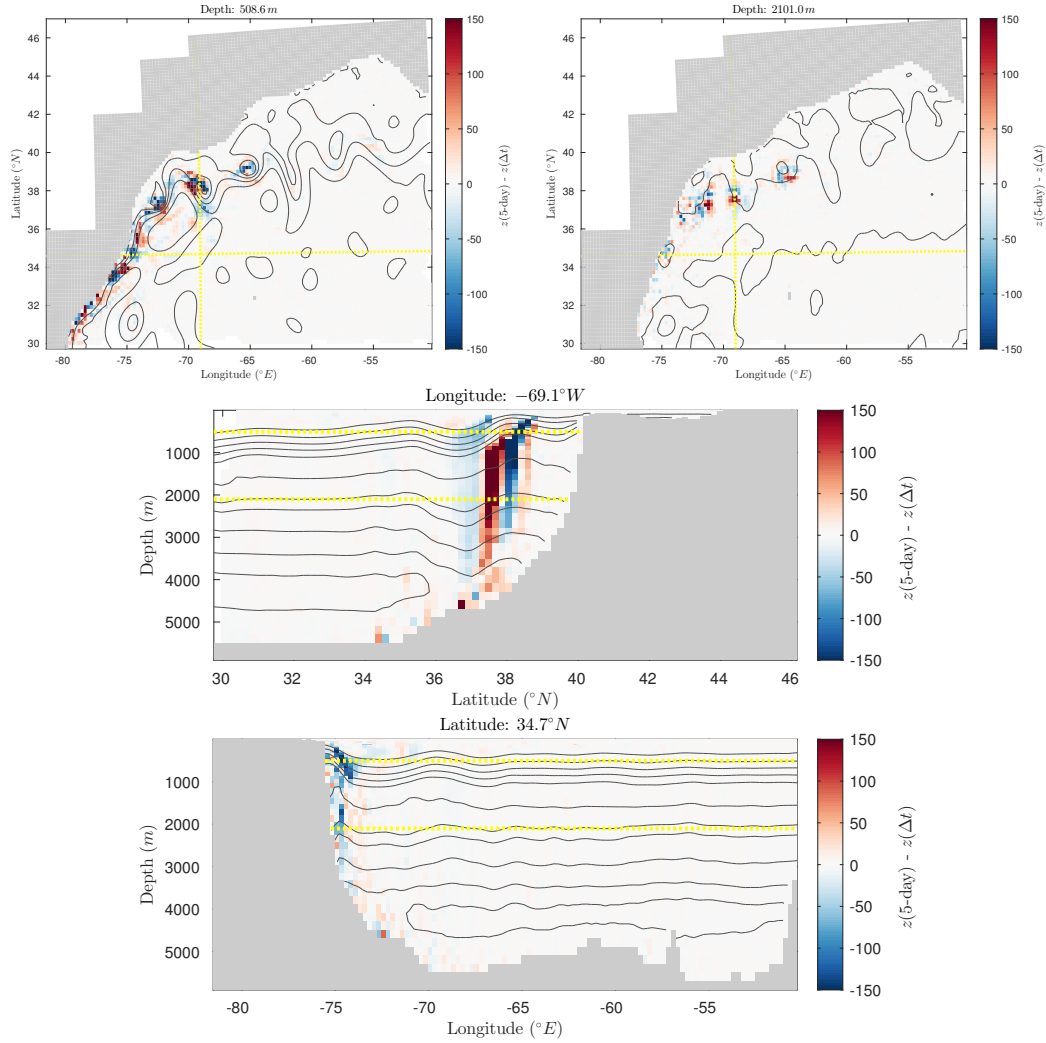


Figure 2.16: Difference in the depth of particles after 5 days when evolved using the 5-day average velocity field, $z(5\text{-day})$, and the velocity field output at the model time-step, $z(\Delta t)$. Particles were initialised at 00:00 on 5th June, 2006, at each tracer point in the Gulf Stream domain of the Arctic-Atlantic mode. Differences are plotted on the particles initial position and shown for two depth surfaces (top panels) and a meridional (middle panel) and zonal (bottom panel) section. Contours of the 5-day average potential density (referenced to the surface) are shown in black. Contour spacing is derived from the mean stratification, taking values every 200 m in the upper 1000 m and every 500 m below that. Yellow dotted lines show the locations of each intersecting section.

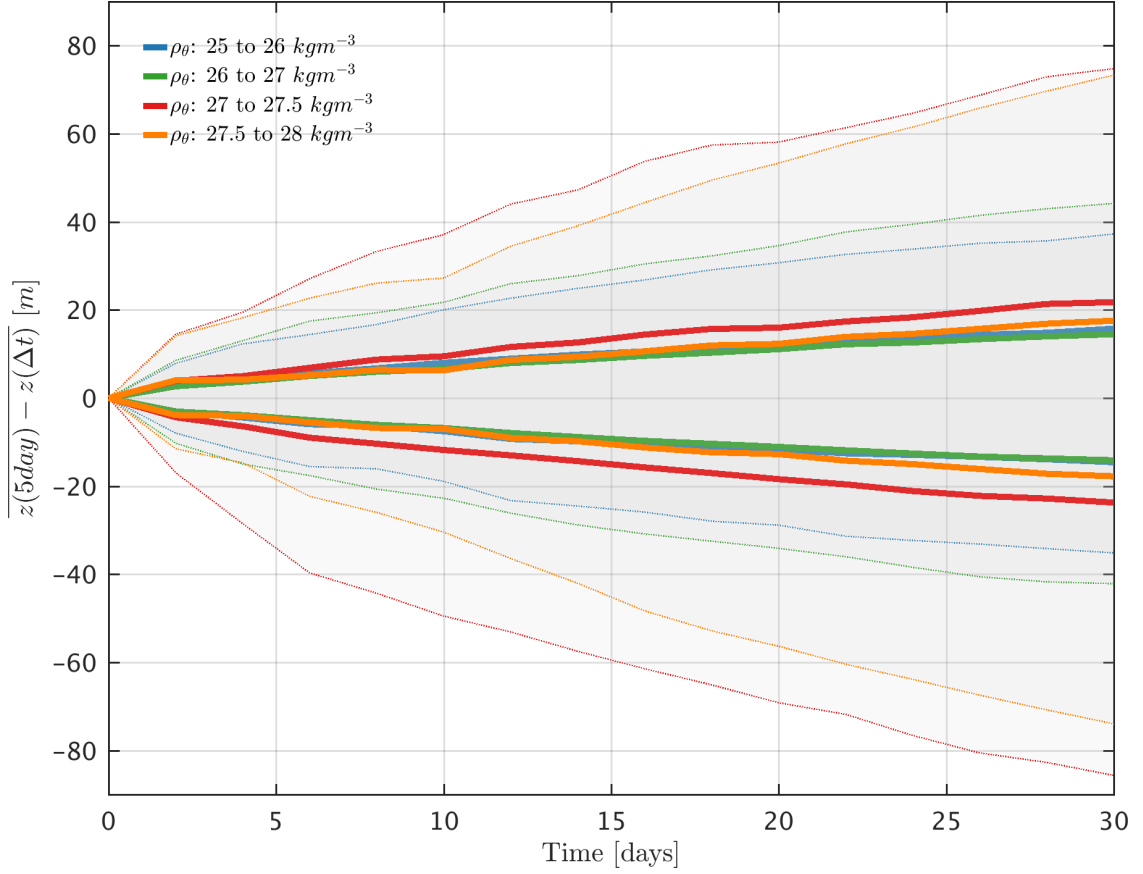


Figure 2.17: Time evolution of the mean difference in depth between trajectories evaluated using 5-day average velocity field and model timestep velocity field, initialised on each tracer point at 00:00 on 1st June, 2006, and evolved forward in time for one month. Positive and negative changes are averaged separately. The trajectory position is output every two days, and the mean (solid line) and standard deviation (grey envelope bounded by thin line) of the difference in depth is determined. Particles are separated into groups based on their initial potential density, ρ_θ , in the 5-day mean density field.

Atlantic domain of the 52-year hindcast simulation, from 5-day to 15-day averages. As for the mixed layer depth sensitivity analysis, we reproduce Figure 2.7 — the mean density change over the lifetime of particles — now with trajectories evaluated using 5-day and 15-day average velocity and tracer fields. This is shown in Figure 2.18. Patterns and magnitudes are broadly similar for the 5-day and 15-day experiments. There is a very slight increase (when the 15-day average fields are used; dashed line) in the magnitude of mean density changes for particles in the thermocline that become more dense over time, coincident with a notable increase in the standard deviation in these same density classes.

Having explored potential sources of error in the Lagrangian trajectory calcula-

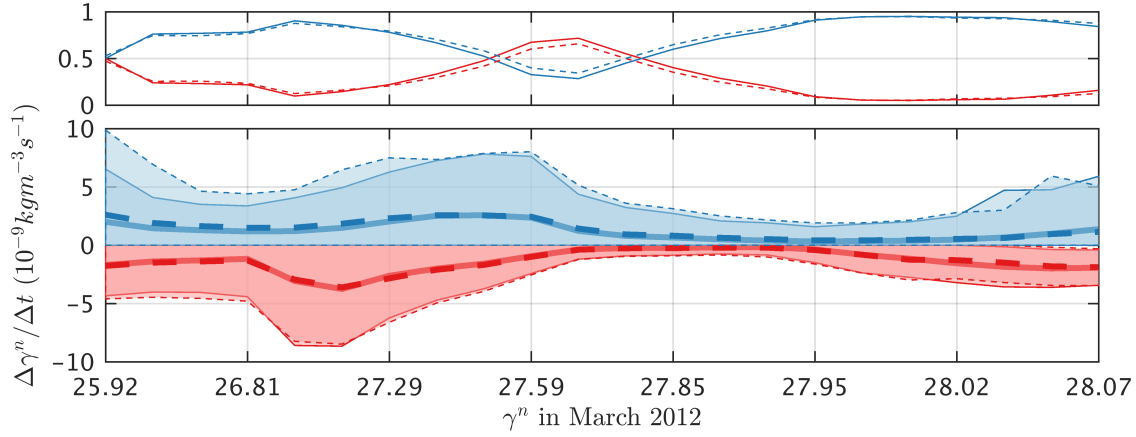


Figure 2.18: As for the upper two panels in Figure 2.7, now showing results corresponding to experiments using 5-day (solid line) and 15-day (dotted line) mean velocity and density fields. (upper panel) The fraction of particles in each neutral density class that became more dense (red) or less dense (blue) since subduction into the subsurface. (lower panel) The average rate of change of neutral density of particles in each density class (evaluated as the density at the end of March 2012 minus the density at subduction, divided by the particle age). Blue and red lines correspond to the average for positive (blue) and negative (red) density changes, with transparent envelopes corresponding to ± 1 standard deviation (limited to not cross the origin of the y -axis for clarity). Density class bin widths are defined based on the stratification in Figure 2.4, such that the x -axis is non-linear.

tion, we now consider sources of diapycnal motion in the simulation itself. The best hope of resolving model-derived diapycnal motion, in the absence of Lagrangian trajectory errors is through the analysis of trajectories evolved for as long as possible using velocity field at the model timestep. Results from these trajectories were previously presented in Figure 2.17 in relation to the accumulation of pathway errors for the 5-day velocity fields. While the density changes associated with this experiment may still be affected by Lagrangian calculation errors, such as from piece-wise timestepping and interpolation of velocity and tracer fields, it is our best estimate of *true* volume pathways through the model and diapycnal motion therein.

A two-dimensional histogram of the rates of change of density over one month, separated into different density classes, is shown in Figure 2.19. The colour represents the probability that particles in that class underwent density change of that magnitude, and rates of change have been separated into positive and negative changes. Overlain are scaling-derived estimates for vertical diffusion with $\log_{10}(k_z) = -3, -4$ and $-5 \text{ m}^2 \text{ s}^{-1}$, and taking the mean stratification within the

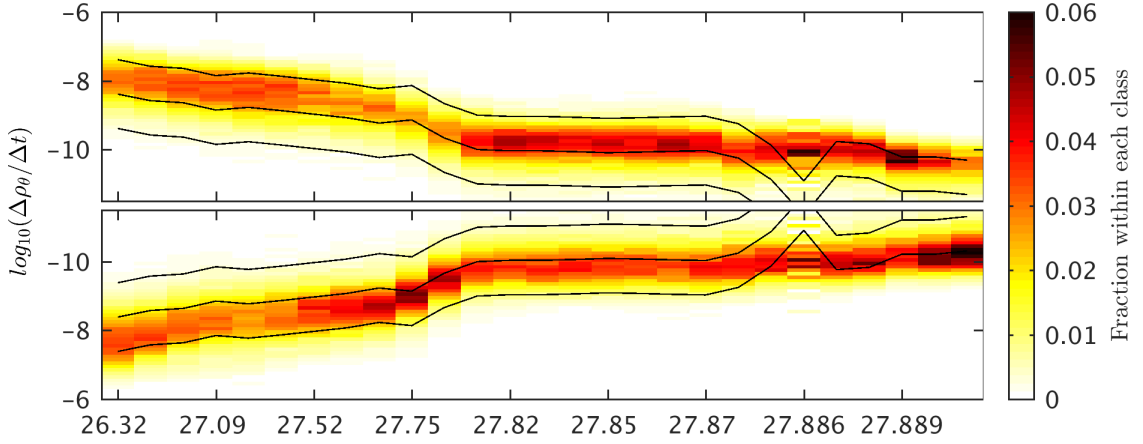


Figure 2.19: Two-dimensional histogram of the rate of density change (evaluated as the difference between the final and initial density, divided by one month) experienced by particles initialised in different density classes, evolved using the velocity field output at the model timestep. Particles were initialised at each tracer point at 00:00 on 1st June, 2006, and evolved forward in time for one month. Positive density changes are grouped in the top panel and negative density changes are grouped in the bottom panel. The y -axis is on a logarithmic scale. The colour scale corresponds to the fraction of each density class that undergoes different magnitudes of the rate of density change, such that each column sums to 1. The bin width of density classes is determined to account for the exponential stratification, such that the x axis is non-linear.

domain. This could be slightly misleading since, as we have seen, most of the density changes occur in the energetic boundary current along the coastline, and in eddying motions, where the stratification is often weaker. In spite of this, we see that most density changes, throughout all density classes, are substantially larger than what would be expected from the background diffusion.

The dominant source of explicit diapycnal mixing in the model is through the implementation of vertical diffusion. In the model, when surface forcing and/or velocity shear act to perturb the static stability of the water column, the magnitude of the diffusivity coefficient increases (over a depth scale that is also a function of the background fields) until stability is restored (Madec, 2008). This is the process behind the parameterisation of convection at the ocean surface. The role of velocity shear however, means that diffusion can also be increased close to the frictional bathymetric boundary, particularly in the deep ocean where stratification is weak. This can be seen in Figure 2.20 where we show the diffusivity coefficient one grid cell above the bathymetry, at the end of June 2012. Bathymetric features, such

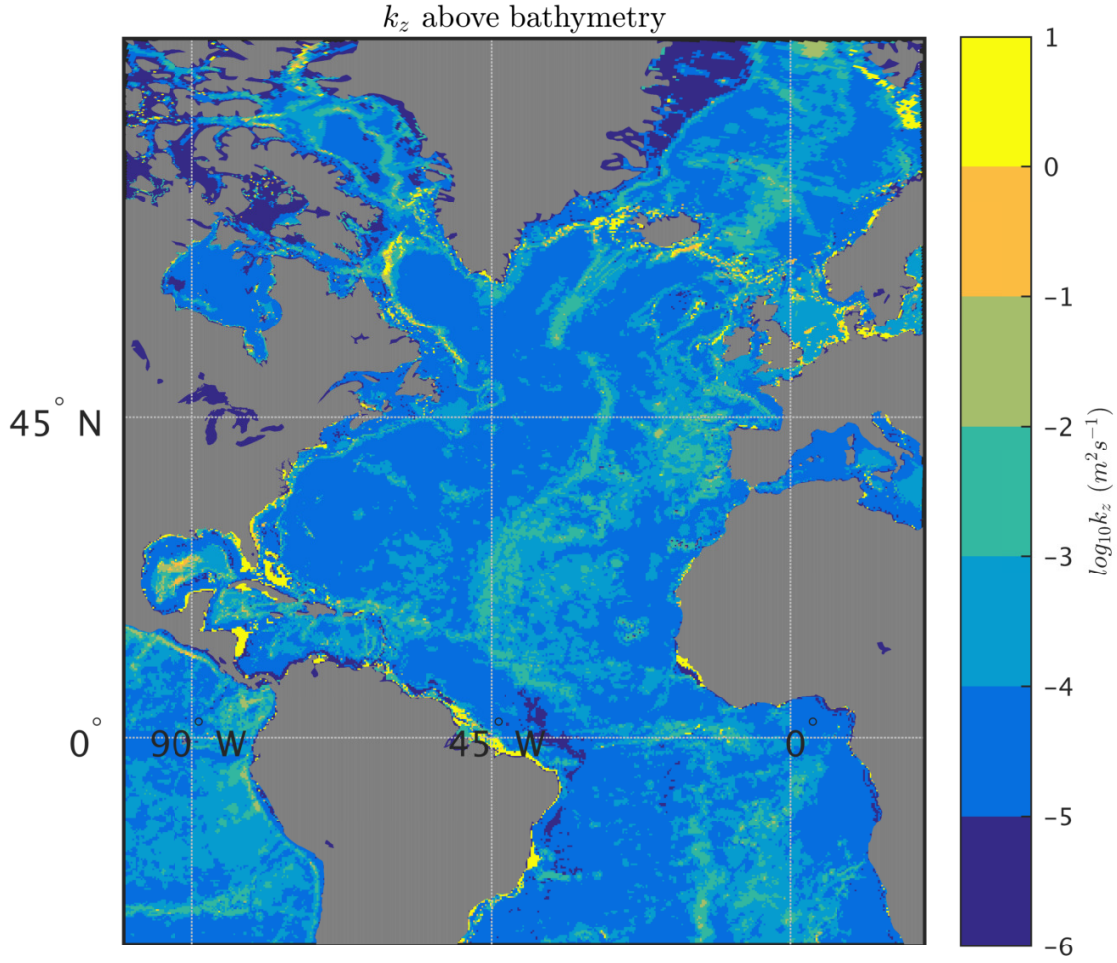


Figure 2.20: Coefficient of vertical diffusion, k_z , one vertical velocity grid point above bathymetry from the Eulerian model output at the end of June 2012. The colour scale is logarithmic.

as the mid-Atlantic ridge, stand out clearly. Elevated values in shallow regions adjacent to coastlines may also be due to surface forcing process. The vertical grid spacing above bathymetry, and thus the vertical scale over which this mixing takes place, is on the order of 100-200 m in the open ocean and over the mid-Atlantic ridge, and 10's of metres on the continental shelves.

In addition to this bottom enhanced mixing, we noted previously (in relation to the mixed layer definitions; Figure 2.14) the persistence of elevated diffusivity in the seasonal thermocline. As such, there are a number of regions where particles moving around in the subsurface could experience elevated vertical diffusivity, and experience changes in their density as a result. To assess the extent of this, we trace

the vertical diffusivity coefficient along trajectories in the experiment conducted with the primary simulation in which particles were initialised throughout the water column in the subtropical and subpolar gyres (Figure 2.8). As for other tracers, k_z was linearly interpolated onto the particle location at each 5-day timestep. In Figure 2.21 we show the *average order of magnitude* of the diffusivity coefficient experienced by particles in the subsurface. We consider the average order of magnitude rather than a simple time average since, due the orders of magnitude variations in k_z , the latter will be skewed toward short amounts of time spent in high mixing environments. Since we wish elucidate the likelihood that particles spend time in regions of elevated mixing, considering the average order of magnitude is more appropriate and indeed proves to be informative. It should be appreciated however, that particles may experience substantial density change over a short period of time spent in a region with elevated k_z . Consequently, the results of this analysis do not reflect the magnitudes of diapycnal motion. Results are presented as a two-dimensional histogram such that each column represents a pdf of the average k_z in that density class.

In the main thermocline, the vast majority of particles are, on average, in low mixing environments, experiencing vertical diffusivity close to background levels. This changes below $\gamma^n = 27 \text{ kgm}^{-3}$, where a higher proportion of particles spend more time in regions of elevated k_z . It is particularly noteworthy that this is the case in the deep ocean waters, around $\gamma^n = 27.6 \text{ kgm}^{-3}$ and denser. It is particles in these density classes that are likely exposed to the elevated mixing close to bathymetry, shown in Figure 2.20.

Elevated levels of diapycnal mixing in the vicinity of bathymetry is thought to be widespread in the ocean. This results from flow over rough topography (Naveira Garabato *et al.*, 2002), which leads to the generation and subsequent breaking of internal waves, and from the generation, radiation and breaking of internal tides (MacKinnon *et al.*, 2017). In the NEMO model, these processes are not included, and the vertical diffusivity coefficient is established by a total kinetic energy closure scheme (Blanke and Delecluse, 1993). Consequently, elevated values of k_z are

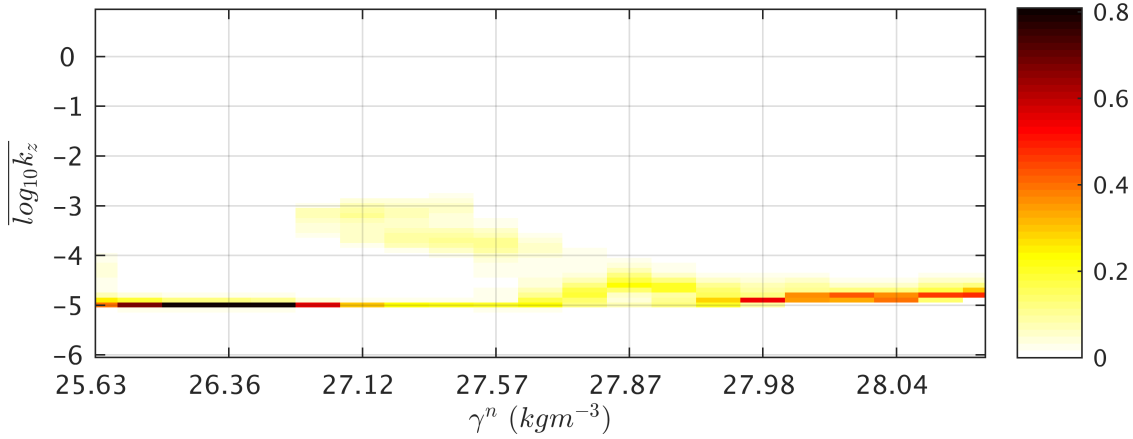


Figure 2.21: Two-dimensional histogram of the mean order of magnitude of the coefficient of vertical diffusion, k_z , experienced by particles initialised in the subtropical and subpolar gyre at the end of June, 1985, in the hindcast simulation. Trajectories are the same as those described in Figure 2.10. The colour scale corresponds to the fraction of each density class that experiences an average $\log_{10}(k_z)$ corresponding to the y -axis value, such that each column sums to 1. The bin width of density classes is determined to account for the exponential stratification, such that the x -axis is non-linear.

likely to be caused by frictionally generated shear in the bottom boundary layer that perturbs the weak local stratification. Thus, while elevated levels of mixing close to the ocean floor may fit with observations, it is unclear whether this is established by physically realistic mechanisms.

Implicit mixing, by its very nature, is difficult to pin down in models. It emerges from numerical truncation errors, as well as the explicitly diffusive nature of some tracer advection and time-stepping schemes. The issue is particularly prevalent in models whose vertical coordinate is depth (Griffies *et al.*, 2000b), as is the case for the model simulations used in this thesis. Approaches to estimate the amount of implicit mixing in numerical simulations focus on the diagnosis of an ‘effective diffusivity’ — the combination of explicit and implicit diffusivity (Griffies *et al.*, 2000b; Lee *et al.*, 2001; Getzlaff *et al.*, 2010, 2012; Ilicak *et al.*, 2012). From a variety of methods, levels of effective diffusivity several times that of the explicitly applied diffusion are consistently diagnosed, resulting in a simulated flow that is considerably more diabatic than observations in the ocean suggest (Ledwell *et al.*, 1993).

Owing to the aggregate manner in which effective diffusivity is evaluated, deriving extensive spatial information is difficult (though depth and latitude dependence

can be inferred from some methodologies; Lee *et al.*, 2001; Hill *et al.*, 2012). From experiments in idealised flow scenarios, however, Griffies *et al.* (2000b) note that particularly high levels of effective diffusivity emerge through inadequate spatial resolution of the model grid in the vicinity of boundary currents and eddying motions.

Following the methodology of Lee *et al.* (2001), who utilise a water mass transformation framework to evaluate effective diffusivity, Megann *et al.* (unpublished work) have diagnosed effective diffusivity in a $1/4^\circ$ configuration of the NEMO model, with similar numerics (including the same advection scheme) as the models used in this thesis. Consistent with aforementioned studies, they find levels of mixing several times the magnitude of background values throughout regions of the ocean interior. They suggest this elevated mixing could be attributed to the large (and often noisy) vertical velocities present close to boundaries and in eddying regions. The evidence in support of this is that a comparable simulation using higher levels of viscosity to damp out these vertical velocities exhibits lower levels of mixing.

2.5 Discussion

In this chapter, we undertook a critical assessment of the representation of water mass transport by Lagrangian trajectory calculation in numerical ocean circulation models. We highlight that the difficulty in establishing accurate levels of diapycnal mixing in numerical simulations, and the possibility for errors in trajectory calculations, could lead to water mass pathways that are more diabatic than what is expected in the ocean.

From a range of experiments and diagnostics, we find that there is indeed significant diapycnal motion associated with trajectories in a $1/4^\circ$ resolution numerical ocean circulation model. Comparison to a simple scaling suggests that this is in excess of what would be expected from observed levels of mixing in the ocean. Furthermore, the diapycnal motion exhibits systematic structure, both in terms of the movement between density classes, and in its spatial distribution across the North Atlantic basin. In the latter case, areas close to bathymetry and

energetic regions such as the Gulf Stream and North Atlantic current, stand out as particularly important in establishing diapycnal motion.

We explored several potential explanations for this observed diapycnal motion, with a particular focus on sources of error in the Lagrangian trajectory calculation. Clear results are impaired by the fact that many explanatory mechanisms are likely to be operating most effectively in the same energetic regions. Nevertheless, our results point toward aspects of both the Lagrangian calculation and explicit model mixing in establishing diapycnal motion (implicit mixing is not assessed directly). For the trajectory calculation, the use of time-averaged velocity fields was shown to be a potentially important source of error, particularly within the thermocline in the boundary current and in detached eddies. However, the long-timescale impact of this is not clear. Density changes exhibit some sensitivity to the definition of the mixed layer depth (a component unique to our experimental approach), but the broad structure and magnitude is largely unaffected. In relation to explicit model mixing, we found that the vertical diffusivity coefficient (established in the model by a total kinetic energy closure scheme) is elevated close to bathymetry. Consequently, particles in deep ocean density classes generally experience levels of mixing that are, on average, elevated relative to the background level. In light of these results, we tentatively suggest that in the energetic regions of the upper ocean and thermocline, a component of the density changes are a consequence of discrepancies in the Lagrangian trajectory calculation. In the deep ocean, on the other hand, diapycnal motion emerges from the model parameterisation of vertical mixing.

It is thus likely that both model mixing and errors in Lagrangian trajectory calculation are responsible for the observed diapycnal motion. Dependent on which of these processes is responsible, different implications may be considered.

If Lagrangian trajectories are in error, caution should be advised in the interpretation of transport timescales and pathways assessed in this way. In particular, many studies infer matter mass transformations from the changing properties of particles along trajectories (Blanke *et al.*, 2001; Lique *et al.*, 2010; Berglund *et al.*, 2017). The results here suggest that these could be grossly in error. The possibility

of errors emerging due to the use of time-averaged velocity fields means that this caution should be extended to any Lagrangian calculations performed ‘offline’, including that of tracers. The presence of diapycnal motion does not rule out the utility of such methods (indeed in this thesis we shall go on to present robust results in spite of it), but it limits to some extent the strength of certain conclusions that can, and have, been drawn.

On the other hand, if model mixing is the major driver of the observed diapycnal motion, this poses important questions on the diapycnal nature of the simulated ocean circulation. While the occurrence of spurious mixing in numerical models has been appreciated for some time (Griffies *et al.*, 2000b), the results here are a good example of the impact that this mixing may have on pathways and timescales of circulation in the subsurface ocean. In the context of ocean ventilation, such diapycnal motion has the potential to be a further significant source of uncertainty in a process that is already a major component of inter-model spread in climate simulations (Boé *et al.*, 2009; Heuze *et al.*, 2013).

3

Characterising the chaotic nature of ocean ventilation

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3.1 Introduction

Ocean circulation is highly turbulent, with the kinetic energy dominated by mesoscale eddies (Ferrari and Wunsch, 2009). In the presence of strong eddy activity, the pathways of water parcels can be highly chaotic (Wiggins, 2005). The chaotic nature of these pathways impacts the transport and distribution of tracers and the spatial scales over which regions of the ocean retain memory

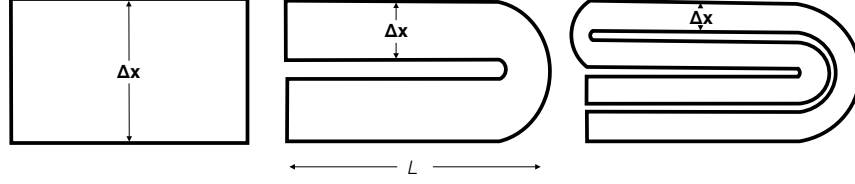
of their upstream properties.

Several studies indicate that the turbulent nature of ocean circulation is of central importance to thermocline ventilation (Robbins *et al.*, 2000; Mecking *et al.*, 2004; Booth and Kamenkovich, 2008; Koch-Larrouy *et al.*, 2010; Abernathey and Ferreira, 2015; Kamenkovich *et al.*, 2017). Quantifying its impact, however, remains challenging due to the difficulty in separating out the effects of different spatial and temporal scales (Booth and Kamenkovich, 2008). Consequently, analyses are often largely qualitative by necessity (e.g. Mecking *et al.*, 2004; Kamenkovich *et al.*, 2017). Notable exceptions to this are attempts to quantify, through a variety of means, a nondimensional Peclet number, which characterises the relative importance of advection and mixing for tracer transport (*e.g.* Rhines and Schopp, 1991; Waugh *et al.*, 2004; Shao *et al.*, 2016).

In this chapter, we propose a novel, kinematic approach to characterise the chaotic nature of ocean ventilation pathways, borrowing concepts from the study of dynamical systems (Strogatz, 1994). We define a nondimensional number that quantifies the reduction in the width of a fluid parcel since leaving the mixed layer. This indicates the extent to which trajectories from the mixed layer into the ocean interior are laminar or chaotic. The approach is complementary to tracer-derived estimates of ventilation pathways (e.g. Haine and Hall, 2002; Waugh *et al.*, 2004; Primeau, 2005; Primeau and Holzer, 2006; Hall *et al.*, 2007; Holzer *et al.*, 2010), and explores the physical processes operating at their heart. Our analysis is focussed on the subtropical thermocline, a region of historical debate on the impact of ventilation and the time-varying flow on the large-scale circulation and stratification (Rhines and Young, 1982; Luyten *et al.*, 1983).

Dynamical systems approaches such as that adopted in this study are often applied to questions of tracer stirring and transport in turbulent (and non-turbulent) geophysical fluids. These range from the investigation of Lagrangian flow maps that are mathematically similar to the advection-diffusion equation (e.g. Pierrehumbert, 1994; Antonsen *et al.*, 1996; Neufeld *et al.*, 2000; Tzella and Haynes, 2010) to evaluation of the dynamical system characteristics of observed or simulated currents

(a) Stretching and folding of puff pastry



(b) Filamentation of fluid parcel

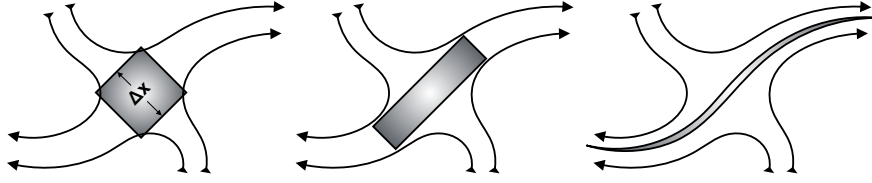


Figure 3.1: Thinning of (a) layers of puff pastry (adapted from Strogatz (1994)) and (b) a patch of fluid at a circulation stagnation point, progressing in time from left to right. In both panels, the filament width is labelled Δx . In (a), the folding length is labelled L .

and tracer fields (e.g. Abraham and Bowen, 2002; Waugh and Abraham, 2008; Haller, 2015; Mukiibi *et al.*, 2016). Oceanographic applications have tended to focus on the surface ocean (see Wiggins, 2005, for a review) and, to our knowledge, this study is the first to apply such an approach directly to the problem of ocean ventilation.

3.2 Theory

As an analogy to the effect of turbulent circulation on ocean ventilation, consider the making of puff pastry (Figure 3.1a). As the dough is repeatedly stretched and folded, the layers become increasingly thin. The change of the layer width, Δx , through time can be expressed as

$$\frac{d\Delta x}{dt} = -\gamma \Delta x, \quad (3.1)$$

where γ is the strain rate — the rate at which the baker rolls the dough. Integrating (3.1), we find that the thinning of the layers occurs exponentially in time:

$$\Delta x(t) = \Delta x(0) e^{-\int_0^t \gamma dt} = \Delta x(0) e^{-\bar{\gamma}t}, \quad (3.2)$$

where $\bar{\gamma}^t$ is the time-mean strain rate. Thus the reduction in the width of the pastry layers is set by the time that the baker has been working for (t) and the vigour with which they roll the pastry (γ), which is averaged over time (Strogatz, 1994). Importantly, it is the strain rate, γ , that impacts the layer width, while the horizontal scale of the pastry (denoted L in Figure 3.1a) is determined by the length scale of the folding.

Analogous to the stretching and folding of puff pastry is the horizontal drawing out and thinning of fluid parcels — so-called filamentation (Figure 3.1b). An infinitesimal fluid parcel of width Δx , aligned perpendicular to the axis of principal strain, will thin exponentially in time according to Eq. 3.2. In this case, the role of the baker is played by the circulation. For a two-dimensional, non-divergent flow, the strain rate, γ , is a function of the horizontal velocity gradients, given by

$$4\gamma^2 = \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right)^2 + \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)^2, \quad (3.3)$$

where symbols have their usual meaning. As is the case for puff pastry, the filament width is affected by the strain rate, while the bounding horizontal scale of the fluid parcel is controlled by the characteristic length scale of the eddy field on which the fluid parcel is folded. Maxima in the strain rate are found at stagnation points in the flow. In a turbulent flow, where stagnation points are a common feature, the width of filaments will collapse to arbitrarily small scale in finite time.

Now consider a fluid parcel ventilated into the ocean subsurface. The time that the baker has been working for corresponds to the time since the fluid parcel left the ocean mixed layer — the ventilation timescale. The vigour with which the baker rolls the pastry is the strain rate of the circulation, which varies in space and time along the parcel's Lagrangian trajectory. Then, from (3.2), the reduction in filament width is a function of the ventilation timescale (τ_{vent}) and the mean strain rate along the Lagrangian trajectory ($\bar{\gamma}^L$; we use the superscript L to distinguish this Lagrangian mean from the Eulerian time-mean strain rate of the puff pastry evaluated at a stationary point). Expressing the latter as a Lagrangian

strain *timescale* ($\bar{\tau}_{\text{strain}}^L = 1/\bar{\gamma}^L$), we can define a nondimensional ‘filamentation number’ as the ratio of these two timescales:

$$F = \frac{\tau_{\text{vent}}}{\bar{\tau}_{\text{strain}}^L}. \quad (3.4)$$

The filament width of a fluid parcel will have been reduced by a factor of order e^{-F} since leaving the mixed layer (Eq. 3.2). For example, in a region where $F = 4$, a ventilated fluid patch with an initial horizontal scale of $\Delta x(0) = 100$ km will have formed filaments of roughly 2 km width (notwithstanding spatial scale considerations outlined below).

In other geophysical fluid applications of concepts from dynamical systems, the filamentation of fluid parcels is characterised by the ‘Lyapunov exponents’ of the system. The finite time Lyapunov exponent (FTLE) is the time mean strain rate following a trajectory. Thus, for individual trajectories, the FTLE is identical to the Lagrangian strain rate defined above. Finite time Lyapunov exponents are evaluated from trajectories initialised across a domain and evolved forwards or backwards for a fixed length of time (e.g. Abraham and Bowen, 2002). Their evolution and distribution as the fixed time increases, and their long time behaviour, has been shown to provide information on the stirring of passive tracers within the domain (Antonsen *et al.*, 1996; Abraham and Bowen, 2002). In the present work, the finite time of integration for each trajectory is the time since the parcel was last in the surface mixed layer, *i.e.* the ventilation timescale. As such, it is unique for each trajectory and each location within the domain. It is for this reason that we identify the Lagrangian strain rate as a distinct measure from the more ubiquitous FTLE.

The formulation of the nondimensional number F assumes that the width of the fluid parcel is infinitesimally small. For F to characterise the filamentation of a finite-size fluid *patch*, the width of the patch must be less than the dominant kinetic energy-containing spatial scale of the circulation. That is to say the fluid patch must be within a ‘nonlocal’ dynamical regime, in which the kinetic energy spectrum of the circulation, and therefore the strain timescale, is dominated by the larger scales (Batchelor, 1959; Bennett, 1984; Keating *et al.*, 2011). The distinction between

‘local’ and ‘nonlocal’ regimes was defined by Bennett (1984) in relation to the dispersion of balloons in the stratosphere. The author argued that characteristics of the dispersion could be identified based on whether the initial separation of balloons was on the same scale as (local), or smaller than (nonlocal), the dominant spatial scale of the flow. So, for example, two balloons positioned close to each other on either side of the mid-point between two counter-rotating eddies would be in a nonlocal regime (their separation being much smaller than the scale of the dominant circulation feature, the eddies) and disperse rapidly in time as they were drawn away from each other by the large-scale flow. The timescale of separation is determined by the strain rate, which would here be associated with the velocity shear between the eddies. On the other hand, two balloons positioned in the centre of each of the eddies would be in the local regime (their separation being on the same scale as the eddies) and their dispersion would be defined by the evolution of the eddies themselves. Now, in relation to filamentation of a fluid patch in the ocean, consider a circulation regime for which the dynamics are nonlocal below 100 km. A ventilated fluid patch with initial horizontal scale of 50 km will be persistently thinned on a strain timescale associated with the nonlocal regime. This timescale is determined by the circulation at the largest scales of the nonlocal regime — 100 km. In this case, F will correctly characterise the reduction in filament width. On the other hand, a ventilated fluid patch with an initial horizontal scale of 500 km — within a ‘local’ regime — will experience a different strain (*i.e.* that associated with a separation of 500 km), the timescale of which is likely to be longer than that within the nonlocal range. Consequently, F will generally overestimate the extent of filamentation of such a fluid patch. Returning briefly to the puff pastry analogy, the baker cannot efficiently roll the dough if its size exceeds their own.

The puff pastry analogy is commonly employed to explain the mechanism by which dynamical systems develop sensitivity to initial conditions, through the stretching and folding of phase space (Strogatz, 1994). Imagine a small drop of food colouring in the pastry dough (Figure 3.1a), representing a cluster of nearby initial conditions in phase space. After a number of iterations of stretching and

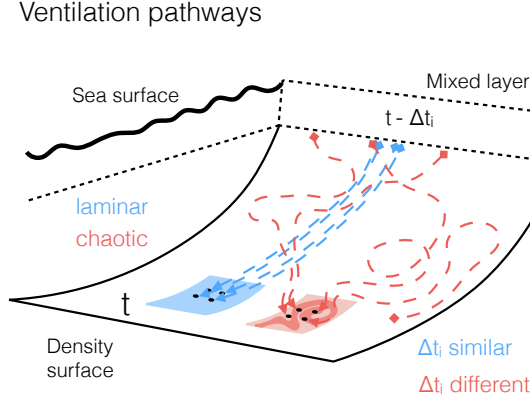


Figure 3.2: Schematic illustration of laminar (blue) and chaotic (red) ventilation pathways of adjacent particles on a density surface. The particles are adjacent at time t and the i^{th} particle left the mixed layer at time $t - \Delta t_i$.

folding, the dye will have spread throughout the pastry, representing the range of possible trajectories of the initially close initial conditions. As the layers thin, trajectories in the system become increasingly sensitive to their initial position — the system becomes increasingly chaotic.

By the same analogy, the value of F in the ocean subsurface characterises the chaotic nature of ventilation pathways. This is illustrated schematically in Figure 3.2, where we consider the ventilation pathways that have been followed by adjacent particles on a density surface. If a region is characterised by a small value of F , implying that it is ventilated on a short timescale (τ_{vent} small) or the flow is predominantly laminar ($\bar{\tau}_{\text{strain}}^L$ large), adjacent particles will have left the mixed layer at similar times and locations (blue pathways). In the context of a passive tracer, its distribution on leaving the mixed layer will be conserved in the ocean interior. If, on the other hand, the region is characterised by large F , suggesting it is ventilated on a long timescale (τ_{vent} large) or the flow is highly turbulent ($\bar{\tau}_{\text{strain}}^L$ small), the particles are more likely to have followed divergent pathways and have left the mixed layer at a range of locations and times (red pathways). In this case, the distribution of a passive tracer will be highly filamented, reflecting these divergent pathways.

In the following, we explore the concept of the filamentation number, evaluating its magnitude within the subtropical thermocline of a numerical ocean circulation model and comparing it to the ventilation pathways in this region.

3.3 Methods

Information on the numerical ocean circulation model and software used for Lagrangian analysis can be found in Chapter 1. Here we provide details of the experimental strategy and calculations that are unique to this chapter.

3.3.1 Timescale Calculations

Both the ventilation and strain timescales are evaluated using Lagrangian trajectories. Particles are initialized across potential density surfaces at a resolution of 25 per grid cell (≈ 5 km apart) in March 2010. They are tracked backwards in time until they intercept the mixed layer (which we define by a density within 0.01 kg m^{-3} of the surface density, following Thomas *et al.* (2015)). Along the trajectory, the local horizontal strain rate, determined from the Eulerian velocity field, is linearly interpolated onto the trajectory location, providing a time series of strain rate for each trajectory. We use the horizontal strain rate under the assumption that flow in the subsurface is predominantly along density surfaces. The error associated with the density surface slope is negligible. To determine $\bar{\tau}_{\text{strain}}^L$, we calculate the inverse of the mean strain rate along each trajectory, and grid this on the particle's initial location on the density surface. For τ_{vent} , the age of each particle (the time between when it left the mixed layer and March 2010) is gridded on its initial location on the density surface. Median values of $\bar{\tau}_{\text{strain}}^L$ and τ_{vent} are determined within each model grid cell (25 particles), and the resulting fields are further smoothed using a two-dimensional, 24 grid cell, spatial moving median. The result is a smoothed map of the ventilation timescale and the Lagrangian strain timescale across the density surface.

3.3.2 Structure Function Calculation

The capacity for F to characterise filamentation of finite-size fluid patches depends on the details of the oceanic energy spectrum, specifically the spatial scales over which the dynamics are nonlocal (Section 3.2). We determine this by analysis of the

Eulerian velocity field, from which we evaluate the variance of separation velocities — the second order structure function — given by:

$$S_2(\mathbf{r}) = \langle [u(\mathbf{x} + \mathbf{r}) - u(\mathbf{x})]^2 \rangle, \quad (3.5)$$

where $\mathbf{r}$ is separation and angular brackets denote the time average. S_2 can be evaluated for velocities and separations in both zonal and meridional directions. From dimensional analysis, the dependence of S_2 on $|\mathbf{r}|$ indicates the dynamical regime of the velocity field (LaCasce, 2002). Where $S_2 \propto |\mathbf{r}|^{2/3}$, the dynamics are local, equivalent to an energy spectral slope of $-5/3$. Where $S_2 \propto |\mathbf{r}|^2$, the dynamics are non-local, equivalent to an energy spectral slope of -3 . In our analysis, second order structure functions are evaluated using horizontal velocities interpolated onto density surfaces in the thermocline.

3.3.3 Comments on the impact of diapycnal trajectories

In Chapter 2 we noted that particles in the subtropical thermocline change their density substantially, becoming more dense over time. The source of these density changes are not clear, and it was concluded that there are likely to be contributions from both the Lagrangian trajectory calculation and mixing in the numerical situation. It should therefore be kept in mind that although we consider particles on specific density surfaces, they have not necessarily moved their adiabatically. Neither the theory outlined in Section 3.2 or the calculation of the ventilation timescale depends on adiabatic movement. The strain timescale may be affected only in the sense that if the particle motion is strongly inclined from the horizontal, a two-dimensional, horizontal strain rate may be inappropriate. We expect this error to be small and not to affect our main results. Related to this, calculation of the structure function also uses horizontal velocities interpolated onto the density surface. Given the qualitative manner in which we consider the structure functions (using them to elucidate the spatial scales of the flow) this will not affect our conclusions. Later in the chapter (Section 3.4.2), we compare the filamentation number to the distribution of properties mapped onto the density surface. Again, this is not dependent on the mapping being adiabatic.

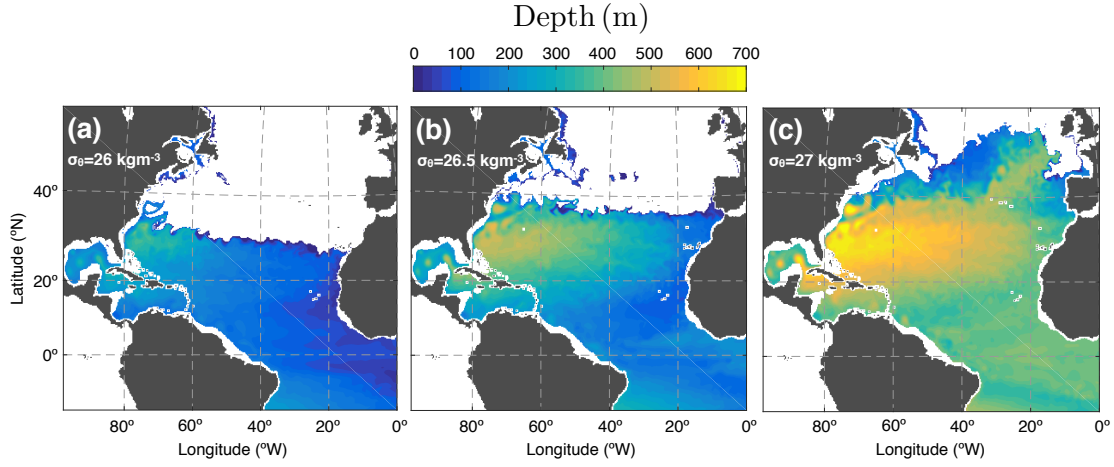


Figure 3.3: Depth of three potential density surfaces in March 2010: (a) $\sigma_\theta = 26 \text{ kg m}^{-3}$, (b) $\sigma_\theta = 26.5 \text{ kg m}^{-3}$ and (c) $\sigma_\theta = 27 \text{ kg m}^{-3}$.

3.4 Results

3.4.1 Quantifying the Filamentation Number

Our analysis considers three potential density surfaces in the North Atlantic subtropical thermocline (Figure 3.3). These surfaces, $\sigma_\theta = 26 \text{ kg m}^{-3}$ ($\sim 100 - 300 \text{ m}$ depth), $\sigma_\theta = 26.5 \text{ kg m}^{-3}$ ($\sim 200 - 600 \text{ m}$ depth) and $\sigma_\theta = 27 \text{ kg m}^{-3}$ ($\sim 300 - 700 \text{ m}$ depth), were chosen to sample a range of dynamically distinct regimes in the subtropical thermocline (Samelson and Vallis, 1997). The shallower two surfaces both outcrop in the downwelling region of the subtropical gyre, while the deeper surface largely outcrops to the north of the Gulf Stream and North Atlantic Current, except at its eastern extent. For the rest of this paper, we refer to these surfaces as σ_{26} , $\sigma_{26.5}$ and σ_{27} .

Ventilation timescales across these three surfaces are shown in Figure 3.4. Across most of the subtropical gyre, σ_{26} is ventilated on timescales less than 5 years (Figure 3.4a). Recently ventilated water, with τ_{vent} less than 2 years, stretches across half of the basin. The intermediate density surface, $\sigma_{26.5}$, is mostly ventilated on timescales between 5 and 15 years (Figure 3.4b). The youngest ventilated fluid is restricted to a relatively small (by comparison with that on the shallow surface) region east of 20°W . On both of these surfaces, longer ventilation timescales are seen in the so-called ‘shadow zone’ — a region of stagnant mean flow off the west coast of Africa

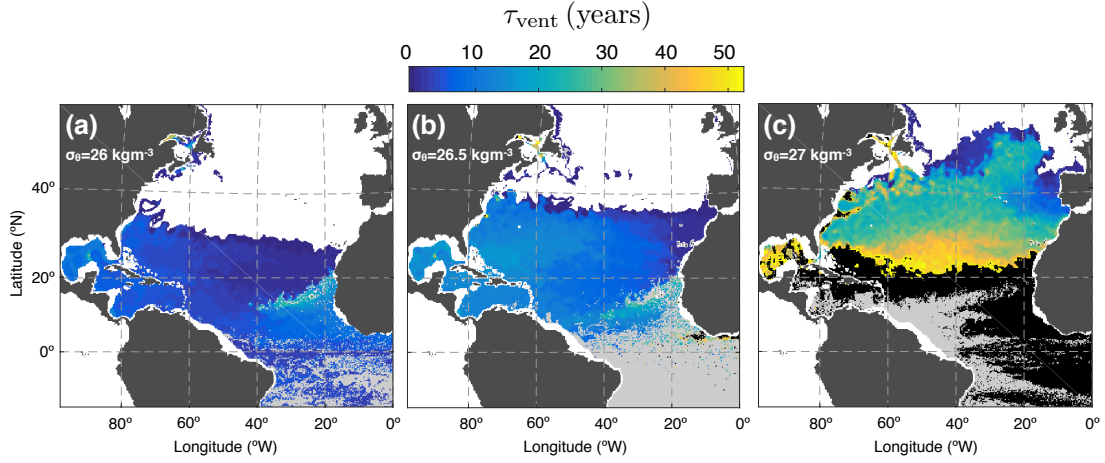


Figure 3.4: The ventilation timescale, τ_{vent} , in years. Values are averaged within each model grid cell and further smoothed by averaging with the adjacent 24 grid cells. Locations in black were unventilated during the model run. Locations in light grey are where more than half of the particles in the region originate outside the experimental domain, thus no ventilation timescale information is obtained.

that is not directly ventilated by the wind-driven gyre (Rhines and Young, 1982; Luyten *et al.*, 1983). The deeper isopycnal, σ_{27} , is ventilated on considerably longer timescales (Figure 3.4c). A gradient exists between comparatively short timescales on the order of 1 to 10 years near the density surface outcrop and longer timescales of 50 years and more to the south west of the gyre. There is a clear signal of long ventilation timescales within the Gulf Stream and its extension, implying that water in this region is recirculated from the poorly ventilated southwest gyre interior. The distribution of τ_{vent} on these surfaces is broadly consistent with observations of tracer-derived ages (Jenkins, 1988) and previous model results (Williams *et al.*, 1995).

Before presenting the Lagrangian strain timescale, $\bar{\tau}_{\text{strain}}^L$, we consider the pattern of the time-averaged, local, Eulerian strain timescale, τ_{strain}^E , across the density surfaces (Figure 3.5a-c). This is determined at each grid cell location using the horizontal Eulerian velocity field interpolated onto the potential density surfaces and averaged over the last 30 years of the simulation. The pattern of τ_{strain}^E on each density surface provides an overall impression of where trajectories will experience high or low strain. To the best of our knowledge, this informative dynamical quantity has not previously been mapped in a realistic ocean circulation model. The magnitude of τ_{strain}^E is similar on the three density surfaces, increasing slightly

with depth in the gyre interior and equatorial region. It ranges from days in energetic regions such as the Gulf Stream and equatorial band, to months in the gyre interior and shadow zone, and is everywhere less than a year. Within the comparatively quiescent gyre interior, there remains considerable spatial structure, with τ_{strain}^E increasing south of the Gulf Stream and decreasing again towards the gyre's southern extent. From observations of a tracer released at $25.6^\circ N$, $28.3^\circ W$, Ledwell *et al.* (1998) estimate a strain timescale of ~ 0.1 years at a potential density of 26.75 kg m^{-3} , consistent with the time-average value in this region presented here. On $\sigma_{26.5}$ and σ_{27} , a band of shorter timescales on the east of the basin at around $35^\circ N$ signals the impact of the Azores current and possibly its interaction with Mediterranean water eddies (Bashmachnikov *et al.*, 2015). There is a notable increase in τ_{strain}^E on all three density surfaces as the boundary between the gyre circulation and shadow zone is crossed.

The Lagrangian strain timescale ($\bar{\tau}_{\text{strain}}^L$; Figure 3.5d-f) is the inverse of the mean strain rate experienced by the fluid parcels along their trajectories from the mixed layer to each of the three density surfaces. Thus, it integrates the local strain rate as trajectories move around the subsurface. Consequently, and consistent with finite time Lyapunov exponents (Antonsen *et al.*, 1996; Abraham and Bowen, 2002; Waugh *et al.*, 2006), values of $\bar{\tau}_{\text{strain}}^L$ should converge at long times. The time for convergence of FTLEs in the surface ocean (~ 1 year Abraham and Bowen, 2002; Waugh *et al.*, 2006) is considerably less than the ventilation timescale across most of the thermocline in our simulation (Figure 3.4). Thus it may be expected that $\bar{\tau}_{\text{strain}}^L$ is relatively uniform compared to τ_{strain}^E . Nevertheless, that $\bar{\tau}_{\text{strain}}^L$ is consistently and uniformly small throughout the thermocline is notable. Given the different possible pathways of ventilation and the difference in strain experienced in the boundary current and interior regions, the small values of $\bar{\tau}_{\text{strain}}^L$ may come about in different ways, for example consistently high levels of strain along the ventilation pathway, or a short time spent in a very energetic region followed by an extended period in the quiescent interior. The remaining basin-scale variation in $\bar{\tau}_{\text{strain}}^L$, and the variation between surfaces, must be due to the large-scale pathways

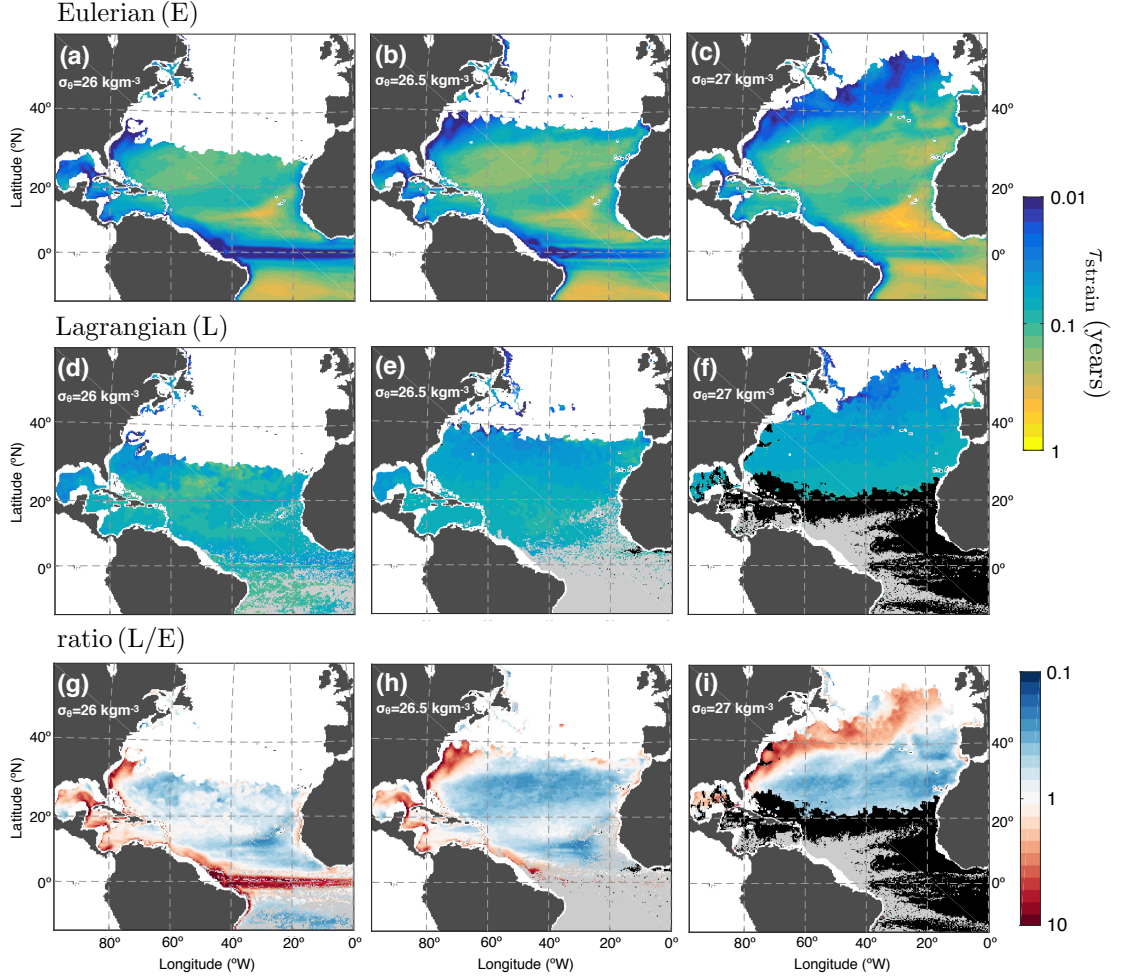


Figure 3.5: (a,b,c) The Eulerian strain timescale in years, evaluated at each horizontal location on the three density surfaces (τ_{strain}^E), averaged over the last 30 years of the numerical simulation. (d,e,f) The Lagrangian strain timescale ($\bar{\tau}_{\text{strain}}^L$) in years, evaluated as the inverse of the mean strain rate experienced along trajectories that are present on the density surfaces in March 2010, and that left the surface ocean within the time of the model simulation. Values are averaged within each model grid cell and further smoothed by averaging with the adjacent 24 grid cells. Locations in black were unventilated during the model run. Locations in light grey are where more than half of the particles in the region originate outside the experimental domain, thus the full strain history could not be determined. Note the logarithmic color scale in both (a) and (b). (g,h,i) The ratio of the Lagrangian and Eulerian strain timescales, presented on a log scale.

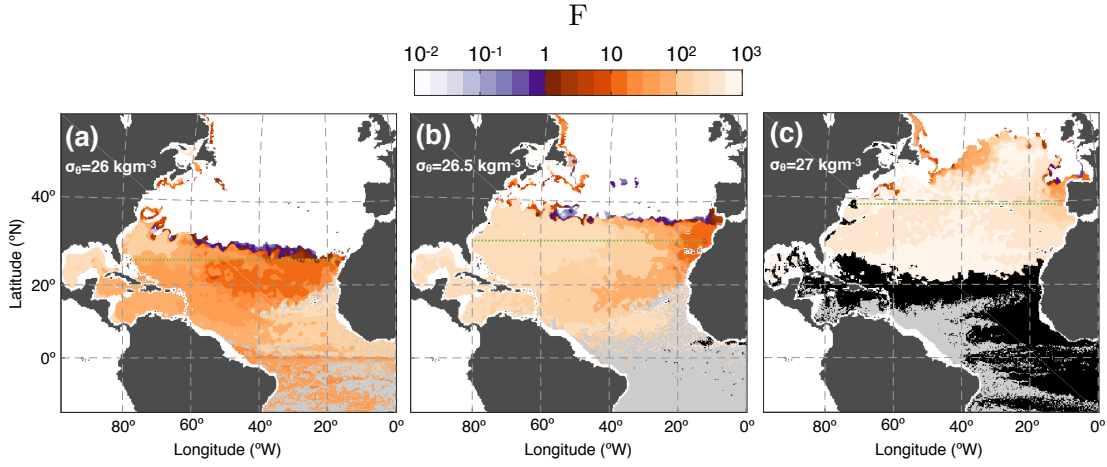


Figure 3.6: The filamentation number, $F = \tau_{\text{vent}}/\bar{\tau}_{\text{strain}}^L$, on the three density surfaces. Locations in black were unventilated during the model run. Locations in light grey are where more than half of the particles in the region originate outside the experimental domain, thus neither the ventilation time or the strain history could be determined. Green, dotted lines show the location of high resolution mappings relevant to Section 3.4.3.

of the trajectories. On σ_{26} , where trajectories have been comparatively recently ventilated, $\bar{\tau}_{\text{strain}}^L$ retains some of the spatial structure of the τ_{strain}^E distribution, with longer timescales in the central gyre. In the older waters present on deeper surfaces, trajectories are more likely to have passed through regions of short local strain timescale, particularly given the outcrop location of $\sigma_{26.5}$ and σ_{27} to the north of the Azores Current and North Atlantic Current (Figure 3.5a-c). This results in a slight decrease in $\bar{\tau}_{\text{strain}}^L$ with depth. By contrast, τ_{strain}^E shows a marginal overall increase with depth. On both of the deeper surfaces, $\bar{\tau}_{\text{strain}}^L$ increases towards the south of the gyre. A large number of particles at the southern extent originate in the ventilation region to the north east of the density surfaces. Their trajectories, therefore, avoid passage through the most turbulent region with shortest strain timescale, *i.e.* the Gulf Stream and North Atlantic Current. It is apparent, therefore, that the distribution of $\bar{\tau}_{\text{strain}}^L$ is strongly influenced by the overall pathways of ventilation, and the strain history along these pathways, rather than being entirely set by the local values of Eulerian strain on each surface.

An Eulerian strain timescale is more easily evaluated than a Lagrangian strain timescale (both in a numerical model and in the ocean). Consequently, it is

instructive to understand the extent to which τ_{strain}^E differs from $\bar{\tau}_{\text{strain}}^L$, and whether the former may be adequate for the purpose of scaling analysis. To this end, their ratio on each density surface is presented in Figure 3.5g-i. On each density surface, differences between $\bar{\tau}_{\text{strain}}^L$ and τ_{strain}^E exist in the quiescent regions (the gyre interior) and energetic regions (such as the Gulf Stream), where the Eulerian value is longer and shorter respectively. Trajectories in these regions have previously experienced longer/shorter strain timescales than the short/long local τ_{strain}^E , and these are incorporated into the calculation of $\bar{\tau}_{\text{strain}}^L$. Nevertheless, the difference between the Eulerian and Lagrangian strain timescale is much less than an order of magnitude across almost all of the area of the density surfaces, implying that an Eulerian measure may be broadly adequate for the scaling analysis in this paper.

The filamentation number, the ratio of ventilation and Lagrangian strain timescales, is shown in Figure 3.6. It is large ($F \gg 1$) throughout the thermocline, except in a narrow strip adjacent to the winter outcrops, and increases markedly with depth. The magnitude of F is a consequence of the considerably longer timescale on which the ocean subsurface is ventilated compared to the timescale over which it is strained. Owing to the relative uniformity of $\bar{\tau}_{\text{strain}}^L$, the spatial distribution of F on each surface and with depth is almost entirely set by that of τ_{vent} . This is highlighted by plotting F against τ_{vent} for all density surfaces in Figure 3.7. As such, the lowest values of F are seen at the eastern end of the outcrops, where waters are recently ventilated, and increase westward. On the shallower surface, F increases from around 10 to more than 100 across the basin, while on the intermediate surface F approaches 300 towards the Gulf Stream region. Across the deeper surface, F exceeds 300 everywhere except in ventilation regions off the coast of Portugal and northward of the North Atlantic Current.

As outlined in Section 3.2, F characterises filamentation of fluid patches with an initial width within the nonlocal dynamical regime. The spatial range of the nonlocal regime can be determined by calculating the variance of separation velocities of the Eulerian velocity field — so-called structure functions (Section 3.3.2). In this numerical simulation, the structure function is proportional to the square of the

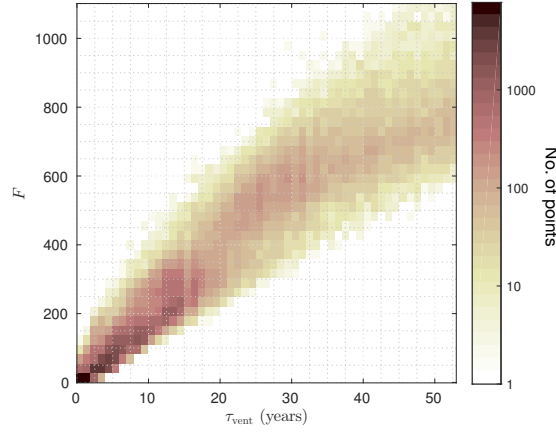


Figure 3.7: Two-dimensional histogram of ventilation timescale (τ_{vent}) and filamentation number (F), where the data are from all three density surfaces. Note the logarithmic color scale.

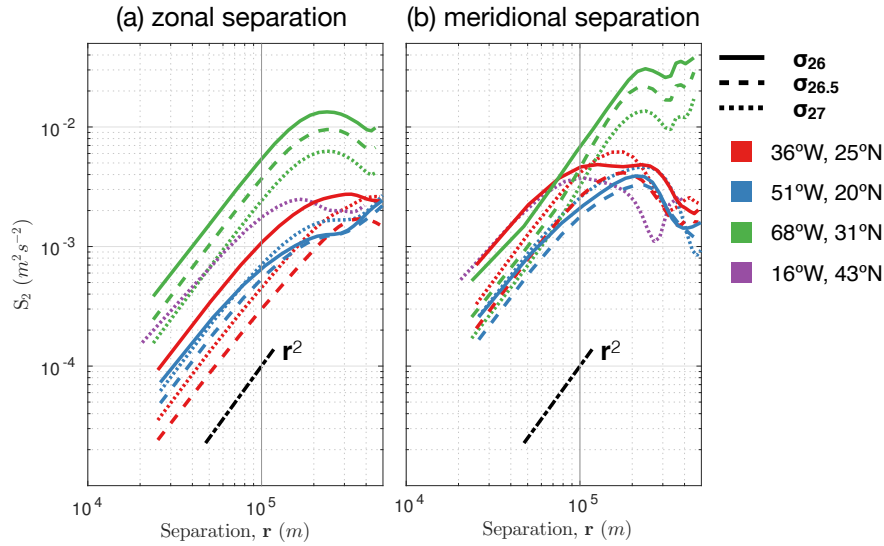


Figure 3.8: Second order structure functions (S_2) at a range of locations (denoted by the line colors) across each of the three density surfaces (denoted by the line styles). See Section 3.3.2 for details of the calculation. A line corresponding to $S_2 \propto r^2$ is also shown.

separation on scales from the grid scale up to around 100 km, as illustrated for a range of locations across the three density surfaces in Figure 3.8. This implies that the dynamics are nonlocal within this range, and that F characterises filamentation for fluid patches with horizontal scales up to at least 100 km.

3.4.2 Mapping Chaotic Pathways

The magnitude of the filamentation number characterises the chaotic nature of ventilation pathways. We now determine these pathways directly by evaluating Lagrangian trajectories backwards in time from an array of points on the three density surfaces to the time and location where they intercept the surface mixed layer. This procedure defines a mapping from each initial position on the density surface to the year and location of ventilation, portrayed schematically in Figure 3.2. The year and location act as non-diffused passive tracers, their distribution set on subduction from the mixed layer and stirred in the subsurface by the circulation. Akin to the mapping of solutions in dynamical systems (see, *e.g.* Strogatz, 1994; Pierrehumbert, 1994; Neufeld *et al.*, 2000), the pattern reveals the chaotic nature of the ventilation pathways.

The mappings are produced in March 2010 across each density surface (Figure 3.9a-c and 3.10a-b). Additionally, we zoom in on interesting regions (Figures 3.9d-f and 3.10c-d). While the horizontal resolution of the velocity field is $1/4^\circ$, the mapping is calculated at higher spatial resolution, which is possible due to the interpolation of velocities between grid cells in Lagrangian analysis (see Chapter 2, Section 2.3). The mapping is purely advective and isolates the role of the model’s resolved scales in producing filamentary structure. In the ocean, the filamentary structure produced by the larger-scale velocity field ceases when local dynamics, such as submesoscale motions, become dominant (Smith and Ferrari, 2009; Callies and Ferrari, 2013).

Most immediately striking in Figure 3.9 is the contrast between the mappings on different density surfaces (panels a, b and c), which becomes increasingly noisy and chaotic with depth. The proportion of the density surfaces occupied by coherent regions of constant ventilation year (a ‘homogenous’ mapping) is sharply reduced between σ_{26} , where recently ventilated ‘2009’ water occupies the eastern third of the basin, and $\sigma_{26.5}$, where it is restricted to the east of $20^\circ W$. On both of these surfaces, the mapping becomes increasingly filamented and chaotic moving westward away from these regions. On σ_{27} , similar homogenous regions are absent, and the

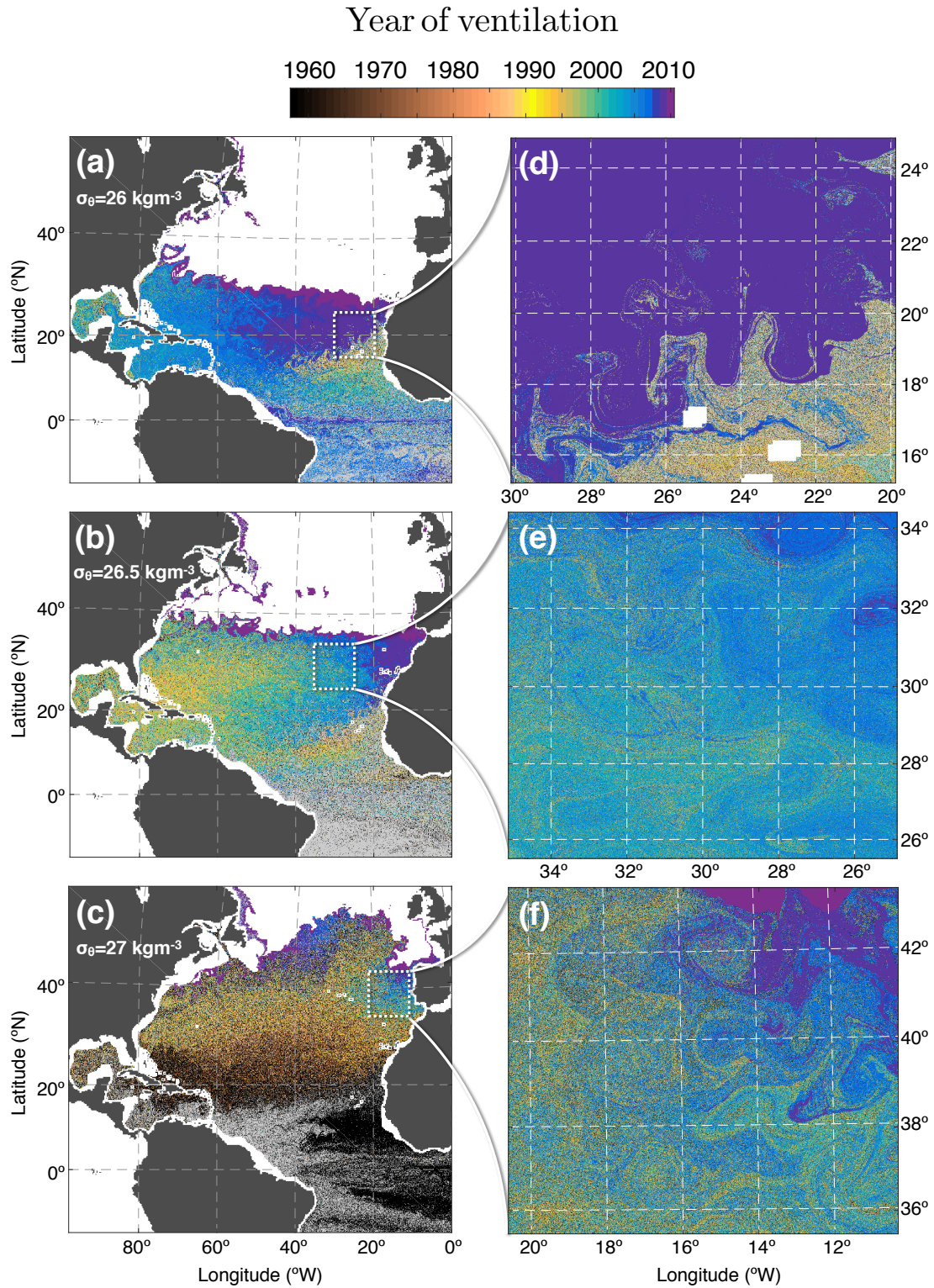


Figure 3.9: Ventilation year of particles on (a,d) $\sigma_\theta = 26 \text{ kgm}^{-3}$, (b,e) $\sigma_\theta = 26.5 \text{ kgm}^{-3}$ and (c,f) $\sigma_\theta = 27 \text{ kgm}^{-3}$ at the end of March 2010. (a,b,c) Entire density surface, 25 particles per model grid cell. (c,d,e) An approximately $10^\circ \times 10^\circ$ box centred on (d) 25°W 20°N , (e) 30°W 30°N and (f) 15.5°W 39.5°N , 625 particles per model grid cell, $\sim 1 \text{ km}$ resolution. Note that the color scale is nonlinear, designed to emphasise gradients in the most recent two decades. Black: particle unventilated during model run. Light grey: Particle originated outside model domain, thus no ventilation year obtained.

mapping is comparatively chaotic across the entire surface. Such variation between surfaces is consistent with our expectations based on a filamentation number that increases with depth (Figure 3.6).

Considering initially σ_{26} , the homogenous nature of the mapping in the eastern half of the basin is perhaps surprising considering the values of F in this region (between 10 and 50) from which one would expect to find smaller scale filaments present. That this filamentation is not present is due to the large spatial scale occupied by recently ventilated 2009 water, which exceeds the scale over which filamentation characterised by F occurs (~ 100 km, Section 3.4.1, Figure 3.8). Consequently, filamentation of 2009 water is confined to its outer edges. This can be seen in the centre of the gyre and, most strikingly, at the boundary between the gyre interior and shadow zone to the south (Figure 3.9a, d). The homogenous mapping of recently ventilated water contrasts starkly with the more filamented, chaotic shadow zone, where adjacent water parcels are often ventilated decades apart. Long, thin filaments of the shadow zone water are drawn out into the newly ventilated gyre interior, and vice versa (Figure 3.9d). This eddy-driven exchange is hypothesised to be crucial for the ventilation of shadow zones (Bettencourt *et al.*, 2015).

Filamentation occurring within the recently ventilated 2009 water on σ_{26} can be visualised by mapping ventilation longitude rather than ventilation year (Figure 3.10). Given the predominantly zonally-aligned nature of the density surface outcrop, and by construction of the color scale, the maximum initial scale of ventilated water in this mapping is 5° longitude (≈ 500 km), and therefore closer to the scales at which the filamentation characterised by F occurs. Consequently, filamentation occurs within a short distance of the outcrop, including within the recently ventilated 2009 water (Figure 3.10a, c). The mapping of ventilation longitude is also indicative of the large horizontal scale over which stirring and filamentation mixes fluid. Regions of the 10° by 10° box on σ_{26} (Figure 3.10c) show trajectories that were ventilated from across a 45° longitude band, within a year of ventilation.

On $\sigma_{26.5}$, recently ventilated water is confined to a comparatively small region at the eastern side of the basin (Figure 3.9b). The mapping becomes increasingly

chaotic within a short distance to the west, where filaments of young and old water are stirred together (Figure 3.9e). The contrasting nature of the ventilation pathways on $\sigma_{26.5}$ and the shallower surface, σ_{26} , is emphasised by considering the mapping of ventilation longitude (Figure 3.10). The high-resolution mappings in Figure 3.10c-d are positioned at the same horizontal location. Consequently, they exhibit the same structure of recent mesoscale stirring on both surfaces. On $\sigma_{26.5}$ the stirring is taking place between already highly filamented water, due to the greater age of the water on this surface and the strain it has experienced since ventilation — characterised by its greater value of F .

The mapping of ventilation longitude gives an impression of the large-scale ventilation pathways on each of these shallower surfaces. On σ_{26} , despite filamentation taking place, there remains a strong signature of the gyre circulation (Figure 3.10a). There is some evidence for the impact of the large-scale gyre circulation on $\sigma_{26.5}$, where fluid ventilated at the eastern edge of the outcrop appears to be preferentially advected around the southern edge of the gyre, though there is evidently significant filamentation and stirring along the way (Figure 3.10b). Both surfaces exhibit increasingly filamented structure towards the western ‘pool’ region, in which eddy stirring is expected to be dominant (Rhines and Young, 1982). On both surfaces, there appears to be eastward movement of water immediately south of the outcrop, which appears to be due to eddy stirring and, on $\sigma_{26.5}$, advection by the Azores current. Finally, the mapping of ventilation year (Figure 3.9) gives the impression that, on both of these surfaces, water is ventilated in the east and ages as it moves westward. In contrast to this view, the western pool region on both density surfaces is at least partly ventilated locally in the west rather than being composed of waters of eastern origin (Figure 3.10a-b). This raises the possibility that the age distribution on these surfaces is, in part, due to stirring between a region in the east that is locally ventilated each year and a region in the west that is ventilated locally, but on much longer long-timescales.

Across the entirety of the deepest surface, σ_{27} , the mapping of ventilation year is highly chaotic, consistent with the large filamentation number, and suggesting

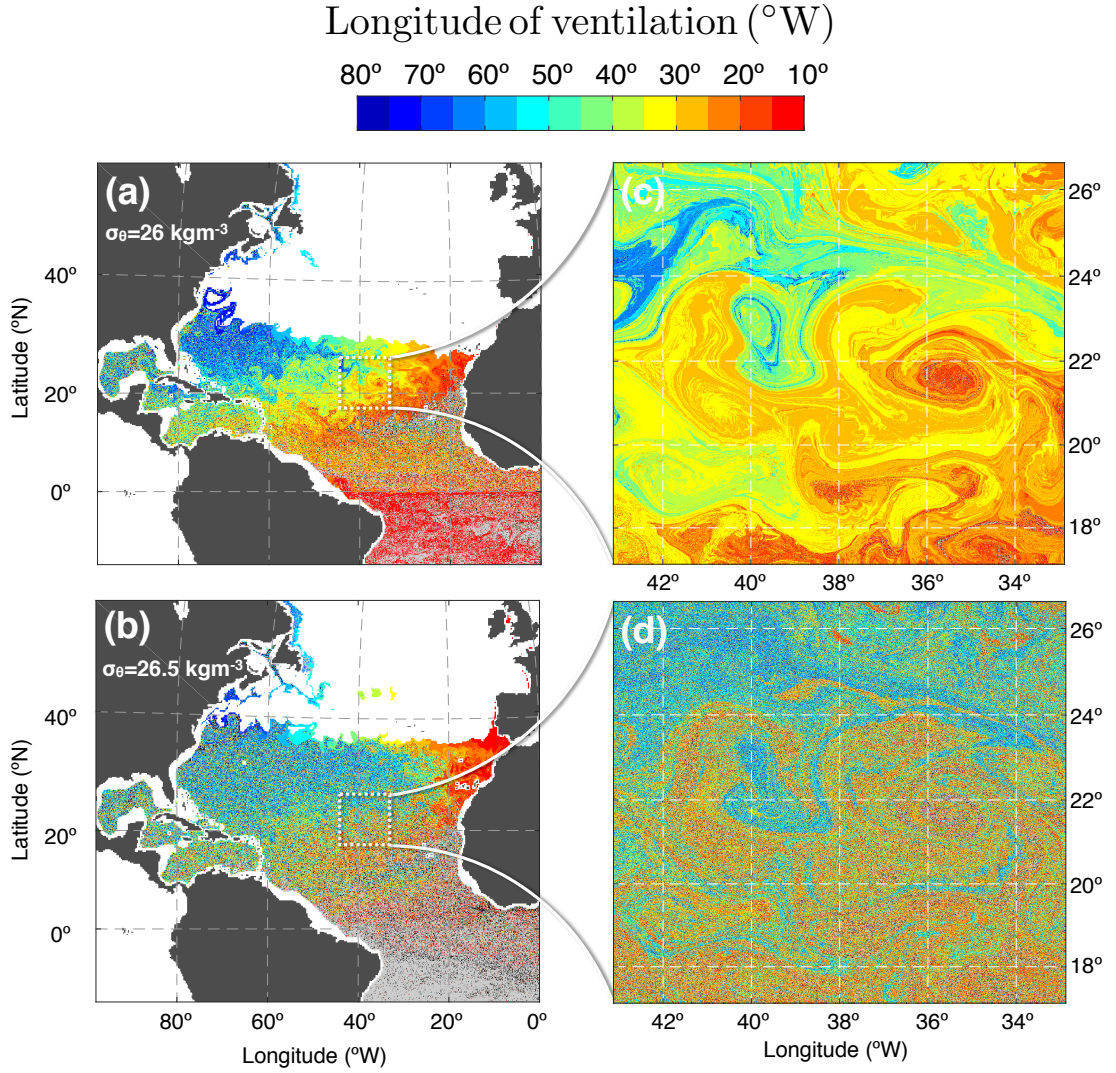


Figure 3.10: Longitudinal band from which particles were ventilated on (a,c) $\sigma_{\theta} = 26 \text{ kgm}^{-3}$ and (b,d) $\sigma_{\theta} = 26.5 \text{ kgm}^{-3}$ at the end of March 2010. (a,b) Entire density surface, 25 particles per model grid cell, and (c,d) approximately $10^{\circ} \times 10^{\circ}$ boxes centred on 38°W 22°N , 625 particles per model grid cell, $\sim 1 \text{ km}$ resolution. Black: particle unventilated during model run. Light grey: Particle originated outside model domain, thus no ventilation longitude obtained.

that the ventilation pathways of this density surface are dominated by eddy-stirring (Figure 3.9c). There persists a large-scale gradient in ventilation year from the northeast to the southwest of the basin, often invoked to hypothesise a dominant role for the gyre circulation (Williams, 1991; Jenkins, 1988). However, such a gradient could feasibly be established by eddy-stirring alone, from the ventilation region in the north east, without any role for the time-mean flow. Such a scenario would be facilitated by the anisotropic nature of eddy-stirring in the North Atlantic, which appears to broadly align with streamlines of the large-scale flow (Rypina *et al.*, 2012).

Even close to the ventilation region in the north east, the mapping is remarkably chaotic, with particles initialised side-by-side often found to have been ventilated decades apart (Figure 3.9f). Recently ventilated water, from 2009, is filamented and stirred into older water close to the density surface outcrop. Within one year, the filaments of 2009 water have been reduced to extremely small scales (Figure 3.9f), emphasising the exponential rate at which this filamentation occurs. The short timescale of filamentation is similarly apparent on the shallowest surface, σ_{26} , at the shadow zone boundary (Figure 3.9d) and in the gyre interior (Figure 3.10c). In both of these regions, the observed filaments have been generated in less than one year.

3.4.3 Validating the Filamentation Number

The theory presented in Section 3.2 indicates that the filamentation number, F , characterises the filament width (and therefore the chaotic nature) of the mappings in Figures 3.9 and 3.10. While obtaining a direct measure of filament width is not straightforward, we can investigate properties of the tracer distribution that may be expected to be related, such as power spectra and tracer gradients. Given the magnitude of F , we expect the filament width to be extremely small — orders of magnitude smaller than the model grid scale. To resolve as much of the filamentation as possible, therefore, we produce a mapping at very high spatial resolution (approximately 1 m) along zonal lines on each of the three surfaces. The location of these zonal lines is shown in Figure 3.6, from which it can be seen that they sample a range of values of F .

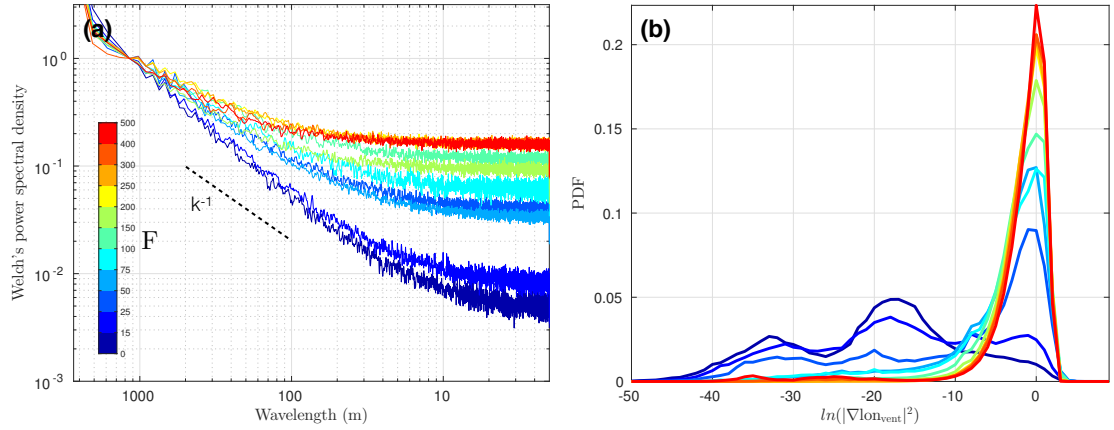


Figure 3.11: (a) Average spatial power spectrum and (b) PDF of gradients (both for longitude of ventilation) for ranges of values of filamentation number, F . See Section 3.4.3 for full details of calculation.

The power spectra of passive tracers in the nonlocal regime are predicted to exhibit power law behaviour, with the power varying as k^α where k is the spatial wavenumber (Batchelor, 1959). Pierrehumbert (1994) found that a slope of $\alpha = -1$ (consistent with the prediction of Batchelor, 1959) emerges in the nondiffusive limit of a dynamical system map developed to simulate chaotic advection. They also note that a flattening of the spectrum occurs when the expected filament width of the tracer is much less than the resolution of the mapping as a result of aliasing from undersampling. That is to say, the presence of increasingly small scales impacts the spectral slope in the resolved range. It logically follows, and indeed Pierrehumbert (1994) found, that the smaller the expected filament scale, the flatter the spectral slope. While this aliasing obscures the signal that Pierrehumbert (1994) were investigating, in our case we would expect its effect to be directly reflected by the filamentation number — a larger value of F implies the presence of smaller scales and consequently a flatter spectral slope. The spatial power spectrum of the ventilation longitude is evaluated within each grid cell (2.5×10^4 data points) using Welch's power spectral method (Welch, 1967). Grid cells are grouped according to their value of F , and the average spatial power spectrum in different ranges of F is determined.

The results of the spectral analysis can be seen in Figure 3.11a. We only show averages for regions with F less than 500. For F less than 25, the spectral slope is

slightly steeper than -1 . This is likely to be due to the fact that the forcing of tracer variance — ventilation — is more similar to a ‘resetting’ forcing (Pierrehumbert, 1994; Neufeld *et al.*, 2000) than an ‘additive’ forcing, adopted in the theory of Batchelor (1959). As we consider regions of larger F , the slope of the average spectrum become increasingly shallow, consistent with smaller filament width, and a more chaotic mapping in these regions.

The filament width should also be related to the gradient of the tracer in the mapping. The tracer gradient, ∇C , scales as $\Delta C/\Delta x$, where Δx is the filament width and ΔC is a typical tracer difference between adjacent filaments. So as Δx decreases, ∇C increases. The PDFs of the squared gradient of the ventilation longitude are shown in Figure 3.11, where the x-axis is on a natural logarithm scale. As for the power spectra, PDFs are grouped and averaged within bands of F . For the ventilation longitude, the relationship between ∇C and F is complicated by the fact that ΔC will also vary depending on the locations where, and scales across which, subduction occurs, as well as the spatial scales of stirring in the subsurface. Close to a ventilation region, ΔC will tend to be small, with water parcels mostly ventilated locally. Deeper in the subsurface, where parcels have originated from a wider range of longitudes, its typical value will be larger. We correct for this by normalising the tracer gradient by the standard deviation of the tracer concentration in each grid cell.

Figure 3.11b shows that at lower values of F , normalized tracer gradients tend to be smaller, consistent with our expectations. If the water were subducted uniformly across the density surface outcrop and not stirred at all during its transport into the subsurface, the squared, normalized tracer gradient would be approximately e^{-20} , which is close to the maximum of the distribution for $F < 15$. As the mapping is produced at greater values of F , there becomes an increasing presence of large gradients. The PDFs converge towards a maximum at e^0 , a value that corresponds to adjacent particles originating from across the width of the basin. As for the power spectra, the PDFs are bounded by the resolution of the mapping, since Δx has a lower bound of around 1 m , meaning that ∇C cannot exceed the width of the basin.

Both power spectra of tracer variance and PDFs of tracer gradients evolve in the expected manner based on our understanding of the filamentation number, F . Future work may seek to elucidate a deeper relationship between F and the properties of the tracer mapping. Such analysis could involve adopting an even higher spatial resolution for the mapping, other metrics of the tracer distribution such as its fractal nature (Pierrehumbert, 1994; Neufeld *et al.*, 2000), or including a form of diffusion along trajectories, as in Abraham and Bowen (2002).

3.5 Discussion

The turbulent nature of ocean circulation is thought to play an important role in the ventilation process, but its impact remains difficult to quantify in both observations and numerical simulations. In this study, we propose that a nondimensional ‘filamentation number’ characterises the chaotic nature of ocean ventilation pathways. The filamentation number is the ratio of a ventilation timescale (the time since a fluid parcel was last in the mixed layer) and a Lagrangian strain timescale (the inverse of the mean strain rate following a water parcel from the mixed layer into the ocean subsurface). It quantifies the extent to which the filament width of a fluid parcel has been reduced since leaving the mixed layer, which, in turn, characterises the extent to which pathways into the ocean interior are laminar or chaotic.

We have shown in an eddy-permitting ocean model that, due to the vastly longer timescale over which the ocean is ventilated compared to that over which it is strained, the filamentation number is large everywhere across three density surfaces in the subtropical North Atlantic thermocline. Consistent with this, mapping surface properties onto these density surfaces reveals highly filamented structure. Consequently, adjacent fluid parcels are found to have followed completely different pathways from the surface mixed layer, and often to have been ventilated decades and great distances apart.

There is a significant increase in the filamentation number with depth (Figure 3.6), implying increasingly chaotic ventilation of the deeper density surfaces, a result confirmed by mapping the ventilation year of individual trajectories (Figure

3.9). This is partly due to the longer ventilation times at depth, but also to the decrease in τ_{strain}^L with depth (Figure 3.5d-f), reflecting the different pathways along which each surface is ventilated. These results are consistent with previous studies that have noted the increased importance of mesoscale variability in the dynamics of the lower thermocline due to the fact that the strength of the time-mean flow decreases more rapidly with depth than does the mesoscale eddy activity (Rhines and Schopp, 1991; Henning and Vallis, 2004). In addition, the outcrop locations of the two deeper density surfaces ($\sigma_\theta = 26.5 \text{ kgm}^{-3}$ and $\sigma_\theta = 27 \text{ kgm}^{-3}$), within and to the north of the Azores current, means that direct subsurface pathways into the subtropical ocean are limited (Robbins *et al.*, 2000). Consequently, much of the ventilation of these density surfaces must be achieved by eddy stirring across the current, leading to filamentation of ventilated fluid parcels and chaotic trajectories.

In the ocean, mesoscale stirring will rapidly reduce the filament width of a coherent fluid patch down to scales at which smaller-scale processes begin to dominate. At this stage, the ventilated fluid patch loses coherence (Rhines and Schopp, 1991). By characterising the reduction in filament width since ventilation, the filamentation number allows us to estimate the distance over which a fluid patch will retain coherence during the ventilation process. Observations of tracers in the thermocline suggest that the filamental structure generated by mesoscale eddies begins to be eroded when the filaments are reduced to widths of around 2 km (Ledwell *et al.*, 1998; Smith and Ferrari, 2009). Thus, for a ventilated fluid patch with initial horizontal scale, $\Delta x(0)$, on the order of 100 km (the upper bound of the nonlocal dynamics in our simulation), a conservative estimate suggests that it would retain coherence only in regions where $F \lesssim 4$. On all three density surfaces, this is within 100 – 300 km of the area where the surface is ventilated (Figure 3.6). This length scale for the loss of coherence is shorter than previous estimates for a gyre circulation (300 – 1200 km) derived from the Peclet number, which characterises the relative impact of advection and eddy mixing on a tracer distribution (O'Dwyer *et al.*, 2000; Rhines and Schopp, 1991). This rapid erosion of the coherence of

ventilated fluid parcels could severely limit the applicability of laminar ventilated thermocline theories, such as Luyten *et al.* (1983).

An alternative framing of the question of coherence is that only a fluid patch with a horizontal scale far exceeding 100 km will remain coherent a significant distance from the ventilation region. This is evident in the mapping of ventilation year, which displays a comparatively vast, coherent region of 2009 water on the shallowest density surface, onto which a large amount of water is ventilated each year. Deeper in the thermocline, the horizontal scale of recently ventilated water decreases and the filamentation occurs within a short distance of the outcrop. Furthermore, in mapping ventilation longitude, for which the initial horizontal scale is limited for all surfaces, filamentation is ubiquitous, as suggested by the large values of F . In the ocean, the same effect is seen in tracer observations. Deser *et al.* (1996) observed the persistence of a cold temperature anomaly during ventilation into the subtropical North Pacific. The anomaly occupied a region of more than 500 km, likely to far exceed the nonlocal regime in the ocean (LaCasce and Ohlmann, 2003; Koszalka *et al.*, 2009), and thus the cold patch retained its signature during ventilation into the ocean interior. On the other hand, in a partially data-constrained numerical simulation of the Southern Ocean, Jones *et al.* (2016) noted erosion of the potential vorticity signature of subantarctic mode waters — with initial horizontal scales between 100 and 200 km — within a few years. Theories for the ventilated thermocline assume that horizontal gradients in potential vorticity are retained as water moves into the ocean interior (Luyten *et al.*, 1983; Huang, 1988; Williams, 1991). If the horizontal scale of these gradients is less than the scale over which rapid filamentation occurs, our results imply that such an assumption would be invalid.

The $1/4^\circ$ ocean model used in the present analysis does not fully resolve mesoscale eddies in the ocean, and is far from resolving submesoscale motions. At higher resolution, both the mesoscale strain and the details of the kinetic energy spectrum (the range of scales over which the dynamics are nonlocal) could be altered. This would affect both the value of F and the scales over which filamentation characterised by F occurs. Given the ongoing debate about the

range over which ocean dynamics are local or nonlocal (LaCasce and Ohlmann, 2003; Lumpkin and Elipot, 2010; McCaffrey *et al.*, 2015), it is not obvious how our results would be altered in a higher resolution simulation or in the ocean. This remains a question for further investigation.

We showed in Figure 3.11 that there is agreement between the properties of an advective mapping and the magnitude of the filamentation number. Such an agreement was expected given the underpinning theoretical basis for the filamentation number establishing the spatial scales of the mapping. However, the quantitative nature of this relationship has not been explored from a theoretical standpoint. There is a rich literature on the distribution of passive tracers stirred by chaotic flows (Pierrehumbert, 1994; Neufeld *et al.*, 2000). In many cases, the tracer distribution is closely determined by properties of the flow, such as the distribution of Lyapunov exponents. In the present case of ocean ventilation, there may be scope to derive a quantitative relationship between the filamentation number and the subsurface tracer distribution.

In conclusion, we have shown that a nondimensional filamentation number characterises the chaotic nature of ocean ventilation. To our knowledge, this is the first attempt to apply a dynamical systems approach to the question of ocean ventilation. We have shown that it is a uniquely appropriate problem for such an approach, providing as it does an inherent timescale over which stirring by the turbulent flow takes place. Further work in this area could prove fruitful in providing deeper understanding of the processes establishing tracer variance (and by extension transit time distributions) in the ocean interior. Our results support the case for a central role for mesoscale strain in setting the properties of the subtropical thermocline. Furthermore, the kinematic approach clarifies the importance of the spatial scales of subduction and of the details of the ocean kinetic energy spectrum in the retention of memory of mixed layer properties during ventilation, with implications for the spreading of atmospherically-derived tracers into the ocean interior.

4

Ventilation of the deep North Atlantic Ocean

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4.1 Introduction

The high-latitude North Atlantic ocean plays a crucial role in global climate. In the first instance, the region has been identified as providing a major contribution to the oceanic uptake of carbon dioxide (Sabine *et al.*, 2004; Khatiwala *et al.*, 2009; Takahashi *et al.*, 2009) and anthropogenic heat (Levitus *et al.*, 2012; Abraham and Baringer, 2013). At the same time, high-latitude surface forcing is thought

to have a substantial impact on the variability of the overturning circulation of the Atlantic Ocean and associated northward heat transport (Stouffer *et al.*, 2006; Robson *et al.*, 2012; Pillar *et al.*, 2016), with wider climatic implications (Zhang and Delworth, 2006; Sutton and Dong, 2012).

The North Atlantic’s prominence is thought to result from the formation and ventilation of intermediate and deep water in the area. Dense water is formed via convective processes in the Labrador, Irminger and Greenland-Iceland-Norway Seas (Lazier *et al.*, 2001; Isachsen *et al.*, 2007; Vage *et al.*, 2011; Yashayaev and Loder, 2016). A component of this water ventilates the wider North Atlantic basin, moving southward as part of the lower limb of the Atlantic overturning circulation. Consequently, heat and carbon exchanged with the atmosphere at the surface can be sequestered in the ocean on timescales from centuries to millennia (Gebbie and Huybers, 2010; Khatiwala *et al.*, 2012). Furthermore, processes implicit in the ventilation of deep waters, primarily deep convection in the Labrador Sea, have been implicated in the variability of the overturning circulation on decadal (Bjastoch *et al.*, 2008; Robson *et al.*, 2012) and centennial (Cheng *et al.*, 2013) timescales, and much longer (Broecker *et al.*, 1985).

In light of this importance, recent decades have seen substantial efforts to understand the connection between variability in surface forcing, deep ocean ventilation, heat and carbon storage, and the large-scale circulation in the North Atlantic (Rhein *et al.*, 2011; Kieke and Yashayaev, 2015). Observations suggest that each of these processes exhibits substantial variability on inter-annual to decadal timescales (Marshall *et al.*, 2001b; Hakkinen and Rhines, 2004; Lozier *et al.*, 2008; Yashayaev and Loder, 2016). Consequently, understanding the nature of this variability, and what drives it, is crucial in distinguishing between internal variations of the climate system from long-term, forced trends. Furthermore, elucidating an oceanic control on the timescale and magnitude of this variability could facilitate decadal predictions of the climate system (Branstator and Teng, 2014; Ortega *et al.*, 2016). On longer timescales, understanding the connection between these processes is central to establishing the response of the North Atlantic, and global climate, to

changes in forcing in a warming world (Vellinga and Wood, 2002; Stouffer *et al.*, 2006). Despite substantial efforts, the manner of the connection between these processes remains poorly understood (Lozier, 2012).

It has often been presumed that variability in dense water formation leads to changes in the ventilation of the deep North Atlantic, as well as the properties of ventilated water. While this is clearly true in a local sense (Van Aken *et al.*, 2011; Yashayaev and Loder, 2016), observational evidence for this link away from the formation regions has been difficult to pin down (Schott *et al.*, 2004; Rhein *et al.*, 2011). This is due to the varied and diffusive pathways of newly formed dense water, which spreads out and erodes the downstream signature of surface forcing (Bower *et al.*, 2009; Zou and Lozier, 2016). In addition, there is considerable uncertainty about the manner in which dense waters are exported from the vicinity of their formation, and the variability of this process (Straneo, 2006; Palter *et al.*, 2008; Jochumsen *et al.*, 2017). Nevertheless, there is increasing evidence for a signature of dense water formation variability being present substantially far downstream of formation sites (Le Bras *et al.*, 2017). In addition, changes in ventilation of the subpolar North Atlantic (inferred from tracer inventories) are seen to reflect changes in the formation process (Rhein *et al.*, 2011; Fine *et al.*, 2002).

In this chapter, we consider the mechanisms and variability of ventilation in the high-latitude North Atlantic of an eddy-permitting, numerical ocean circulation model. In particular, we focus on the processes exporting dense water from its location of formation, and the variability therein. We adopt an approach that directly links water in the deep North Atlantic ocean to the time and location that it left the mixed layer, via backwards-in-time, non-diffused Lagrangian trajectories. This approach is akin to a purely advective evaluation of the transit time (and formation location) distribution (Holzer and Hall, 2000; Primeau, 2005), with the advantage that signatures of variability are not eroded in the subsurface as in the diffusive, tracer-derived case (Waugh *et al.*, 2004).

The questions we address are twofold:

1. How is ventilation of the deep Atlantic Ocean achieved in a $1/4^\circ$ numerical ocean circulation model?
2. How is variability in surface forcing translated into the ocean interior?

In the methods section, we establish a mathematical notation to be used in the rest of the chapter, outline our experimental procedure and justify our selection of ‘North Atlantic Deep Water’ in the numerical simulation used. We separate the results into three sections considering the locations at which ventilation occurs in the model, the pathways along which that ventilated water flows, and the variability in the properties of the ventilated water.

4.2 Methods

Details of the numerical simulation and Lagrangian code used for the following analysis are given in Chapter 2. Here we provide details of the experimental strategy and methodology unique to this chapter.

4.2.1 Mathematical notation

We establish a consistent mathematical notation to assist the interpretation and accuracy of the following work. In particular, we use the mathematical notation in each figure caption to clarify precisely what is being shown. The nomenclature is based on set notation, with additional shorthands for our purposes. A summary of the notation is found in Table 4.1.

We define longitude, latitude coordinates as $\mathbf{x} = (\lambda, \phi)$, depth as z , and time as t , in units of decimal years. We begin with the set of all points in space and time, constrained by the timespan and spatial domain of our numerical model:

$$P(\mathbf{x}, t) = \{\mathbf{x} \in \text{NA}, t \geq 0\}, \quad (4.1)$$

where NA is the North Atlantic domain of our model and $t = 0$ corresponds to the start of the numerical simulation (00:00 on 1st January 1958). From t , we define an alternative time coordinate corresponding to the decimal year: $y = 1958 + t$.

In the Eulerian frame, we can derive a subset of P from the local *properties*. These could be the space and time coordinates themselves, or other quantities that depend on these, such as temperature or density. Having established the full set, P , we denote a subset using conditional statements. For example, the set of all points, with space and time within P , and with neutral density greater than 27.8 kgm^{-3} is written:

$$S(\gamma^n > 27.8) = \{(\mathbf{x}, t) \in P : \gamma^n(\mathbf{x}, t) > 27.8\}. \quad (4.2)$$

For properties for which conditions are not explicitly stated, points are included across their entire range.

The benefit of Lagrangian trajectory analysis is to establish further properties of the points in the set, distinct from their local, Eulerian properties. This allows us to subsample the set P in novel ways. In particular, for this study, we establish the time and location where each point left the surface ocean mixed layer. We denote these variables $\mathbf{x}_v$ and t_v , respectively (where v denotes ventilation). From this we also define the *ventilation year*, $y_v = 1958 + t_v$, and the age, $a = t - t_v$. The essence of Lagrangian analysis means that, because we apply no stochastic noise (see Chapter 2), these trajectory-derived variables are invariant quantities associated with each point in space and time that have been labelled with the coordinates $(\mathbf{x}, t)$ (Bennett, 2006). So, for example, the subset of all points ventilated since 1st January 1958 is written:

$$S(y_v > 1958) = \{(\mathbf{x}, t) \in P : y_v(\mathbf{x}, t) > 1958\}, \quad (4.3)$$

where the colon should be read as “such that” or “given”.

We can also derive subsets from multiple conditions. For example, the subset of points with neutral density greater than 27.8 kgm^{-3} and ventilated in the year 2000 is written:

$$S(\gamma^n > 27.8, y_v = 2000) = \{(\mathbf{x}, t) \in P : \gamma^n > 27.8 \cap 2000 \leq y_v < 2001\}, \quad (4.4)$$

where the $\cap$ symbol denotes “and”. Note that in the shorthand, we have dropped the inequality for simplicity, such that $y_v = 2000$, means that the point was ventilated at any time during the year 2000.

We introduce further notation to define the properties of the points in a subset. For example, the potential temperatures associated with points ventilated in the year 2000 would be written:

$$\Theta(y_v = 2000) = \{\theta(\mathbf{x}, t) : (\mathbf{x}, t) \in S(y_v = 2000)\}. \quad (4.5)$$

Properties for which we use this notation in this study include local volume (variable notation: v , set notation: $\mathcal{V}$), age (a , $\mathcal{A}$), and latitude (ϕ , Φ).

We denote the sums and volume-weighted means of the properties of points in a subset using tildes and overbars, respectively. Using the above example,

$$\tilde{\Theta}(y_v = 2000) = \sum_{(\mathbf{x}, t) \in S(y_v = 2000)} \theta(\mathbf{x}, t) \quad (4.6)$$

$$\bar{\Theta}(y_v = 2000) = \frac{1}{\tilde{\mathcal{V}}(y_v = 2000)} \sum_{(\mathbf{x}, t) \in S(y_v = 2000)} v(\mathbf{x}, t) \theta(\mathbf{x}, t). \quad (4.7)$$

A significant component of the following analysis is the arrangement of points into distributions, based on their properties. We denote the distribution by $\mathbb{D}$. The arguments correspond to the subset of points across which the distribution is derived. The property into which the subset is divided is denoted in the subscript. For example, the age distribution of points with neutral density greater than 27.8 kgm^{-3} would be written:

$$\mathbb{D}_a[S(\gamma^n > 27.8)], \quad (4.8)$$

for which the entry corresponding to age a_i would be

$$S(\gamma^n > 27.8, a - \frac{\Delta a}{2} \leq a_i < a + \frac{\Delta a}{2}), \quad (4.9)$$

where Δa is the bin-width of the distribution. For simplicity, the limits and bin-width of the distribution are not explicitly labelled in the notation. Unless otherwise stated, the limits will include the whole range of possible values and the bin width

will be a value that adequately resolves the components of the distribution that we wish to highlight. An anomalous distribution, *i.e.* a distribution minus its mean value, is annotated with a prime: *e.g.* $\mathbb{D}'_a$.

If we wish to determine the distribution of a *property* of the points in a subset, we replace S in equation 4.9 with the property subset notation given in equation 4.5, for which we can also specify that we are taking the sum or mean. For example, the *volumetric* distribution of density for all points ventilated in the year 2000, would be written:

$$\mathbb{D}_{\gamma^n}[\tilde{\mathcal{V}}(y_v = 2000)]. \quad (4.10)$$

Finally, we notate the mean of distributions over a property using an overbar. This is required when, for example, we wish to determine the time-mean age distribution on a density surface. So, the volumetric age distribution, evaluated in different years and then averaged, would be written:

$$\overline{\mathbb{D}}_a[\tilde{\mathcal{V}}]. \quad (4.11)$$

Again for brevity, we do not specify the range over which the average is taken. This will be explicitly stated in the text.

There are some further things that, for clarity, are implicitly assumed in the notation. Unless otherwise stated, if a subset or distribution depends on a ventilation property (*e.g.* neutral density at the time of subduction, γ_v^n), then the points included are only those that were ventilated since January 1958 *i.e.* unventilated points are not included. Also, if it is not otherwise stated, we are considering points in the final year of the simulation, *i.e.* at the end of June 2012.

4.2.2 Experimental strategy

We wish to determine the Lagrangian properties, namely the time and location of subduction, of the points in the deep North Atlantic throughout time in our numerical ocean simulation. That is, we wish to establish the Lagrangian properties of the set P . To this end, we evaluate backwards-in-time trajectories from a volume

Table 4.1: Summary of mathematical notation

Notation	Description
P	Set of all points in the model domain and timespan
$S(\delta \geq \delta_i)$	Subset of P based on the value of the property δ
$\Delta(\epsilon \geq \epsilon_i)$	Property δ (set notation Δ) of the points in subset defined by property ϵ
$\tilde{\Delta}, \overline{\Delta}$	Sum and volume-weighted mean of properties of points in a subset
$\mathbb{D}_\epsilon[S]$	Distribution by property ϵ of subset S
$\mathbb{D}'_\epsilon[S]$	Anomalous distribution (distribution minus mean value)
$\mathbb{D}_\epsilon[\Delta]$	Distribution by property ϵ of property δ of points in subset S
$\overline{\mathbb{D}}_\epsilon^\zeta[\Delta]$	Mean of distribution across range of property ζ

within the deep North Atlantic, and determine the last time and location that that water was in the mixed layer. Particles were initialised at each model tracer point (located in the centre of the grid cell) at the end of June every year between 1975 and 2012 (we avoid the early, spin-up years of the simulation). Because we are interested in inter-annual and longer timescales in the ventilation process, and because ventilation into the ocean interior happens over a limited time period in the annual cycle, it is sufficient to evaluate the Lagrangian characteristics at only one point in time each year. Trajectories were evaluated backwards in time until reaching a density that was within 0.01 kgm^{-3} of the density at 10 m, following Thomas *et al.* (2015). The sensitivity of our results to this definition of mixed layer depth is assessed in due course.

We complement the backwards-in-time experiments with some forwards-in-time experiments. These were conducted using the points identified from the backwards experiments as having been ventilated in the years 1975 to 2012, *e.g.* we initialise particles in 1975 at the points that were found to be ventilated in 1975: $S(y = 1975, y_v = 1975)$. Again, these trajectories were evaluated until they intersected the mixed layer (defined by the same density-difference criteria) or left across a lateral boundary.

The use of purely advective trajectories enables us to link points in the subsurface to unique properties associated with their subduction from the mixed layer. However, the absence of a stochastic parameterisation for sub-gridscale motion (*e.g.* Shah *et al.*, 2011; Koszalka *et al.*, 2013; Shah *et al.*, 2017) could mean that the pathways

of these trajectories are inaccurate. On the other hand, recent work suggests that the resolved scales in eddy-permitting models (such as that used in this study) are sufficient to capture much of the diffusive spreading of tracers (Gary *et al.*, 2011; Kamenkovich *et al.*, 2017). Furthermore, as we shall see in Section 4.3.2, the age distribution derived from purely advective trajectories is broadly consistent with that derived from tracer observations in the ocean. This suggests advection by the resolved velocity field captures the main components of the ventilation pathways. As such, we are confident that the absence of a diffusive parameterisation in our trajectories does not affect our main results or conclusions.

4.2.3 Identifying North Atlantic Deep Water

The boundary surfaces of the volume were chosen to capture all of the deep ocean ventilation in the North Atlantic, which we hereafter collectively label North Atlantic Deep Water (NADW). It does not make sense to choose these boundaries based on observations of ventilated surfaces in the North Atlantic ocean, since model hydrography can deviate substantially from the real ocean. Instead, we chose to consider the volume bounded between $\gamma^n = 27.7$ and 28 kgm^{-3} , and present the justification for this below.

The time-mean surface density distribution at high northern latitudes during late winter in the model simulation is shown in Figure 4.1. Outcropping density surfaces between $\gamma^n = 27$ and 28.5 kgm^{-3} are present in the region, with the deepest surface outcropping in the Greenland-Iceland-Norway (GIN) seas and along the west coast of Greenland. A local maximum in surface density is also apparent in the Labrador Sea. Notably lighter densities coincide with the Arctic outflows along the east coast of Greenland and from Baffin Bay along the south west of the Labrador Sea. Outcrops corresponding to our definition of NADW are also shown, with the thickness of the contour reflecting the density. The contours bound the Labrador Sea, with the lighter surfaces outcropping around the boundary and the outcrop for $\gamma^n = 27.9 \text{ kgm}^{-3}$ appearing in the north west region. The upper bound of the

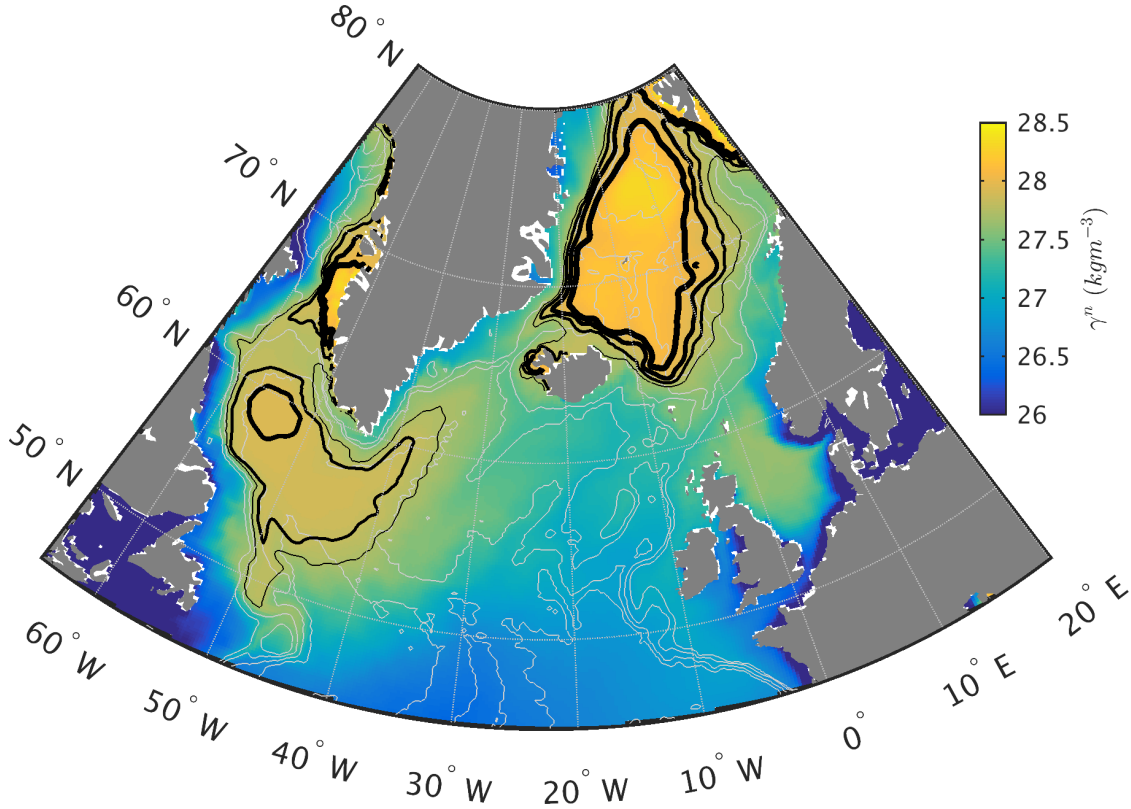


Figure 4.1: Distribution of neutral density in the high-latitude North Atlantic surface ocean. Black contours of increasing thickness correspond to values of $\gamma^n = 27.7, 27.8, 27.9$ and 28 kgm^{-3} . Bathymetric contours at $z = 509, 1516, 2956$ and 3898 m are shown in light grey.

volume ($\gamma^n = 28 \text{ kgm}^{-3}$) excludes the central GIN seas, such that the dense water in that region is not included in our definition of NADW.

The neutral density distribution of volume in the whole of the Atlantic sector of the model (30°S to 80°N 100°W to 30°E) is shown in Figure 4.2, where we only show densities greater than $\gamma^n = 27 \text{ kgm}^{-3}$. Most of the volume is contained between $\gamma^n = 27.7$ and 28.2 kgm^{-3} , with three distinct peaks at around 27.85, 27.95 and 28.05. Also shown is the neutral density distribution of the volume ventilated in an experiment in which particles were initialised throughout the entire sector in the final winter of the simulation. Over the 54 years of the simulation, $\sim 10\%$ of the model domain was ventilated from the mixed layer and, in the deep ocean, this was concentrated between $\gamma^n = 27.7$ and 28 kgm^{-3} , with a single peak at $\gamma^n = 27.85 \text{ kgm}^{-3}$.

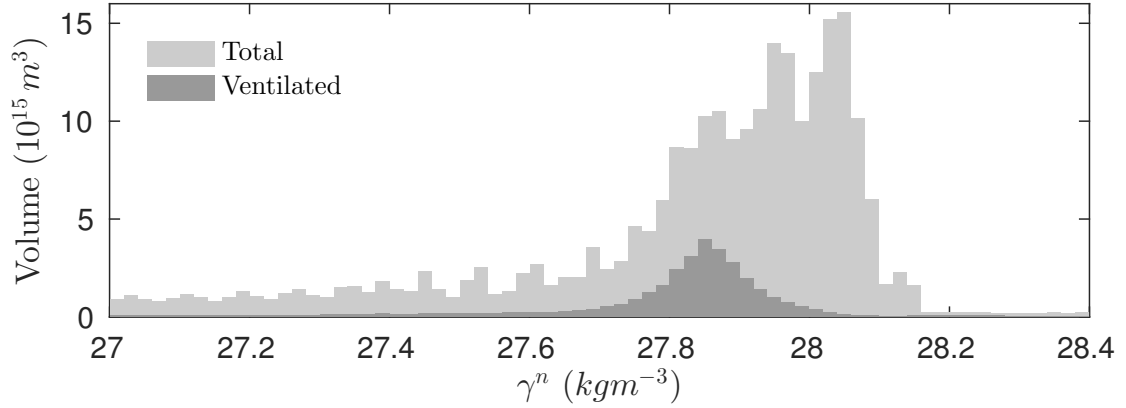


Figure 4.2: Volumetric histogram of the density distribution in the Atlantic domain in March, 2012, of the simulation. Light grey bars correspond to the distribution across the total volume: $\mathbb{D}_{\gamma^n}[\tilde{\mathcal{V}}]$. Dark grey bars correspond to the volume that is ventilated over the 52 years of the simulation: $\mathbb{D}_{\gamma^n}[\tilde{\mathcal{V}}(y_v > 1958)]$

Another aspect that we wish to capture in our selection of the volume boundaries is the southward flow of NADW as the lower limb of the Atlantic Meridional Overturning Circulation (AMOC). Figure 4.3 shows the AMOC streamfunction at the end of June in the final model year. This is overlain with contours of neutral density, averaged across the main North Atlantic basin (*i.e.* excluding the Mediterranean), at $\gamma^n = 27.7, 27.8, 27.9$ and 28 kgm^{-3} . This shows clearly that the volume bounded between $\gamma^n = 27.7$ and 28 kgm^{-3} captures the major component of the southward limb of the AMOC. The upper boundary at $\gamma^n = 27.7$ sits marginally below the northward flowing limb at subtropical latitudes and thus it makes sense not to consider lighter water masses.

There is ventilation in density classes greater than $\gamma = 28 \text{ kgm}^{-3}$ (Figure 4.2) that we omit in our main experiments. To ensure that this does not result in us missing an important component of deep North Atlantic ventilation, we look more closely at this water mass. Figure 4.4 shows cumulative histograms of the latitude at which water with $\gamma > 28 \text{ kgm}^{-3}$ is ventilated, and where it ends up at the end of the simulation. The ventilation latitude shows that this volume is mainly formed between 65 and 75°N , implying that it is from the Greenland-Iceland-Norway (GIN) Seas. The bottom panel shows, however, that only a very small fraction (less than 5%) of this water mass exported south of 60°N and into

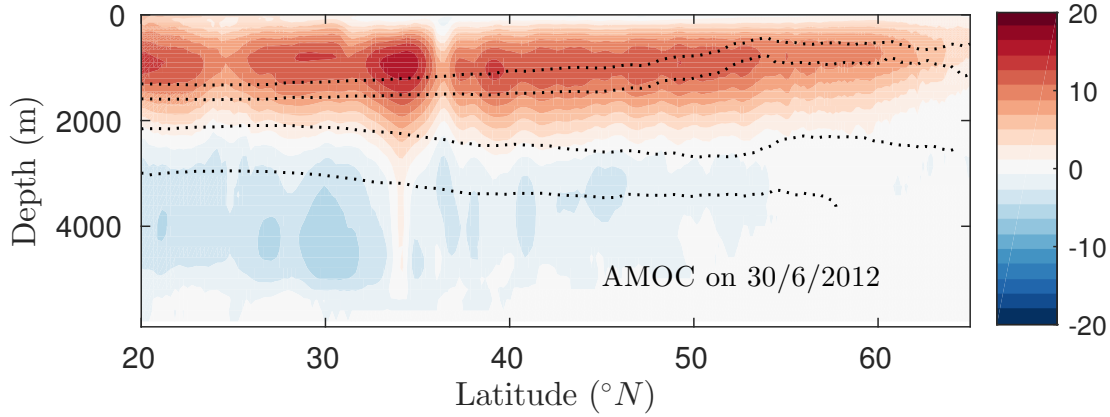


Figure 4.3: Atlantic meridional overturning circulation (AMOC), in units of Sverdrups (Sv ; $1 Sv = 10^6 m^3 s^{-1}$), evaluated in depth space at the end of June, 2012. Black dotted lines correspond to neutral density contours at $\gamma^n = 27.7, 27.8, 27.9$ and $28 kg m^{-3}$.

the main North Atlantic basin. This ventilated water mass is GIN seas water that remains mostly within the GIN seas and as such is not a significant contribution to the NADW that this study focusses on.

4.2.4 Water mass transformation

At the ocean surface, the movement of water between density classes (and therefore the formation of dense water) is established by fluxes of heat and freshwater. The combination of these, the surface buoyancy flux, $\mathcal{D}_{surf}(\lambda, \theta, t)$ is given by

$$\mathcal{D}_{surf} = -\frac{\alpha}{c_p} Q_{net} + \rho \beta (E - P) S \quad (4.12)$$

where α is the coefficient of thermal expansion, Q_{net} is the total heat flux (incoming shortwave radiation, outgoing longwave radiation, latent and sensible heat fluxes), c_p is the specific heat capacity of water, ρ is density, β is the haline contraction coefficient, $(E - P)$ is evaporation minus precipitation and S is salinity.

Using the water mass formation theory of Walin (1982), which combines the mass and buoyancy conservation equations, we can derive the flux of water across a density surface at the ocean surface based on the surface distribution of buoyancy fluxes and density. This surface-forced water mass *transformation*, $F(\rho)$, is given by

$$F(\rho) = -\frac{\partial}{\partial \rho} \mathcal{D}_{surf}(\rho). \quad (4.13)$$

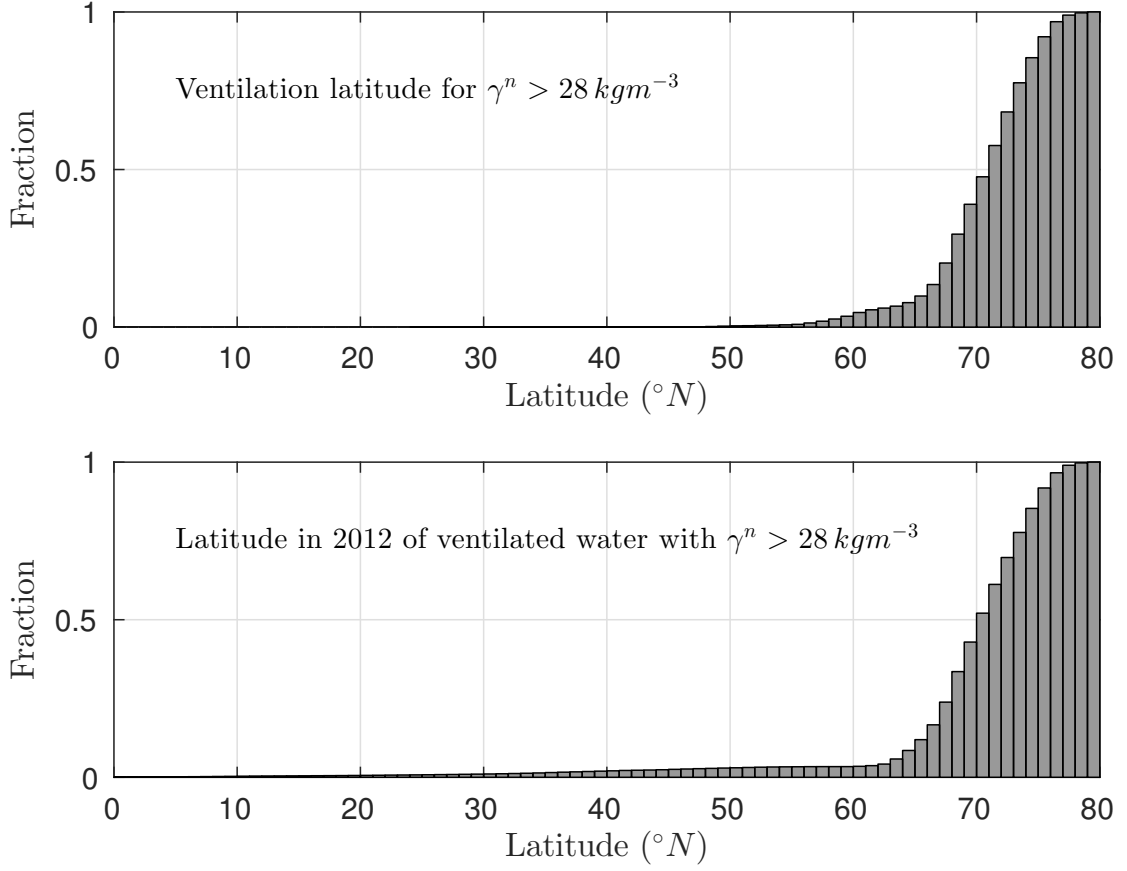


Figure 4.4: Volumetric histogram, presented as a cumulative distribution function, of (top panel) the latitude at which water more dense than $\gamma^n = 28 \text{ kgm}^{-3}$ is subducted: $\mathbb{D}_{\phi_v}[\tilde{\mathcal{V}}(\gamma_v^n > 28)]$, and (bottom panel) final latitude (in March, 2012) of water initially subducted with a density greater than $\gamma^n = 28 \text{ kgm}^{-3}$: $\mathbb{D}_{\phi}[\tilde{\mathcal{V}}(y = 2012, \gamma_v^n > 28)]$

That is, the surface-forced water mass transformation is equal to the diapycnal divergence of the surface buoyancy flux. We can go another step to derive the movement of water into specific density classes, the surface-forced water mass *formation*:

$$M(\rho) = -\frac{\partial}{\partial \rho}(F) = \frac{\partial^2}{\partial \rho^2} \mathcal{D}_{surf}(\rho). \quad (4.14)$$

The formation of these water masses at the ocean surface does not mean that they will be translated into the ocean interior, or retain the same density structure when there. This is because mixing processes, both in the surface mixed layer and in the ocean interior, also enact a buoyancy flux on the water mass, denoted $\mathcal{D}_{int}$. The full form of the Walin (1982) water mass formation theory (in a steady

state and closed domain) is then

$$G(\rho) = -\frac{\partial}{\partial \rho} \mathcal{D}_{surf}(\rho) - \frac{\partial}{\partial \rho} \mathcal{D}_{int}(\rho). \quad (4.15)$$

Thus the volume of water moving between density classes G is a balance between the surface forced water mass transformation and interior mixing. In practice, the interior mixing term is difficult to establish, both in the ocean and even in numerical simulations (Nurser *et al.*, 1999).

We complement our main Lagrangian-based analysis with calculations of the surface forced water mass transformation and its variability. In particular, we consider the extent to which variability in the surface forcing is reflected in the subsurface water masses.

The volume of NADW that we consider is established based on neutral density, γ^n . However, water mass transformations are calculated with respect to potential density referenced to the surface ρ_θ . Iudicone *et al.* (2008) derived a means of evaluating water mass transformation in neutral density coordinates. This requires the calculation of a highly uncertain variable at each point in space and time corresponding to the local slope of neutral and potential density. We opt instead to follow the approach of Abernathey *et al.* (2016) and derive a mapping between ρ_θ and γ^n and attribute the transformation into γ^n bins accordingly. While Abernathey *et al.* (2016) claim that there was a simple, linear relation between these two variables in their region of interest (the Southern Ocean), we do not find such a straightforward situation. This is exemplified in the top panel of Figure 4.5 which shows the difference between ρ_θ and γ^n close to the ocean surface in March 2012. There are substantial variations in the relationship between ρ_θ and γ^n that appear to be related to the presence of freshwater, and the subtropical or high-latitude source of the surface waters. A two-dimensional histogram of γ^n and ρ_θ in March 2012, over the γ^n range of NADW, is shown in the bottom panel of Figure 4.5. A straightforward averaging of γ^n in each ρ_θ bin (blue line) results in a noisy relationship. Our approach, therefore, is to establish both the buoyancy flux and the neutral density along the ρ_θ outcrop for which transformation is being evaluated.

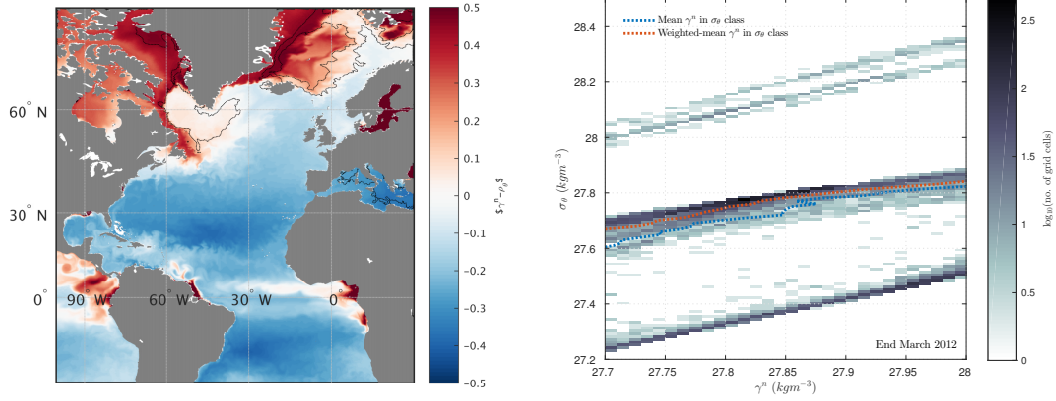


Figure 4.5: (left panel) Difference between neutral density (γ^n) and surface-referenced potential density (σ_θ) at a depth of 10 m across the Atlantic basin at the end of March 2012. Black dotted lines correspond to surface neutral density contours at $\gamma^n = 27.7$ and 28 kg m^{-3} . (right panel) Two-dimensional histogram of neutral density (γ^n) and surface-referenced potential density (σ_θ) at a depth of 10 m within the neutral density range for which we define North Atlantic Deep Water. The colour scale is logarithmic and corresponds to the number of grid cells in each bin, *i.e.* no area weighting is applied. Dotted lines correspond to the estimated relationship between the two variables for the purpose of water mass transformation calculations (Section 4.2.4). The blue line corresponds to taking the mean value of γ^n in each σ_θ class, while the red line corresponds to weighting this mean by the distribution of buoyancy fluxes in each σ_θ class.

We then attribute that transformation to the buoyancy flux-weighted mean γ^n . The buoyancy flux-weighted mean γ^n exhibits a much smoother relationship to ρ_θ in March 2012 (red line in the bottom panel of Figure 4.5).

4.2.5 Comments on the impact of diapycnal trajectories

In Chapter 2, we noted that Lagrangian trajectories in the subsurface ocean, including within the deep water masses, have a substantial diapycnal component. This would pose a problem to the results of this chapter if (a) density changes are in excess of what would be expected in the deep ocean, and (b) the source of these density changes was errors in the Lagrangian trajectory calculation. From the analysis of Chapter 2, we find two main reasons to expect that this is not the case. First, density changes taking place in the deep water masses of the North Atlantic were noted to be close to plausible values derived from a scaling analysis (Figure 2.7). Second, there is evidence to suggest that density changes along trajectories

in the deep ocean are the result of explicit vertical mixing in the model, close to bathymetry (Figure 2.21). This implies that density changes in the deep ocean are consistent with the diabatic nature of the numerical simulation. Nevertheless, we take steps to ensure that our results are not dependent on a presumption of isopycnal motion. In particular, it is for this reason that we initialise particles within a volume rather than on a surface, since it would be difficult to assess processes of ventilation on a surface if many of the particles had arrived from different densities. In contrast, we find that 80% of particles within our NADW volume are subducted within the same volume, such that even if there is diapycnal motion between density classes in the volume, we can still consider processes ventilating NADW as a whole.

4.3 Results

4.3.1 Ventilation locations

Dense waters of North Atlantic origin are formed primarily by convective processes that act to deepen the surface mixed layer (Lazier *et al.*, 2001). As such, the spatial distribution of the mixed layer depth is diagnostic of the regions where dense water is formed. The time-mean, late-winter (mid-March to mid-April) mixed layer depth is shown in Figure 4.6 (top panel). By far the deepest mixed layers are found in the central Labrador Sea and extending south eastward into the Irminger Sea. The colour scale is limited to 1500 *m* so that the spatial pattern outside the deep Labrador Sea can be seen. Black contours, included in the saturated range at 1800 and 2100 *m*, show that, within the Labrador Sea, the deepest mixed layers are found in the north west. North east of this region, the winter mixed layer shoals sharply to depths of less than 500 *m*. At the northern extent of the Labrador Sea, towards the entrance to Baffin Bay, mixed layer depths of ~ 1000 *m* are found in a band that broadly follows bathymetric contours. Across the rest of the subpolar gyre, the deepest mixed layer depths tend to be close to the basin boundaries.

The depth of the winter mixed layer in the model Labrador Sea is substantially greater than that observed in the ocean (Yashayaev and Loder, 2016). In Figure 4.6 (bottom left panel), we show the climatological mixed layer depth in March, derived

from all profile data between 1941 and 2002 (threshold criteria of $\Delta\rho < 0.03 \text{ kgm}^{-3}$; de Boyer Montégut *et al.*, 2004). In addition, we show (bottom right panel) the climatological *maximum* mixed layer depth in March, derived from Argo data between 2004 and 2017 (algorithmic definition of Holte *et al.*, 2017). The late-winter mean mixed layer depth in the model far exceeds even the maximum value in observational estimates (Argo data does not cover the time periods of deepest Labrador Sea convection in the early 1990s, but this is unlikely to explain the substantial difference). We note, however, that the spatial distribution, particularly in relation to the region of deepest mixed layers and extension into the Irminger Sea, shows broad agreement between the model and both sets of observations. On the other hand, there is no evidence in the observations for the deep mixed layers seen in the model at the entrance to Baffin Bay.

Regions in which mixed layers extend into the deep ocean do not necessarily correspond to the regions that are ventilating the ocean interior on inter-annual timescales and longer. To contribute to the latter, water must also be advected away from the region of deep mixed layers before the following winter. The volume of water ventilated into the ocean subsurface at each grid cell, derived from our Lagrangian analysis — $\mathbb{D}_{\mathbf{x}_v}[\tilde{\mathcal{V}}(y = 2012, y_v \leq 2011)]$ — is shown in Figure 4.7. Note that the distribution is derived for ventilated water present in NADW in the final year of the simulation, and thus does not include contributions from water that, since subduction, has been re-entrained to the mixed layer, has moved diapycnally out of NADW, or has been exported out of the North Atlantic domain.

Ventilation occurs close to the boundary around the west and south of the Labrador Sea, in the open ocean to the north east of the Labrador Sea, and at a spread of locations across the rest of the Labrador, Irminger and GIN seas. Broadly speaking, the distribution does not reflect the spatial pattern of the winter mixed layer depth, emphasising that the pathways of water following subduction are crucial to the ventilation process. Relatively high levels of ventilation are present across the western boundary of the Labrador Sea, with intermittent ‘hotspots’ (around $57^\circ\text{W } 56^\circ\text{N}$ and $60^\circ\text{W } 61^\circ\text{N}$) at which there is up to 3 times more ventilation

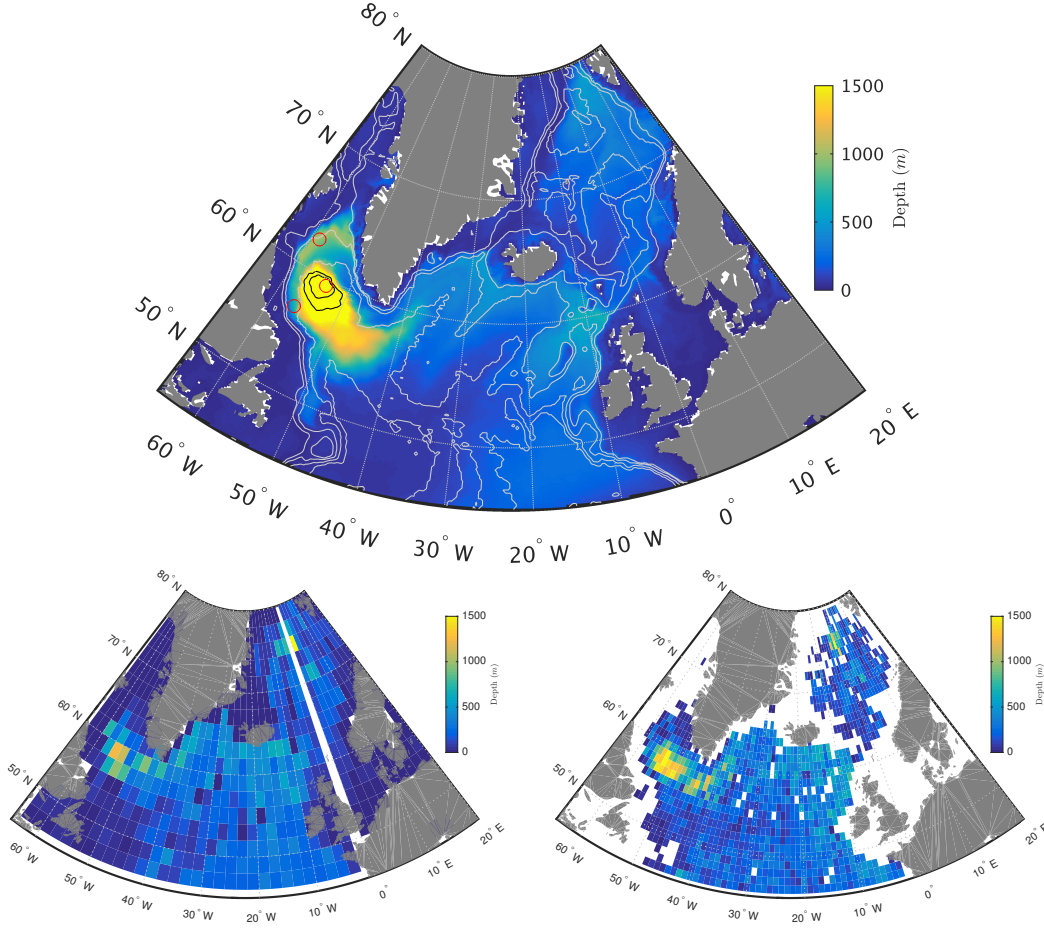


Figure 4.6: Late winter mixed layer depths in the subpolar North Atlantic. (top) Hindcast simulation, mid-February to mid-April time-mean (1975 to 2012) mixed layer depth, defined by a threshold criteria of within 0.01 kgm^{-3} of the density at 10 m . The colour bar is saturated at 1500 m and black contours within the saturated region are for depths of 1800 m and 2100 m . Red circles correspond to the regions where the winter mixed layer depth variability was computed for Figure 4.34. (bottom left) Average March mixed layer from profile data between 1941 and 2002, defined by a threshold criteria of 0.03 kgm^{-3} (de Boyer Montégut *et al.*, 2004). (bottom right) Time average of the maximum March mixed layer depth between 2002 and 2016 from Argo float data, using an algorithmic mixed layer definition to derive the depth from each profile (Holte *et al.*, 2017). In all plots, bathymetric contours at $z = 509, 1516, 2956$ and 3898 m are shown in light grey.

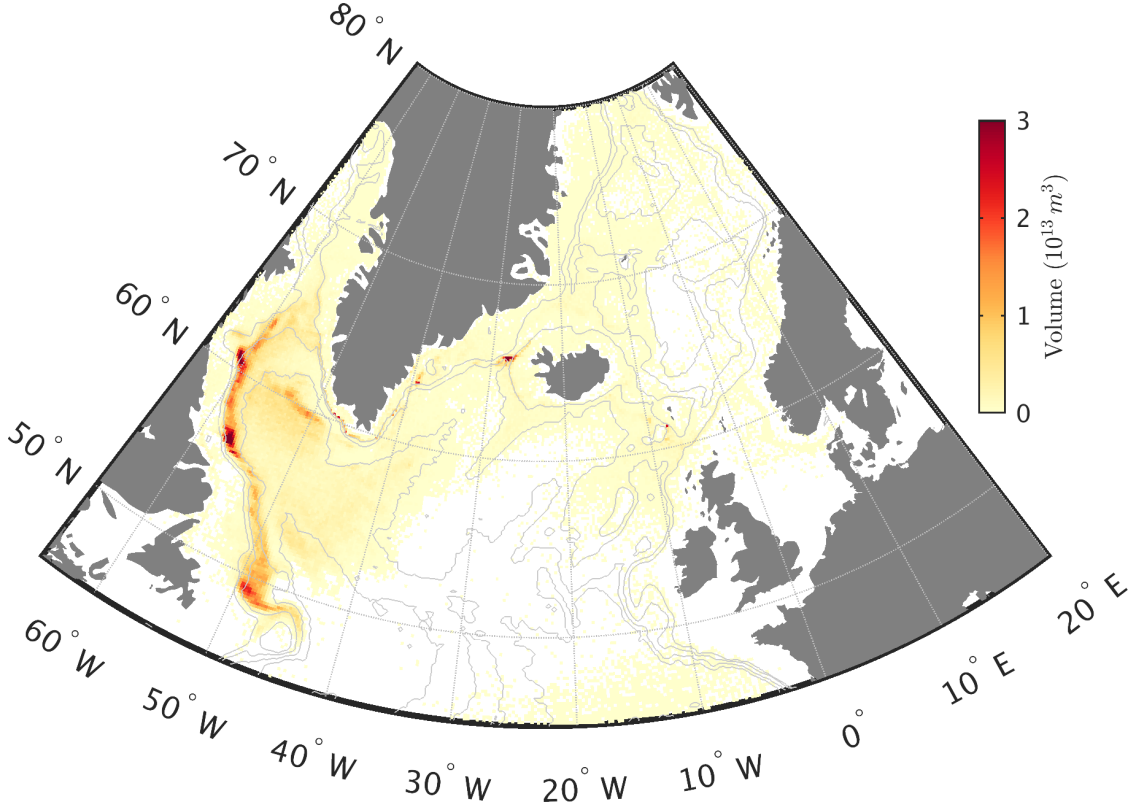


Figure 4.7: Volume of North Atlantic Deep Water subducted at each model grid cell by the final year of the simulation: $\mathbb{D}_{\mathbf{x}_v}[\tilde{\mathcal{V}}(y = 2012, y_v \leq 2011)]$. Subduction in the final year is not included so as to not dominate the figure. Bathymetric contours at $z = 509, 1516, 2956$ and 3898 m are shown in light grey.

(as much as $6 \times 10^{13} \text{ m}^{-3}$) over a few grid cells than in adjacent regions. This localised ventilation is also present in a narrow region at the southwestern extent of the Denmark Straits overflow, at $28^\circ\text{W } 66^\circ\text{N}$, and at various points around the continental shelf south of Greenland.

To confirm that this pattern of ventilation is not biased by the time at which we evaluate the Lagrangian trajectories (*i.e.* the end of the simulation), in Figure 4.8 we also show the pattern for water ventilated before 1984, 1994 and 2004, as evaluated from the Lagrangian properties of NADW in those years. That is $\mathbb{D}_{\mathbf{x}_v}[\tilde{\mathcal{V}}(y = 1984, y_v \leq 1983)]$, $\mathbb{D}_{\mathbf{x}_v}[\tilde{\mathcal{V}}(y = 1994, y_v \leq 1993)]$ and $\mathbb{D}_{\mathbf{x}_v}[\tilde{\mathcal{V}}(y = 2004, y_v \leq 2003)]$. These distributions are presented as PDFs, dividing the volume subducted at each location by the total subduction, to account for the fact that less of the NADW has been ventilated earlier in the simulation. The spatial arrangement of ventilation location is highly persistent, and not biased by the time

at which we observe it. That is to say, the pattern in Figure 4.7 is not influenced by ventilation in specific years, or by the fact that re-entrained water, or water that has left the domain, are not included.

The distribution of ventilation as a function of bathymetric contour, $\mathbb{D}_{b_v}[\tilde{V}]$, is shown as a cumulative histogram in Figure 4.9. The vertical grey lines correspond to the bathymetric contours displayed in Figure 4.7, with the percentage of the volume ventilated between these contours also shown. The majority of ventilation of NADW in the model (71%) takes place shallower than 3000 m, with most of this occurring between 1500 and 3000 m. Open ocean ventilation, deeper than ~ 3000 m, accounts for around 29% of the total ventilation. Consideration of the bathymetric contour locations in Figure 4.7 suggests that most of the open ocean ventilation occurs in the Labrador Sea, while a proportion of the shallower ventilation can be attributed to the GIN seas and Baffin Bay.

Given the dominance of the Labrador Sea in 4.7, these bathymetric contours were chosen to delineate the open ocean from the boundary current in that region. The boundary current system in the Labrador Sea comprises the Labrador Current, with its core above the shelf break around the 1000 m isobath, and the deep Labrador Current, with a core that sits approximately above the 2500 m isobath (Lazier and Wright, 1993; Pickart *et al.*, 2002; Cuny *et al.*, 2005). The 3000 m isobath is commonly adopted as the oceanward extent of the Deep Western Boundary Current (Palter *et al.*, 2008). Figure 4.10 shows the winter mean barotropic streamfunction across the subpolar gyre (mid-February to mid-April mean in the final 30 years of the simulation). In the Labrador Sea, the grouping of streamlines between the 1500 and 3000 m isobaths confirms the presence of a strong boundary current. The maximum transport of around 35 Sv at the western side of the basin is consistent with the observed value of ~ 30 Sv (Hall *et al.*, 2013). It is not possible to clearly distinguish between a shoreward Labrador Current and deep Labrador Current, though the strongest transport coincides with the expected location of the deep current (above the 2500 m isobath). Along the western side of the basin, streamlines closely follow bathymetric contours. In the open ocean, the cyclonic recirculation in

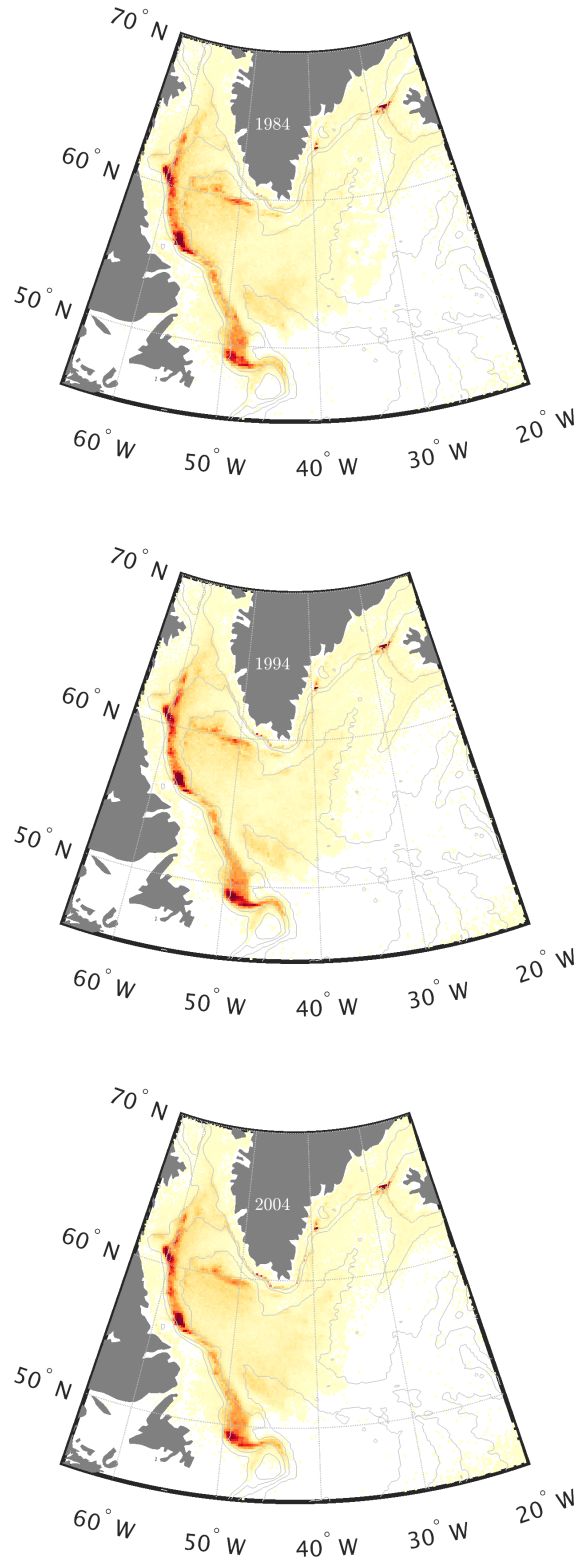


Figure 4.8: As for Figure 4.7 but with the colourscale corresponding to the fraction of the total ventilation and evaluated for subduction before (top) 1984: $\mathbb{D}_{\mathbf{x}_v}[\tilde{\mathcal{V}}(y = 1984, y_v \leq 1983)]$, (middle) 1994: $\mathbb{D}_{\mathbf{x}_v}[\tilde{\mathcal{V}}(y = 1994, y_v \leq 1993)]$ and (bottom) 2004: $\mathbb{D}_{\mathbf{x}_v}[\tilde{\mathcal{V}}(y = 2004, y_v \leq 2003)]$.

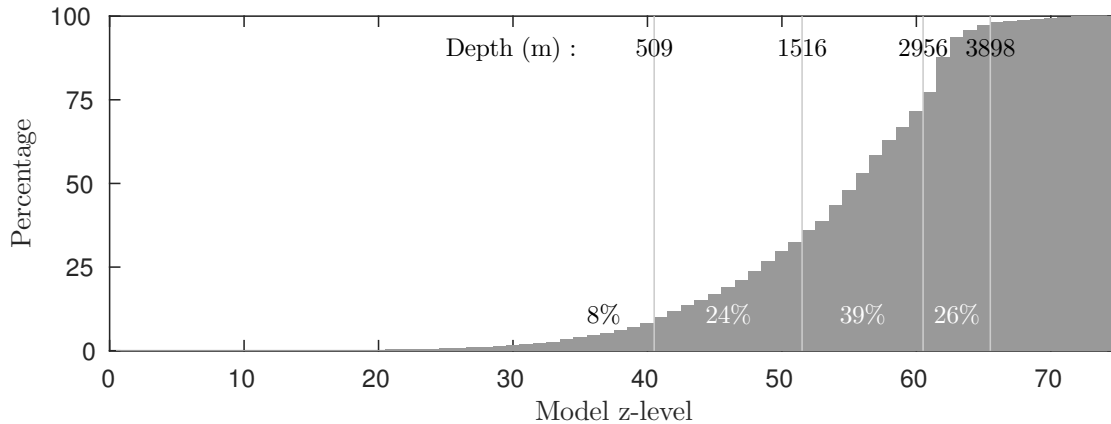


Figure 4.9: Volumetric distribution, presented as a cumulative distribution function, of the model depth level over which subduction occurs: $\mathbb{D}_{b_v}[\tilde{\mathcal{V}}]$. Vertical grey lines are placed at levels corresponding to the bathymetric levels shown in the map-view figures: $z = 509, 1516, 2956$ and 3898 m . Percentages of subduction occurring between each of these contours (except for the very deepest levels) are displayed toward the bottom of the figure.

the west of the basin is consistent with observations (Lavender *et al.*, 2000; Straneo *et al.*, 2003; Faure and Speer, 2005; Palter *et al.*, 2016). In contrast, there is less clear observational evidence for the weak but persistent anticyclonic circulation off the south west coast of Greenland, whereby a component of the flow leaves the coast, circulates around the interior basin and rejoins the boundary current upstream. Palter *et al.* (2008) do calculate a relatively strong shoreward flux across the 3000 m isobath in this region. The coincidence of this anticyclonic circulation with the peak in open ocean ventilation (Figure 4.7) suggests that it may be important for the export ventilated water from interior basin.

Observations in the Labrador Sea and downstream tend distinguish between two ‘classes’ of water formed in the region, based on their density: upper Labrador Sea Water and classical or deep Labrador Sea Water (Stramma *et al.*, 2004; Kieke *et al.*, 2006). The lighter of the two classes, upper Labrador Sea Water, is formed persistently in the Labrador Current (Pickart *et al.*, 1997), as well as in the interior basin during years of relatively moderate surface buoyancy loss (Kieke *et al.*, 2006). Deep Labrador Sea Water is formed in the interior basin during periods of deep convection, when mixed layer depths can exceed 2000 m (Yashayaev and Loder, 2016). A water mass with the same density and almost indistinguishable

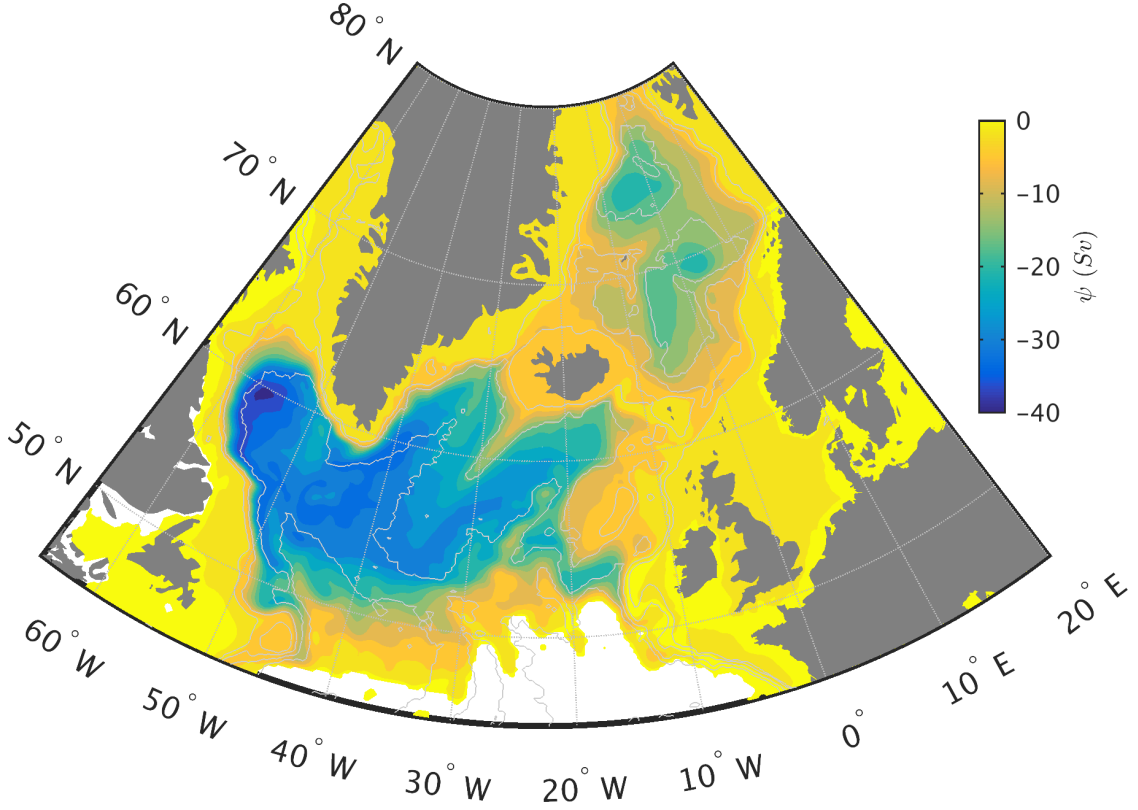


Figure 4.10: Late winter (mid-February to mid-April) time-mean (1982 to 2012) barotropic streamfunction (ψ) in Sverdrups. Only negative contours are displayed. Bathymetric contours at $z = 509, 1516, 2956$ and 3898 m are shown in light grey.

temperature and salinity properties, has also been observed to form directly within in the deep Labrador Current under extreme winter-time forcing (Pickart *et al.*, 2002; Cuny *et al.*, 2005).

To establish the regions of formation of different density classes within ventilated NADW in the model, we consider the distributions in density at the time of subduction, separated over different bathymetric ranges: $\mathbb{D}_{\gamma_v^n}[b_v^i < b_v < b_v^j]$, where b_v^i and b_v^j are the lower and upper limit of the bathymetric range. In Figure 4.11, these are presented as probability distribution functions of the total ventilated volume over that bathymetric range. Bear in mind that these bathymetric range definitions are fixed and quasi-arbitrary (defined broadly based on the time-mean barotropic stream function), such that they do not necessarily imply distinct ventilation mechanisms. We find that, consistent with observations and reflecting the distribution of surface outcrops (Figure 4.1), predominantly lighter density

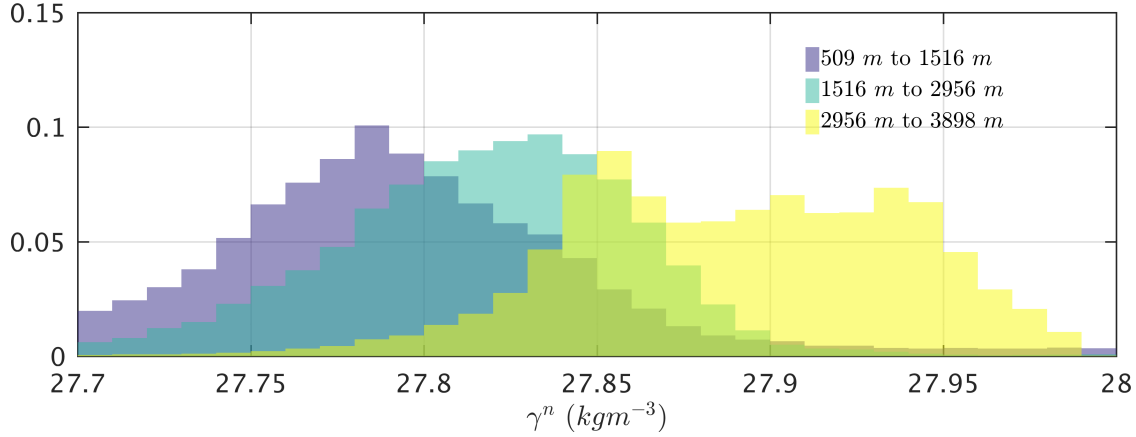


Figure 4.11: Volumetric distribution, presented as a probability distribution function, of the neutral density (γ^n) at which subduction occurs over different bathymetric ranges: $\mathbb{D}_{\gamma^n}[\tilde{\mathcal{V}}(b_v^l < b_v < b_v^u)]$, where b_v^l and b_v^u are the lower and upper limits of the bathymetry range.

classes are formed close to the boundary, while denser classes are formed offshore. It is notable that two distinct classes are formed in the open ocean region, with peaks around $\gamma^n = 27.85 \text{ kgm}^{-3}$ and between $\gamma^n = 27.9$ and 27.95 kgm^{-3} , that suggests consistency with observations of the formation of both upper and deep Labrador Sea Water in the interior basin (Stramma *et al.*, 2004). The lighter of these two open ocean classes closely coincides with the peak density class for water formed in the main boundary current region, somewhat consistent with the suggestion of Pickart *et al.* (2002) that boundary current and open ocean ventilation are almost indistinguishable. On the other hand, the densest classes formed in the open ocean are clearly distinct from those formed in the boundary currents.

We consider more closely the ventilation in the boundary current region by evaluating the upstream pathways of water ventilated between 500 and 3000 *m*. Exchange between the boundary current and open ocean, usually by eddy driven processes, is a crucial component of the formation and export of Labrador Sea Water (Straneo, 2006; Palter *et al.*, 2008). Thus, we wish to establish whether the ventilation apparent in this region is derived from subduction within the boundary current itself, or from exchange with the ocean interior. We follow trajectories for one month further back in time from their time of subduction and a random subset of these pathways is shown in Figure 4.12. For the most part,

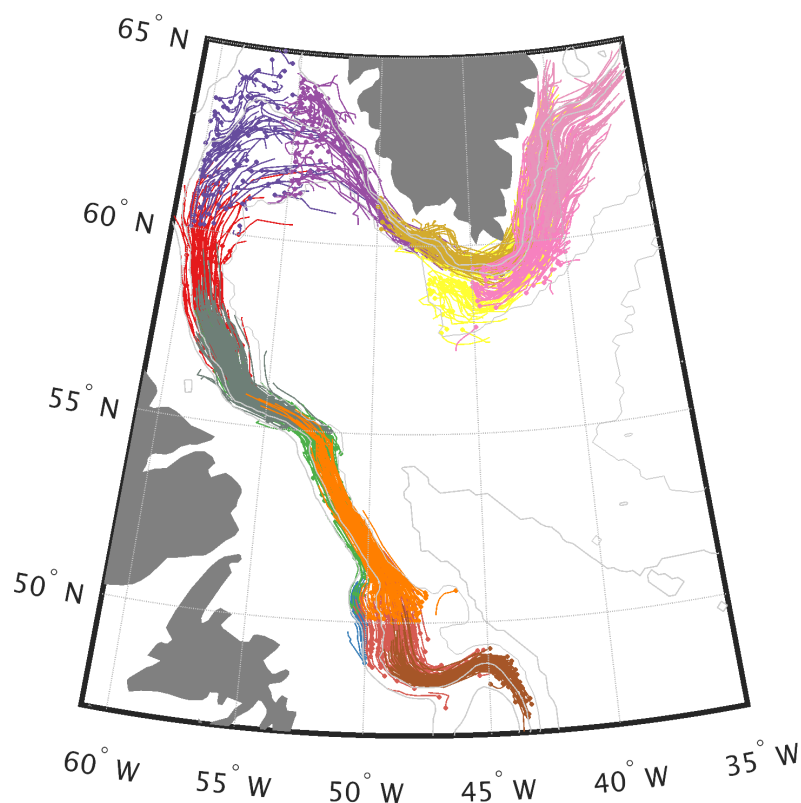


Figure 4.12: One month long trajectories, backwards in time from the time of subduction, of water subducted over bathymetric levels between 500 and 3000 *m* in the Labrador Sea. A random subset of particles is displayed, and coloured differently based on the latitude and longitude of subduction, in $5^\circ \times 5^\circ$ subregions. The end of the trajectory corresponding to the subduction location is denoted by a dot. Bathymetric contours at $z = 509, 1516, 2956$ and 3898 *m* are shown in light grey.

pathways are closely confined to the boundary current, with only a few having come from offshore. There is some degree more variability in the pathways of water ventilated in the north (purple and red trajectories in Figure 4.12), where the time-mean circulation is less strong and coincides with the re-entry of the cyclonic interior recirculation (Figure 4.10).

To be ventilated into the ocean interior on timescales longer than one year, newly subducted water must move to a region of shallower winter mixed layer depth (Stommel, 1979). Consequently, lateral gradients in the winter mixed layer depth, and their coincidence with the direction of circulation, are often good indicators of important subduction locations (*e.g.* Liu and Huang, 2012; Sallée *et al.*, 2010). The late winter mixed layer depth in the Labrador Sea, sampled on bathymetric contours, is shown in Figure 4.13, is overlain with a red contour corresponding to

the regions of elevated ventilation volume (taken from Figure 4.7). Distances, in kilometres starting from the north east, along the shallowest bathymetric contour are also shown. This figure is complemented by Figure 4.14 (top panel) where we plot the same information, but now as a function of the distance around the Labrador Sea. We consider the mixed layer depth along bathymetric contours rather than along streamlines of the barotropic stream function because the two closely coincide in the region of interest. In the north east of the Labrador Sea, where streamlines deviate more substantially from bathymetric contours, evaluating the mixed layer depth along streamlines may reveal more about the subduction process.

Deepening of the mixed layer from around 200 m to greater than 1000 m in the north of the basin occurs between ~ 200 and 1000 km along the bathymetric contours (there are differences between contours for where the deepening begins, but the magnitude of change is approximately similar). From around 1000 km , the mixed layer begins to shallow again as the contours curve round to the south west boundary of the basin. On each of the contours, shallowing of the mixed layer occurs relatively quickly at first, decreasing by as much as $\sim 700\text{ m}$ over a distance of 200 km . The decrease in mixed layer depth continues to around 1500 km around the basin. Across all of the bathymetric contours considered, but most consistently for those shoreward of 2700 m , the mixed layer depth shallows by between 800 to 1000 m over a distance of around 600 km . On the bottom panel of Figure 4.14, we show the volume of ventilation at each grid cell along the same bathymetric contours. Elevated levels of ventilation are seen across the region where the mixed layer depth is shallowing. Furthermore, peaks in subduction volume, at around 1000 km and 1300 km (corresponding to the 'hotspots' of ventilation identified in Figure 4.7), coincide with regions where the mixed layer shallows most rapidly. The relationship between the volume of ventilation and shallowing of the mixed layer depth is clearly not linear, and further investigation is required. However, these results provide substantial evidence that the spatial pattern of ventilation around the boundary current is established by a variable mixed layer depth along the path of boundary current. Furthermore, it appears that deep mixed layers

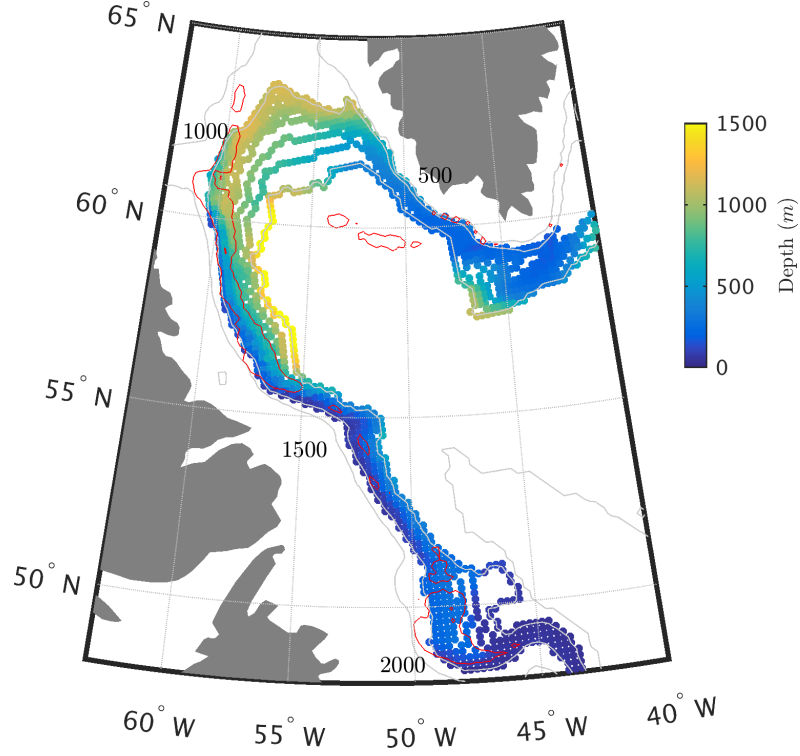


Figure 4.13: Time-mean, late-winter mixed layer depth (as in Figure 4.6), sampled on bathymetric contours for each model level between $z = 1516$ and 2956 m. Red lines are the $1 \times 10^{13} \text{ m}^3$ contour of the subduction volume, taken from Figure 4.7. Numbers around the edge of the basin correspond to the distance along the shallowest contour, initially referenced to $X^\circ\text{N}$, $Y^\circ\text{W}$. Bathymetric contours at $z = 509$, 1516 , 2956 and 3898 m are shown in light grey.

in the north of Labrador Sea play a substantial role in establishing the variable mixed layer depth around the boundary.

Over deeper bathymetry ($b_v > 2956$ m), ventilation takes place across a spread of locations in the interior basin of the Labrador Sea, and extending south-eastward and into the Irminger Sea. In the Labrador Sea, the largest volume is ventilated in the north east corner (Figure 4.7). This region coincides with the shoreward branch of the recirculations identified in the time-mean barotropic stream function (Figure 4.10), suggesting that water subducted here could be transported into the boundary current and exported from the Labrador Sea on relatively short timescales. Furthermore, the region corresponds to an area where the time-mean deep winter mixed layer shoals substantially (Figure 4.6), such that water subducted in this region need not move far before escaping re-entrainment in the following

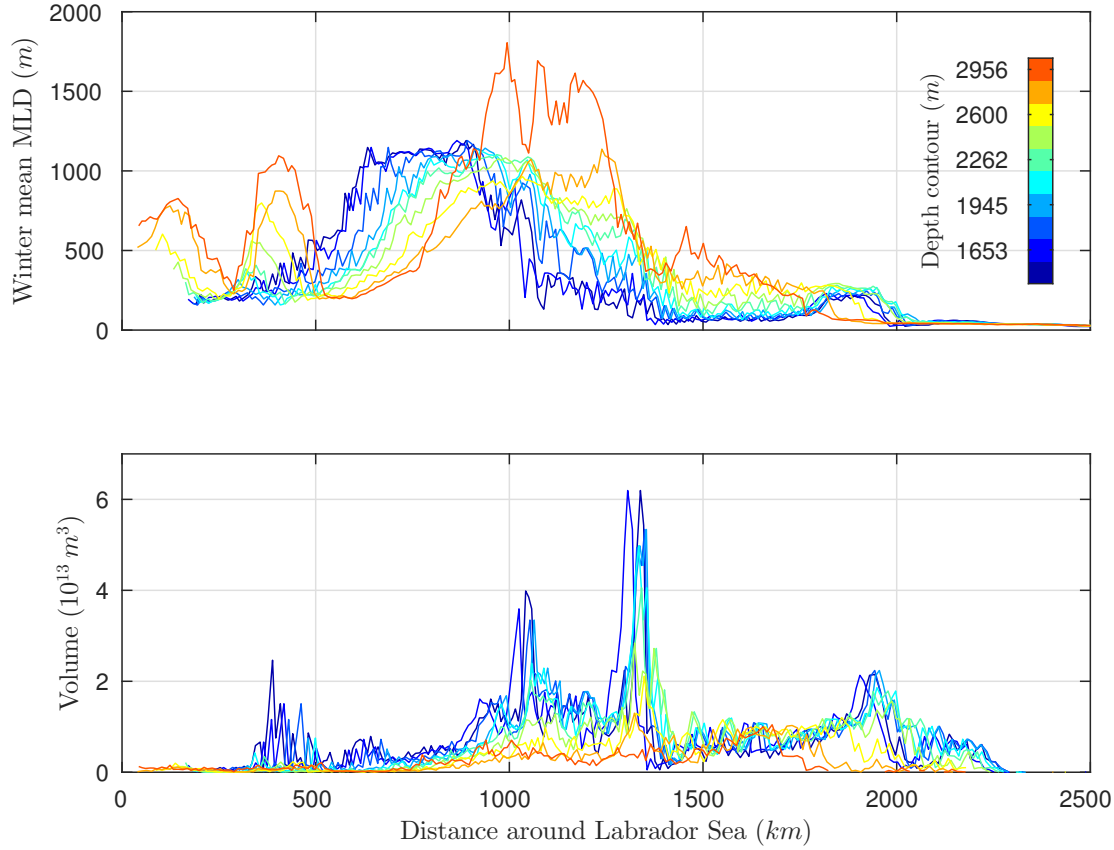


Figure 4.14: (top panel) Time-mean, late-winter mixed layer depth (as in Figure 4.6) on bathymetric contours between $z = 1516, 2956 \text{ m}$, presented as a function of distance along the contour (which we interpret as the distance around the Labrador Sea, since all of these contours circumvent the basin). (bottom panel) Volume of subduction, taken from Figure 4.7, along the same contours. The distance is initially referenced to 60°N , 35°W to ensure that, for each contour, it corresponds to approximately the same location around the Labrador Sea.

year. From float observations, Palter *et al.* (2008) investigated how and where Labrador Sea Water was exported from the interior basin to the boundary current. They found that both eddy-driven exchange and divergence of the time-mean flow played a role, although their estimate of the latter is uncertain. Furthermore, they found no preferential location where the water in the interior enters the boundary current. Further analysis of the pathways followed by water following subduction in this region will enable us to assess the processes facilitating export from the interior basin into the boundary current.

In identifying NADW (Section 4.2.3), we noted that water denser than $\gamma^n = 28 \text{ kgm}^{-3}$ formed in the Greenland-Iceland-Norway Seas, but was not exported

into the main North Atlantic basin. Similarly, in our main investigation of the NADW volume, a very small fraction has come from subduction in the GIN seas (Figure 4.7). During export from the GIN seas into the main North Atlantic basin, dense water must overflow shallow sills between Greenland, Iceland and Scotland. At these sills, overflowing dense water mixes vigorously with the ambient fluid in the North Atlantic, entraining it into the dense water plume such that its transport increases approximately two-fold (Girton and Sanford, 2003; Mauritzen *et al.*, 2005). The resulting water masses (called Denmark Straits Overflow Water and Iceland-Scotland Overflow Water, depending on the region that they descend into the Atlantic basin) form the major constituent parts of the deep layers of NADW throughout most of the Atlantic (de Carvalho Ferreira and Kerr, 2017). Consequently, it is surprising that Lagrangian trajectories reveal little evidence of ventilation in the area of their source waters.

The reasons for the lack of GIN seas ventilation in the NADW of this simulation are investigated using forwards-in-time trajectory calculations, in which particles are initialised in the GIN seas below the winter mixed layer in late March, 1975, and stopped when they intersect the mixed layer at some future time. Note that we only initialise particles in one year so that our results could be biased for the specific conditions of 1975. As we shall see, however, re-entrainment of the initialised particles occurs over a wide area and decadal timescale, thus we believe the main results would be very similar for particles initialised in different years. The location of the initialised volume is outlined by the black contour in Figure 4.15. Of this volume, 6% leaves the domain to the north, 66% remains in the GIN seas, and 28% is exported southward into the subpolar North Atlantic. Of the volume that remains in the GIN seas, 38% is re-entrained into the mixed layer, while the rest remains in the deep parts of the basin. The locations of re-entrainment can be seen in Figure 4.15. The majority of this re-entrainment occurs over the first 5-7 years, Figure 4.16, and the remaining volume is re-entrained steadily until the end of the simulation. For the volume that is exported to the North Atlantic, 64% is re-entrained to the mixed layer, predominantly in the boundary current and open

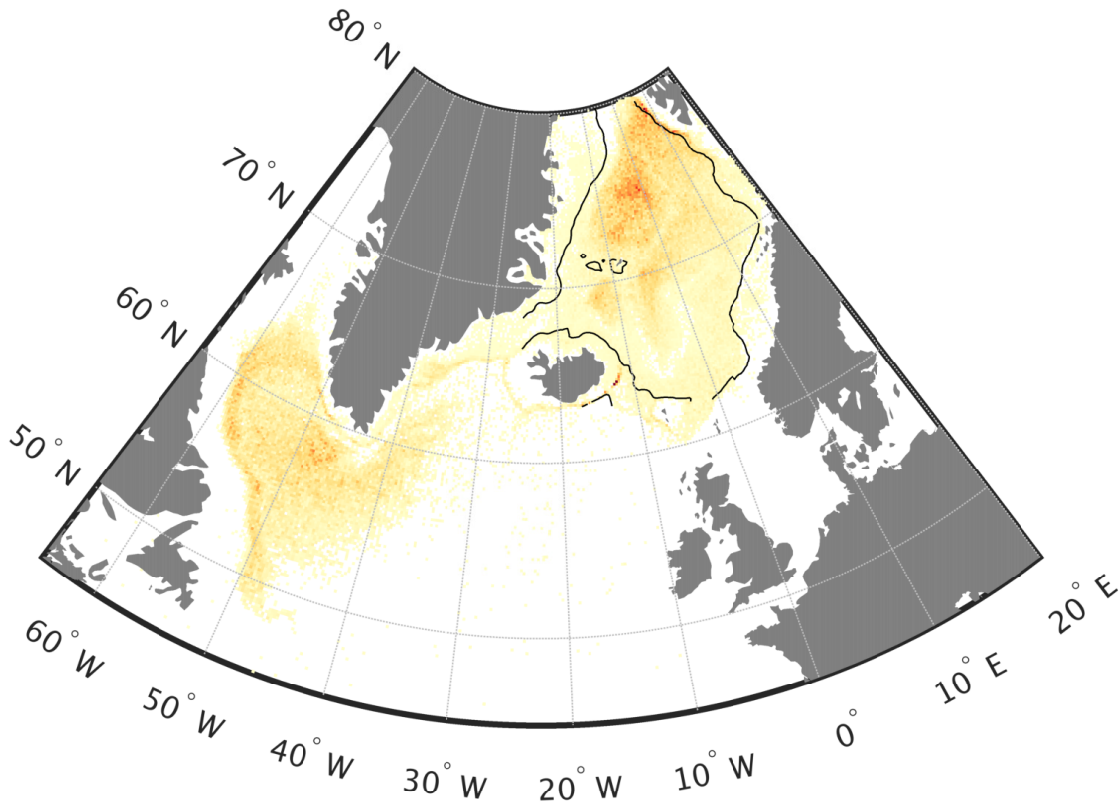


Figure 4.15: Fraction of water re-entrained into the surface mixed layer at each model grid cell, following initialisation in the Greenland-Iceland-Norway Seas at the end of March, 1975. Only water re-entrained after half a year is included. The initial location of water contributing to the picture of re-entrainment is shown by the black contour.

ocean of the Labrador Sea (Figure 4.15). The majority of the re-entrainment of water exported from the GIN seas occurs within 15 years.

To elucidate why the majority of dense waters in the GIN seas are re-entrained to the mixed layer before ever being exported south of the Labrador Sea, we consider the density distribution of water when it is initially in the GIN seas, and its distribution when it is re-entrained (Figure 4.17). For the volume re-entrained within the GIN seas, there is an overall decrease in density between initialisation and re-entrainment, particularly for the deepest density classes. There is a substantially more extreme shift in the density distribution for the volume re-entrained outside the GIN seas. There is a 0.6 kgm^{-3} shift of the distribution peak towards lighter classes at the time of re-entrainment, and a narrowing in the density range between $\gamma^n = 27.6$ and 27.8 kgm^{-3} .

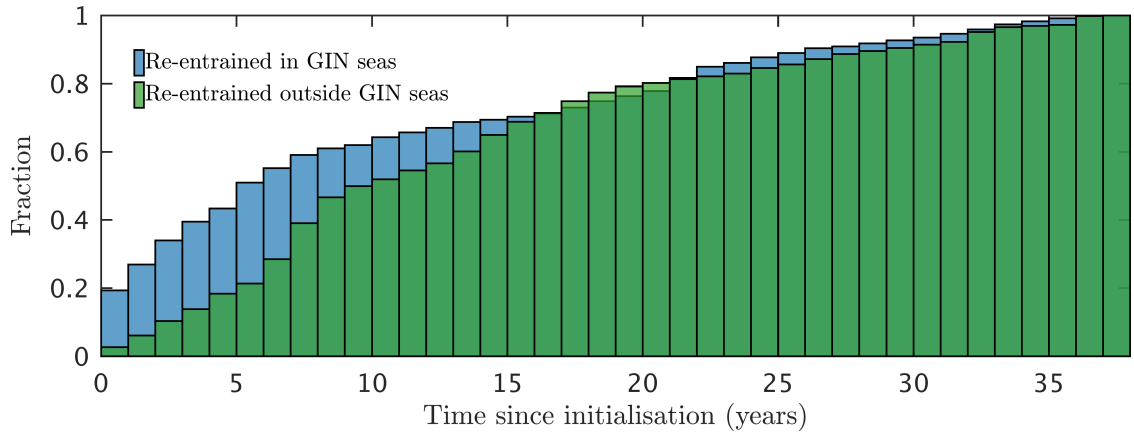


Figure 4.16: Volumetric histogram, presented as a cumulative distribution function, of the age of water, released in the GIN seas March, 1975, when it is re-entrained into the ocean mixed layer. The distribution is separated into water that was re-entrained within the GIN seas (north of $65^\circ N$; blue bars) and that re-entrained outside the GIN seas (green bars).

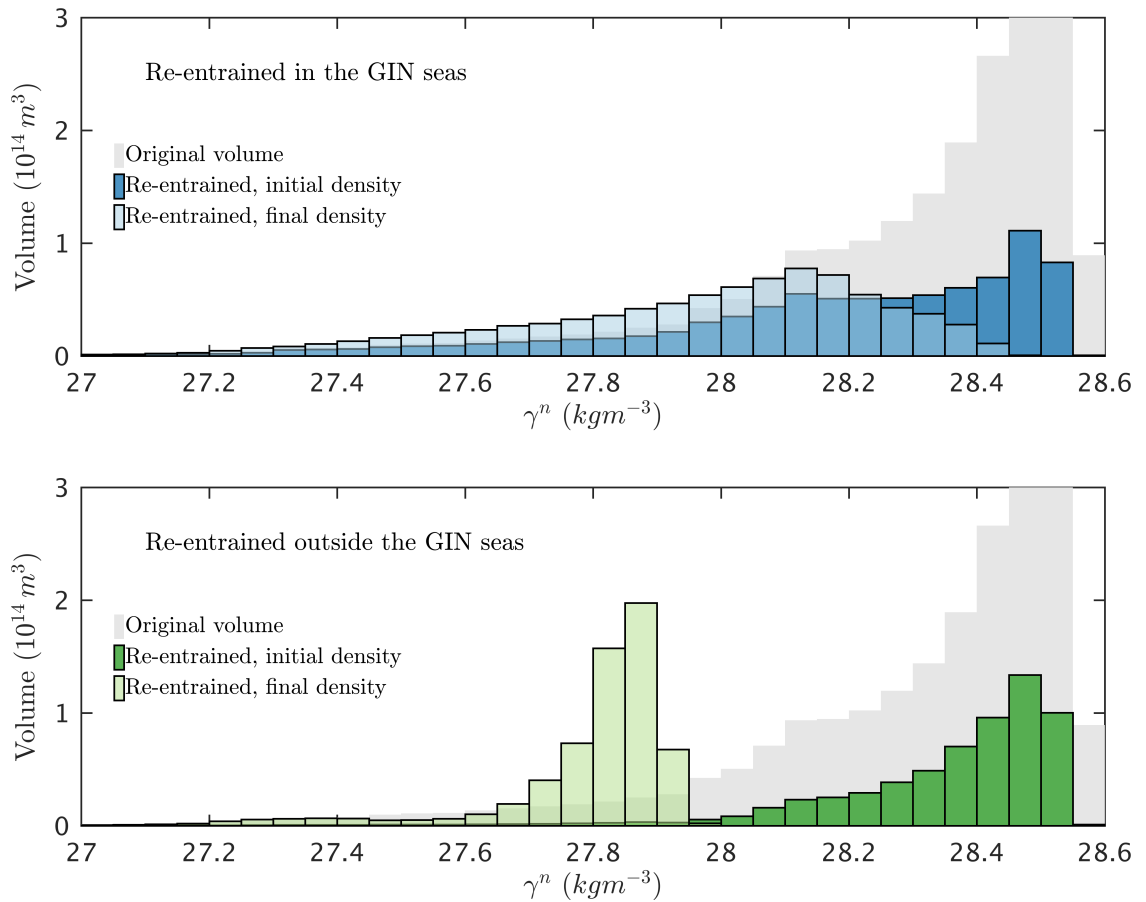


Figure 4.17: Volumetric distribution of neutral density (γ^n) at the time of initialisation in March 1975 (solid colours) and at the time of re-entrainment (transparent colours) for re-entrainment that occurs within the GIN seas (top panel) and outside the GIN seas (bottom panel). Grey bars show the distribution of neutral density for all of the water initialised in the GIN seas.

We expect that much of the density decrease in exported GIN seas water occurs during the passage of this dense water over the overflows between Greenland, Iceland and Scotland. Representation of gravity-driven downslope flow is notoriously difficult in numerical ocean circulation models (Legg *et al.*, 2009). This is particularly true of z -coordinate models, where adjacent bathymetric levels are separated in a discrete manner, such that it is difficult for dense water to flow between them. Particular challenges exist in achieving appropriate levels of exchange between the downslope flow and the ambient surrounding water, such that the eventual properties of water masses can be poorly represented (Legg *et al.*, 2009). In our configuration of the NEMO ocean model, gravity-driven flow is parameterised by a ‘bottom boundary layer’ scheme, following Beckmann and Döscher (1997). In this scheme, grid cells above bathymetry are configured such that when denser water is present in the upslope cell, they can communicate directly via advection and diffusion of tracer values (Madec, 2008). Importantly, the entrainment process — exchange between the gravity-driven flow and surrounding water — is not explicitly parameterised, but rather is left to the implicitly diffusive nature of the tracer advection scheme between the nearby cells. In addition, the scheme is known to be particularly diffusive when neighbouring bathymetric grid cells are of variable thickness (Beckmann and Döscher, 1997).

4.3.2 Ventilation timescales and spreading pathways

Ventilation of the NADW in this simulation is dominated by water formed in the Labrador Sea (Figure 4.7). The spreading pathways of Labrador Sea Water (LSW) have been well established in recent years from analysis of dynamic and passive tracers (Talley and McCartney, 1982; Rhein *et al.*, 2015) and real and ‘synthetic’ (evolved in numerical simulations) floats (Lavender *et al.*, 2000; Bower *et al.*, 2009; Gary *et al.*, 2011). The picture that has emerged is of three dominant pathways: recirculation in the Labrador and Irminger Seas, transport to the eastern subpolar gyre via the North Atlantic Current, and southward export to the subtropics via the Deep Western Boundary Current (DWBC) and interior ocean pathways.

To consider the ventilation pathways in the model, we show the time-average of the volume-weighted median age of water throughout the simulation: $\overline{\mathbb{D}}_{\mathbf{x}}^y[\mathcal{A}]$ (Figure 4.18). Calculating the median means that we also include unventilated points (marked with an age corresponding to the length of the simulation) in this average. We separate the volume into three further density groups, to consider density-dependent differences in spreading pathways.

The overall picture is remarkably close to the distribution of ages in Labrador Sea Water derived from recently-compiled passive tracer observations (Rhein *et al.*, 2015). The pathways in all density ranges adhere to the established picture from other studies, with the youngest water in the Labrador and Irminger Seas, ageing to the eastern half of the subpolar gyre, and exported southward via the DWBC and interior pathways.

Within the shallowest density class, the youngest water (less than 5 years old) extends across much of the of the subpolar gyre. The boundary of this young water closely coincides with the inner streamlines of the barotropic streamfunction (Figure 4.10). Furthermore, there is a marked increase in mean age between the inner and outer gyre circulation (from ~ 5 in the inner circulation to $\sim 10 - 15$ years in the outer), suggesting that strong mean flow results in substantial confinement of the youngest waters within the inner circulation. In the deeper density classes, the lateral extent of recently ventilated water shrinks westward markedly, and in the deepest water is confined to the boundary and interior of the Labrador Sea. Gradients across the subpolar gyre are notably less sharp than in the shallow density class.

Export of young water around and to the south of the Grand Banks within a narrow DWBC is apparent in both the upper and intermediate density classes, though the signature is eroded within a few hundred kilometres. Interior pathways to the west of the mid-Atlantic ridge are evident within each of the density classes. Mean ages within these interior pathways are somewhat younger than those in the western boundary, particularly in the densest class. This is somewhat in contrast to tracer observations (Rhein *et al.*, 2015), which show the youngest waters consistently along the western boundary, albeit with only a marginal west-to-east

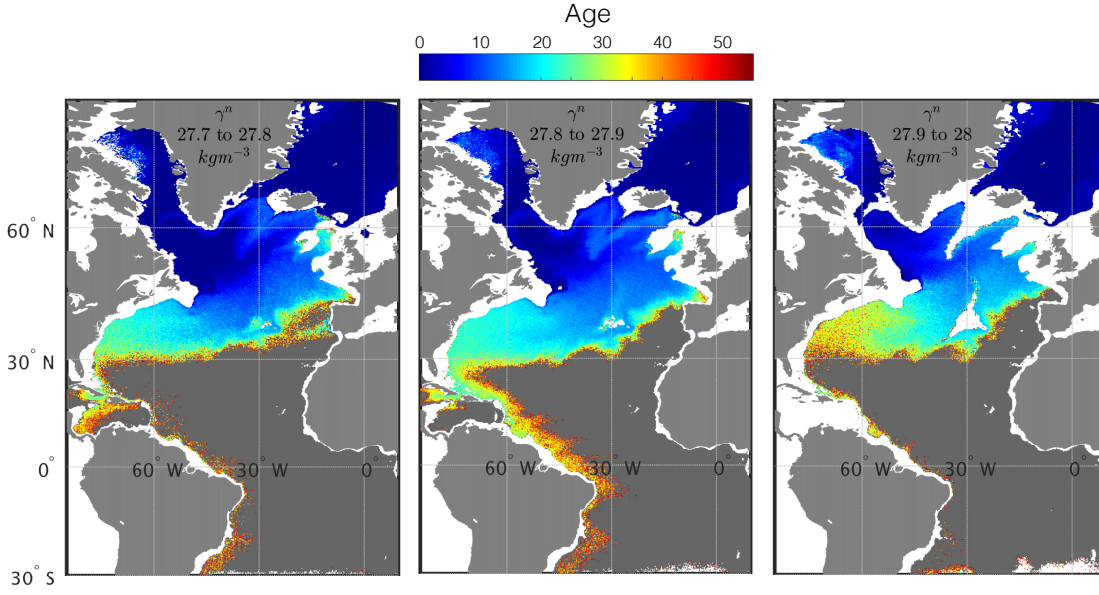


Figure 4.18: Time-mean of the median age distribution in North Atlantic Deep Water, separated into three neutral density volumes: $\mathbb{D}_{\mathbf{x}}^y[\mathcal{A}(\gamma_a^n < \gamma^n \leq \gamma_b^n)]$, where γ_a^n and γ_b^n are the upper and lower limits of the neutral density volume. Unventilated waters are included in the depth median calculation. Dark grey areas correspond to regions with a median age greater than the length of the simulation.

gradient in age. South of $30^\circ N$, interior pathways cease, and ventilation further south is confined to the western boundary. Southern ventilation is most apparent in the intermediate density class, in which water reaching the equator has an average age between 35 and 45 years.

Ventilation to the east of the mid-Atlantic ridge (MAR) in Labrador Sea Water is a persistent feature in many observational and modelling studies (Gary *et al.*, 2011; Rhein *et al.*, 2015). However, by comparison to the spreading pathways on the western side of the North Atlantic basin (Lozier, 1997; Gary *et al.*, 2011), attempts to explain the dynamics of the eastern basin ventilation have been lacking. In Figure 4.19 we show the region more closely, overlain with bathymetric contours. Assuming at this stage that water is penetrating southward from the subpolar gyre, the age distribution implies that at approximately $45^\circ N$ and 10 to $20^\circ W$, relatively recently ventilated water is diverted westward, along a slight bathymetric high, toward the eastern flank of the MAR along which it is closely confined as it travels further south. The sharp transition between these relatively young waters and

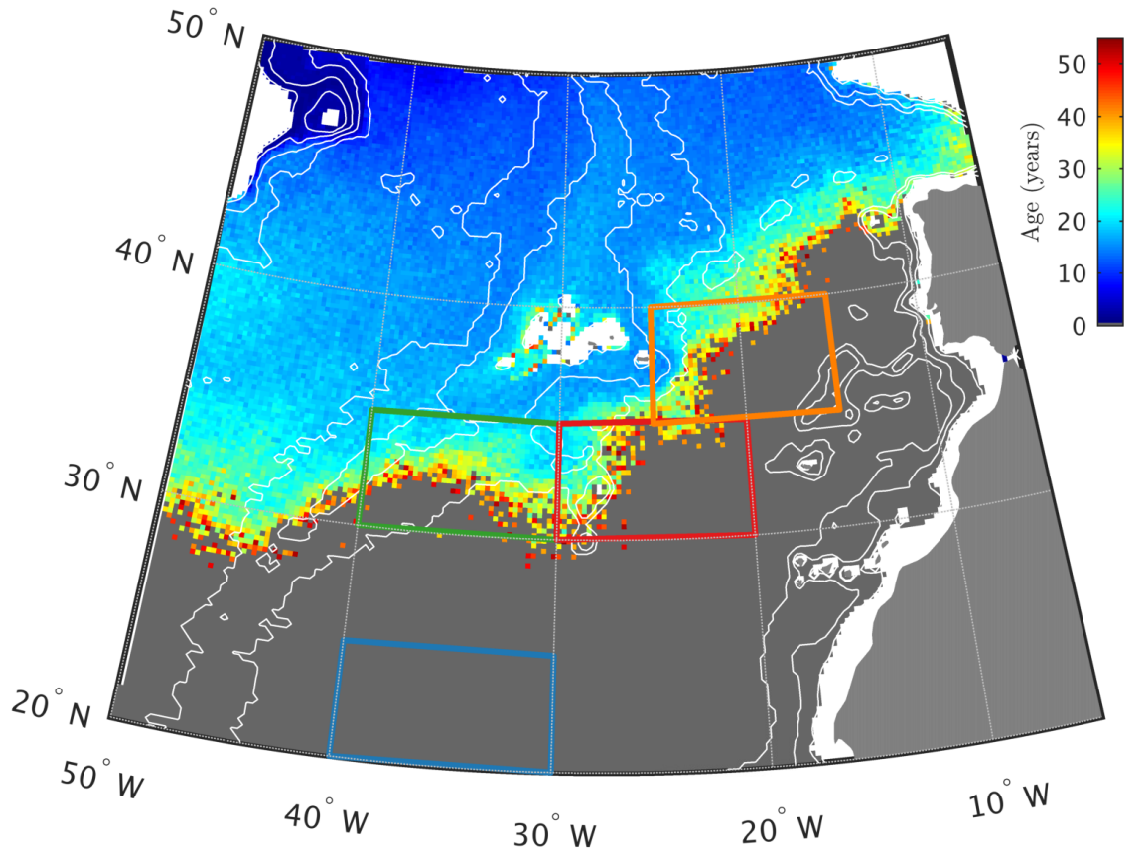


Figure 4.19: Time-mean of the depth median age for the middle density range in Figure 4.18 — $\mathbb{D}_x^y[\mathcal{A}(27.8 < \gamma^n \leq 27.9)]$ — zoomed in to the east of the mid-Atlantic ridge. Coloured boxes correspond to the initialisation regions for the tracked experiments outlined in the text, the pathways to which are shown in Figure 4.22.

the unventilated region extends southwestward from the north of Portugal to the eastern flank of the MAR at $30^\circ N$ and from there, zonally to the western boundary. In this region, hydrography is strongly influenced by the outflow of dense water from the Mediterranean (Talley and McCartney, 1982; Baringer and Price, 1999). Thus, while there is a clear influence of bathymetric steering in the ventilation pathways, we investigate a possible role for the Mediterranean outflow in establishing and sustaining the region of poor ventilation in the eastern Atlantic.

Before pursuing this, however, it should be noted that this region is one in which the labelling of water mass by neutral density is problematic. Figure 4.20 shows a zonal section at around $37^\circ N$ of contours of neutral density (dotted black lines), as used in our NADW definition, and potential density referenced to 2000 m (dashed black lines). The slopes of the surfaces match closely on the western side of

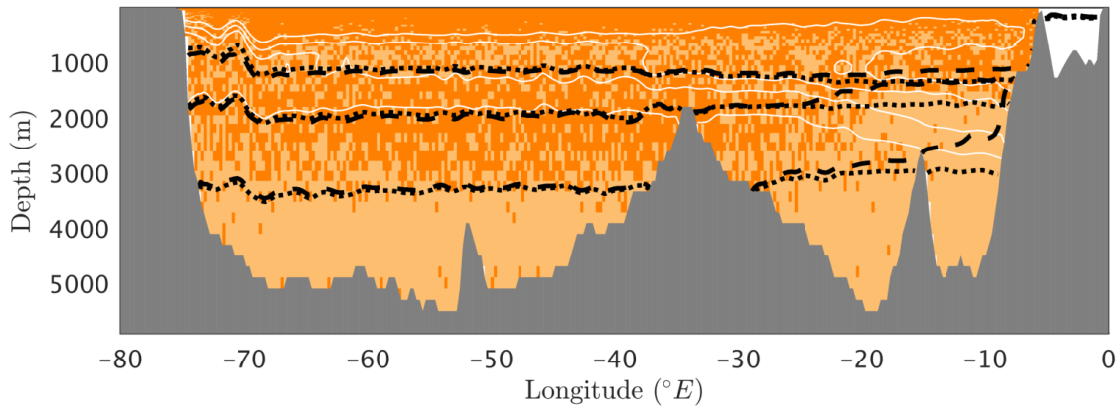


Figure 4.20: Ventilation and stratification across a zonal section at $37^\circ N$. Colours correspond to ventilated (dark orange) and unventilated (light orange) points across the section. Black lines are neutral density (dotted) and potential density referenced to 2000 m (dashed) contours. Neutral density contours correspond to values of $\gamma^n = 27.7, 27.85$ and 28 kgm^{-3} . Potential density contours correspond to $\sigma_2 =$. White lines are contours of salinity, decreasing away from the Mediterranean outflow in the east.

the basin, but diverge significantly in the east, where contours of neutral density remain flat while those of potential density shoal upwards. The likely reason for this divergence is the outflow of Mediterranean water (hereafter MW) from the Strait of Gibraltar, which introduces a high-salinity signature, the contours of which are also shown in Figure 4.20. The colours in Figure 4.20 identify the ventilated (dark orange) and unventilated (light orange) water across this section, as derived from the experiment in which particles were initialised throughout the model domain (previously referred to in Section 4.2.3). North Atlantic Deep Water, as defined by neutral density, clearly coincides with a region of poorly ventilated water on the eastern side of the basin, as was previously noted in Figures 4.18. However, the potential density surfaces that correspond to the same water mass on the west of the basin extend upward into ventilated waters. This raises the possibility that the poor ventilation in neutral density-defined NADW is an artefact of the volume definition.

We address this concern by comparing the distribution of ventilation ages in Figure 4.19 with those around a corresponding potential density surface referenced to 2000 m . We choose a surface with $\sigma_2 = 27.8\text{ kgm}^{-3}$, which corresponds to the core of NADW on the west of the basin. The age was determined in late winter of the last simulation year and was again extracted from the experiment in which

particles were initialised throughout the model domain. Figure 4.21 shows the depth median age on this potential density surface: $\mathbb{D}_x[\overline{\mathcal{A}}(27.74 < \sigma_2 < 27.86)]$. Note that this is the age at a single point in time, and thus is more noisy than the time-average age distribution in Figure 4.19. The pattern is broadly consistent with that seen in the neutral density volume, particularly in relation to southward penetration of young water along the eastern flank for the MAR from around $45^\circ N$. The main difference between this picture, and that in the volume defined by neutral density, is a pool of recently ventilated water off the coast of Portugal. The ventilation location of this water confirms that it was ventilated directly from the Mediterranean. Thus, we conclude that in establishing the pathways of southward ventilation to the east Atlantic, poor approximation of the local neutral surface by neutral density, and our choice to initialise particles within this volume, is not critical.

To investigate what established and maintains the ventilation pattern on the east of the mid-Atlantic ridge, we evaluate the full trajectories (*i.e.* establishing the Lagrangian position every 5 days) of water in both the ventilated and unventilated regions. The locations of these regions are shown in Figure 4.19. In the left panel of Figure 4.22, we show contours of pathway probability for each of the four regions. These are constructed by counting the number of times a trajectory intersects a grid cell, and dividing by the total number of intersections, which establishes the most likely pathways water in a certain region has taken to get there. The region furthest south (blue contours) is entirely unventilated. Water arriving at this region has originated from both the north east and the south west. The northern extent of these pathways coincides with the boundary of the ventilated NADW (Figure 4.19). The equal distribution of contours to the north east and south west is indicative of diffusive spreading, with a preferential direction along that curvature. In the south west, the depth of the MAR increases and it ceases to encroach on the base of NADW volume. Consequently, trajectories spread freely over the ridge. Pathways to regions in the north and east (green, red and orange contours), which have both ventilated and unventilated waters present, show a more substantial component of advection from the north. As with the unventilated region, water has arrived

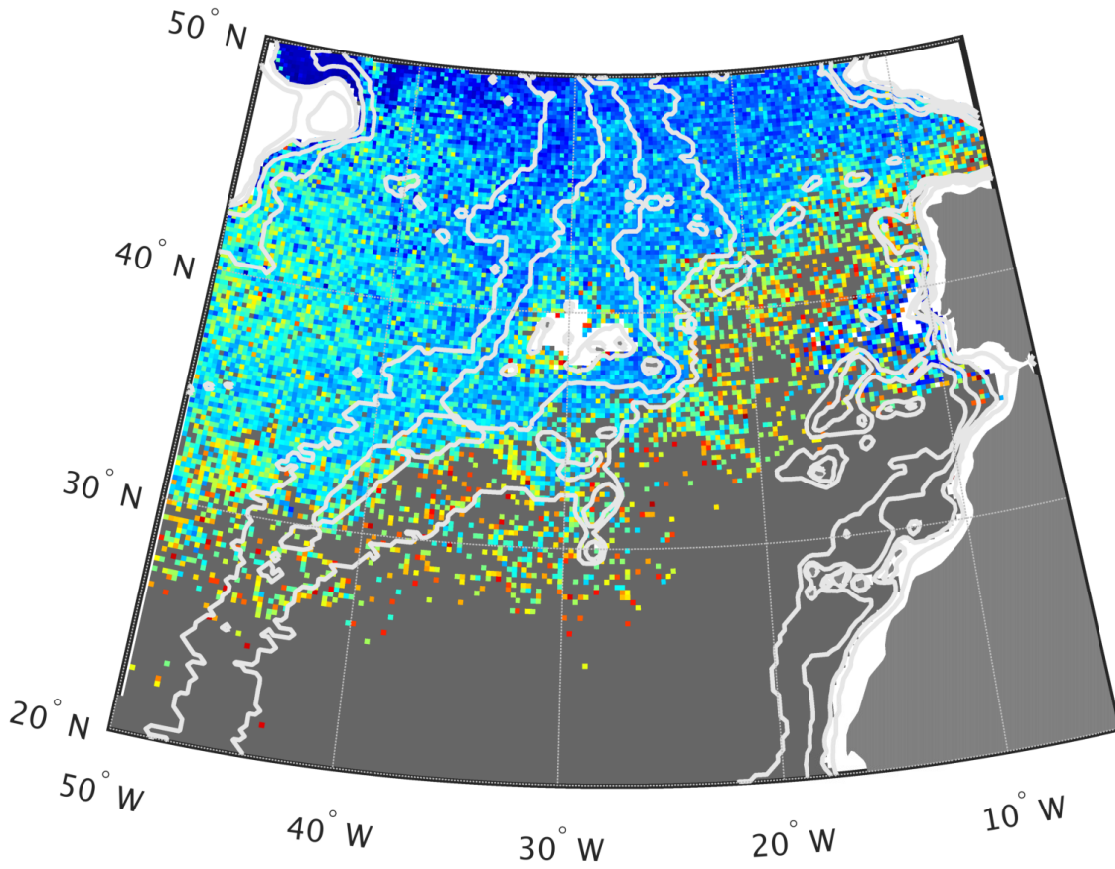


Figure 4.21: Median ventilation age at the end of March, 2012, between $\sigma_2 = 27.74$ and 27.86 kgm^{-3} — $\mathbb{D}_x[\bar{A}(27.74 < \sigma_2 < 27.86)]$ — derived from the experiment in which particles were initialised everywhere in the North Atlantic domain. Dark grey regions were unventilated during the simulation.

from both the north and south, but the preferential stretching of contours into the subpolar gyre suggests that there is a dominant southward component to the flow into these regions. To the west, pathways are strongly constrained by bathymetry.

Pathway probabilities to all of four of the highlighted regions, now including only the pathways of ventilated waters, are shown in the panel on the right in Figure 4.22. The pattern suggests an advective ventilation pathway closely constrained by bathymetry. Following subduction in the Labrador Sea, water moves across the subpolar basin, crossing the mid-Atlantic ridge at a distinct depression at around $32^\circ\text{W}, 52^\circ\text{N}$. This is the Charlie-Gibbs Fracture Zone, frequently noted as the main place where Labrador Sea Water crosses the MAR (Palter *et al.*, 2016). Water then transits southward, to the east of the MAR across a swath of the basin, though

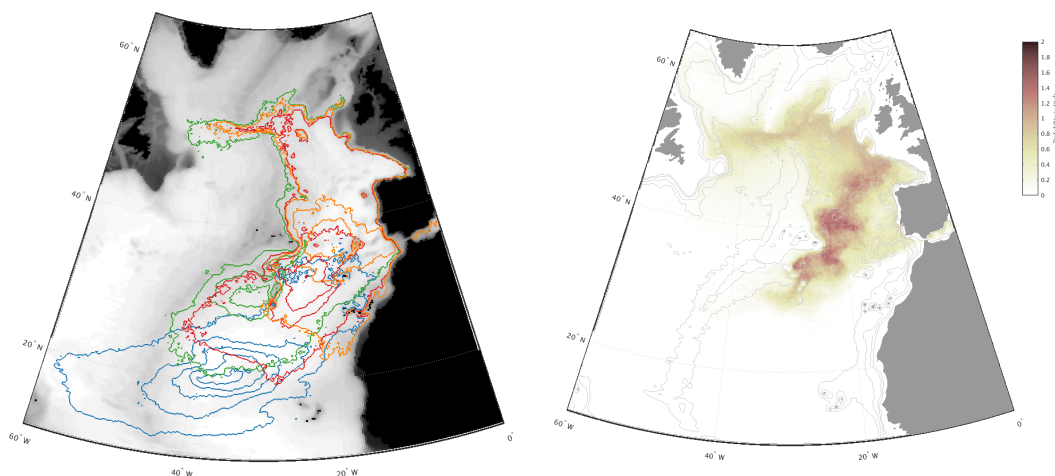


Figure 4.22: (left panel) Contours of the pathway probability distribution for the experiment tracing the origins of water that ends up on east of the mid-Atlantic ridge in June, 2012, overlain on grayscale bathymetry. Colours are consistent with the boxes shown in Figure 4.19 which display the regions where the water ends up. (right panel) Pathway probability distribution of water ending up on the east of the mid-Atlantic ridge that was ventilated during the 52-year numerical simulation.

preferentially through narrow bathymetric channels (*e.g.* at 20°W , 52°N) and along the eastern continental slope. At around 50°N , the main pathway separates from the continental slope and traverses the basin in a south westward direction until it meets the eastern flank of the MAR, along which it is exported south. As noted in pathways to the unventilated region (Figure 4.22), spreading pathways are no longer constrained by the MAR from around 25 to 30°N , where the depth of the ridge increases. Consequently, from this latitude, recently ventilated water can spread zonally, rather than continuing further south (Figure 4.18).

In summary, pathways to the east of the mid-Atlantic ridge have an advective component, aided by bathymetric steering, that brings ventilated water from the subpolar gyre. South of 45°N , this ventilated water is strongly confined close to the MAR. Away from the influence of the MAR, pathways are largely diffusive in nature, preferentially spreading along a northeast-southwest axis, and for the most part remain unventilated during the model simulation.

The outflow of high-salinity water from the Mediterranean is a key component of the hydrography in this region (Baringer and Price, 1999; Bashmachnikov *et al.*, 2015). Its influence can be seen in the zonal section of Figure 4.20. The main,

high-salinity tongue penetrates into the open ocean at around 1000 *m* but distortion of salinity contours is evident down to at least 3000 *m*. Thus, we consider what role the presence of MW plays in defining the observed ventilation pathways and structure of the unventilated region. To assess this, we consider the distribution of large-scale potential vorticity:

$$q = \frac{f}{\rho} \frac{\partial \rho}{\partial z}, \quad (4.16)$$

where $f = 2\Omega \sin(\phi)$ is the Coriolis parameter, and Ω is the rotation rate of the earth. In using the low potential vorticity signature of Labrador Sea Water as a passive tracer, Talley and McCartney (1982) noted that to the east of the MAR, contours of potential vorticity and salinity were closely aligned, and attributed this to the influence of MW.

Figure 4.23 shows the depth-mean salinity around $\sigma_2 = 27.8 \text{ kgm}^{-3}$ overlain with contours of potential vorticity. We consider a potential density surface rather than a neutral density surface because of the aforementioned issues with the latter in this region. As observed by Talley and McCartney (1982), the potential vorticity distribution coincides closely with that of MW, with contours substantially diverted away from a zonal direction throughout the region of elevated salinity. This is most evident close to the outflow, but continues far to the southwest. From around 30°N , potential vorticity contours are more zonal. Thus it appears that the MW influence is a source of relatively high potential vorticity into the NADW volume layers. The extent of the MW influence in the north coincides with the region where water ventilated in the subpolar gyre ceases to penetrate further south and is instead diverted westward to the MAR. The potential vorticity gradient between NADW and MW in this region is likely to inhibit mixing of ventilated water across the bathymetric high, and thus may be important in sustaining an unventilated pool in eastern Atlantic.

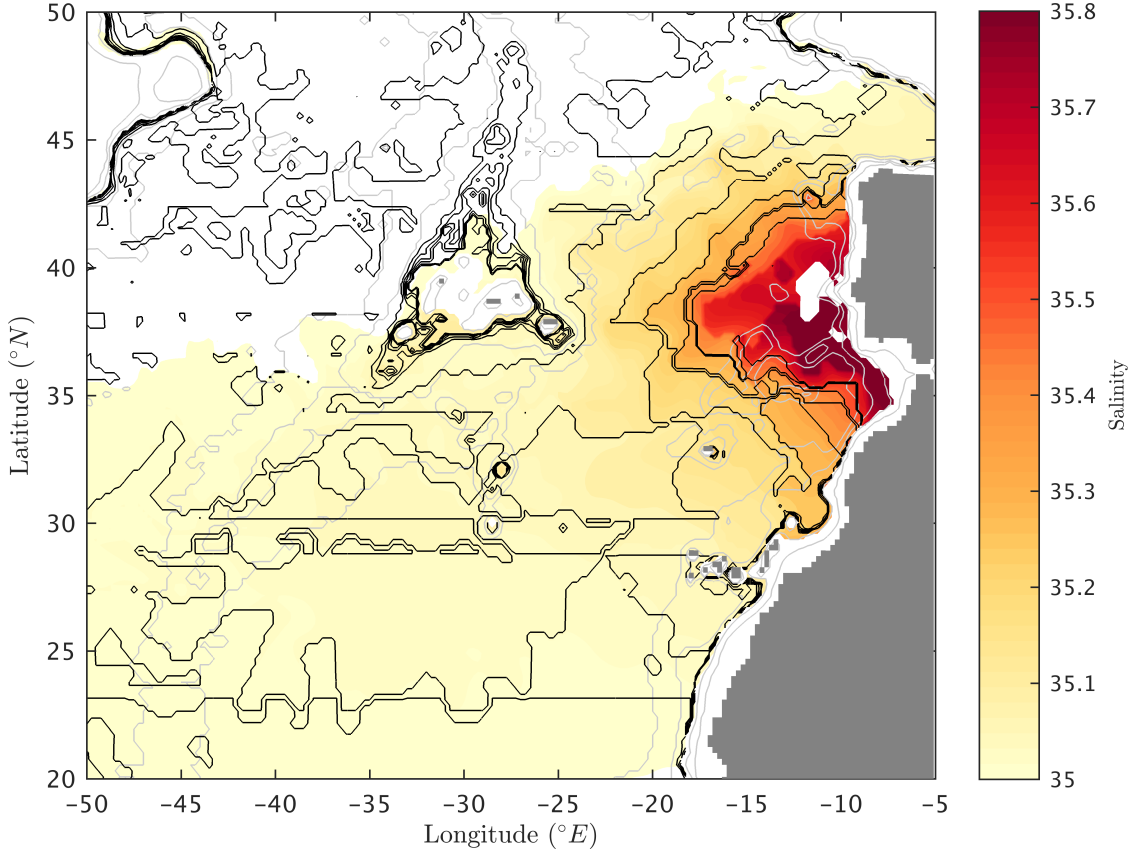


Figure 4.23: Depth-mean salinity between $\sigma_2 = 27.74$ and 27.86 kgm^{-3} (colours) overlain with contours (black) of large-scale potential vorticity ($q = f/\rho\partial\rho/\partial z$).

4.3.3 NADW age distribution and ventilation variability

Time-mean NADW age distribution

Variability in the ventilation of NADW will be manifest in variations of the age distribution, evaluated from the Lagrangian analysis. Before considering this, we evaluate the *average* age distribution within NADW during the simulation: $\overline{\mathbb{D}}_a^y[\tilde{V}]$, where we average distributions evaluated between 1975 and 2012 (Figure 4.24). Note that due to the finite timespan of the simulation, values at the tail of the distribution become less reliable, *e.g.* there is only 1 year (2012) when we establish a volume of 54 year old water.

This distribution can be interpreted as the evolution of an average NADW volume over time. A peak at ages less than one year is associated with water remnant in the subsurface after dense water formation. At $\sim 20 \times 10^{14} \text{ m}^3$, this represents around 2% of the total NADW volume in the model domain. By the

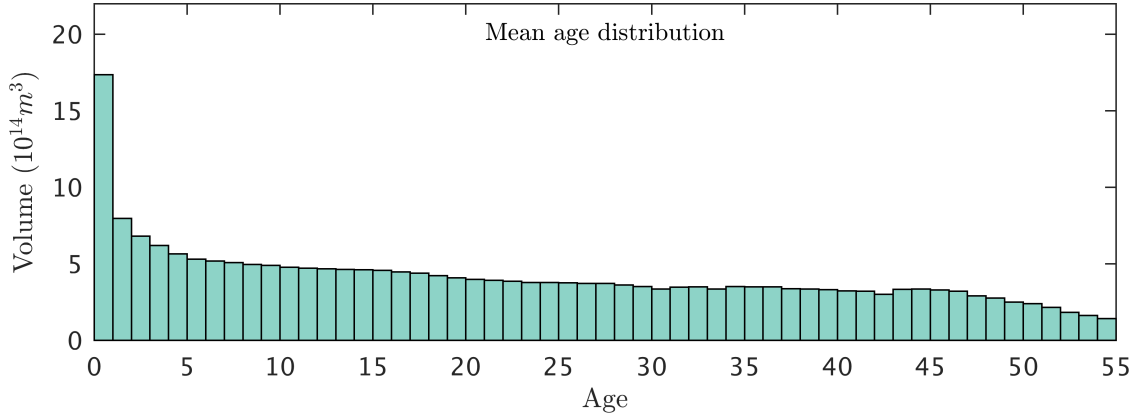


Figure 4.24: Average volumetric age distribution in NADW, for initialisations between 1975 and 2012: $\mathbb{D}_a^y[\tilde{\mathcal{V}}]$

end of the 2nd year, this has been reduced by more than half to $\sim 8 \times 10^{14} m^3$, or $\sim 1\%$ of the NADW volume. This reduction is the effect of Stommel’s demon re-entraining a large fraction of the recently ventilated water back to the surface before it escapes to regions of shallower winter mixed layer depth. The average volume of water present after a full annual cycle, $\sim 8 \times 10^{14} m^3$, implies an annual formation rate for NADW of $25 Sv$.

Following initial re-entrainment, the NADW volume continues to decrease over time. The rate of reduction is substantial up to around 5 years, with a further $2 \times 10^{14} m^3$ lost over this time period — 10% of the initial volume. After this the rate of attrition decreases, but the volume continues to be eroded at a rate of $0.05 \times 10^{14} m^3 yr^{-1}$ or $\sim 0.2 Sv$. This reduction over time could be due to water leaving across the lateral boundaries of the model domain, or being re-entrained back to the surface mixed layer.

We establish the processes responsible for the reduction in NADW volume by running complementary forwards-in-time experiments. Details of these experiments can be found in Section 4.2.2. In the forwards-in-time experiments, we can establish whether, after some time, water has been re-entrained into the surface mixed layer, has left the domain across a lateral boundary, or is still be present in the subsurface. In Figure 4.25 we present the time-mean distribution of this ‘fate’ of ventilated

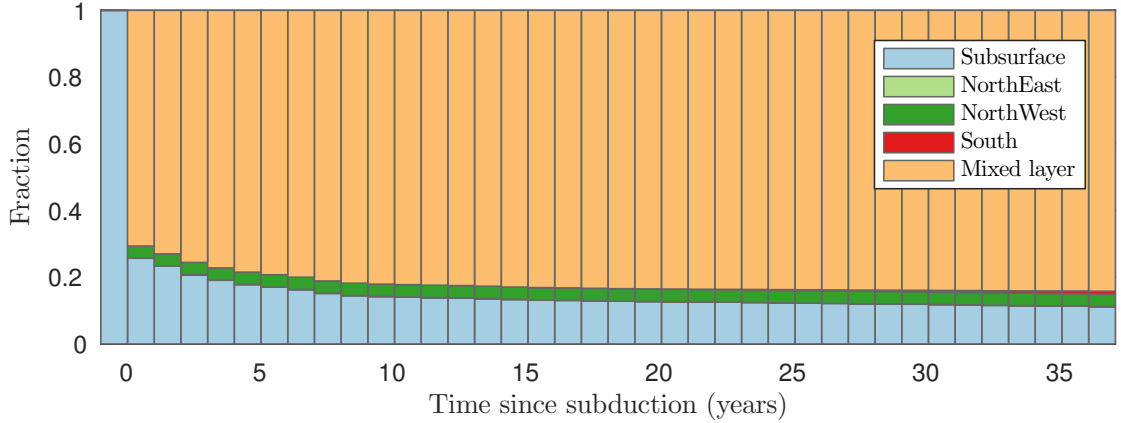


Figure 4.25: Cumulative distributions of the average fate of ventilated NADW as a function of time. Each column, presents the fraction of the initial volume that has either been re-entrained to the surface mixed layer, been exported across a lateral boundary, or remains in the subsurface. Each contribution is cumulatively summed from left to right (with the subsurface contribution being evaluated as the residual).

NADW as a function of age, for initialisations between 1975 and 2012. We present the results as cumulative distributions, summing up contributions from left to right.

The shape of the distribution of subsurface water shows reasonable agreement with that derived from the backwards trajectories. However, the volume reduction over the first year is larger when considering the forwards case ($\sim 75\%$ compared to $\sim 60\%$). The precise reason for this difference is unclear, but is likely to be due to the nature in which volumes are assigned in the forwards and backwards experiments. It is evident from Figure 4.25 that almost all of the volume reduction (except for a small amount lost to the north west in the first year) is due to re-entrainment in the mixed layer. This process continues for several years after the initial re-entrainment. From around 25 years, a small contribution from export of NADW volume across the southern boundary of the domain emerges.

NADW age distribution in 2012

In Figure 4.26, we show the distribution of ages in NADW in 2012: $\mathbb{D}_a[\tilde{\mathcal{V}}(y = 2012)]$. There are substantial differences in the volume of water present for different ages, suggesting that ventilation varies considerably over time. Before considering the variability of this distribution relative to that of the average age distribution, however, we assess its sensitivity to components of our analysis.

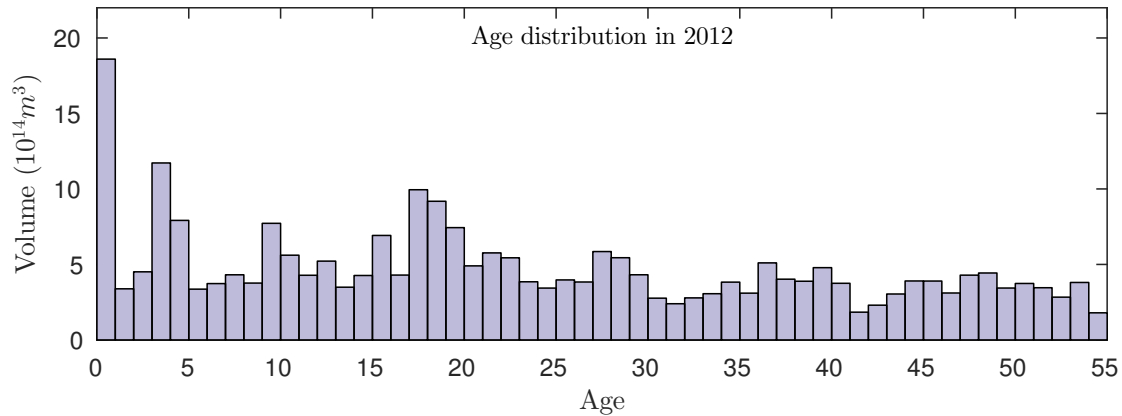


Figure 4.26: Age distribution in NADW in June, 2012: $\mathbb{D}_a[\tilde{\mathcal{V}}(y = 2012)]$

In the first instance, we consider the effect of our mixed layer definition. In Figure 4.27, we show the volumetric distribution of ages in the final model year from our standard definition (threshold criteria of density within 0.01 kgm^{-3} of the density at 10 m) and from two further definitions: one which increases the density threshold to 0.1 kgm^{-3} and another that uses a relaxed density threshold (0.4 kgm^{-3}) combined with a condition on the coefficient of vertical diffusion ($k_z > 10^{-4} \text{ m}^2 \text{ s}^{-1}$), which we can also trace along trajectories. Results from these experiments were previously shown in Chapter 2 in relation to subsurface density changes, and differences in the depths of the mixed layer from these definitions, in summer and winter, can be seen there (Figures 2.13 and 2.14). Figure 4.27 shows that multi-annual timescale variations in the volumetric distribution are largely unaffected by the density definition, but that there are some differences in inter-annual variations. Since our subsequent analysis and conclusions do not rely heavily on the quantitative details of variability on these timescales, we do not expect this level of sensitivity to be important.

We wish to attribute variability in the distribution of ages in 2012 to variations in ventilation from a particular year. That is to say that, for example, we wish to attribute an anomalously high volume of 20 year old water in 2012 to an anomalously large amount of ventilation in 1992. To do this, however, requires that peaks and troughs attributed to particular years remain steady over time, *i.e.* they are insensitive to the time at which we evaluate Lagrangian properties. In Figure

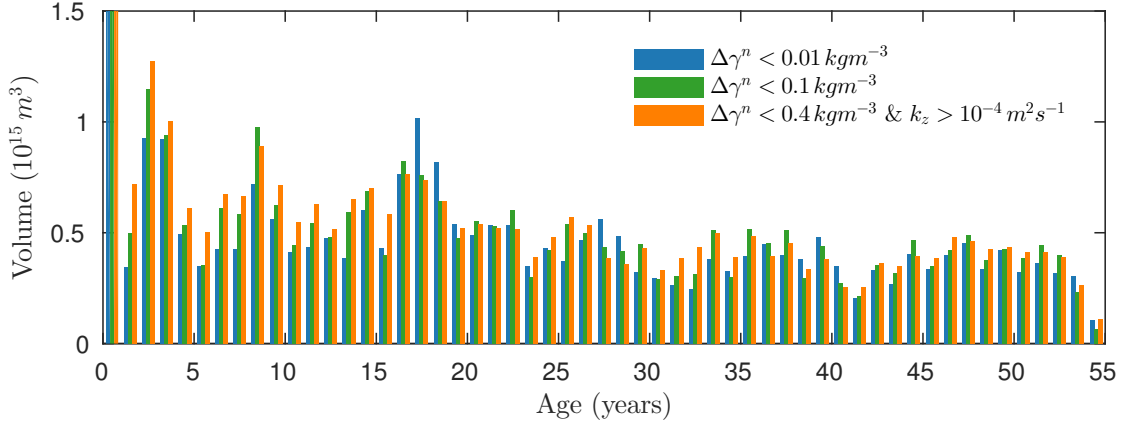


Figure 4.27: Age distribution in NADW in June, 2012, for experiments using three different definitions of mixed layer depth: (blue) threshold criteria of density within 0.01 kgm^{-3} of the density at 10 m — the standard definition used for all other experiments; (green) increased threshold density of 0.1 kgm^{-3} ; (orange) increased threshold density of 0.4 kgm^{-3} and vertical diffusion coefficient criteria of values greater than $10^{-4} \text{ m}^2 \text{ s}^{-1}$.

4.28, we present the volumetric distribution of ventilation year for initialisations in each year between 1975 and 2012, represented by the colours of the bars. So, if the volume of water from, say, 1970 were completely constant over time, then the height of the bars would remain the same, progressing from blue (1975) to yellow (2012) initialisations. That volumes continue to decrease over time is evidence for progressive re-entrainment, as seen in the average age distribution, as well as perhaps loss out of the volume from diapycnal motion. Spikes in ventilation years from 1975 onwards are showing subduction volumes in the year of initialisation, and elevated volumes for the following year or two. The volumes set after a year or two (*i.e.* after initial re-entrainment) are relatively constant over initialisation years and variability between years is conserved.

Having established the robustness of variations in the age distribution in 2012, and their attribution to ventilation in specific years, we now compare this distribution to the average age distribution in NADW (Figure 4.24). To account for the loss of volume over time, as seen in the average age distribution, we take the difference between the 2012 distribution and the average distribution, and normalise by the average distribution. We hereafter refer to this as the normalised 2012 age distribution.

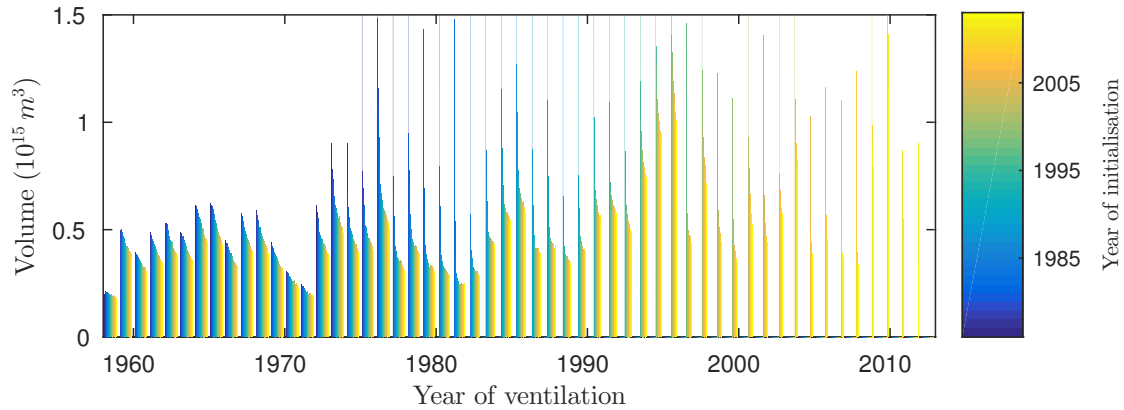


Figure 4.28: Distributions of ventilation year for different initialisation years: $\mathbb{D}_{y_v}[\tilde{\mathcal{V}}(y = i)]$, for i between 1975 and 2012. A decrease in the magnitude of a peak at a certain year, moving from blue to yellow, implies a loss of volume over time of water ventilated in that year.

In Figure 4.29, the top panel shows the mean age distribution, reversed in direction so that age now corresponds to year of ventilation. Overlain as black dots is the volumetric age distribution in 2012 from Figure X. The bottom panel shows the normalised 2012 age distribution, similarly recast in terms of ventilation year. A value of ± 1 means that the volume of water present in NADW ventilated in year $y_v = i$ is 100% greater or less than the volume of water of the same age that is present *on average* in NADW. As such, the normalised 2012 age distribution acts as a proxy for the years in which ventilation into the NADW volume is anomalously high or low. Importantly, it represents only the variability that is retained in the subsurface on timescales of a year and longer. In Figure 4.29, the substantial variability on inter-annual timescales and longer, suggests that there is preferential subduction and retention of water from certain years in the simulation. Positive peaks in the 1990s stand out clearly, as do sustained periods of negative anomalies in the early 1970s, 1980s and mid-2000s.

Inter-annual variability in NADW ventilation

We wish to understand the mechanism by which variability in the normalised 2012 age distribution is established. We consider this first in the context of the timescale over which the variability is set. Observed anomalies must be the net result of

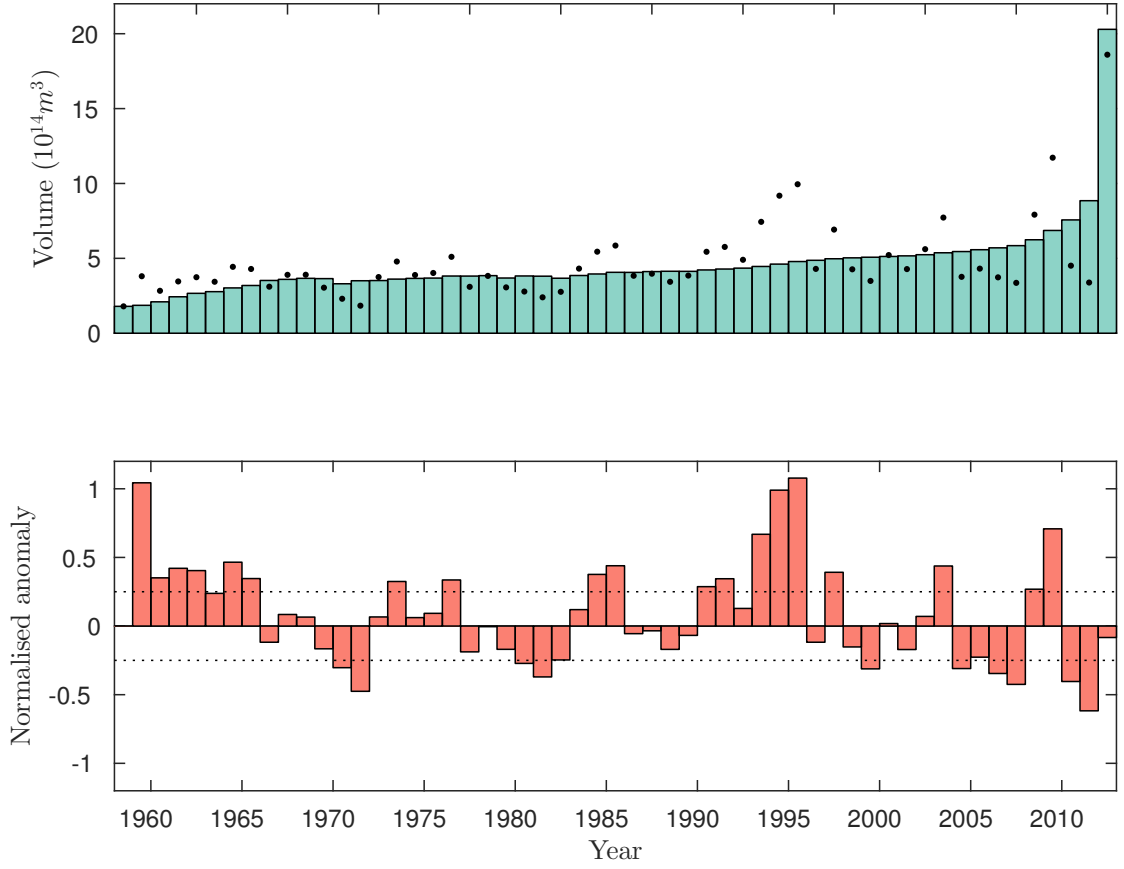


Figure 4.29: (top panel) Average age distribution for NADW, $\overline{\mathbb{D}}_a^y[\tilde{\mathcal{V}}]$, reversed in direction and overlain with black dots corresponding to the age distribution in 2012, $\mathbb{D}_a[\tilde{\mathcal{V}}(y = 2012)]$. (bottom panel) Normalised 2012 age distribution: $(\mathbb{D}_a[\tilde{\mathcal{V}}(y = 2012)] - \overline{\mathbb{D}}_a^y[\tilde{\mathcal{V}}]) / \overline{\mathbb{D}}_a^y[\tilde{\mathcal{V}}]$. Horizontal dotted lines correspond to ± 0.25 .

subduction and re-entrainment (noting that the contribution from lateral export is small; Figure 4.25). A positive anomaly in a given year may be established either by an anomalously large amount of subduction in that year, or an anomalously small amount of re-entrainment in the following year or indeed in subsequent years. Similarly for a negative anomaly being the result of low subduction or high re-entrainment. Temporal variability in one or both of these processes will be establishing the distribution in Figure 4.29.

To establish how subduction and re-entrainment interact to set the age distribution in NADW, we consider how the volume of water subducted from the mixed layer in a particular year changes over time. In Figure 4.30 we show, in the top panel, the anomalous distribution of the volume of newly subducted water in the

years that the subduction takes place: $\mathbb{D}'_y[\tilde{\mathcal{V}}(a < 1)]$, normalised by the mean. This is a measure of the years in which there is more or less subduction than average. We are thus interested in the extent to which this distribution matches that of the normalised 2012 age distribution, which is overlain as black dots.

The broad, multi-annual, timescale of variability of the normalised 2012 age distribution is apparent, with anomalously high volumes in the mid-70s, mid-80s and the early-to-mid 90s offset by low volumes in the late 70s to early 80s and mid-2000s. However, there are years in which the subduction anomaly does not capture the apparent shorter timescale variability, such as in the early to mid-80s and throughout the 90s and at times in the 2000s. These shorter timescales are more clearly captured in the anomalous distribution one year after subduction: $\mathbb{D}'_y[\tilde{\mathcal{V}}(1 < a < 2)]$, normalised by the mean (second panel), *i.e.* after re-entrainment in the following winter. Note that the volume anomaly distributions shift back in time as we consider longer timescales due to the finite length of the simulation: we don't resolve the 2012 distribution after 1 year, or the 2011 distribution after two years *etc.* The distribution of volume anomalies after one year closely match the normalised 2012 age distribution during the 1980s and 2000s. However, during the 1990s, the two do not match up until several years after subduction, suggesting that these anomalies are established on a long timescales. The third panel of Figure 4.30 shows the distribution of volume anomalies 13 years after subduction — $\mathbb{D}'_y[\tilde{\mathcal{V}}(12 < a < 13)]$, normalised by the mean — by which time it closely covaries with the normalised 2012 age distribution. There is an apparent systematic offset that reflects the different manner in which the two distributions are evaluated.

In the bottom panel of Figure 4.30, we show how the correlation coefficient between the anomalous volume distributions and the normalised 2012 age distribution evolves over time since subduction. This shows the timescale over which the age distribution in 2012 is established. The largest increase in the correlation coefficient occurs after 1 year, as expected, but it continues to increase notably over the following 4 years up to a value of ~ 0.95 . This ongoing increase is presumably the result of the long timescale re-entrainment process of waters circulating the

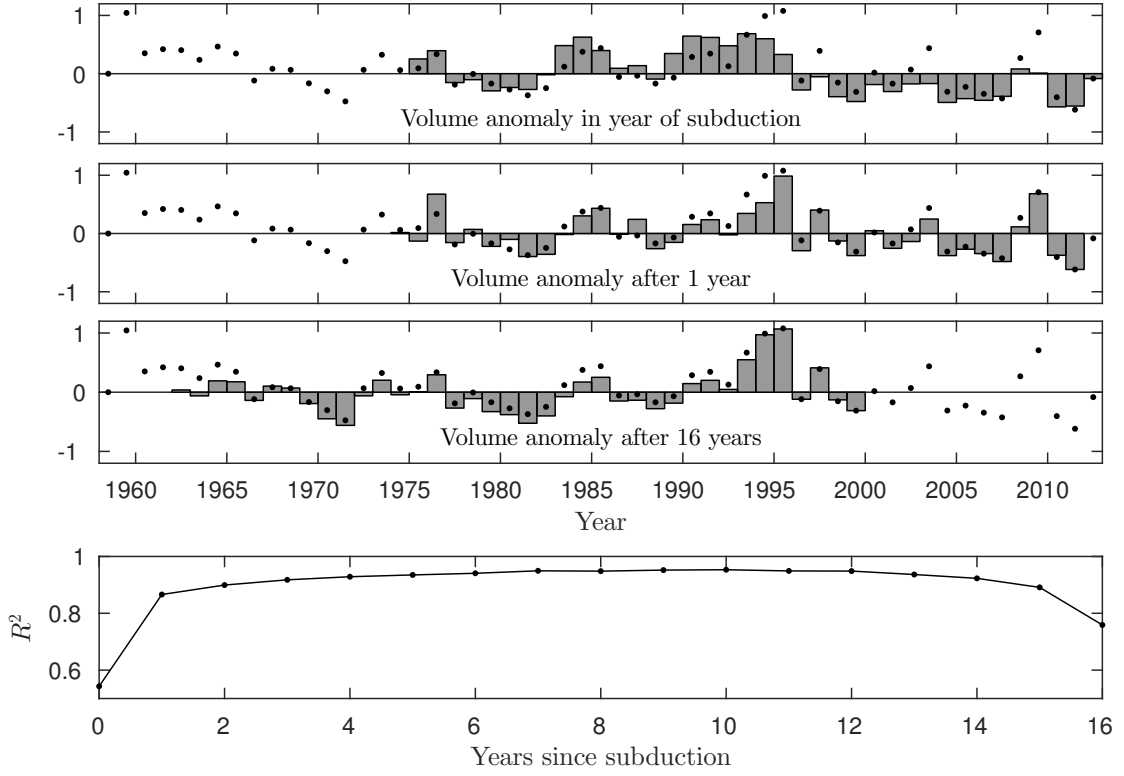


Figure 4.30: (top panel) Distribution of the volume anomalies of water that is less than one year old in the year that it is initialised, $\mathbb{D}'_y[\tilde{\mathcal{V}}(a < 1)]$, *i.e.* anomaly in subducted volume. (second panel) Distribution of the volume anomalies of water that is between one years old in the year *after* it was initialised, $\mathbb{D}'_y[\tilde{\mathcal{V}}(1 < a < 2)]$, shifted left to place it on the year in which it was form, *i.e.* anomaly in volume retained after one year. (third panel) As for previous panels, but for ages between 12 and 13 years. (bottom panel) Correlation coefficient for a linear regression between volume anomaly distributions and the normalised 2012 age distribution, overlain as black dots in each of the upper panels.

subpolar gyre, as noted in the forwards-in-time experiments. The drop in the correlation coefficient after 13 years comes from the inclusion of the very early spin-up years of the model.

It is evident, therefore, that the process of re-entrainment is important in establishing variations in the age distribution of subsurface waters. Variability in the re-entrainment process is displayed in Figure 4.31, in which we show the change in the volume of water subducted in a particular year over the first and second year, as a percentage of the original subducted volume. We label these the first and second year demons. For each year, i , we calculate:

$$\frac{[\tilde{\mathcal{V}}(y = i + 1, y_v = i) - \tilde{\mathcal{V}}(y = i, y_v = i)]}{\tilde{\mathcal{V}}(y = i, y_v = i)} \quad (4.17)$$

and

$$\frac{[\tilde{\mathcal{V}}(y = i + 2, y_v = i) - \tilde{\mathcal{V}}(y = i + 1, y_v = i)]}{\tilde{\mathcal{V}}(y = i, y_v = i)}. \quad (4.18)$$

The average percentage volume reduction, after the first and second year, is shown as horizontal dotted lines.

The first year demon shows substantial variation, with the volume reduced in the first year after subduction by anywhere between 25% and 75%. The largest first year volume reductions occur in the early 1980s and early to mid-1990s, the latter corresponding closely with the time of anomalously large subduction (Figure 4.30). The exception is in the final year of this period, 1995, when there is anomalously large subduction, but anomalously low re-entrainment in the first year. There is a notable shift, after 1994, to lower volume reduction — a less effective demon — but inter-annual variability remains substantial.

There continues to be a significant level of volume reduction by what we call the ‘second year demon’. The average percentage volume reduction is around 8% of the initial volume subducted. There is also substantial variability, with values ranging from < 5% to > 15%. Over some years, there is the suggestion of a negative correlation between the first and second year demons, with anomalously high volume reduction in the first year corresponding to anomalously low volume reduction in the second year and *vice versa*. See, for example, 1975 to 1980. This would be expected simply from the fact that less volume left in the subsurface after one year means less to be re-entrained in the second.

In summary, multi-annual variation in the subsurface age distribution in NADW is set by changes in subducted volume. However, a large percentage of this volume is re-entrained to the surface mixed layer in the following winter. Inter-annual variations in the subsurface age distribution, then, are established by variability in this re-entrainment process. Finally, we note that this picture is not changed when we consider only ventilation that occurs in the Labrador Sea, suggesting that it is processes in this area that are responsible for establishing variations in the age distribution of NADW.

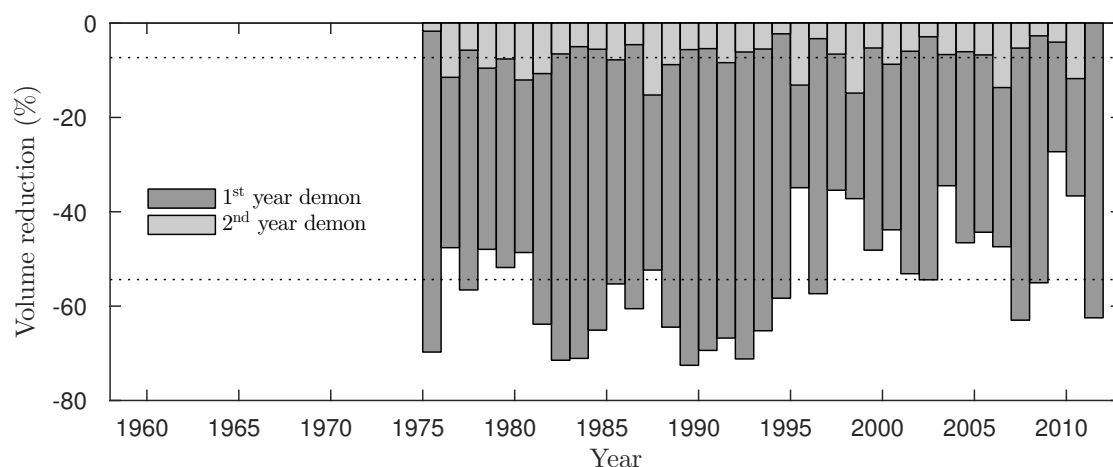


Figure 4.31: Percentage volume reduction of subducted water in the first year after subduction (dark grey, 1st year demon), and in the second year after subduction (light grey, 2nd year demon). Horizontal dotted lines correspond to the mean volume reduction after the first and second years.

The effectiveness of Stommel's demon in the ventilation of the permanent thermocline has been argued on the basis of the relative distances over which a migrating density outcrop and a parcel of subducted water move in one year. Williams *et al.* (1995) notes that, in the subtropical gyre, the former is almost an order of magnitude greater than the latter, supporting the hypothesis that only fluid subducted at the southern extent of the outcrop migration (*i.e.* in late winter) will escape re-entrainment. This raises the question of whether a similar length-scale argument can be made in relation to the effectiveness of Stommel's demon in the subpolar gyre, and its inter-annual variability.

In the subtropical gyre, the direction of the large-scale, time-mean flow in the ocean interior (where much of the subduction occurs) and that of the migrating outcrops are broadly similar. Thus the choice of directly comparable length-scales is clear. In the subpolar gyre on the other hand, the large-scale, time-mean flow in the interior subpolar gyre is northward, moving any subducted parcels back toward regions of deeper mixed layers. Movement away from deep mixed layers rather occurs within southward flowing western boundary currents, as evidenced by the prevalence of ventilation in the boundary current of the Labrador Sea (Figure 4.7). Consequently, the distance travelled by subducted water parcels in the subpolar

gyre is of a comparable order of magnitude to the north-south migration of density outcrops, both being on the order of 1000 km (assuming an average southward velocity in the boundary currents of 0.1 ms^{-1}). More problematic for a length-scale argument in the subpolar gyre perhaps, is that the seasonal migration of outcrops does not follow a strictly north-south path, being strongly influenced by freshwater outflow from the Arctic and the intermittent occurrence of deep convection. Thus it is apparent that a length-scale argument for the effectiveness of Stommel's demon is much less straightforward in the subpolar than in the subtropical gyre.

In relation to inter-annual variability, the southward extent of late-winter density outcrops in the subpolar gyre varies by distances on the order of hundreds of kilometres from year to year. This is an order of magnitude less than the distance travelled by water subducted in southward-flowing western boundary currents. While the caveats associated with a length-scale argument in this region still hold, this large difference broadly implies that inter-annual migrations will not dominate the timing of ventilation into the subsurface. On the other hand, water subducted in the open ocean (*e.g.* by deep convection in the central Labrador Sea) will move southward at a slower rate, its export requiring exchange into the boundary current or eddy-driven dispersion. Thus it may be expected that ventilation of this water will be subjected to more substantial variability that results from the inter-annual migration of late winter density outcrops. In the following section, we explore this possibility directly in our Lagrangian experiments.

Density and subduction location variation in NADW ventilation

Thus far, we have considered variability in the NADW volume as a whole. We noted in Section 4.3.1, however, that ventilation of NADW occurred in distinct regions, particularly in the boundary current and interior basin of the Labrador Sea, and further, that different density classes were ventilated in each of these regions. Differences in regional circulation (Figure 4.10), as well as winter mixed layer depths (Figure 4.6), are likely to impact the variability of both subduction and re-entrainment in these regions, and the density classes into which water is subducted.

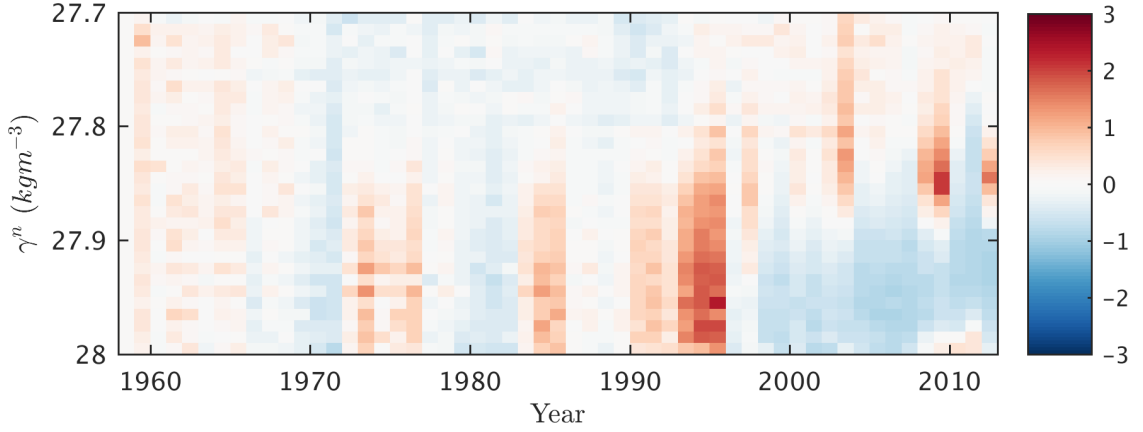


Figure 4.32: Age-density distribution in 2012, $\mathbb{D}_{a,\gamma^n}[\tilde{\mathcal{V}}]$, evaluated as the normalised anomaly relative to the mean distribution, $\overline{\mathbb{D}}_{a,\gamma^n}^y[\tilde{\mathcal{V}}]$.

In Figure 4.32 we show the variability of the NADW age distribution, now separated to show the variability spread across different density classes: $\mathbb{D}_{a,\gamma^n}[\tilde{\mathcal{V}}]$. As for the whole NADW volume, this is presented as the normalised volume anomaly, having subtracted and divided by the time-average joint distribution: $\overline{\mathbb{D}}_{a,\gamma^n}^y[\tilde{\mathcal{V}}]$, where the average is calculated between 1975 and 2012. Again, we have reversed the direction of the x -axis so that it corresponds to the year of subduction. The decrease in variability in early years may be due to the decrease in the number of realisations as we go further back in time, as well as the influence of diapycnal motion (Chapter 2) smoothing out the signature of variability within the volume.

The most immediately striking aspect of Figure 4.32 is that almost all of the variability in the 1970s, 80s and first half of the 1990s is apparent in classes denser than around $\gamma^n = 27.83 \text{ kg m}^{-3}$, with almost no variation in the lighter classes. After 1995, the opposite is true, with the lighter density classes exhibiting more substantial inter-annual variability, and the volume in denser classes being anomalously and consistently low.

From Figure 4.11, we noted that the densest classes of NADW in the model were formed in the open ocean, while intermediate and lighter density classes were formed close to the boundary. On the other hand, density distributions within bathymetric ranges are broad, particularly in the open ocean, suggesting that the variability in the ventilation of a particular class could arise from subduction in

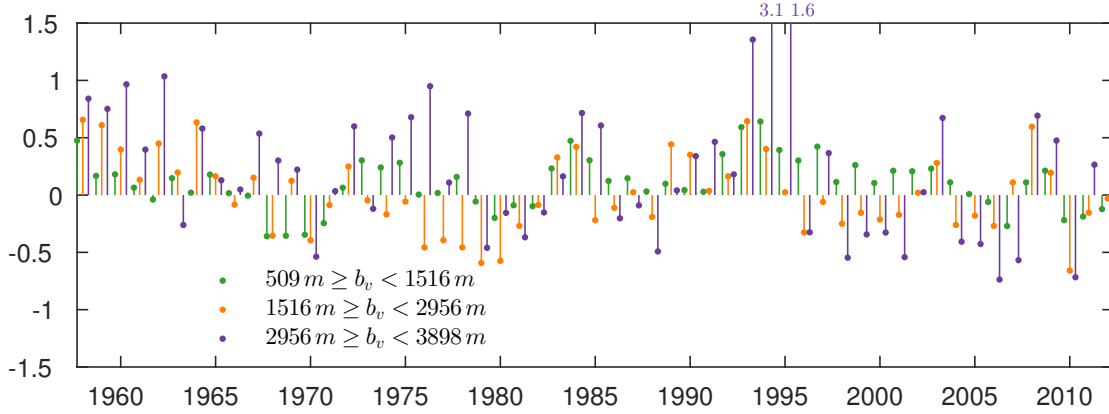


Figure 4.33: Joint age and subduction bathymetry distribution in 2012, $\mathbb{D}_{a,b_v}[\tilde{\mathcal{V}}]$, for the three bathymetric ranges considered previously, evaluated as the normalised anomaly relative to the mean distribution, $\mathbb{D}_{a,b_v}^y[\tilde{\mathcal{V}}]$.

either the boundary regions or the interior basin. Figure 4.33 shows the normalised 2012 age distribution, now separated by bathymetric range over which subduction occurs. Anomalies associated with subduction over the open ocean (purple) show the most extreme variability over the time-series. Anomalies in the deep boundary region (orange) are sometimes seen to be broadly in-sync with those of the deep ocean (albeit with smaller magnitude), such as from the start of the simulation to the mid-1960s and from 1995 to 2012. At other times, however, the distributions diverge for periods of a few years, such in the mid-1970s and mid-1990s. The implication is that, at these times, which correspond to periods of large open ocean anomalies, the processes establishing variability in ventilation in the boundary current and open ocean become decoupled. Anomalies in ventilation over the shallowest bathymetric range, have a similar range of variability to that in the deep boundary current region, but are frequently decoupled, suggesting that they are controlled by quite different processes.

Relating anomalies to surface forcing

Research into ventilation of the deep water in the North Atlantic ocean focusses on linking variability in surface forcing to its signature in the subsurface (Schott *et al.*, 2004; Rhein *et al.*, 2011; Le Bras *et al.*, 2017). We have shown that, within the NADW volume, there is substantial inter-annual to multi-annual variations in

the volume of water associated with ventilation in particular years. Furthermore, variations are seen in the density classes in which that volume appears, and the locations at which it was subducted. We now wish to establish the extent to which the subsurface anomalies reflect Eulerian measures of surface forcing, namely mixed layer depth, atmospheric modes and surface buoyancy flux variability.

We saw in Section 4.3.1 that the majority of NADW ventilation takes place via subduction in the boundary current and open ocean of the Labrador Sea. Thus we evaluate the variability in the winter-mean (mid-February to mid-April) mixed layer depth between 1975 and 2012 in three locations in the Labrador Sea, as an indication of the local dense water formation variability. These locations are shown by red circles in Figure 4.6 and correspond to the interior basin where the largest mixed layers are observed, the northern boundary region where there are relatively deep mixed layers, and on the south west boundary, where high levels of ventilation are observed (Figure 4.7). The mixed layer depths in these regions are shown in Figure 4.34.

In the open ocean, periods of sustained deep mixed layers in the mid 1970s, mid 80s and early 1990s match the periods when volumes of water in the year of subduction (top panel of Figure 4.30) exhibit sustained positive anomalies, implying that a component of these is be due to deep convection in the open ocean. Mixed layers are generally deep throughout the 1970s, 80s and early 90s, before a substantial change in the mid-1990s to persistently shallower depths. The timing of this change corresponds to the time when there is a shift in the efficiency of the re-entrainment process (Figure 4.31). Winter mixed layers in the south west boundary region do not show much agreement with those of the open ocean until the early 1990s, after which they closely covary. In the northern region, mixed layer depths are generally more steady, at a depth of around 1000 *m* and show little evidence of consistency with the mixed layers elsewhere in the Labrador Sea.

In the bottom panel of Figure 4.34 we show the DJF-index of the North Atlantic Oscillation (NAO; Hurrell and Deser, 2009), the dominant mode of atmospheric variability in the North Atlantic. A positive anomaly in the NAO index coincides

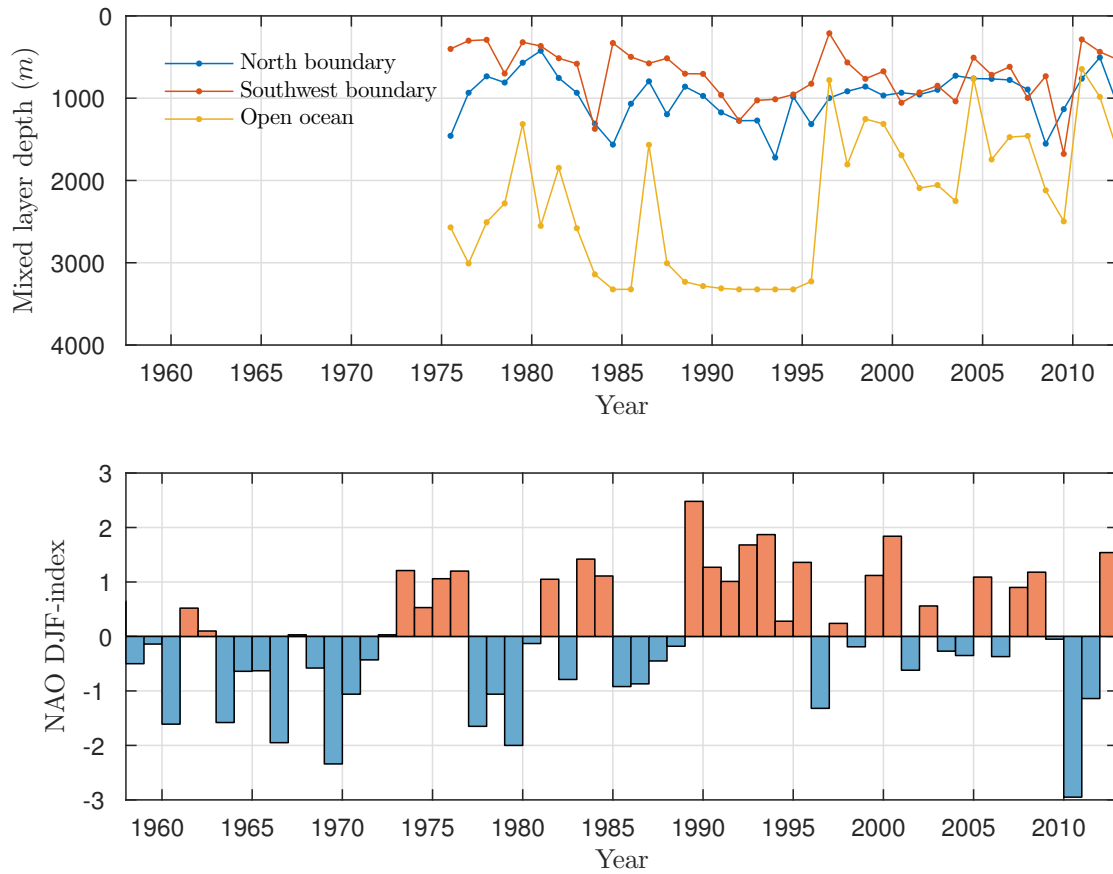


Figure 4.34: Time series of (a) mid-February to mid-April mean mixed layer depths at three locations in the Labrador Sea (shown in Figure 4.6), and (b) the December-January-February North Atlantic Oscillation index (Hurrell and Deser, 2009).

with strong heat loss over the Labrador Sea and higher occurrence of deep convection, particularly in the open ocean (Marshall *et al.*, 2001a; Yashayaev and Loder, 2016). In the model, we see that the mixed layer depths in the open ocean indeed show consistency with this, particularly during the period of deepest convection in the 1970s, 80s and 90s, although convection appears to start in the 1990s before the onset of positive NAO anomalies. Furthermore, comparison of the NAO index with the normalised 2012 age distribution (Figure 4.29) shows good agreement over multi-annual timescales.

To consider variability in the densities of water being formed over time, as noted in subsurface NADW (Figure 4.32), we evaluate anomalies in the water mass transformation in the North Atlantic, derived from surface buoyancy forcing (Section 4.2.4). Figure 4.35 shows the anomaly in the annual-mean water mass transformation,

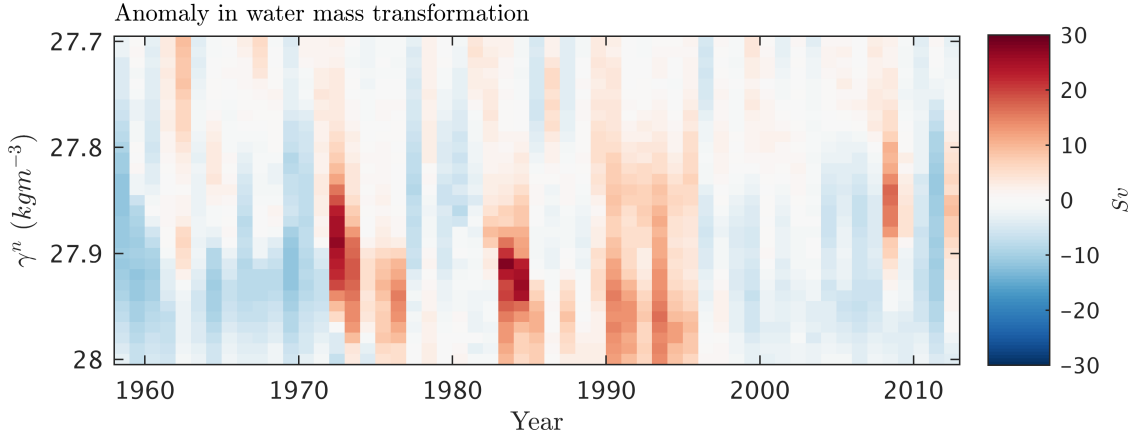


Figure 4.35: Anomaly in the surface-forced water mass transformation, F , for the NADW volume during the simulation. See Section 4.2.4 for details of the calculation.

F , for the neutral density range corresponding to NADW. There is broad agreement between F and the normalised 2012 anomaly. Peaks in transformation to greater densities in the 1970s, 80s and 90s closely match the years in which an anomalously large volume of dense water ventilated in those years was retained in the subsurface. There is also agreement in more recent years, in 2008 and 2012, when transformation at lighter densities is observed. We note that due to both the manner in which neutral density and potential density must be matched up to calculate F (Section 4.2.4), and the possible imprint of diapycnal motion on the normalised 2012 age-density distribution (Chapter 2), we cannot precisely match the two. We thus interpret the consistency between the two measures as evidence that the broad pattern of surface-forced dense water formation is retained in the subsurface of NADW. This is noteworthy in itself since it implies that buoyancy forcing by interior mixing, both in the mixed layer and subsurface, is of secondary importance in setting the properties of these dense water masses, a result previously suggested by Nurser *et al.* (1999) based on a quite different, Eulerian approach in a coarse resolution, isopycnal model.

In summary, Eulerian diagnostics of dense water formation variability capture the multi-annual and longer timescale component of NADW ventilation in the model, *i.e.* that which is established by variations in subduction. They fail, on the other hand, to capture differences on inter-annual timescales related to variability in the subsequent re-entrainment of subducted water.

The impact of ventilation variability

We have shown that the distribution of ages in NADW in 2012 reflects variability in the subduction and re-entrainment process over the model simulation. Is there any impact of this variability on the ventilation pathways and timescales of export of newly ventilated water? Figure 4.36 shows the volume-weighted mean latitude of water as a function of age: $\overline{\mathbb{D}}_a^y \Phi$ (black dots, grey shading). This is a measure of the average southward movement of the centre of mass (in our case volume) of ventilated water. In addition, we show the same distribution but subsetting to include only years with anomalously low and high values (magnitude greater than 0.25) in the normalised 2012 age distribution (Figure 4.29). Over the first 15 years, the distributions are broadly similar. Only after this time, corresponding to export across $\sim 42^\circ N$ do the southward spreading rates diverge, with water ventilated in years with a high volume anomaly moving southward at a faster rate. The divergence in rates only persists over a few degrees of latitude (between ~ 42 and $37^\circ N$) south of which the rates appear similar. The impact however, is that the centre of mass of water ventilated in years with a high volume anomaly are exported to, for example, $30^\circ N$ approximately 4 to 5 years earlier, on average, than water ventilated in years with a low volume anomaly. Given the relatively small number of distributions used to derive these distributions, it is possible that the slight divergence in export rate at $\sim 42^\circ N$ is a biased signal. However, if robust, this result provides evidence for an impact of ventilation variability on southward export that has previously been elusive (Lozier, 2012; Zou and Lozier, 2016).

4.4 Discussion

In this study, we have used a novel Lagrangian approach to explore the nature of North Atlantic Deep Water ventilation in a $1/4^\circ$ resolution ocean circulation model. We directly link, via non-diffused Lagrangian trajectories, water throughout NADW in the subsurface to the time and location that it left the surface ocean mixed layer.

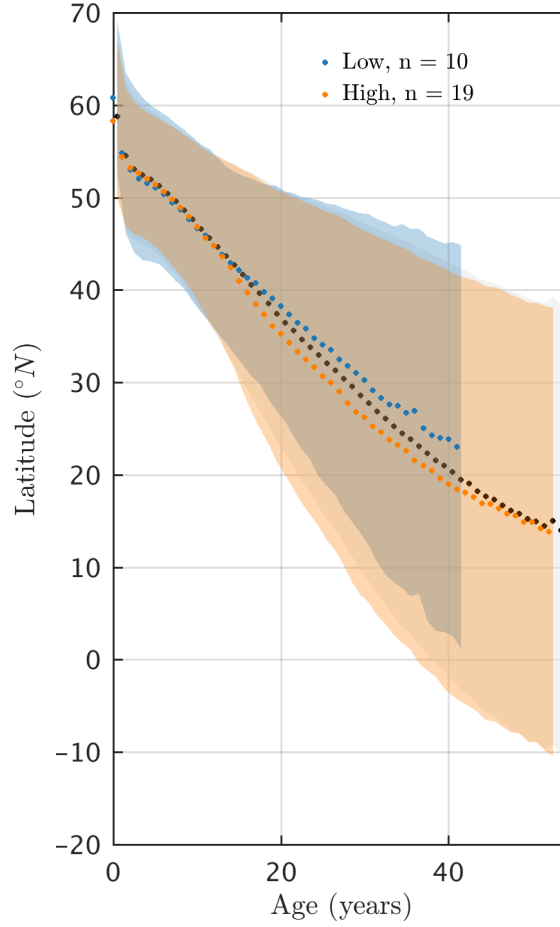


Figure 4.36: Average latitude for water of each age, $\overline{\mathbb{D}}_a^y \Phi$, for (black) all initialisations between 1975 and 2012, (blue) years for which the normalised 2012 age anomaly is less than -0.25 and (orange) years for which the normalised 2012 age anomaly is greater than 0.25 . Shaded areas show the standard deviation.

Our analysis reveals that, in this simulation, NADW ventilation is dominated by subduction in the Labrador Sea (Figure 4.7). This is not in keeping with observations, that suggest important contributions from ventilation in the GIN seas (leading to the formation of overflow water) and Irminger Seas (Lazier *et al.*, 2001). Note, however, that evidence for the latter is based on observations of local deep convection (Vage *et al.*, 2011) rather than a distinct signature of this region in downstream water mass properties (since the properties are indistinguishable from that formed in the Labrador Sea). Consequently, dense water may be formed in the Irminger Sea and subsequently re-entrained to the mixed layer in the Labrador Sea, before being subducted again, making the Irminger Sea important for water mass transformation but not the final location of NADW ventilation. Since our

analysis considers only the last time that water was in the mixed layer, we have not yet investigated upstream water mass transformations.

Denmark Straits Overflow Water (DSOW), on the other hand, has a distinct hydrographic signature in the deep North Atlantic that suggests its last point of surface contact was in the GIN seas (Isachsen *et al.*, 2007; de Carvalho Ferreira and Kerr, 2017). Analysis with forwards-in-time trajectories suggests the water that is formed in the GIN seas and exported across the sills into the subpolar North Atlantic is re-entrained into the mixed layer during its passage through the Labrador Sea (Figure 4.15), such that very little is exported south of the subpolar gyre continuously within the subsurface. In the ocean, stratification resulting from the greater density of DSOW prevents penetration of the mixed layer into this water mass in the Labrador Sea, even during periods of intense deep convection (Yashayaev and Loder, 2016). In the model, however, water exported from the GIN seas experiences a substantial shift towards lighter densities between formation and re-entrainment (Figure 4.17). In the absence of deep ocean stratification, therefore, convection in the Labrador Sea is persistently widespread and deep (Figure 4.6), and consequently re-entrains any water that previously left the mixed layer further north. The impact of an absence of DSOW on the representation of Labrador Sea convection in models was also inferred by Kösters *et al.* (2005). The decrease in density of GIN seas water is likely to have occurred close to and downstream of the sills. In these regions, mixing between gravity-driven downslope flow and ambient water is represented by a fairly crude parameterisation (Madec, 2008) that is likely to be overly diffusive (Legg *et al.*, 2009; Graham *et al.*, in review).

Dominance of the Labrador Sea as the site of NADW ventilation in this simulation carries important implications for the model’s representation of ventilation, particularly in relation to its use in coupled climate simulations and projections (Williams *et al.*, 2015a). In the first instance, surface buoyancy forcing in the region is insufficient to form the densest classes of NADW found in the ocean (Pickart *et al.*, 1997; Marsh *et al.*, 2000). Downstream, this could result in misrepresentation of the location where, and timescale on which, this water is re-entrained back into

the surface mixed layer and re-exposed to the atmosphere (Talley, 2013). This has evident consequences for the storage of heat and carbon dioxide in the deep ocean, and the timescales of their exchange with the atmosphere, potentially eroding the accuracy with which this is represented in climate projections. In addition, the localisation of NADW formation could make the model overly sensitive to forcing in this region. Countless studies have explored the sensitivity of the ocean circulation, and global climate, to forcing changes in the high-latitude North Atlantic Ocean, with a particular focus on its effect on the Atlantic Meridional Overturning Circulation and its associated northward heat transport (Vellinga and Wood, 2002; Stouffer *et al.*, 2006). In many of these studies, the Labrador Sea stands out as critical region of sensitivity. On the other hand, observations suggest that the region is much less important for the overturning circulation, and indeed water mass transformations, than has been previously considered and that these model sensitivities suggest (Pickart and Spall, 2007). It is plausible that the discrepancy between these results is, in part, related to the models' over-representation of NADW ventilation in the Labrador Sea.

For ventilation in the Labrador Sea, the majority takes place within the boundary current (Figure 4.9), forming water in the upper and intermediate density classes of NADW (Figure 4.11). Observations of ventilation in the boundary current system are increasingly widespread (Pickart *et al.*, 2002; Cuny *et al.*, 2005; Palter *et al.*, 2008). However, it is not generally considered to be a dominant source of Labrador Sea Water (Lazier *et al.*, 2001; Rhein *et al.*, 2011), with convection in the interior basin believed to be the main formation region and subsequent exchange into the boundary current leading to its export (Straneo, 2006; Palter *et al.*, 2008). This perspective, however, is mostly derived from downstream properties (Rhein *et al.*, 2011), from which it is likely impossible to distinguish between water formed in the deep boundary current and that formed in the interior basin (Pickart *et al.*, 2002). Furthermore, Palter *et al.* (2008) note from float observations that formation in the boundary current is at least as important as exchange with the interior in setting the properties of exported water.

Given the distinct hydrographic properties of the model relative to observations, it is difficult to establish the realism of the model's boundary current ventilation. Our analysis suggests that its prevalence is related to a shallowing of the mean winter mixed layer along the pathway of the boundary current. This shallowing is due to the presence of deep winter mixed layers in the north of the Labrador Sea, near the entrance to Baffin Bay, that are relatively constant over time (Figure 4.34). Observations of climatological mixed layer depths (Figure 4.6) do not suggest that this takes place in the ocean (though the observational resolution could be insufficient). Thus, while our analysis emphasises the important role of ventilation within the Labrador Sea boundary current, it also serves to show how this process could be over-represented in the simulation.

In the ventilation of the eastern side of the mid-Atlantic ridge, we noted alignment between ventilation pathways and the salinity and potential vorticity signature of the Mediterranean outflow, consistent with observations (Talley and McCartney, 1982). We suggest that the presence of the outflow is an important component, along with bathymetric steering, in slowing southward propagation of recently ventilated upper layers of Labrador Sea Water in the eastern Atlantic, by establishing a potential vorticity gradient at this depth. In terms of its salinity signature, the influence of Mediterranean water extends far below the main outflow tongue, through vertical diffusion enhanced by salt-fingering (Schmitt, 2003; Jia *et al.*, 2007). We have not yet assessed whether this influence is also felt in the potential vorticity of the dense classes of NADW. In an assessment of climatological potential vorticity in the abyssal ocean, O'Dwyer and Williams (1997) do not find clear evidence for this, although there is some distortion of the potential vorticity contours at depths of around 2.6 km, to the west of the Mediterranean outflow.

The age distribution in NADW (Figure 4.29) points toward substantial variations in the formation of NADW, and its retention in the subsurface, on inter-annual to decadal timescales. A multi-annual timescale is established from sustained levels of subduction (Figure 4.30), which show good agreement with atmospheric forcing variability (in the form of the NAO index), mixed layer depths in the Labrador

Sea, and surface-forced water mass transformation, particularly during the 1970s through to the mid-1990s. This is consistent with observations, which have found signatures of Labrador Sea Water variability in remote locations after the period of sustained deep convection in the 1990s (Schott *et al.*, 2004; Rhein *et al.*, 2011).

Variations in the age distribution of NADW on shorter timescales reflect variability in the re-entrainment process — the ‘effectiveness’ of Stommel’s demon. An insightful example occurs during the 1990s, when sustained, atmospheric forcing results in the annual formation of large volumes of NADW. During this time period, from around 1989 to 1995, the amount of dense water formed is approximately equal between years (Figure 4.30). However, an anomalously large percentage of water in the early years is re-entrained to the mixed-layer in the following winter (Figure 4.31). Consequently, it is only dense water formed in the later years (from 1993 to 1995), that show particularly large anomalies present in NADW. It is notable that the initial amount of NADW formed in 1995 is around half that formed in 1990, but around 4 times as much is retained in the subsurface.

These shorter timescale variations are not reflected in the Eulerian diagnostics of dense water formation. Consequently, it is likely that these measures would overestimate the overall formation rate if they assumed no (or even constant) annual re-entrainment, as is commonly done in observations (Marsh *et al.*, 2000; Rhein *et al.*, 2011). In addition, comparison of the timing of advected downstream signals with the onset of dense water formation (Le Bras *et al.*, 2017) could misrepresent the timescale of propagation, particularly during periods of sustained formation.

In assessing the sources of this variability, we considered its distribution between density classes and between subduction locations. Variability during the 1970s to mid-1990s is concentrated in the denser classes of NADW. This points towards open ocean convection (where the densest water masses are formed) being largely responsible for these variations. In fact, anomalies in ventilation over both the boundary regions and open ocean are present during this time, but the most extreme positive anomalies do appear to be the result of ventilation in the open ocean (Figure 4.9). This is particularly true in the 1990s, when it is also the case

that open ocean ventilation exhibits much larger anomalies in latter years (1993 to 1995) relative to early years (1989 to 1992) by comparison to ventilation in the boundary region. Consequently, the mechanism establishing short timescale variations in the ventilation of NADW appears most effective for ventilation in the open ocean, at least during the time period of anomalously deep open ocean winter mixed layers. This makes intuitive sense in the context of re-circulations in the Labrador Sea (Lavender *et al.*, 2000), which make it more difficult for water to be exported towards regions of shallower winter mixed layers depths than if they are ventilated in the boundary current. Furthermore, pre-conditioning of the water column makes it more likely that deep convection will occur in consecutive years in the open ocean (Yashayaev and Loder, 2016) leading to perpetual re-entrainment of dense water. Only when the conditions change markedly (such as in 1995) will dense water be afforded sufficient time to escape the region in large quantities.

After 1995, anomalies shift towards lighter density classes, consistent with observations (Kieke *et al.*, 2006), and reflected in surface-forced water mass transformation (Figure 4.35). During this time, anomalies are shared between ventilation in the boundary current and the open ocean, although variability is more substantial in the latter.

An obvious caveat to the conclusions drawn here is the length of the model simulation. We have explored these mechanisms in a much longer (375 years) simulation, and initial results (shown in Chapter 6) agree favourably with the results presented here. However, further exploration in this long simulation would be beneficial.

5

The polar Southern Ocean carbon cycle

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5.1 Introduction

Throughout this thesis, we have investigated the physics of ocean ventilation. Namely, the processes facilitating the movement of water into and around the ocean interior. These processes are broadly sufficient to describe the transport of atmospherically-derived passive tracers, such as CFCs. When we are instead interested in the movement of a chemically and/or biologically active tracer, such as carbon dioxide, the physics of ventilation only tells half (or indeed some other

fraction) of the story. The remaining fraction belongs to the biogeochemical processes that act to modify the concentration of such a tracer within water masses as they are ventilated into, re-entrained from, or simply transported around, the ocean interior. In the following chapter, we present one such scenario related to the uptake and sequestration of carbon dioxide in the polar Southern Ocean, in which the purely physical process of ocean ventilation is only part of the story.

The polar Southern Ocean, south of the Antarctic Circumpolar Current (ACC), is arguably the most important region on the planet for the centennial to millennial timescale cycling of carbon (Sigman *et al.*, 2010). Atmospheric carbon dioxide (CO_2) exhibits strong sensitivity to the physical and biogeochemical dynamics in the region on glacial timescales in paleoclimatic observations (Gottschalk *et al.*, 2016), low-complexity box models (Sarmiento and Toggweiler, 1984; Stephens and Keeling, 2000) and fully three-dimensional numerical simulations (Bernardello *et al.*, 2014; Watson *et al.*, 2015; Ferrari *et al.*, 2014). Furthermore, in the present day, the regional uptake of anthropogenic carbon could be a major contributor to its millennial-timescale storage in the deep ocean (Sandrini *et al.*, 2007; Arrigo *et al.*, 2008; van Heuven *et al.*, 2014). Consequently, understanding the operation and variability of the regional carbon cycle, and its propensity for change, are fundamental challenges facing modern climate research.

The circulation of the polar Southern Ocean is characterised by intense water mass transformations. Water transported across the ACC at intermediate depths, so-called Circumpolar Deep Water (CDW), is upwelled towards the surface ocean as a result of wind-driven divergence (Gordon and Huber, 1990; Hoppema *et al.*, 1999; Jullion *et al.*, 2014). Along the coast of Antarctica, cooling under ice-shelves and brine rejection from continuous sea-ice formation leads to the formation of extremely dense water on the continental shelves (Gill, 1973; Whitworth *et al.*, 1994). Cascading off the shelves, entraining CDW along their path, these waters form Antarctic Bottom Water (AABW) (Gill, 1973; Nicholls *et al.*, 2009; Jullion *et al.*, 2014), which goes on to flood the global abyssal ocean (Orsi *et al.*, 1999; Naveira Garabato *et al.*, 2002).

These intense water mass transformations have important implications for the regional cycling of carbon. Circumpolar Deep Water, entering the region at intermediate depths, is rich in dissolved inorganic carbon. Outgassing of this carbon to the atmosphere via upwelling, or translation into the abyssal ocean via bottom water formation, would have a substantial impact on the partitioning of carbon between the atmospheric and oceanic reservoirs. Following this perspective, the conceptual framework of the polar Southern Ocean carbon cycle has traditionally collapsed onto a two-dimensional, latitude-depth plane, shown schematically in Figure 5.1. Consequently, the vertical overturning circulation, particularly the formation of AABW, has been central in attempts to explore the role of the polar Southern Ocean carbon cycle in global climate (Sarmiento and Toggweiler, 1984; Ferrari *et al.*, 2014; Watson *et al.*, 2015).

In the overturning-centric framework, the operation of the polar Southern Ocean as a net source or sink of atmospheric carbon dioxide is established by the interaction of water mass transformations with biogeochemical processes and sea-ice dynamics (Shadwick *et al.*, 2014; Delille *et al.*, 2014). Research efforts have largely focussed on the regions of the most intense water mass transformations, biological activity and sea-ice dynamics: the continental shelves (Arrigo *et al.*, 2008; Wang *et al.*, 2010; Roden *et al.*, 2013; Shadwick *et al.*, 2014; Legge *et al.*, 2015; Hauri *et al.*, 2015; Tortell *et al.*, 2015). Present understanding holds that the air-sea exchange of CO₂ in these regions is set by the coastal upwelling of carbon-rich CDW and a careful balance in the relative timing of biological activity and sea-ice advance and retreat (Wang *et al.*, 2010; Roden *et al.*, 2013). Importantly, carbon observations in these regions suggest that dense shelf waters, which will go on to form AABW, have consistently lower levels of inorganic carbon than the upwelling CDW (Sandrini *et al.*, 2007; Shadwick *et al.*, 2014). In addition, carbon concentrations in surface water are low relative to that of CDW as a result of biological activity (Stoll *et al.*, 1999; Bakker *et al.*, 2008). From the two-dimensional perspective therefore, both wind-driven upwelling and the formation of AABW in the polar Southern Ocean domain should lead to the outgassing of CO₂ to the atmosphere. Several studies note, however, that both

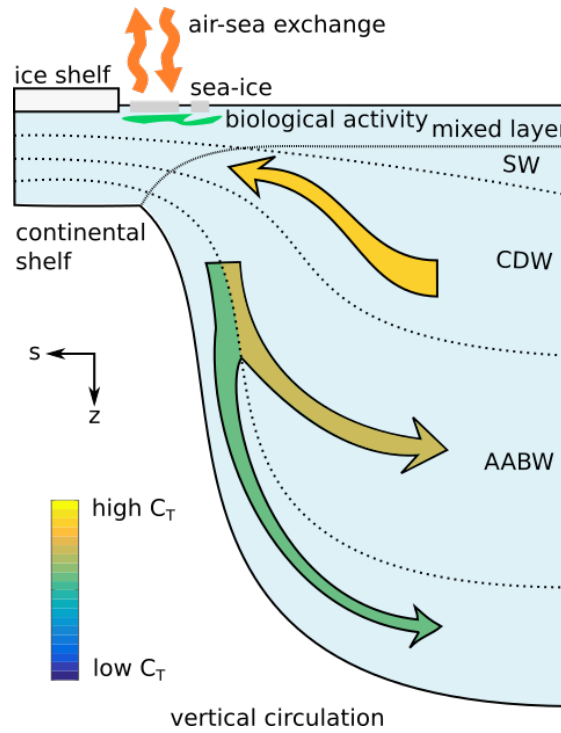


Figure 5.1: Schematic illustration of a two-dimensional, overturning-centric perspective of the polar Southern Ocean carbon cycle. Dotted lines delineate Surface Water (SW), Circumpolar Deep Water (CDW), and upper and lower layers of Antarctic Bottom Water (AABW).

the continental shelves (Arrigo *et al.*, 2008; Legge *et al.*, 2015; Roden *et al.*, 2013) and wider regions of the polar Southern Ocean (Hoppema *et al.*, 2007; Bakker *et al.*, 2008; Takahashi *et al.*, 2009; Brown *et al.*, 2015) act as sinks for atmospheric CO_2 in the present-day. This suggests, therefore, that processes separate to the overturning circulation are acting to take up atmospheric CO_2 in the polar Southern Ocean.

An alternative perspective of the polar Southern Ocean carbon cycle has placed more attention on open ocean processes (Stoll *et al.*, 1999; Hoppema *et al.*, 1999, 2002; Bakker *et al.*, 2008). These regions are characterised by large, cyclonic gyres, particularly in the Ross and Weddell Seas (Dellnitz *et al.*, 2009), within which carbon uptake is determined by a balance between wind-driven upwelling and biologically drawdown (Hoppema *et al.*, 1999). Despite relatively low levels of primary production (Hoppema *et al.*, 2007), observations suggest that these open ocean regions are sinks of atmospheric CO_2 (Stoll *et al.*, 1999; Hoppema *et al.*, 1999) and furthermore that the biologically-fixed carbon is sequestered, via horizontal

transport, into the deep ocean (Hoppema, 2004a).

In this chapter, we assess the carbon budget in the Weddell Gyre (Figure 5.2), an important region of the polar Southern Ocean, using observations around its boundary. We show that the regional net uptake of CO_2 from the atmosphere is the result of a balance between a source of carbon from the overturning circulation and a sink of carbon from the horizontal circulation. We show that the horizontal sink is due to the enrichment of carbon in CDW by the remineralisation of organic matter during its residence in the cyclonic Weddell Gyre, placing open ocean biological processes at the heart of the story. This shifted perspective changes our conception of the important parameters in the polar Southern Ocean carbon cycle. We argue that these must include the residence time of the horizontal circulation and open ocean biological processes such as export production and remineralisation rates.

5.2 Materials and Methods

5.2.1 Hydrographic and chemical data

Data were collected on three oceanographic transects, plotted in Figure 5.2, that took place over a period of two years, from 2008 to 2010. Two of the cruises were conducted as part of the Antarctic Deep Water Rates of Exchange (ANDREX) project in 2008 and 2010, from the Antarctic Peninsula to 30°E around the northern rim of the Weddell Sea (Bacon and Jullion, 2009; Meredith, 2010). A third cruise was completed as part of the US CLIVAR project in 2008 along the quasi-meridional I6S section at 30°E (Speer and Dittmar, 2008). Temperature and salinity were measured in 2 db pressure bins across the full depth range at each station. Water was collected at an array of depths for onboard measurement of a number of chemical species. Relevant for this study are total dissolved inorganic carbon, total alkalinity, dissolved oxygen, silicate and phosphate. Full details of the procedure for hydrographic and chemical measurements can be found in the cruise reports, as well as in Jullion *et al.* (2014) and Brown *et al.* (2015). Bottle measurements were optimally interpolated (Roemmich, 1983) onto the hydrographic data points.

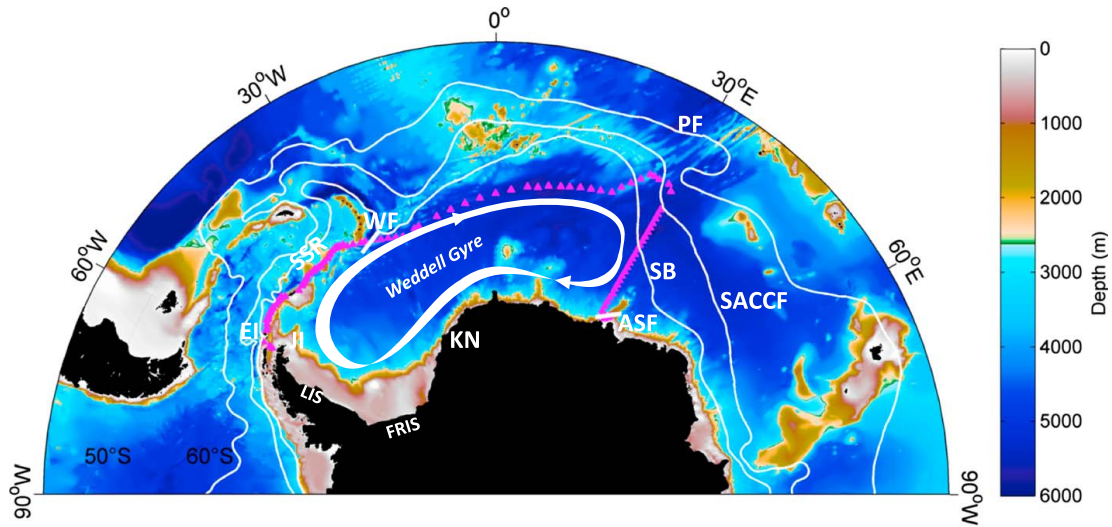


Figure 5.2: Illustration of the location and oceanographic setting of the Weddell Gyre, used with permission from Brown *et al.* (2015). Pink triangles show the station locations of the hydrographic sections used in this analysis. White contours illustrate the climatological positions of Southern Ocean fronts (Orsi *et al.*, 1995), used to illustrate the location of the Antarctic Circumpolar Current and where it intersects the sections. Abbreviations relevant for this study: ASF = Antarctic Slope Front, SSR = South Scotia Ridge. Other abbreviations: EI = Elephant Island, FRIS = Filchner Ronne Ice Shelf, JI = Joinville Island, KN = Kapp Norvegia, LIS = Larsen Ice Shelf, PF = Polar Front, SACCF = Southern Antarctic Circumpolar Current Front, SB = Southern Boundary, and WF = Weddell Front.

5.2.2 Box inverse model solution

The velocity field used in this analysis was derived by Jullion *et al.* (2014) via a box-inversion. Box inverse modelling (Wunsch, 1996) allows the estimation of large-scale ocean circulation from observations, within a theoretical framework in which conservation of mass, heat, salt and any other measured tracer can be imposed. Observations of potential temperature and salinity, from which potential density is calculated, are used to derive the vertical shear of the cross-section velocity through thermal wind balance. The box inverse method allows the estimation of reference velocities (for each hydrographic station pair) that achieve conservation of heat, freshwater and mass (equivalently temperature, salinity and volume, assuming incompressibility) across the full depth and within each of the model layers, with the minimal perturbation (in a least squares sense) to an *a priori* approximation. Jullion *et al.* (2014) used 10 vertical layers based on neutral density (Jackett and

McDougall, 1997), chosen to delineate the major water masses in the Weddell Gyre region. In this inversion, an additional constraint was placed on the net transport of the ACC ($0 \pm 5 Sv$), between stations 82 and 11, to improve the solution. The solution of Jullion *et al.* (2014) also allows for the transport of volume, temperature and freshwater by eddying motions. These terms were derived from time averaging of the Southern Ocean State Estimate (Mazloff *et al.*, 2010) at the location of the sections in Figure 5.2. In this study, we apply a small correction to the solution of Jullion *et al.* (2014) to impose full-depth conservation of mass as opposed to volume (the previous solution assumed incompressibility). In applying this correction, we constrain the full-depth carbon transport so that it remains consistent with that of (Brown *et al.*, 2015). The correction invokes minimal change in the velocity field but mass conservation is important for the decomposition of the overturning and horizontal circulation.

5.2.3 Carbon framework

Carbon concentration in a water parcel can be separated into constituent parts using coincidentally measured hydrographic and chemical data (Williams and Follows, 2011). The primary separation is between preformed carbon (the concentration present in the water parcel on leaving the surface) and regenerated carbon (carbon added to the water parcel since leaving the surface ocean). The carbon framework is written as

$$C_T = \underbrace{C_{sat}^{pi} + \overbrace{C_{sat}^{ant} + \Delta C}^{C_{res}}}_{\text{preformed}} + \underbrace{C_{soft} + C_{carb}}_{\text{regenerated}} \quad (5.1)$$

The saturated component ($C_{sat}^{pi} + C_{sat}^{ant}$) is a measure of the carbon concentration that would have been present in the water at the surface were it at equilibrium with the overlying atmosphere. It is separated into a ‘preindustrial’ and ‘anthropogenic’ component to account for the changing levels of atmospheric CO₂ since the industrial revolution. The preindustrial saturated component, C_{sat}^{pi} , was determined from temperature, salinity and an approximation of the pre-formed alkalinity, silicate and phosphate (see below). It was evaluated using the CO2SYS Matlab program (van

Heuven *et al.*, 2009) assuming a preindustrial atmospheric CO_2 level of 278 ppm. We do not attempt to evaluate the anthropogenic saturated component directly, but instead gather it into a residual C_{res} along with the disequilibrium component, ΔC , which accounts for the extent to which the water parcel was not at equilibrium with the overlying atmosphere when it left the surface ocean.

Preformed nutrients were approximated as the difference between observed and regenerated values, where the latter was estimated from the apparent oxygen utilisation using stoichiometric ratios for silicate and phosphate to oxygen of 15 : -170 and 1 : -170 respectively (Anderson and Sarmiento, 1994). Apparent oxygen utilisation was derived from an estimate of the preformed oxygen concentration ($AOU = \text{O}_2 - \text{O}_{2,pre}$), which is a function of potential temperature and salinity. We assume 100% saturation of oxygen in the surface ocean. Preformed alkalinity is estimated from salinity, using its close-to-linear relationship with alkalinity in the surface ocean (Figure 5.3).

The regenerated components comprise contributions from the remineralisation of soft tissue organic matter, C_{soft} , and the dissolution of the hard shell carbonates, C_{carb} . The remineralisation of organic carbon utilises oxygen. Hence, the soft tissue component is established from apparent oxygen utilisation, using an oxygen to carbon ratio of 117 : -170 (Anderson and Sarmiento, 1994). The dissolution of carbonates releases alkalinity and dissolved inorganic carbon in a 2 : 1 ratio. Thus, the dissolved carbonate contribution can be established from the difference between the measured alkalinity and its preformed value, as well as an additional term associated with regenerated nitrate (using AOU and a stoichiometric ratio of 16 : -170). The additional term corrects for the fact that alkalinity is also released, in the form of nitrate, from the remineralisation of organic matter.

This carbon framework is a widely used diagnostic tool for understanding the operation of the oceanic carbon cycle (*e.g.* Ito and Follows, 2005; Kwon *et al.*, 2011; Lauderdale *et al.*, 2012). Nevertheless, there are substantial uncertainties in its implementation. These exist primarily in the estimation of regenerated carbon and nutrients, both in the necessity to assume a level of oxygen saturation (Ito

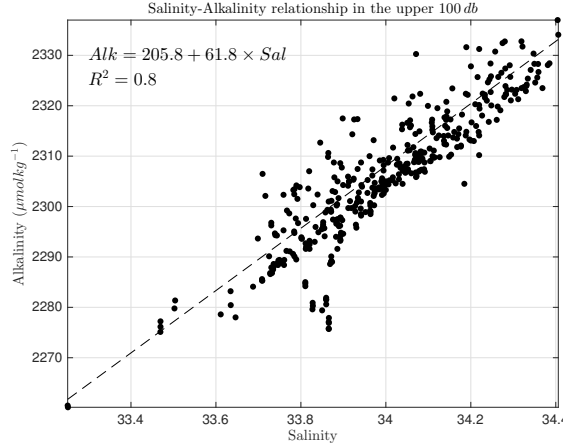


Figure 5.3: Scatter plot of the alkalinity and salinity collected in the upper 100 m across the hydrographic sections. The dashed line shows the result of a linear regression, used to derive an expression for preformed alkalinity.

et al., 2004) and in the prescription of fixed stoichiometric ratios (Giddy *et al.*, 2012). In addition, the salinity-alkalinity relationship in the surface ocean can vary widely (Fry *et al.*, 2015). We adopt the simplest approximations possible (100% oxygen saturation, standard stoichiometric ratios, and the local salinity-alkalinity relationship), accepting that there could be quantitative differences in the results if other values were used.

5.2.4 Uncertainties

For layer-wise and full-depth volume and carbon transport uncertainties, we use the same values as Jullion *et al.* (2014) and Brown *et al.* (2015). These were determined using Monte Carlo simulations of the inversion-derived velocity field and carbon concentration section. Reference velocities for the inversion were perturbed based on 5-day variability of the velocity field in the Southern Ocean State Estimate. Carbon concentrations were perturbed within measurement uncertainty (Brown *et al.*, 2015). By far the largest source of uncertainty comes from the volume transport (Brown *et al.*, 2015), and we use this fact to approximate uncertainties for carbon transports due to the overturning and horizontal circulation. For the overturning, we use the same uncertainty as for the total carbon transport for each layer and the full depth transport. We divide this uncertainty by the area-weighted

mean carbon concentration in each layer to derive an approximation of the layer-wise volume transport uncertainty. We approximate the uncertainty for the horizontal transport as this volume transport uncertainty multiplied by the variance of the carbon concentration anomaly in each layer. This approach is applied to transports of the total carbon concentration and the components of the carbon framework.

5.3 Physical and biogeochemical setting

The Weddell Gyre is a large, wind-driven, cyclonic gyre located to the south of the Atlantic sector of the Southern Ocean, spanning the region to the east of the Antarctic peninsula (Figure 5.2). The gyre is bounded to the north by the South Scotia Ridge and ACC, and to the south by the Antarctic continent. To the southwest, and along the Antarctic peninsula, the west Antarctic ice sheet terminates in the ocean, forming extensive ice shelves. Offshore winds in these regions support continuous ice production, and the resultant brine rejection, along with surface cooling, leads to the formation of AABW (Gill, 1973; Nicholls *et al.*, 2009). The region plays a central role within the polar Southern Ocean in the formation and northward export of AABW, and the closure of the lower limb of the global overturning circulation (Orsi *et al.*, 1999; Naveira Garabato *et al.*, 2002; Jullion *et al.*, 2014).

From hydrographic sections and moorings that enclose the Weddell Gyre (Figure 5.4a), (Jullion *et al.*, 2014) approximated the circulation in the region using a box inversion. The horizontal and vertical components of this circulation are shown in Figures 5.4b and c. The horizontal circulation, presented as the cumulative sum of transports moving clockwise around the box (and displayed such that upwards implies export from the region), is dominated by the cyclonic gyre, with a volume transport of $40 - 50 Sv$ ($1 Sv = 10^6 m^3 s^{-1}$). Jullion *et al.* (2014) identified a large throughflow ($13 \pm 4 Sv$), with water entering the region primarily in the Antarctic Slope Front (ASF; Figure 5.2) next to the Antarctic continent (station pairs 110-123), and exits to the north between station pairs 50 and 75. The ACC crosses the north east corner of the box, between station pairs 80 and 100. In the vertical, the

box is divided up into 10 layers, defined by neutral density (Jackett and McDougall, 1997), representing the major water masses in the area. For simplicity, we collect these layers into three major watermasses: surface water (SW, $\gamma^n < 27.7$, layers 1 – 2), which includes the mixed layer at the time of measurement and the mixed layer in the previous winter; Circumpolar Deep Water (CDW, $\gamma^n = 28$ to 28.27 kgm^{-3} , layers 3 – 5); Antarctic Bottom Water (AABW, $\gamma^n > 28.27$, layers 6-10), which, in the figures, is further separated into a lighter and denser class. The circulation consists of a dual overturning cell, with water imported in CDW and the upper two layers of AABW and exported within both the surface waters and deep waters. The upper cell ($2 \pm 2 \text{ Sv}$) is the result of Ekman upwelling in the centre of the cyclonic gyre. The lower cell ($8 \pm 2 \text{ Sv}$) is the result of water mass transformation in the ice shelf regions to the southwest.

What is the impact of this circulation pattern on the regional carbon cycle? Circumpolar Deep Water imported into the region is rich in dissolved inorganic carbon (C_T ; Figure 5.4d, e). The fate of this water mass, along with the biogeochemical interactions in the region, will determine whether this carbon is outgassed to the atmosphere or sequestered in the deep ocean. A variety of methods, including calculation of atmosphere-ocean CO_2 differences (Bakker *et al.*, 2008), vertical chemical mass balance (Hoppema *et al.*, 1999; Hoppema, 2004b) and lateral budget estimates (Brown *et al.*, 2015), have found that the Weddell Gyre is a present day CO_2 sink. The study Brown *et al.* (2015) combined the velocity field of Jullion *et al.* (2014) with the coincident measurements of C_T described in Section 5.2.1. They found a transport of C_T of $-53 \pm 10 \text{ TgCyr}^{-1}$ out of the Weddell Gyre region, resulting in an air-sea CO_2 uptake up $58 \pm 10 \text{ TgCyr}^{-1}$ (having accounted for dissolved inorganic carbon storage within the box) and validated this number against two further independent methods. Advancing this approach, we can probe a deeper understanding of what sets the export of carbon from the Weddell Gyre. In particular, we assess the relative contributions to this export from the overturning and horizontal circulation.

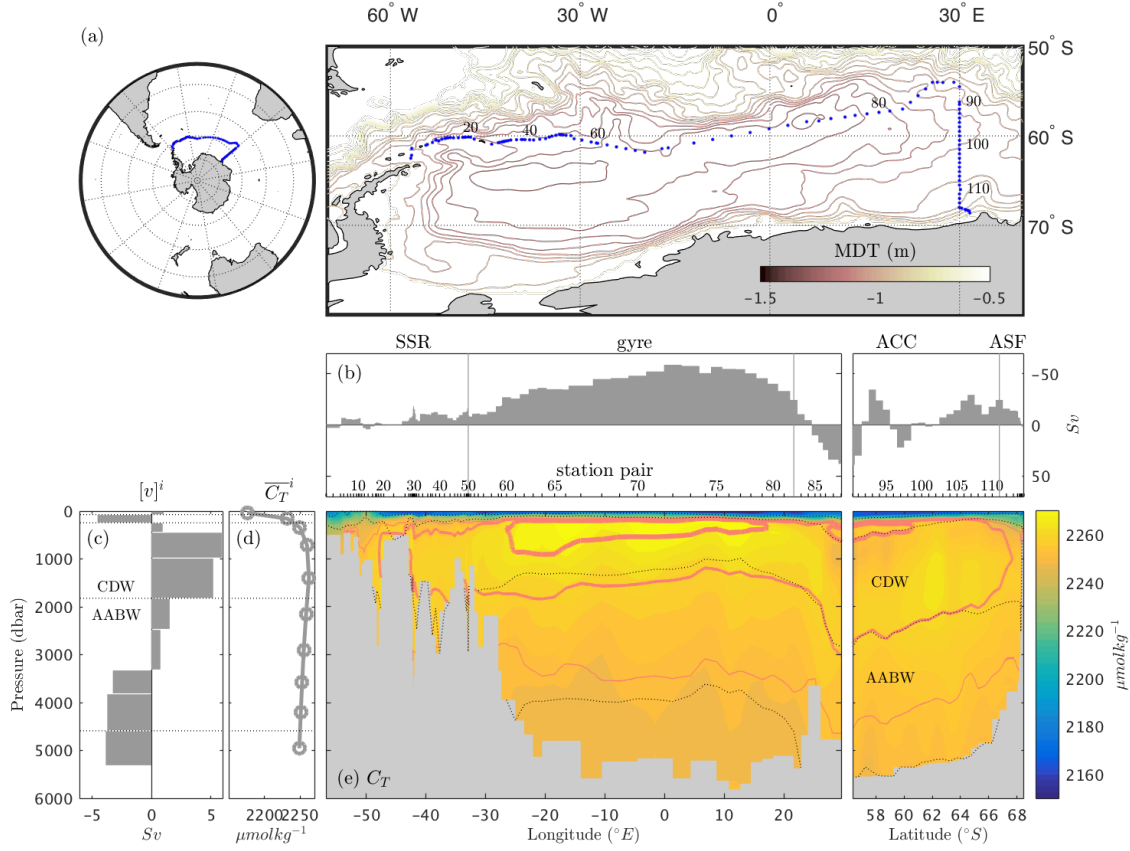


Figure 5.4: Circulation and dissolved inorganic carbon in the Weddell Sea. (a) The horizontal circulation of the Weddell Sea. Mass transports for each station pair are integrated from left to right. Note the reversed direction of the y-axis, such that export is upwards. (b) The overturning circulation in the Weddell Sea, in neutral density layers. Bars correspond to the mass transport in each layer ($[v\rho]^i$). The centre location and thickness of each bar corresponds to the mean depth and thickness of that layer. Horizontal dotted lines denote the interfaces between major water masses. (c) The area-weighted mean carbon concentration in each layer ($\overline{C_T}^i$). (d) The carbon concentration, C_T , around the Weddell Sea. As for (b) and (c) dotted lines denote the interfaces between the major water masses. Grey contours correspond to the 80, 90 and 100 $\mu\text{mol kg}^{-1}$ concentrations of the remineralised organic matter component (C_{soft}) of the carbon framework (see 5.2.3), with thicker contours denoting larger concentrations.

5.4 Results

5.4.1 Separating overturning and horizontal carbon transports

A qualitative look at the vertical profiles of mass transport and carbon concentration (Figure 5.4c, d) indicates immediately that the overturning circulation should be a source of carbon to the Weddell Gyre region. Concentrations of C_T in the imported

CDW and upper AABW exceed those in the exported water both in the surface ocean and deep ocean, in the lower layers of AABW. This vertical perspective indicates that the overturning circulation imports C_T to the region and is therefore a source of CO_2 to the atmosphere. A similarly straightforward picture for the horizontal circulation is less obvious. However, in CDW layers in particular, the C_T concentration of imported water in the Antarctic Slope Front is low relative to that of water exported across the northern rim. This would support an export of carbon from the box, associated with the horizontal through-flow. A qualitative perspective, therefore, suggests that the transport of carbon across the boundaries of the Weddell Gyre could result from a balance between carbon imported by the overturning circulation and exported by the horizontal circulation.

Following Bryden and Imawaki (2001), who applied the approach to oceanic heat budgets, the mass flux, layer thickness, and carbon concentrations across the boundaries of the Weddell Gyre can be written as the sum of the temporal (t) and along-section (x) average value within each neutral density layer (n) and the deviation from this average:

$$\begin{aligned} v\rho &= \overline{v\rho}^{x,t}(n) + (v\rho)'(x, n, t) \\ h &= \overline{h}^{x,t}(n) + h'(x, n, t) \\ C_T &= \overline{C_T}^{x,t}(n) + C'_T(x, n, t), \end{aligned} \tag{5.2}$$

where v is velocity, ρ is *in situ* density and h is layer thickness. Overbars denote temporal and along-section area-weighted means in each layer and primes denote deviations. Then the total carbon transport across the section can be written as

$$T_C = \sum_{i=1}^{10} [v\rho h C_T]^i = \underbrace{\sum_{i=1}^{10} [\overline{v\rho} \overline{h} + (v\rho)' h']^i \overline{C_T}(i)}_{T_C^o} + \underbrace{\sum_{i=1}^{10} [(v\rho h)' C'_T]^i}_{T_C^h}, \tag{5.3}$$

where square brackets denote the along-section integrated value within layer i , and we have dropped the overbar superscripts for clarity. The first term on the right hand side is the overturning component, T_C^o , being the product of the mass transport and the mean carbon concentration in each layer. This term includes contributions

both from time- and along-section average mass transports ($\overline{v\rho h}$), and ‘bolus’ mass transports ($((v\rho)'h')$) that arise from temporal and along-section correlations between the mass flux and layer thickness. As noted in Section 5.2.2, the temporal component of the bolus mass flux was evaluated as part of the inverse model solution and is included in our calculations. Inclusion of the along-section component is implicit in the integration. Within each neutral density layer, the contribution of the bolus mass flux to the total carbon transport is small relative to the time and along-section mean transport due to large time-mean mass fluxes (Jullion *et al.*, 2014). However, in the full summation, the carbon transport associated with the bolus mass flux is of leading-order importance, as noted by (Brown *et al.*, 2015). The second term, evaluated as the residual of the total transport and the overturning component, arises from the correlation between the mass flux and the carbon concentration within each layer. We call this the horizontal component, T_C^h . Note that this component is not strictly ‘horizontal’ (that is, aligned with pressure surfaces), since neutral density layers can vary in depth across the section, but we use the term for simplicity.

The total carbon transport, along with the overturning and horizontal components, are shown in Figure 5.5. Being associated with large mass transports, T_C and T_C^o are large within each layer, and differences between the two are barely visible. However, in the mass-conserved full-depth transport, the difference becomes apparent. The overturning circulation imports $18 \pm 10 \text{ TgCyr}^{-1}$ to the region and is a source of CO_2 to the atmosphere, as the vertical profiles of carbon concentration and mass transport suggest. This import of carbon by the overturning circulation leaves the total full-depth export of $-53 \pm 10 \text{ TgCyr}^{-1}$ to be achieved by the horizontal transport, which consequently exports $-72 \pm 4 \text{ TgCyr}^{-1}$ from the Weddell Gyre. In the vertical profile of T_C^h , it is clear that a large fraction of this export is achieved in CDW layers, with further smaller contributions in the surface water and upper AABW layers.

The horizontal transport arises from correlations between mass transport and carbon concentration within each layer (equation 5.3). For the export of carbon seen in Figure 5.5, C_T in imported water must be anomalously low, while C_T in exported

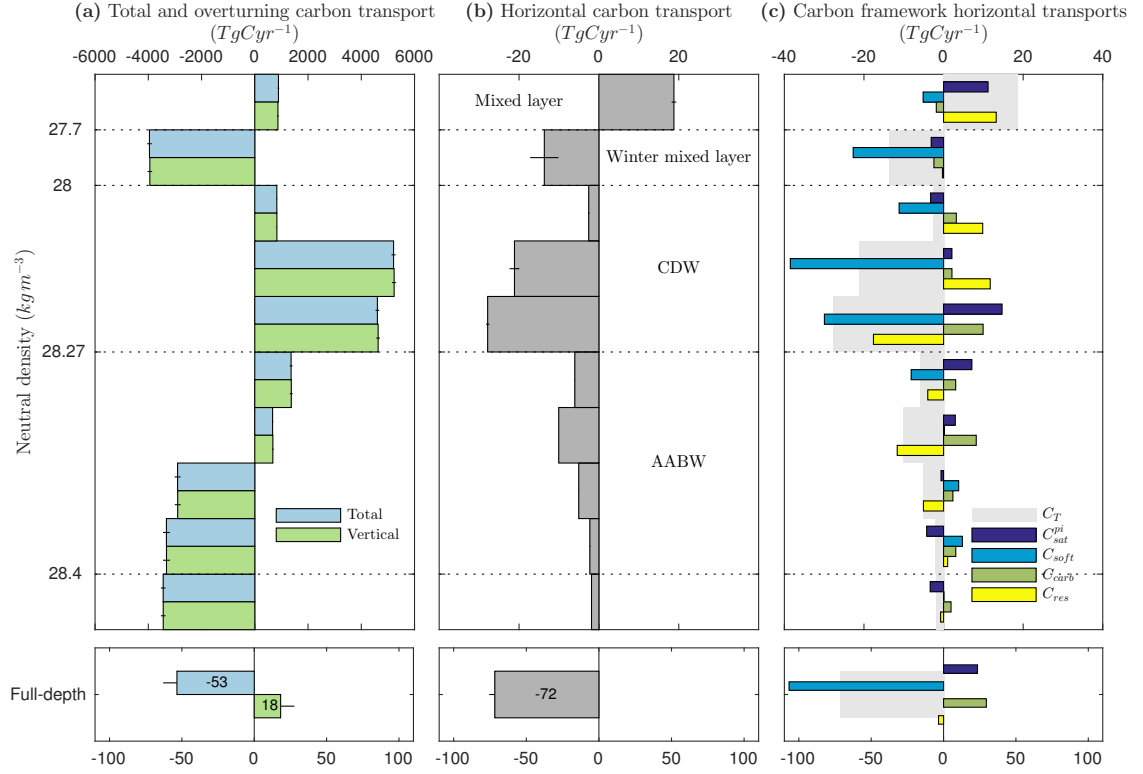


Figure 5.5: Total, overturning and horizontal transports of carbon from the Weddell Sea. (a) The total transport of carbon in the Weddell Sea by (blue) and the component achieved by the overturning component of the circulation (green), for each layer (top panel) and summed throughout the full depth (bottom panel). Positive values denote transport into the region, while negative values denote transport out of the region. Full-depth transports include export of carbon in sea-ice, assuming a sea-ice carbon concentration of $600\ TgC\ yr^{-1}$. (b) The horizontal transport of carbon in the Weddell Sea, for each layer (top panel) and summed over the full depth (bottom panel). (c) The residual transport of carbon (grey bars; same as in panel b) broken down into contributions from each component of the carbon framework, for each layer (top panel) and summed over the full depth (bottom panel). Note for all panels, the different scales of the x -axes between the layer-wise and the full-depth transports. All of the full depth transports have the same scale.

water must be anomalously high. These correlations may exist over a range of horizontal scales, from adjacent station pairs importing and exporting low and high carbon concentrations respectively, to the gyre scale, with carbon concentrations correlated with the broad horizontal circulation pattern. Our qualitative perspective, observing that the carbon content of water imported in the Antarctic Slope Front is low relative to water exported to the north, suggests that the large-scale correlations dominate the horizontal transport.

We can consider this more closely by evaluating the transport of the carbon

anomaly ($C'_T = C_T - \overline{C_T}^i$) within each layer (Figure 5.6). Non-zero carbon anomaly transports highlight the regions that contribute to the horizontal component of total carbon transport since, for example, export of high C_T water and import of low C_T water have the same sign in terms of C'_T transport. Consistent with the figure of horizontal mass transport (Figure 5.4b), the carbon anomaly transport is presented as a cumulative sum of transports moving clockwise around the box, and the y -axis is reversed such that upwards implies export. In the CDW layers, major regions of carbon anomaly export coincide with mass export across the northern rim and import in the Antarctic Slope Front. This strongly supports the suggestion that the horizontal component of total carbon transport is associated with the throughflow of the large-scale circulation.

Further contributions to the transport of carbon anomalies appear across the South Scotia Ridge and around the stations coincident with the crossing of the ACC. The former is associated with discrete jumps, particularly in the winter mixed layer and CDW, suggesting that it is related to complex flow pattern in the narrow channels of this region (Jullion *et al.*, 2014), and could result from uncertainty in the interpolation of carbon concentration from discrete measurements. Across the ACC there is net import in CDW and export within the winter mixed layer. The compensatory nature of these transports points toward a possible discrepancy in the neutral surface definition in this region (Jackett and McDougall, 1997). There is a distinct dip in the neutral density surface in this region. Subsequent analysis of the carbon framework (Figure 5.8) implies that this dip does not entirely follow chemical signatures across the ACC, with a possible interpretation being that the neutral density surface does not accurately capture the direction of adiabatic flow across this region. If winter mixed layer water is incorrectly ascribed to CDW, this would explain the compensatory transports. There are similar changes in the upper levels of AABW across the ACC but with no net effect. In both the winter mixed layer and the upper layers of AABW, much of the export is achieved across the meridional section, mostly in the region of Antarctic Slope Front.

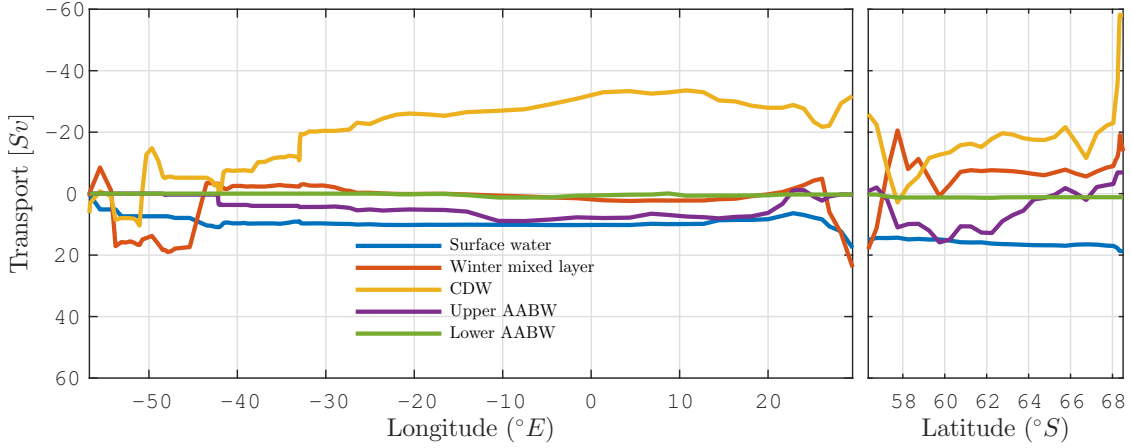


Figure 5.6: Depth integrated transport of the carbon anomaly ($C'_T = C_T - \overline{C_T}^i$) in different water masses. The transport is shown as a cumulative sum clockwise around the bounding sections, *i.e.* from left to right. Note that the direction of the y-axis is reversed so that upward implies export from the region.

In Figure 5.7, we consider more closely the horizontal transport in the lower two layers of CDW, which dominate the carbon export, by plotting the carbon anomaly and mass flux anomaly separately, along with the cumulative sum of their product. The figure reinforces much of what was noted for CDW in Figure 5.6. In particular there is a small export of carbon across the gyre circulation in both layers (largest for lower layer), which results from the outward flux of water with anomalously high carbon concentration. Contrastingly, export of carbon at the Antarctic Slope Front results from the inward flux of low carbon water. Across the South Scotia Ridge (SSR), alternating flow leads to a relatively large net export of carbon in both layers, being particularly pronounced in the upper layer. This export results predominantly from the inward flux of low carbon water across only one or two station pairs. There are substantial changes in the anomalous carbon concentration within both layers across the ACC, leading to a non-zero net transports across this region, in spite of the imposed no net volume flux across this section in the inversion (Section 5.2.2). The compensatory nature of carbon transports between the upper and lower layers across the ACC, with a net import of carbon in the upper layer partially cancelled out by export in the lower layer, again suggests that this may be an artefact of the neutral density definitions in this region.

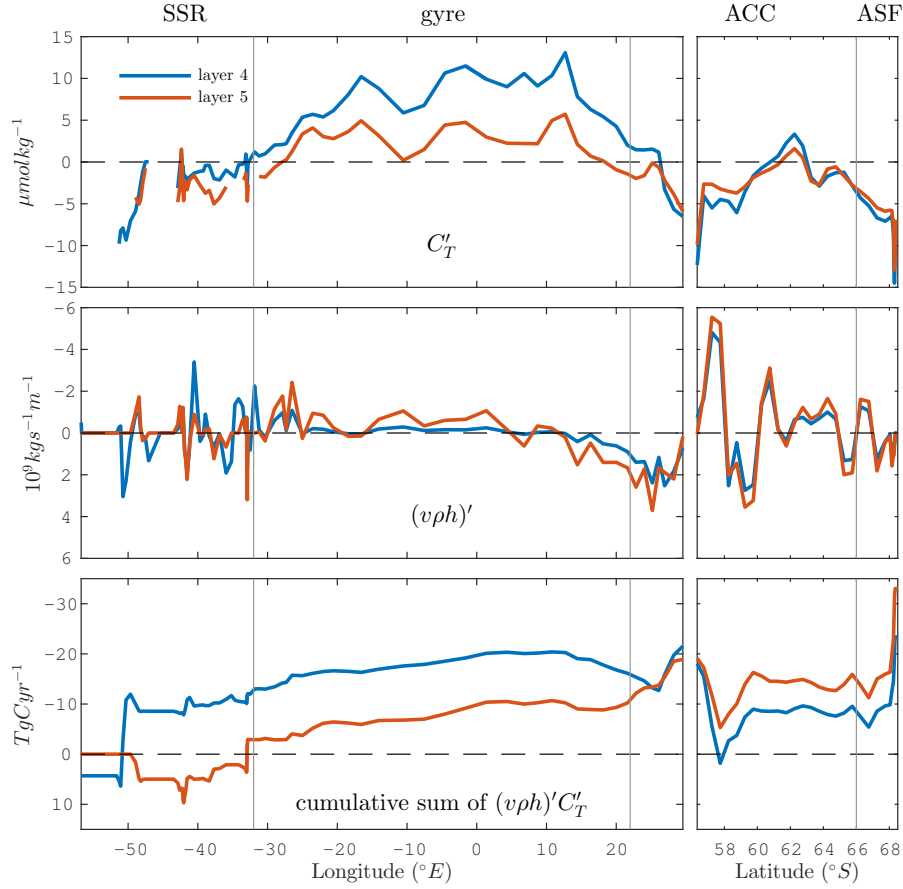


Figure 5.7: (top) Carbon anomaly, (b) mass flux anomaly, and (c) cumulative sum (summing from left to right) of the carbon anomaly transport, for the lower two layers of CDW. Vertical grey lines delineate circulation features of interest, including flow across the South Scotia Ridge (SSR), the gyre circulation, the Antarctic Circumpolar Current (ACC), and Antarctic Slope Front. Note that in the bottom two panels, the direction of the y-axis is reversed so that upward implies export from the region.

5.4.2 The role of biology in carbon uptake

We have shown that the transport of carbon out of the Weddell Gyre is predominantly the result of export by the horizontal circulation in CDW. This is due to the difference in C_T between water entering in the Antarctic Slope Front and exiting across the northern rim. This begs the question: what causes the carbon concentration to increase between the time that it enters and exits the Weddell Gyre?

We can address this question through the use of a carbon framework (Williams and Follows, 2011; MacGilchrist *et al.*, 2014), through which we attribute carbon concentrations to various physical and biogeochemical processes that have estab-

lished them. The components of the carbon framework are shown in Figure 5.8. Of these, only remineralised carbon C_{soft} shows a pattern consistent that of total carbon in CDW, with low concentrations in the Antarctic Slope Front, and high concentrations across the northern rim. There is some evidence of this pattern in dissolved carbonates, C_{carb} , but the signal is much smaller ($\sim 5 \mu\text{mol kg}^{-1}$ difference relative to $\sim 20 \mu\text{mol kg}^{-1}$ for C_{soft}). The coincidence of the patterns in C_{soft} and C_T is exemplified in Figure 5.4, in which contours of C_{soft} at 80, 90 and $100 \mu\text{mol kg}^{-1}$, with respectively increasing thickness, are overlaid on the distribution of C_T . Agreement between the spatial distributions indicates that elevated C_T in CDW across the northern rim relative to the Antarctic Slope Front is due to the additional presence of remineralised organic matter.

This pool of biologically-enriched carbon concentration in CDW has been consistently observed in the centre of the Weddell Gyre and is given the name Central Intermediate Water (Whitworth and Nowlin, 1987; Orsi *et al.*, 1993; Hoppema *et al.*, 2002). It is enriched with C_{soft} by open ocean biological production which exports organic matter beneath the surface layers (Hoppema, 2004b). The remineralisation of this organic matter occurs at relatively shallow depths (Fischer *et al.*, 2000; Usbeck *et al.*, 2002), meaning that the carbon is suspended within the CDW layer. Hoppema (2004b) identified that the lateral transport of this water out of the Weddell Gyre was a significant contributor to global deep ocean carbon sequestration.

With the enrichment of C_T set by the addition of remineralised C_{soft} , the horizontal export of carbon in the CDW should be accounted for by the export of C_{soft} (MacGilchrist *et al.*, 2014). We apply the overturning-horizontal separation to each constituent of the carbon framework, and the horizontal component, T_C^h , is shown in Figure 5.5c. The export of carbon in the CDW layers is indeed due to the export of C_{soft} . Export in these layers dominates the overall transport, with a transport of $-107 \pm 9 \text{ TgCyr}^{-1}$ of C_{soft} balanced by an import of preformed carbon (C_{sat}^{pi} ; $23 \pm 1 \text{ TgCyr}^{-1}$) and dissolved carbonates (C_{carb} ; $30 \pm 1 \text{ TgCyr}^{-1}$).

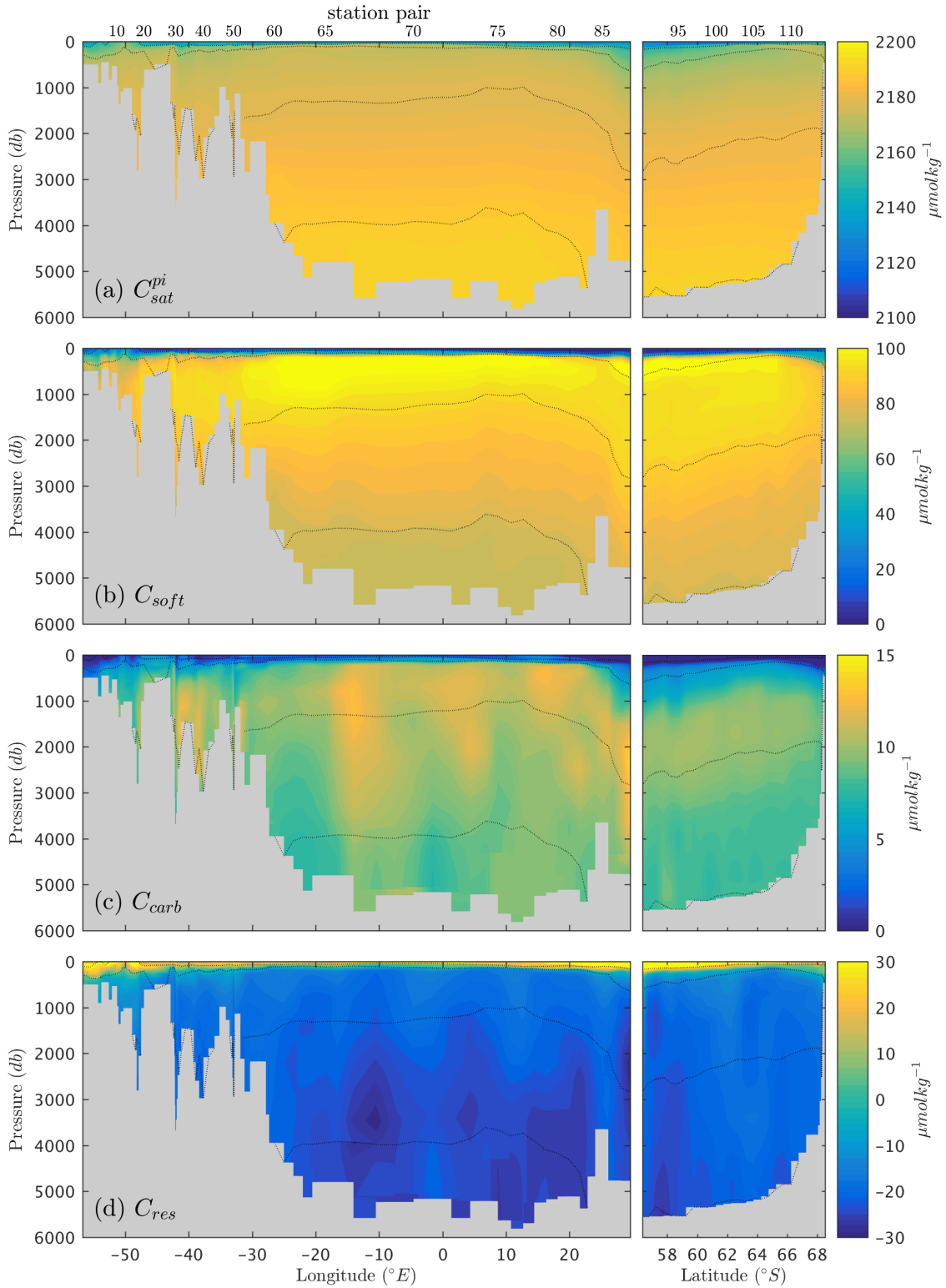


Figure 5.8: Concentrations around the hydrographic sections of the constituents of the carbon framework: (a) pre-industrial saturated carbon (C_{sat}^{pi}), (b) remineralised soft tissue carbon (C_{soft}), (c) dissolved carbonates (C_{carb}), and (d) residual carbon (C_{res}), including saturated anthropogenic carbon (C_{sat}^{ant}) and the disequilibrium component (ΔC). Dotted lines denote the interfaces between surface water, Circumpolar Deep Water and upper and lower layers of Antarctic Bottom Water.

5.4.3 Observations in the Ross Sea

Much of the horizontal circulation in the polar Southern Ocean is characterised by cyclonic gyres similar to the Weddell Gyre, including the Ross and Kerguelen Gyres (Park and Gambroni, 1995; Gouretski, 1999; Dellnitz *et al.*, 2009). It stands to reason that the mechanism of carbon export associated with the horizontal circulation could also be playing a leading-order role in these regions. (Hoppema, 2004b) speculated that this could be the case in the Ross Gyre, since observations suggest relatively shallow organic matter remineralisation (Nelson *et al.*, 1996), similar to that in the Weddell Sea, with the possibility that it leads to local enrichment of CDW.

In Figure 5.9, we show C_T and oxygen (O_2) measurements, made in 2011, along hydrographic sections around the outer edge of the Ross Gyre and through the centre of the region (Millero *et al.*, 2013). Mid-depth concentrations of C_T do not show the same elevated signal as in the Weddell Gyre, either around the boundary, or in the central region. As such, it is not possible to make any qualitative arguments for the overturning and horizontal carbon transports, as was possible for the Weddell Gyre, without knowing the specific details of the regional circulation. We note though that there is a minimum in O_2 between ~ 100 and 1000 m , suggesting the presence of older waters and the likelihood of elevated C_{soft} . In light of this, the relative depth invariance of C_T is somewhat surprising, since it must be sustained by a source of carbon to the deep waters that is not due to respiration. An obvious candidate for this source is anthropogenic carbon, and indeed Sandrini *et al.* (2007) found relatively high concentrations in dense shelf waters in the Ross Gyre. On the other hand, in the shelf-slope region to the west (between stations 2 and 15) and to some extent at the shelf slope in the central region (stations 77 to 82), newly ventilated dense waters (as identified by the relatively high O_2 concentration) have a distinctly lower C_T concentration than the overlying water. This confounds the previous suggestion and rather indicates a C_T difference between CDW and AABW that is similar to that observed in the Weddell Gyre, implying a role for the regional overturning circulation as a source of carbon to the atmosphere.

Application of the carbon framework to the Ross Sea data may bring greater clarity to this issue, but has not yet been attempted.

Hoppema (2004a) note that even if the Weddell Gyre is the only region in which the horizontal circulation translates carbon into the deep ocean, it still represents a globally significant term in the deep ocean carbon budget. This argument is amplified in this study, which suggests around twice as much export in the CDW layers ($\sim 45 \text{ TgCyr}^{-1}$) than was estimated Hoppema (2004a) using mass balance arguments (19 TgCyr^{-1}). Nevertheless, the operation of the carbon cycle, and the potential for export by the horizontal circulation mechanism in the Ross Sea merits further investigation.

5.5 Discussion

A two-dimensional perspective places the overturning circulation and water mass transformations at the heart of the polar Southern Ocean carbon cycle (Figure 5.1). Consequently, studies on the role of the polar Southern Ocean in long timescale climate variability have uniquely focussed on carbon cycling within the context of the overturning circulation, particularly related to the formation of AABW (Sarmiento and Toggweiler, 1984; Stephens and Marshall, 2000; Ferrari *et al.*, 2014; Watson *et al.*, 2015), while observational campaigns have largely focussed on the shelf seas (Shadwick *et al.*, 2014). In contrast to this view, we have shown that for the present day sink of atmospheric carbon in the Weddell Gyre, the horizontal circulation plays a central role. Consistent with Hoppema (2004a), we found that the importance of the horizontal transport is established by the cyclonic gyre circulation coupled to open ocean biological production and export. The carbon cycle in the Weddell Gyre can thus be considered as a balance between overturning and horizontal components, with both components being of leading-order importance in establishing the region as a source or sink of atmospheric CO_2 . If a similar mechanism operates in the other cyclonic gyres of the polar Southern Ocean (for which present evidence is inconclusive; Section 5.4.3), this suggests a broad reframing

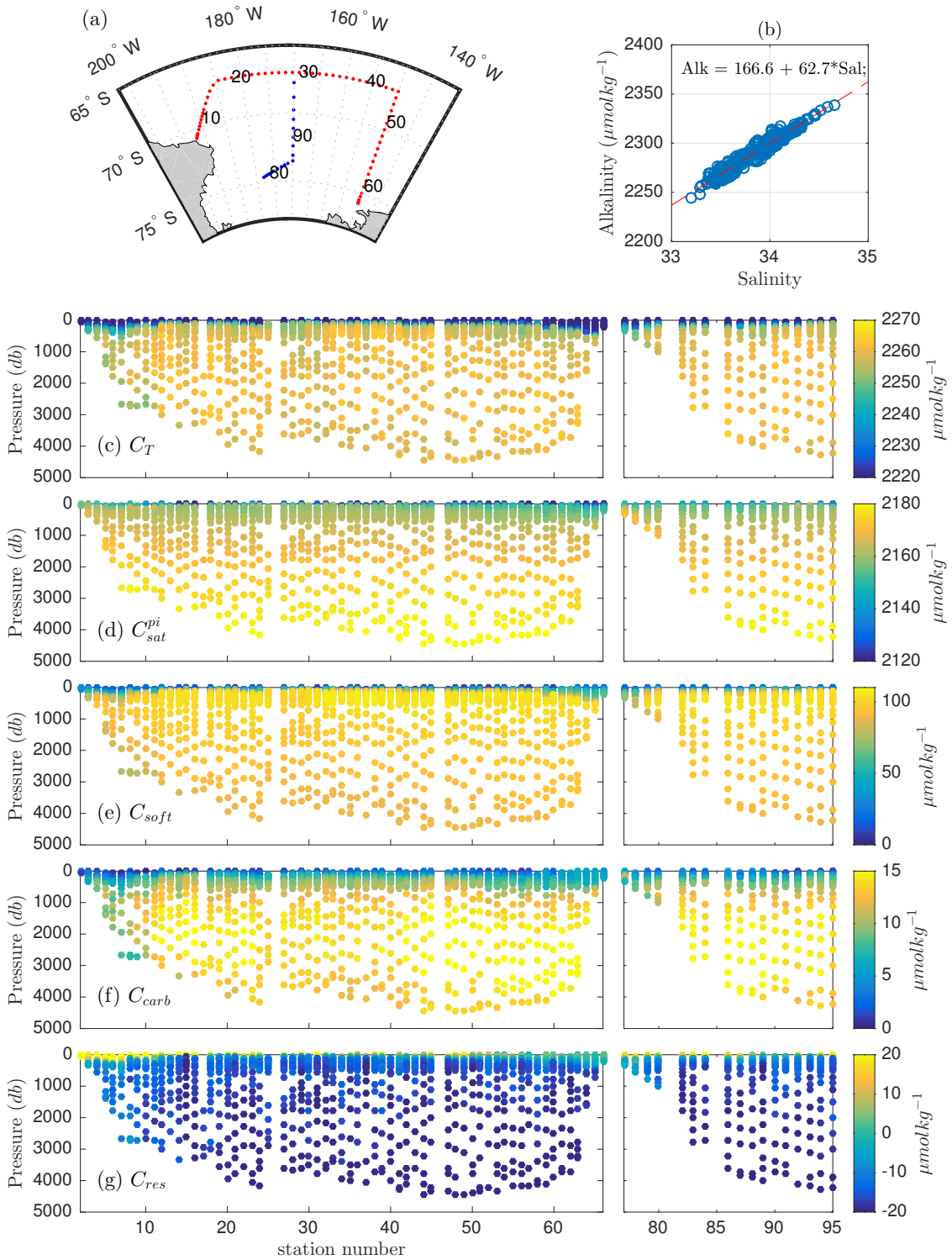


Figure 5.9: (map) Location of hydrographic sections around and through the Ross Gyre, along with station numbers that correspond to those of the figures below. Sections of (a) dissolved inorganic carbon, C_T , and (b) dissolved oxygen, O_2 . The sections show the distribution of measured data only, with no interpolation. The section on the left (station numbers 2 to 66) goes around the outside of the Ross Gyre (red dots in the map), and the section on the right (station numbers 77 to 95) goes through the gyre centre, towards the continental shelf (blue dots in the map).

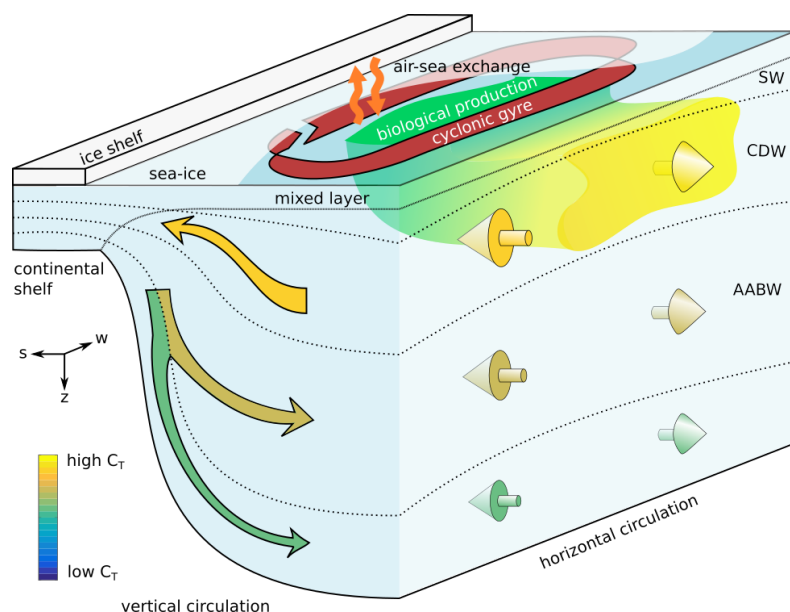


Figure 5.10: Schematic illustration of the polar Southern Ocean carbon cycle, extended to include a role for the horizontal circulation and enrichment of outflowing water by open ocean biological production and remineralisation. Dotted lines delineate Surface Water (SW), Circumpolar Deep Water (CDW), and upper and lower layers of Antarctic Bottom Water (AABW).

of the conceptual framework of the polar Southern Ocean carbon cycle. We outline this new framework in a revised schematic in Figure 5.10.

In the present day, transport of carbon by the horizontal circulation is related to its accumulation and export in CDW (Figure 5.5). The enrichment of carbon within this layer is thought to be due to the shallow remineralisation of organic detritus originating from open ocean biological production (Usbeck *et al.*, 2002; Hoppema *et al.*, 2002; Hoppema, 2004a). Consequently, the magnitude of the horizontal carbon sink is set by the open ocean export production, together with the remineralisation profile, and the residence time of water in the central Weddell Gyre (Hoppema, 2004a) with this, in turn, dependent on surface momentum fluxes. This means that the parameters of importance for the horizontal component are substantially distinct from that of the overturning component, which rather include rates of dense water formation, residence time of water in the shelf seas and the relative timing of sea-ice retreat and biological activity (Shadwick *et al.*, 2014; Hauri *et al.*, 2015). Consequently, the two components are likely to respond quite

differently to system changes.

The operation of the overturning circulation as a present-day source of CO₂ to the atmosphere (Figure 5.5) is established by the difference in area-weighted mean C_T between incoming CDW and outgoing AABW (Figure 5.4c). The difference is small, being on the order of only a few $\mu\text{mol kg}^{-1}$. Mechanisms by which this difference might be eroded or enhanced are the basis for many arguments on the role of AABW in long-timescale atmospheric CO₂ variability (Sigman *et al.*, 2010). One such mechanism would be the uptake of carbon released to the atmosphere during the industrial age, so-called anthropogenic carbon, in bottom waters. In the absence of other changes to the system, the human-induced increase in atmospheric CO₂ inhibits outgassing and favours air-to-sea gas-exchange. Recent work has found enrichment of recently ventilated AABW with anthropogenic carbon (van Heuven *et al.*, 2011; Shadwick *et al.*, 2014). We do not explicitly calculate anthropogenic carbon concentration in the carbon framework and the distribution of C_{res} does not give any qualitative impression of its presence in AABW. This could be because anthropogenic carbon is not yet present at the boundaries of the Weddell Gyre in concentrations greater than the uncertainty of the carbon framework, or because a large negative disequilibrium (ΔC) dominates the signal. Nevertheless, it is plausible that continued accumulation of anthropogenic carbon in AABW, in the absence of other regional changes, will result in the overturning circulation acting as a net sink of CO₂ from the atmosphere, in addition to the horizontal sink.

6

Conclusions

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The uptake and storage of climatically important substances, such as heat and carbon, is arguably the most important role of the ocean in the climate system. Ventilation — the subduction and spreading of water, along with its properties, from the surface mixed layer into the ocean interior — is at the heart of this process. While ocean ventilation has been observed and considered important for decades, the governing mechanisms remain poorly understood. As with many oceanographic processes, understanding is inhibited by a scarcity of observations and the difficulty of representation in numerical simulations.

The aim of this thesis is to contribute understanding to some of the outstanding questions around the ventilation processes. Specifically, we address questions pertaining to mechanisms and pathways of spreading, the representation and evaluation of ventilation in numerical ocean circulation models, and mechanisms establishing variability in ventilation. Our analysis has focussed on numerical simulations, adopting a predominantly Lagrangian approach, complemented with

some Eulerian diagnostics. Here, we summarise the analysis, main results and their implications for each chapter in turn. Subsequently, we address some of the questions left open in this work and points towards areas of further research.

6.1 Summary

The thesis is introduced with a critical assessment of the representation of water mass transport by Lagrangian trajectory calculation in numerical ocean circulation models, specifically in relation to diapycnal motion. The difficulty in controlling levels of mixing in numerical simulations (Griffies *et al.*, 2000b) means that mass transport in the model could be more diapycnal than that expected in the ocean. On the other hand, potential for errors in Lagrangian trajectory calculation could lead to the evaluated pathways being more diapycnal than mass transport in the model. We considered this problem through a series of experiments in which we traced the density along trajectories in two eddy-permitting models, comparing changes to what would be expected in the ocean, and exploring several potential causes.

In a hindcast simulation, we found that particles in the ocean subsurface on the whole change density by an amount that exceeds our expectations based on a scaling analysis. These changes have a systematic structure both in terms of the density classes in which they emerge, and in their horizontal spatial distribution, which is concentrated along bathymetry and in energetic regions. Analysis of a subdomain of a similar numerical model revealed that the use of time-average velocity fields in trajectory calculations could be a source of spurious diapycnal motion, particularly in the upper ocean. In the deep ocean, we found that the parameterisation of vertical mixing, with elevated levels close to bathymetry, explains a component of the observed density changes.

The results of Chapter 2 highlight the difficulty in sustaining low levels of mixing in oceanic mass transports both during their numerical simulation and their subsequent assessment. The sensitivity of Lagrangian pathways to time-averaging of velocity fields in particular carries implications for the fidelity of offline trajectory analysis (as well as that of tracer transports by solving of the

advection-diffusion equation), as simulated flows become increasingly energetic and non-linear. On the other hand, the clear impact of mixing on the pathways and timescales of ventilation (with implications simulating ocean storage of climatically-relevant quantities, particularly in deep ocean water masses) emphasises the need to ensure realistic parameterisations of mixing processes and negligible levels of numerical mixing, as well as for observations that will clarify what constitutes an ‘appropriate level’ of modelled mixing.

The impact of the ocean’s turbulent nature on the ventilation pathways of the subtropical thermocline was considered in Chapter 3. Mesoscale eddies are ubiquitous in the ocean (Chelton *et al.*, 2011; Ferrari and Wunsch, 2009) and likely play an important role in the spreading of tracers in the subsurface (Kamenkovich *et al.*, 2017), but their importance in this respect is unknown and difficult to quantify (Mecking *et al.*, 2004; Booth and Kamenkovich, 2008). We adopt a dynamical systems approach to this problem, defining a non-dimensional ‘filamentation number’ that quantifies the reduction in the width of filaments of a ventilated fluid parcel (from the ratio of the ventilation timescale and the time-mean strain along the trajectory), thereby characterising the chaotic nature of ventilation pathways.

We showed that the filamentation number is large ($\gg 1$) across three density surfaces in the thermocline of the subtropical North Atlantic in a $1/4^\circ$ numerical ocean circulation model, suggesting highly chaotic ventilation pathways. Lagrangian mapping from the density surfaces to surface mixed layer properties (year and longitude of subduction) allowed us to directly resolve filament widths in the subsurface and establish that the filamentation number does indeed capture their spatial variability.

A dynamical system approach provides novel perspective on the role played by the turbulent ocean circulation in ventilation. The short timescale of mesoscale strain, by comparison to that of ventilation, results in substantial filamentation and chaotic trajectories within a short distance of density surface outcrops. Implications for the spreading of tracers in the subsurface, and the retention of subducted tracer gradients, depend on the relative spatial scales of tracer gradients compared to

that of mesoscale stirring. Further investigation along dynamical systems lines, including seeking a quantitative relationship between the filamentation number and the distribution of passive tracers, could lead to a deeper understanding of the role of turbulence in ocean ventilation.

In Chapter 4, we assess the mechanisms and variability of ventilation of the deep North Atlantic Ocean. Ventilation of intermediate and deep waters in the subpolar North Atlantic, and variability therein, is thought to have substantial climatic importance, through the uptake and storage of heat and carbon dioxide in the ocean (Sabine *et al.*, 2004; Levitus *et al.*, 2012). By connecting the deep waters of the subsurface Atlantic with their properties at subduction (*e.g.* time, location and depth of subduction) via non-diffused (purely advective) Lagrangian trajectories in a numerical simulation, we explore the processes contributing to their formation and variability.

In the model, almost all of the North Atlantic Deep Water (NADW) was last in the surface mixed layer in the Labrador Sea, with the majority of this within or shoreward of the Deep Western Boundary Current. Subduction in the boundary, forming light and intermediate density NADW, was found to reflect the shallowing of the winter mixed layer along the path of the barotropic stream function in a time-mean sense. Ventilation of NADW showed substantial variability on inter-annual to multi-annual (3-5 year) timescales, reflected in the anomalous age distribution in the subsurface. We found that the longer timescales of variability reflected that of surface-forced dense water formation, while shorter timescales were set by inter-annual variations in re-entrainment.

The role of Stommel’s demon in setting the properties of the ocean interior on an annual basis is well known (Williams *et al.*, 1995). Our results show that, at least in the high-latitude North Atlantic, variability in its effectiveness can play a role in setting the properties on inter-annual timescales as well. It may be that the Labrador Sea is a region where the signal of this variability is particularly pronounced, with intermittent deep convection and the potential for rapid export

in the boundary currents both exerting a control on the demon's operation and effectiveness from year to year.

In Chapter 5, we explore how the interplay between circulation and biogeochemistry establishes carbon uptake in the Weddell Gyre. Perspectives of the carbon cycle in the Weddell Gyre (and wider polar Southern Ocean) — thought to be critical in mediating contemporary (van Heuven *et al.*, 2011) and historical (Sigman *et al.*, 2010) levels of atmospheric carbon dioxide — have historically adopted a two-dimensional view, focussed predominantly on regional water mass transformations and deep ocean ventilation (Stephens and Keeling, 2000; Watson *et al.*, 2014). We decompose carbon transports, derived using measurements of dissolved inorganic carbon and a mass-balanced, box-inversion velocity field, into overturning and horizontal components (Bryden and Imawaki, 2001; Pickart and Spall, 2007) and explore their relative role, along with that of biological processes, in exporting carbon from the region.

Decomposition of the carbon transport into overturning and horizontal components showed that, in contrast to a two-dimensional perspective, both terms play a leading-order role in the carbon cycle of the Weddell Gyre. We showed that the operation of the Weddell Gyre as a present-day sink of atmospheric carbon dioxide ($-58 \pm 10 \text{ TgCyr}^{-1}$) is established by a balance between an overturning source ($18 \pm 10 \text{ TgCyr}^{-1}$) and a horizontal sink ($-72 \pm 4 \text{ TgCyr}^{-1}$). Using a framework to attribute carbon concentrations to their physical and biogeochemical origins, we show that the sink of carbon associated with the horizontal circulation is predominantly due to the enrichment of exported Circumpolar Deep Waters with remineralised organic matter. Following Hoppema (2004b), we argue that this enrichment is due to the shallow remineralisation of open ocean biological production. Further work is required to establish whether, and to what extent, the horizontal sink operates in the other cyclonic gyres of the polar Southern Ocean.

Based on our results, we propose augmenting the overturning-centric paradigm of the polar Southern Ocean carbon cycle to include the horizontal circulation and open ocean biological production and export. In this frame, the system will

exhibit different sensitivities to external forcing, with implications for the role of the polar Southern Ocean in past and future climate change. Investigation of idealised models that include the important parameters of the horizontal transport may help to elucidate these sensitivities.

6.2 Outstanding questions and further analysis

The results presented in this thesis have opened up many avenues for further analysis. In addition, the Lagrangian methodology adopted here for the North Atlantic can be applied to explore related questions in other important and interest regions of the global ocean. In concluding this thesis, we present some preliminary results along these lines.

A longer timescale analysis of NADW formation

The results of Chapter 4, concerning mechanisms establishing variability in the ventilation of NADW, would benefit from analysis over a longer timescale. We present preliminary results from investigation of the control simulation of the U.K. Met Office fully coupled atmosphere-ocean-sea-ice-land climate model, GC2 (Williams *et al.*, 2015a). The ocean core of this model is same as that used in Chapter 4, in a configuration described in Megann *et al.* (2014). It has the same horizontal and vertical resolution and numerics as that of Chapter 4. The control simulation is 375 years long and output is saved as monthly-means.

Results are presented from an experiment in which particles were initialised on a neutral density *surface* (rather than volume) at $\gamma^n = 27.8 \text{ kgm}^{-3}$. In this coupled simulation, the deep North Atlantic has altogether lower densities than in the hindcast simulation, such that this surface is close to the centre of the southward flowing NADW in this simulation. Particles were initialised on this surface during March, every 5 years for the last 100 years of the simulation. As in Chapter 4, particles were run backwards-in-time until they reached the surface mixed layer, defined as being within a density of 0.01 kgm^{-3} of the density at 10 m depth.

We present figures pertaining to the three main components of the analysis in Chapter 4, namely the locations of ventilation, the pathways of ventilation and the variability in the age inventory in the subsurface. Figure 6.1 shows the locations where water was subducted from the surface mixed layer, presented as a fraction of the total number of ventilated particles (note that in this preliminary analysis we have not weighted particles based on the area they represent on the density surface, as was done with volume in Chapter 4). The pattern is notably distinct from that of the NADW volume in the hindcast simulation (Figure 4.7). In particular, there is a complete absence of ventilation around the western boundary. On the other hand, the pattern in the open ocean Labrador Sea, increasing to the north east, and the absence of GIN seas water are consistent with the results of Chapter 4. The difference could be because we are looking at a specific surface, one that is not ventilated around the boundary current region. However, we note that this pattern of high-latitude ventilation, particularly the absence of ventilation in the boundary current, persists in experiments for different density surfaces, although more comprehensive analysis is required. It could be the case that the coupled nature of this simulation leads to a markedly distinct pattern of surface forcing, and/or sea-ice extent, around this boundary region, which inhibit the formation of the deep mixed layers that develop in the hindcast simulation. Investigation of the regional wintertime mixed layer depth, surface buoyancy forcing, sea-ice extent and the local circulation will help to elucidate the mechanisms establishing this ventilation pattern.

Spreading pathways and timescales (Figure 6.2) show broad consistency with the known pathways of Labrador Sea Water, as in Chapter 4. Given the consistency of the ocean model configuration, this is perhaps not surprising. Ventilation to the east of the mid-Atlantic ridge, discussed at length in Chapter 4, shows a similar pattern as in the hindcast. We see, however, that the region west of Portugal is ventilated on timescales of between 100 and 200 years, presumably by eddy mixing across the potential vorticity front, or direct ventilation from the Mediterranean Sea. On the other hand, the poorly ventilated region to the west of North Africa persists even after 375-years, although there is evidence of some ventilation over this

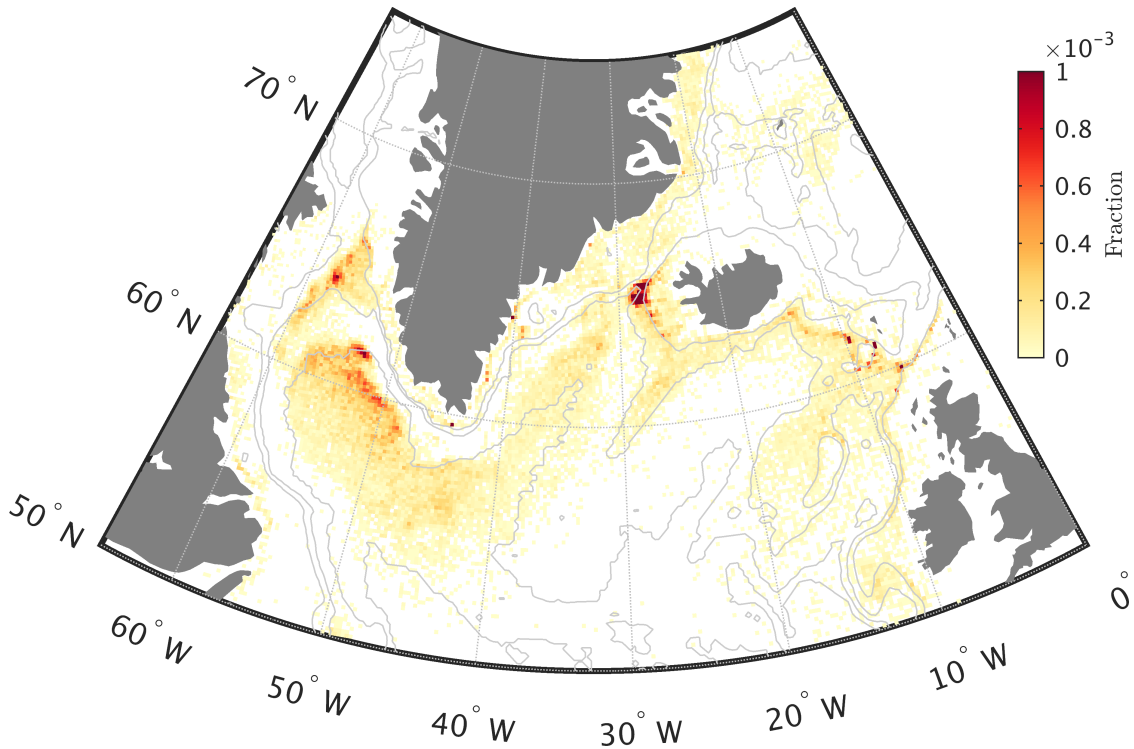


Figure 6.1: The fraction of the ventilated particles that left the mixed layer at each model grid cell. Bathymetric contours at $z = 509, 1516, 2956$ and 3898 m are shown in light grey.

timescale. This supports the case that a persistent meridional asymmetry exists in the ventilation of the deep subtropical North Atlantic ocean, that may be established by bathymetric steering (or lack thereof from 30°N) with a further role for the Mediterranean outflow. On the other hand, this long simulation reveals that a similar region of poorly ventilated water also exists in the Southern hemisphere subtropics.

In Figure 6.3, we show the time-mean age distribution (top panel; distribution evaluated every 5 years for last 100 years of simulation) and normalised anomaly for the age distribution in the final year of the simulation (bottom panel). In the mean distribution, we note that a substantial decrease in volume occurs over the first 10 years, which may correspond to the erosion of GIN seas water. As was noted for the hindcast simulation, there appears to be a combination of multi-year to decadal timescales, with prolonged periods of higher or lower anomalies, as well as substantial inter-annual variability. It is interesting to note that negative anomalies are more common and seemingly more persistent, while positive anomalies are often

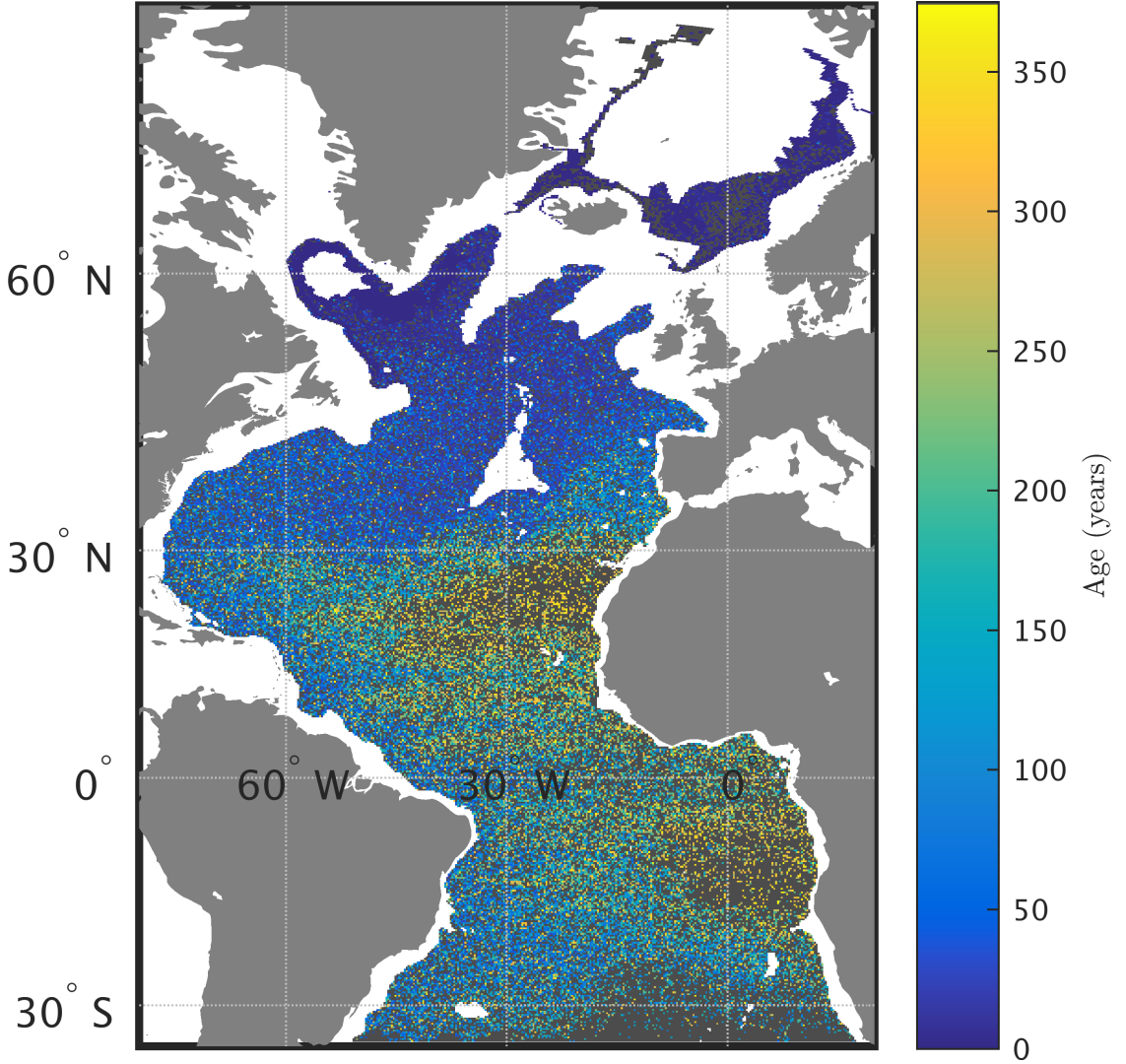


Figure 6.2: Age of particles initialised on $\gamma^n = 27.8 \text{ kgm}^{-3}$ in the final year of the coupled numerical simulation. Dark grey regions were unventilated during the simulation.

more extreme. The persistence of low anomalies could be indicative of prolonged periods without deep convection, while the positive extremes could indicate the sharpening effect of Stommel's demon following periods of persistent deep convection (as observed during the 1990s in Chapter 4). More comprehensive analysis, including the initialisation of particles in subsequent years throughout the simulation, and the evaluation of surface-forced water mass transformation, will facilitate better understanding of what establishes these timescales.

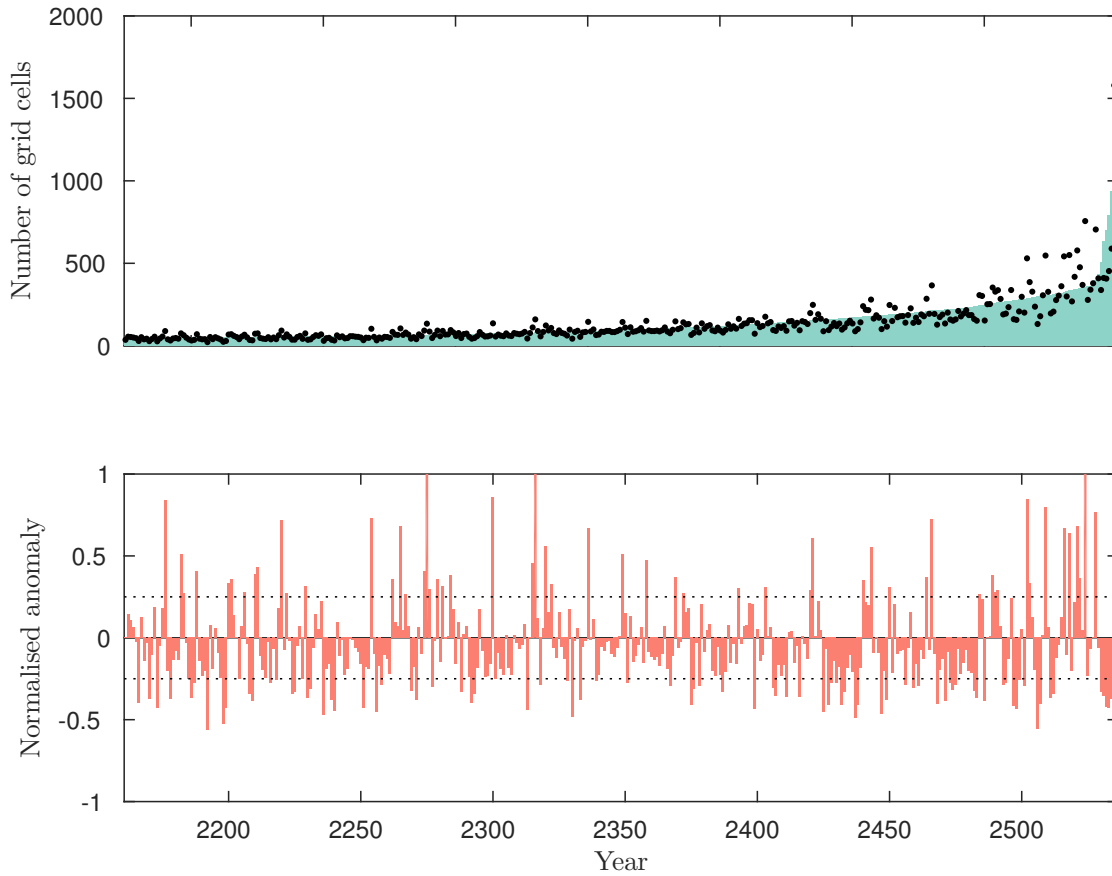


Figure 6.3: (top panel) Time-mean age distribution on $\gamma^n = 27.8 \text{ kgm}^{-3}$, evaluated by averaging the age distributions every 5 years for the last 100 years of the simulation. Black dots correspond to the age distribution in the final year of the simulation. (bottom panel) Anomaly in the age distribution, calculated as the distribution in the final model year minus the time-mean age distribution, normalised by the time-mean age distribution. Horizontal dotted lines correspond to ± 0.25 .

The inter-annual variability of volume storage in the high-latitude North Atlantic

It is increasingly well-established that high-latitude buoyancy forcing impacts the Atlantic meridional overturning circulation at subtropical latitudes on decadal timescales and longer (Bjastoch *et al.*, 2008; McCarthy *et al.*, 2015; Pillar *et al.*, 2016). The mechanisms of this connection are poorly understood but numerical simulations suggest it is related to the propagation of density anomalies along the western boundary (Johnson and Marshall, 2002; Getzlaff *et al.*, 2005; Zhang, 2010). On the other hand, buoyancy forcing at high latitudes exhibits substantial seasonal to inter-annual variability. This was noted in Chapter 4, when we introduced the

concept of surface-forced water mass transformation (Figure 4.35), and indeed we found that some of the signature of this variability was retained in the subsurface water mass inventory. In investigating the connection between high-latitude surface forcing and the overturning circulation, therefore, it is intuitive to question why none of the short-timescale variability is translated between the two.

The relationship between surface buoyancy forcing and the overturning circulation can be considered in terms of the water mass formation framework (Walin, 1982), shown schematically in Figure 6.4. Mass balance dictates that water transformed across an isopycnal, G (established by surface and interior buoyancy fluxes; see Section 4.2.4), can contribute either to the overturning circulation in latitude-density coordinates, ψ_γ , or to a local change in the volume of water denser than that isopycnal, $\partial V/\partial t$. We can write this as:

$$G(\gamma^n, \phi) = \frac{\partial V}{\partial t}(\gamma^n, \phi) - \psi_\gamma(\gamma^n, \phi). \quad (6.1)$$

As noted in Section 4.2.4, G can be separated into contributions from surface forcing, F , and from interior mixing, $\partial \mathcal{D}_{in}/\partial \gamma$. We evaluate separately the terms in equation 6.1 across the North Atlantic in the hindcast simulation used in Chapter 4, for $\gamma^n = 27.85 \text{ kg m}^{-3}$ and $\phi = 40^\circ \text{N}$, and calculating only the surface-forced component of G . Note that, as in Chapter 4, we evaluate the transformation for potential density referenced to the surface, and assign it to the appropriate, corresponding neutral density class.

In this frame, the absence of high-frequency (seasonal to inter-annual) variability shared between high-latitude surface buoyancy forcing, G , and overturning circulation, ψ_γ , must be due to absorption of the signal into either volume storage or subsurface mixing (or both). This latter point is an intriguing possibility, namely that when a greater volume of water is formed by buoyancy forcing, more is eroded by interior mixing before being exported further south. We do not explore this further at this stage. Instead we focus on the variability in volume storage.

Variability in volume storage is straightforward in relation to the seasonal cycle (Figure 6.5), since it relates to the migration of surface outcrops and the generation

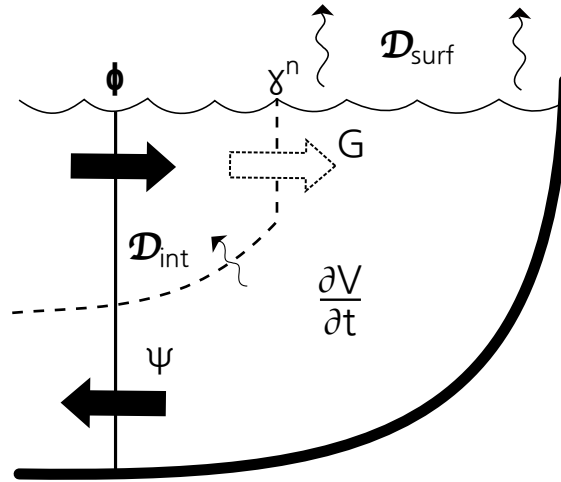


Figure 6.4: Schematic representation of the water mass formation framework, showing mass balance between water mass transformation, G , volume storage rate, $\partial V/\partial t$, and the overturning circulation, ψ_γ . Water mass transformation is set by the diapycnal derivatives of surface, $\mathcal{D}_{surf}$ and interior $\mathcal{D}_{int}$.

of a seasonal pycnocline. As water is made more dense by surface forcing from September, the isopycnal outcrop migrates southward, leaving more water to the north and resulting in positive $\partial V/\partial t$. The sign reverses in late March when the migration back northward begins. The residual of F and $\partial V/\partial t$ (yellow line) is due to steady southward export by the overturning circulation and by interior mixing. Note that the tracking of the surface forcing and changing volume storage is imperfect, such that there is remnant seasonality and shorter timescale variations in the residual. The variability is shared by the overturning circulation (purple line). It could be indicative of temporal variability in mixing, but is more likely to be related to the imperfect manner in which we assign transformation to neutral density classes (see Section 4.2.4), such that transformation and storage are not perfectly aligned. Furthermore, we note that the difference in the absolute magnitude between the residual and the overturning, 10 to 15 Sv , is larger than we would expect from an interior mixing contribution (Nurser *et al.*, 1999). This merits further investigation to ensure that we are closing the budget accurately.

In Figure 6.6 we show the variability in the annual transformation, volume storage rate and overturning circulation over the full simulation. We can see clearly that F and $\partial V/\partial t$ covary on inter-annual, and indeed longer, timescales. Consequently,

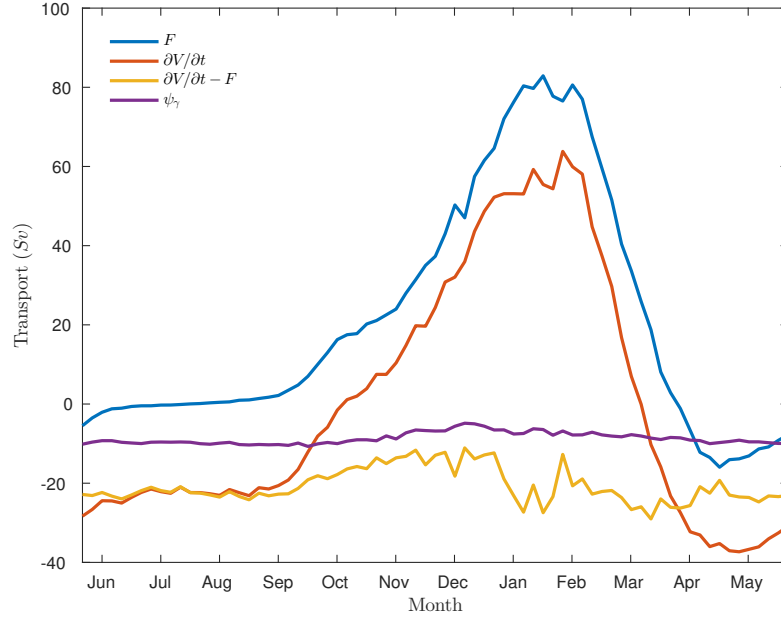


Figure 6.5: Seasonal climatology (presented from June to June) of the terms in the water mass formation framework (equation 6.1) for $\gamma^n = 27.85 \text{ kg m}^{-3}$ and $\phi = 40^\circ \text{ N}$, evaluated over the full model simulation. Terms include surface-forced water mass transformation (F ; blue) volume storage rate ($\partial V/\partial t$; red), their difference (yellow) and the overturning circulation (ψ_γ ; purple).

their residual (yellow line) has much reduced short-timescale variability, and a multi-decadal variation that matches, to some extent, the overturning circulation. We note that volume transport across the northern boundary of the domain is approximately $1 \pm 1 \text{ Sv}$ during this time period. Short timescale variations in transformation and volume storage do not match up perfectly, particularly in years such as 1975, meaning that there is still a substantial amount of short timescale variability in the residual that is not reflected in the overturning circulation. As for the seasonal cycle, this could be related to uncertainty in the potential to neutral density relation. We note, however, that the discrepancy is magnified in the early, spin-up years of the model, which could have a large effect on the mass balance (Lee *et al.*, 2001). Irrespective, Figure 6.6 supports the hypothesis that much of the inter-annual and multi-annual variability in water mass transformation goes into volume storage at high-latitudes, and therefore does not contribute to the large-scale overturning circulation.

We note that the relationship between F and $\partial V/\partial t$ is less clear in other density

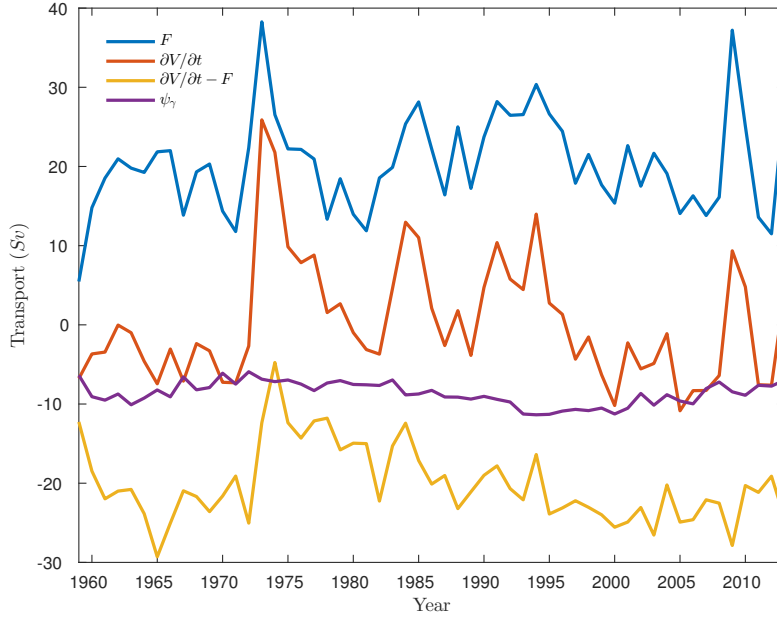


Figure 6.6: Variability over the model simulation of the annual average (January to December) of terms in the water mass formation framework (equation 6.1) for $\gamma^n = 27.85 \text{ kgm}^{-3}$ and $\phi = 40^\circ \text{N}$, evaluated over the full model simulation. Terms include surface-forced water mass transformation (F ; blue) volume storage rate ($\partial V/\partial t$; red), their difference (yellow) and the overturning circulation (ψ_γ ; purple).

classes, suggesting an important water mass dependence. That the relationship holds for $\gamma^n = 27.85 \text{ kgm}^{-3}$ makes sense in the context of work that has identified substantial recirculation and slow, diffusive pathways for Labrador Sea Water in the subpolar gyre (Lavender *et al.*, 2000; Bower *et al.*, 2009), as well as long timescales of exchange between the ocean interior and boundary currents (Straneo, 2006), resulting in relatively little variability in the export of this water to the subtropics (Zou and Lozier, 2016).

Further consideration of this problem in a water mass formation framework will allow us to establish where storage occurs, through annual undulations in the upper interface of a deep ocean volume, with the potential to discern why anomalies do not propagate southward. In particular, matching up of inter-annual anomalies in subsurface storage with anomalies in the spatial distribution of surface-forced transformation maps (Brambilla *et al.*, 2008; Maze *et al.*, 2009), derived by rearrangement of the Walin (1982) formulation, will allow us to establish where anomalies are generated, where they move to, and where they are eroded. In

the hindcast simulation used here, this is likely to be focussed around the annual occurrence of deep convection in the Labrador Sea. Perhaps more interestingly, however, such an approach could be readily applied to observations, utilising buoyancy fluxes from atmospheric reanalyses (bearing in mind caveats on their reliability, *e.g.* Renfrew *et al.*, 2002) and subsurface hydrography from Argo floats and other high-resolution measurements. Importantly, only the upper interface of the density volume need be resolved, without any need to determine the full-depth stratification.

Global thermocline ventilation: a two-headed demon

Williams *et al.* (1995) investigated the operation of Stommel’s demon in the subtropical North Atlantic ocean. Using an idealised age tracer in numerical simulations, they showed that, due to the seasonal migration of density surface outcrops, only water subducted from the mixed layer in late winter (March and April) penetrates into the permanent thermocline.

In the Southern Hemisphere, the seasonality is reversed, such that the deepest mixed layers occur in September and October. It follows therefore, that water from both March/April and September/October should alternately enter the permanent thermocline during the annual cycle. On the other hand, it is not obvious that Stommel’s demon will operate in the same manner in the Southern Hemisphere, particularly for density surfaces that outcrop in the Southern Ocean, where substantial mesoscale eddy activity and a strong zonal flow could affect the mechanisms and timing of subduction from the mixed layer (Sallée *et al.*, 2010; Kwon, 2013).

Using the same Lagrangian approach as has been adopted throughout this thesis, we consider the operation of Stommel’s demon across the entire global ocean. Figure 6.7 shows the depth-median month of ventilation for particles initialised in September, 2015, at tracer points throughout a neutral density range corresponding to the mid-to-lower thermocline. The use of advective Lagrangian trajectories means that months are not diffused, as was the case in the tracer calculations of Williams

et al. (1995). It is for a similar reason that we take the median in depth rather than the mean, since the latter could lead to spurious months (*e.g.* for example, the mean of March and September subduction would suggest ventilation in June). Note that since the purpose is to consider the month of ventilation rather than the absolute age, the median is taken over ventilated particles only, meaning that unventilated regions are less extensive — if any particle in the volume is ventilated then the grid cell will be shown ventilated. Consequently, regions such as the subtropical shadow zones appear ‘well-ventilated’, in contrast to the age distributions in Chapter 3. Note that the use of the month of ventilation is a purely model-derived diagnostic. We are not suggesting that one could measure this in the ocean and use it to identify a Northern or Southern Hemisphere source of thermocline water. Rather we simply use it to explore the operation of Stommel’s demon in the Southern Hemisphere, and the mixing of water in equatorial regions.

Across the Southern Hemisphere, water is seen to have left the mixed layer in September and October, suggesting that a demon does indeed operate within this density range. This results in a broad, hemispheric divide, with northern-sourced waters subducted in March and April and southern-sourced waters subducted in September and October. There are interesting, basin-dependent differences in what happens in equatorial regions, where waters from the two hemispheres meet. In the Pacific Ocean (particularly in the east) and northern Indian Ocean, a much broader range of months is present, with more water that was ventilated between June and August. It is likely that this is due to a longer period of local subduction, since the equatorial seasonality is less pronounced. However, it is notable that ventilation is still not year-round, with no water present that was ventilated between October and February. In the Atlantic basin, there is clear penetration of Southern Hemisphere water into the Northern Hemisphere, consistent with cross-equatorial mean flow (Kirchner *et al.*, 2009). Finally, in the Arctic Ocean there is a notably wide range of ventilation months, between January and May, suggesting a longer annual subduction period compared to other locations in the Northern Hemisphere, perhaps associated with sea-ice dynamics.

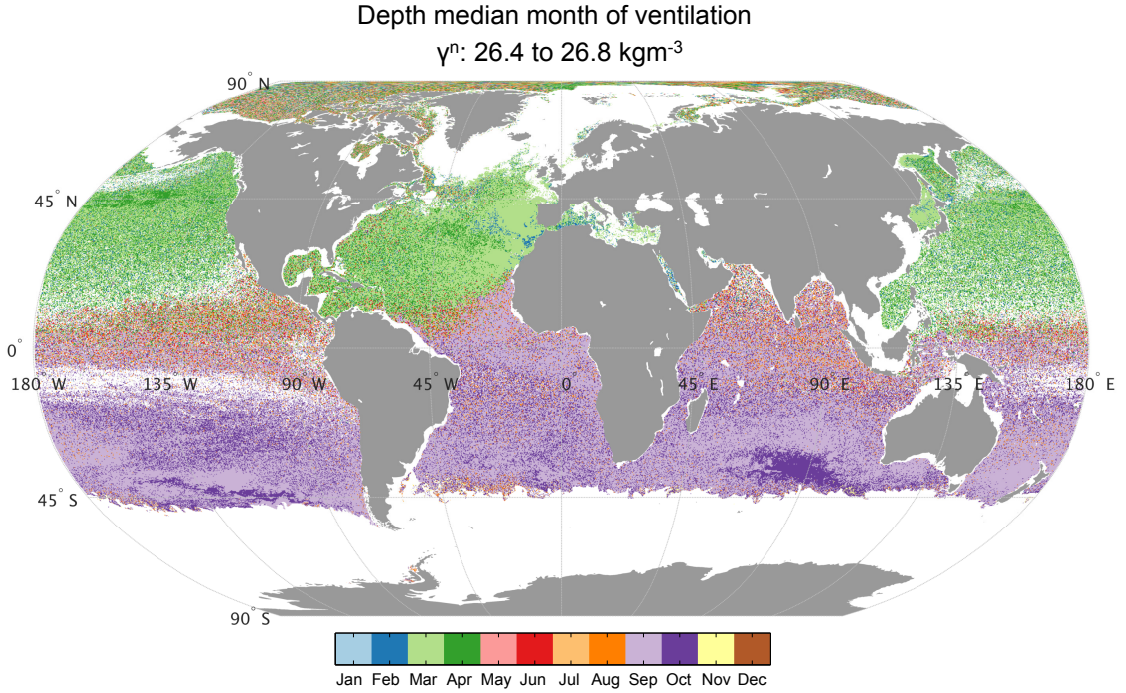


Figure 6.7: Depth median month of ventilation for particles initialised in September, 2015, between $\gamma^n = 26.4$ and 26.8 kgm^{-3} across the global ocean. White regions correspond to where the density range was not present in September, 2015, (northern and southern high latitudes and in coastal regions) and to regions that were not ventilated during the simulation.

Ventilation of the Southern Ocean

This thesis has focussed predominantly on the North Atlantic, using a Lagrangian approach to understand the mechanisms, pathways and variability of ventilation in subtropical and subpolar regions. The approach has proved useful both in exploring mechanisms and variability of ventilation, as well as assessing its representation in numerical simulations, by comparison to observations.

The Southern Ocean is a region of equal, if not greater, importance in the ventilation of intermediate and abyssal waters (Gebbie and Huybers, 2010). In addition, the Southern Ocean is the region where much of the deep water formed in the North Atlantic returns to the ocean surface (Liu and Huang, 2012; Talley, 2013), making it is a critical region for the two-way exchange between the atmosphere and the deep ocean. The importance of the region in this respect was highlighted in Chapter 5, when we investigated the role of the circulation in the operation of the

carbon cycle. Under greenhouse gas forcing, ventilation of the Southern Ocean, with associated heat and carbon exchange, is likely to play a central role in establishing the extent and timescale of future climate change (Sallée *et al.*, 2012; Bopp *et al.*, 2015)

For ventilation into the thermocline of the Southern Ocean, mesoscale eddies are thought to be crucial in both the subduction (Marshall, 1997; Sallée *et al.*, 2010; Kwon, 2013) and spreading (Jones *et al.*, 2016; Kamenkovich *et al.*, 2017) of water masses. Such is the role of eddies in the Southern Ocean, that it has been seen to operate against the direction of time-mean, upwelling flow in the centre of the Antarctic Circumpolar Current in a numerical simulation (Abernathey and Ferreira, 2015). A dynamical systems approach, applied to the subtropical North Atlantic in 3, could be used to assess the role of ocean turbulence in the region. In particular, there is substantial vertical structure in both ventilation timescales (Waugh *et al.*, 2013) and eddy energy (Klocker *et al.*, 2012) in the Southern Ocean, such that vertical variations in the filamentation number could prove insightful.

Ventilation into the abyssal ocean involves complex formation processes in the shelf seas around Antarctica, as well as gravity-driven overflows and entrainment during export (Nicholls *et al.*, 2009). Accurate representation of so-called Antarctic Bottom Water is therefore notoriously difficult in numerical simulations (Heuze *et al.*, 2013). The approach of Chapter 4 would be useful in assessing this.

In Figure 6.8, we present some preliminary results from a Lagrangian experiment in the Atlantic sector of the Southern Ocean. Using the same model simulation as in Chapters 3 and 4, we initialise particles in the deep ocean in late September, 2015, and run them backwards in time to the mixed layer (same definition as previously). In the top panel of Figure 6.8, we show the depth median ventilation month, averaged within the volume that we identified in Chapter 4 as North Atlantic Deep Water ($\gamma^n = 27.7$ to 28). The month of ventilation reveals (as a result of the two-headed demon) the southward penetration of water formed in the Northern Hemisphere along the western boundary, and a substantial zonal component to this flow at around $20^\circ S$. A strong signature of southward penetration stops at around $40^\circ S$, where mixing between Northern and Southern Hemisphere water

ensues. The northward spreading of Southern Hemisphere-sourced water is broadly zonally symmetric, with no clear advective pathway. This noisy, diffusive spreading is reminiscent of the deeper surfaces of the subtropical thermocline (Chapter 3, Figure 3.9), suggesting that it could be largely achieved by eddying processes. In the bottom panel of this figure, we show the zonal median ventilation month for all water denser than $\gamma^n = 27.7$. Northern Hemisphere-sourced water is again seen penetrating southward, along isopycnals (dashed white contours), between 2000 and 3000 m, and mixing with Southern Hemisphere water at the southern extent, between 40 and 50°S. Above and below this are northward penetrating waters of Southern Hemisphere origin. These preliminary results provide motivation that much can be learnt from adopting this Lagrangian approach in the Southern Ocean.

6.3 Concluding remarks

Observations in the last several decades have revealed widespread changes in the ocean content of oxygen (Stramma *et al.*, 2008; Schmidtke *et al.*, 2017), carbon (Sabine *et al.*, 2004; van Heuven *et al.*, 2011) and heat (Purkey and Johnson, 2010; Levitus *et al.*, 2012) in both the upper and deep ocean. Ventilation of water from the surface ocean into its interior is implicated as an important process in all three (Gruber, 2011). Understanding these changes and predicting their future evolution, therefore, depends on robust understanding of the physical processes involved in ventilation, their variability, and their propensity to change. The results of this thesis have served to emphasise the complexity of these components, both in the spatial and temporal scales involved, and their interaction with tracers that we are motivated to consider, such as carbon dioxide.

We have shown in the course of this thesis the benefits that can be derived from a Lagrangian perspective of ocean ventilation. Although there are substantial challenges, such an approach has enabled quantitative assessment of the processes involved in ocean ventilation, offering insight that could not have been gained from Eulerian diagnostics, or indeed diffusive tracers.

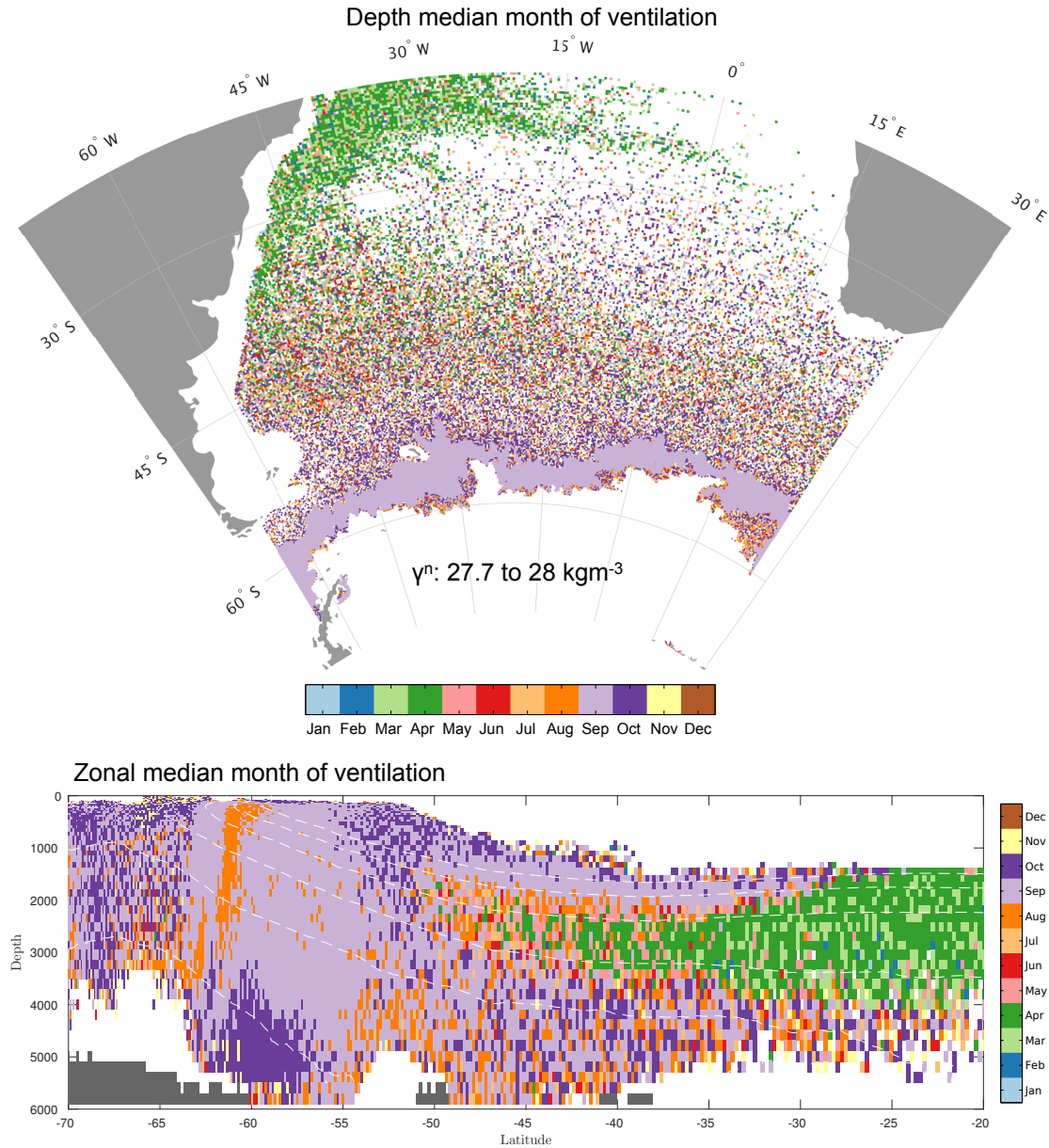


Figure 6.8: Median month of ventilation for particles initialised in September, 2015, in the Atlantic sector of the Southern Ocean. (top) Depth average between $\gamma^n = 27.7$ and 28 kgm^{-3} . (bottom) Zonal average for $\gamma^n > 27.7 \text{ kgm}^{-3}$. White regions correspond to where the density range was not present in September, 2015, (southern high latitudes and in coastal regions) and to regions that were not ventilated during the simulation.

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