Dynamic and Double-Diffusive Instabilities in a Weak Pycnocline. Part I: Observations of Heat Flux and Diffusivity in the Vicinity of Maud Rise, Weddell Sea

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ABSTRACT

An expedition to study the stability of the weakly stratified water column in the eastern Weddell Sea was undertaken in the austral winter of 2005. A regional CTD survey around Maud Rise delineated water mass boundaries associated with flow around the seamount and identified areas most susceptible to overturning. A downstream region of the seamount Taylor column was found least stable, with a potential density difference across the pycnocline less than 0.018 kg m\(^{-3}\). Intensive water column measurements, including 1300 profiles of temperature, conductivity, and fast-response microconductivity, were made during a series of 13 drift stations to investigate vertical turbulent transports and the evolution of water column stability. The dependence of pycnocline turbulent diffusivity \(k_T\) on Froude number \(F_r\) (turbulence generated by internal wave shear) and density ratio \(R_r\) (turbulence generated by diffusive layering and possibly diapycnal cabbeling) is investigated. The \(F_r\) alone cannot explain completely the observed \(k_T\) variability. Instead, there is also a strong dependence on \(R_r\). Turbulent diffusivity is an order of magnitude larger in the weakly stratified Taylor cap over Maud Rise (where \(R_r\) approaches one) than in the surrounding water column that is unaffected by flow around Maud Rise. In terms of water column stability, diffusive heat flux across the pycnocline inhibits winter ice growth and densification of the surface layer. The observed \(R_r\) dependence of \(k_T\) thus provides a strong negative feedback on the winter evolution of the Maud Rise area water column toward overturning instability.

1. Introduction

In the austral winter, the Weddell Sea water column is marginally stable. The intermittent occurrences (as observed during the satellite era) of large polynyas in the eastern Weddell are usually interpreted as signatures of deep, open-ocean convection ventilating the deep waters. Although there has been much interest, we do not yet have a firm understanding of the processes and perturbations that control the intermittency of the climatically significant polynyas and convection in this area.

This paper is the first in a two-part study on turbulent diffusion in the winter Weddell Sea pycnocline near the Maud Rise seamount, a 200-km diameter seamount that rises from the 5000-m-deep abyssal plain to within 1800 m of the sea surface (Fig. 1). In late winter, the water column is expected to be the least stable as the result of salt rejection during sea ice growth. Here, we use field observations from the Maud Rise Nonlinear Equation of State Study (MaudNESS) to examine mixing mechanisms and the role of fluxes across the pycnocline in moderating water column stability. The second paper, Flanagan et al. (2013, manuscript submitted to J. Phys. Oceanogr., hereafter referred to as Part II), uses numerical experiments to gain further insight into the turbulent mechanisms in weak stratification that is susceptible to diffusive layering instability.

The Weddell Polynya, a large expanse of open water that formed near Maud Rise and persisted through the winters of 1974–76 (Carsey 1980; Martinson et al. 1981), is the prime example of deep-reaching convection in the open Weddell Sea. Immediately following the polynya years, Gordon (1978) observed a cold, fresh, and nearly homogeneous “deep chimney” to 3000-m depth in the area of the polynya. Although there have been no persistent (i.e., multiyear) openings in the sea ice since the 1970s, large, transient (i.e., single winter) openings are common (Comiso and Gordon 1987; Drinkwater 1996). In fact, a band of reduced-concentration winter ice cover surrounds Maud Rise in the long-term time mean (Lindsay et al. 2004).
The vigorous air–sea interaction and deep convection that accompany expansive polynyas in the Weddell Sea affect global climate. Large open water areas allow direct coupling between ocean and atmosphere, affecting short-term atmospheric changes while the open-ocean convection produces a long-term cooling in the deep water of the World Ocean. Based on CTD observations before and after the polynya, Gordon (1982) documented decreased stability and substantial cooling (0.2°C over 2500-m depth range) and estimated that Weddell Polynya convection contributed 2.6–3.2 Sverdrups (Sv; $1 \text{ Sv} = 10^6 \text{ m}^3 \text{ s}^{-1}$) of surface water to deep-water formation during its existence, a significant fraction of total deep-water formation rate estimates for the Weddell Sea (2–5 Sv; e.g., Jacobs 2004). Using a longer period of CTD profile observations, McPhee (2003) documented a decade-scale recovery time for ocean heat content to the levels present before the polynya and noted that the observed ocean heat loss corresponds to a 4.6 GJ m$^{-2}$ ventilation of heat to the atmosphere.

Weddell surface layer densification, and hence water column stability, is primarily driven by brine rejection during winter sea ice growth. Although the ice cover is thin (e.g., Wadhams et al. 1987) and the pycnocline is weak (e.g., Martinson et al. 1981), the limited occurrence of open-ocean polynyas and deep convection indicates that the Weddell ocean/sea ice system is robust to a range of wintertime conditions including large heat loss to the atmosphere and severe storm forcing. The inherent robustness of the system is related to the fact that as pycnocline strength decreases, heat contained in the pycnocline and underlying Weddell Warm Deep Water (WDW) is more readily transported to the surface layer, where it inhibits further ice growth (Martinson 1990). This negative feedback associated with the phase change at the ocean–ice interface is known as the “thermal barrier” (Martinson 1990). The strength of the thermal barrier negative feedback depends critically on the parameter dependencies of surface-forced entrainment and pycnocline diffusion mechanisms, which together determine the magnitude of the ocean-to-ice...
heat flux in the winter Weddell water column. Potential forcing mechanisms of pycnocline turbulence include internal wave shear, the diffusive-layer form of double diffusion, and diapycnal cabbeling.

Internal wave–driven mixing is likely controlled by the Froude number

$$\text{Fr} = \frac{|d\vec{u}/dz|}{N},$$

which is the ratio of destabilizing shear magnitude to stabilizing density gradient. Here, $\vec{u}$ is the horizontal velocity vector, $z$ is depth, and $N$ is the buoyancy frequency. At sufficiently fine scales, Fr characterizes the onset of shear instability (Miles 1961; Howard 1961), and the critical condition in terms of Froude number is $\text{Fr}_{cr} = 2$. Oceanic studies have found a correlation between large values of Fr and the occurrence of overturns (e.g., Alford and Pinkel 2000). Kunze et al. (1990) found that 1-m resolution was necessary to resolve critical values of Fr. Various forms of Fr are also the most important parameters in the successful diffusivity parameterizations developed for mixing driven by internal waves following the Garrett and Munk (GM) spectral form (e.g., Gregg 1986). In and environments where the internal wave field departs from the GM form, such as the continental shelf (MacKinnon and Gregg 2003). These parameterizations, which use shear and stratification at relatively large scales (on the order of 10 m), are based on the idea that large-scale waves interact with smaller waves in a predictable manner to produce shear instability at small scales.

In the Weddell Sea, relatively cold and fresh surface water overlies relatively warm and salty WDW, an arrangement susceptible to the diffusive layering form of double diffusion instability. Classical theoretical and laboratory results on diffusive layering (e.g., Turner 1973) indicate that heat flux and the ratio of heat flux to salt flux is determined by the density ratio

$$R_p = \frac{\beta}{\alpha} \frac{dS}{dT},$$

which is the stabilizing salt component of the density gradient compared to the destabilizing thermal component of the density gradient. Here, $T$ is temperature, $S$ is salinity, and $\alpha$ and $\beta$ are the thermal expansion and haline contraction coefficients, respectively. Double diffusion has the unusual property of increasing water column stability. For the diffusive layering form, this is accomplished by the preferential transport of heat upward. The staircase structures observed above the warm Atlantic layer of the Arctic Ocean (e.g., Padman and Dillon 1987; Timmermans et al. 2008) are well-known examples of diffusive layering.

Cabbeling is an equation of state effect that arises from thermal nonlinearity of density, primarily the temperature-dependent variation in the thermal expansion coefficient for water near the freezing point. For the case of an interface separating cold and freshwater from relatively warm and salty water, such as the weak pycnocline in the Weddell Sea that separates the surface layer from underlying WDW, vertical mixing can produce negatively buoyant parcels within the pycnocline, which would be a source of turbulent kinetic energy to support pycnocline turbulence and mixing (Harcourt 2005). Like double diffusion, susceptibility to diapycnal cabbeling is controlled by $R_p$, as the instability occurs when the linear salinity contribution to the density gradient is small enough to “expose” the thermal nonlinear contribution to the density gradient [see Fig. 5 of Harcourt (2005)].

Interaction between Weddell Gyre circulation and bathymetric features affects the local Froude number, density ratio, and water column stability. In the southeastern portion of the gyre, a core of incompletely mixed Circumpolar Deep Water (CDW) and WDW impinges on the Maud Rise (e.g., Muench et al. 2001). The topographic interaction accelerates the incoming flow in a jet around the flanks of the seamount and creates an isolated Taylor column (referred to hereafter as the Taylor cap) above the seamount (e.g., de Steur et al. 2007). The circulation around the flanks of Maud Rise containing the relatively warm CDW will be referred to as the warm water “Halo.” Outside of the Halo, above the Weddell abyssal plain, the deep water is cooler and fresher and the water column is more stable than in the areas affected by the flow around Maud Rise. We will refer to this area as the “Ambient” water column.

Regional numerical simulations (Holland 2001; de Steur et al. 2007) emphasize the dynamical impact of eddies that are generated by the flow impinging on Maud Rise. De Steur et al. (2007) showed that warm-core eddies spin off from the jet, but tend to adhere to the flanks, that these eddies statistically make up the warm Halo feature, and that eddies that do detach are the likely source for 100-km scale “warm pools,” which are the warmer water masses observed to the west and southwest of Maud Rise (e.g., Gordon and Huber 1995; Muench et al. 2001). The warm-core eddies impart a divergent Ekman stress to the base of the sea ice, providing a potential explanation for open water areas observed around Maud Rise (Holland 2001).

MaudNESS was conceived to investigate the processes controlling water column stability in the vicinity of Maud Rise, including the onset and maintenance of deep-reaching convection. A major component of the
program was an expedition to the eastern Weddell Sea aboard the research vessel (R/V) Nathaniel B. Palmer during late austral winter of 2005. De Steur et al. (2007) have described aspects of the regional hydrography, with an emphasis on the dynamics of the warm Halo regime on the flanks of Maud Rise. Sirevaag et al. (2010) describe surface layer turbulence measurements.

The present analysis quantifies the regional water column stability using the regional CTD dataset described by de Steur et al. (2007), but is primarily based on observations from a combined CTD and microstructure package that are used to estimate turbulent diffusivity in the weak and diffusively unstable pycnocline around Maud Rise. The remainder of the paper is organized as follows: The MaudNESS dataset is described in section 2. The pycnocline diffusivity analysis is described in section 3, and the results are presented in section 4. The significance of the results in the context of the surface layer buoyancy budget is discussed in section 5. Conclusions are stated in section 6.

Results of this paper are extended in Part II, where small-scale numerical results provide additional insight into the interaction of shear and double-diffusive instabilities.

2. Observations

Overview of MaudNESS operations

Upper-ocean measurements were made from 2 August to 4 September 2005 during three sampling “Phases.” In Phase 1, a regional CTD survey (Fig. 1) mapped the variability in the upper ocean. In Phases 2 and 3, intensive water column turbulence observations were collected during 13 “drift stations” (referred to as D1–D13 for the remainder), during which the ship was held stationary with respect to an ice floe. In Phase 2, two “ice station” drifts were performed during which measurement systems were deployed from the ship and from the sea ice. The first of the Phase 2 drifts, D1, started near the summit of Maud Rise and drifted in a northeast direction for 34 h before the floe began to break up. The 100-h-long D2 was located in the Halo region to the west of Maud Rise’s summit. During Phase 3, 11 “ship” drifts were executed in which measurement systems were deployed only from the ship. These drifts lasted between 9 and 36 h. Most of them (D3–D11) took place in Taylor cap water southwest of the summit (Fig. 1), where the Phase 1 survey indicated the water column was the least stable. D12 was executed in the transition area between Taylor cap and Halo water, and D13 was executed in Ambient water (Fig. 1). Throughout the area of operations, the ocean was covered by a 40–80-cm-thick layer of sea ice and about 10 cm of snow.

The CTD/microstructure profiler comprised a pumped, dual-sensor Sea-Bird Electronics (SBE) 911plus and a custom shear and scalar microstructure package. The microstructure instrumentation, referred to hereafter as the lowered microstructure package (LMP), was suspended from the bottom of the CTD cage by a spring that was designed to isolate the microstructure sensors from cable vibrations. The profiler entered the ocean through the vessel’s moon pool, which allowed for rapid and continuous deployment in a variety of ice conditions. A computer-controlled winch cycled the profiler from 17-m depth down to 300–350-m depth at a wire speed of approximately 0.6 m s\(^{-1}\). At this speed, a round trip profile required about 16–18 min, depending on how deep the profile went. Only data from the down-going portions of the profiles are used in this analysis, because the microstructure sensors were obstructed by the CTD in the up-going portions. During the Phase 2 and 3 drifts, 1302 down casts were obtained.

The LMP was not deployed with the CTD during most of D2 because it suffered a small leak. For this reason, D2 profiles are not included in the analysis.

Profiler observations were supplemented with simultaneous observations of water column velocity profiles from the ship’s hull-mounted, 150-KHz broadband ADCP. ADCP data collected during the expedition were processed and quality controlled by the University of Hawaii Data Acquisition System. The final product had 5-min temporal resolution in 49 8-m depth bins between 35- and 419-m depth.

Resolving the small temperature gradients and extremely small salinity gradients in the Maud Rise region is a technical challenge. The CTD data were processed using the alignment, filtering, and thermal lag correction techniques recommended by Sea-Bird Electronics. The temperature signal was sharpened following the procedure described in Johnson et al. (2007), although we employed a sensor time constant of 0.056 s appropriate for the SBE 3plus sensor on the profiler. Conductivity cell lag corrections were optimized to minimize salinity spiking. This was achieved by calculating salinity profiles for a range of test lags and choosing the lag that minimized salinity variance. The combination of temperature signal sharpening and optimal estimation of lags effectively ameliorated salinity spiking, allowing estimation of salinity and density at 10-cm vertical scales. Salinity and density were calculated using standard formulas, and potential temperature and density were calculated at a reference pressure of 100 dbar.

Averaging procedures for turbulence quantities (see next section) required robust estimates of the depth of the surface layer base. For our purposes, we defined the pycnocline as the high-gradient region separating the surface mixed layer from underlying WDW. After experimenting with standard techniques for identifying
the depth of the base of the surface mixed layer, we concluded that a nonlinear, profile-fitting approach provided the most robust estimate of the depth of the mixed layer base and the vertical extent of the pycnocline. The potential density (referenced to 100 dbar) profile is assumed to consist of a linear profile in the surface layer and an exponential–linear profile through the pycnocline and into the WDW:

\[
\rho_a(d) = \begin{cases} 
\rho_{\theta_s} + a_1 d, & \text{for } d \leq d_{\text{ml}} \\
\rho_a(d_{\text{ml}}) + a_2 \left[ 1 - e^{-(d-d_{\text{ml}})/d_{\text{pyc}}} \right] + a_3 (d - d_{\text{ml}}), & \text{for } d > d_{\text{ml}}. 
\end{cases}
\]

The six unknowns in the profile, \(\rho_{\theta_s}, d_{\text{ml}}, d_{\text{pyc}}, a_1, a_2,\) and \(a_3\) (including the surface density \(\rho_{\theta_s}\), the depth of surface mixed layer base \(d_{\text{ml}}\), and the \(e\)-folding depth scale of the pycnocline \(d_{\text{pyc}}\), were calculated using an iterative least squares estimation algorithm [Seber and Wild 2003; performed with matrix laboratory (MATLAB) function “nlinfit”] applied to the entire profile. We found that such a complex profile form was required to accurately and robustly describe the depth of the surface layer base. Examples of the profile-fitting technique to density profiles from the Phase 1 survey (Fig. 3, described in greater detail below) demonstrate that the technique robustly identifies the mixed layer base (visible as the discontinuity of slope in the profile fits).

The LMP was equipped with an airfoil-type shear sensor, a fast-response, glass-coated bead thermistor [Thermometrics Fastip Probe (FP) 07], and a fast-response, dual-needle conductivity sensor (SBE 7). The shear and thermistor data were acquired at 100 Hz, and the fast-response conductivity data were acquired at 200 Hz. Throughout the experiment, the microconductivity sensor had better signal-to-noise ratios than the shear probe and the thermistor, so turbulent diffusivities were estimated using the conductivity data.

Output from the conductivity sensor was preemphasized (e.g., Mudge and Lueck 1994) to reduce the discretization noise floor of that signal. For each downcast, conductivity sensor calibrations were obtained by regression against CTD values, and a microconductivity spectral noise model was estimated using the most quiescent sections of the cast (typically near the bottom). These noise spectra were subtracted from observed spectra. Microconductivity data were edited using a combination of automated algorithms and manual inspection to remove spikes that resulted, most likely, from collisions with small organisms.

3. Estimating turbulent diffusivity and stability parameters

The fundamental quantity estimated from the conductivity measurements is the rate of destruction of the thermal variance by mixing, defined by

\[
\chi_T = 6\kappa_T \left( \frac{dT^*}{dz} \right)^2 = 6\kappa_T \int_0^\infty S_{T,T}\, dk
\]

for vertical measurements in an assumed isotropic turbulent field. Here, \(\kappa_T\) is the molecular diffusivity of heat, \(dT^*/dz\) is the vertical derivative of the turbulent temperature field, and the overline notation indicates Reynolds averaging, which is fully defined below. The vertical temperature gradient spectrum \(S_{T,T}\) is a function of the vertical wavenumber \(k\). The temporal measurements are translated into spatial measurements along the vertical profile using Taylor’s frozen turbulence hypothesis, with the sensor fall speed as the advection speed.

Interpreting the conductivity signal in terms of the temperature relation is linear, then \(\chi_T\) would equal a normalized integral of the conductivity gradient \(S_{CC}\) given by

\[
\chi_C = \frac{6\kappa_T}{C_0^2 A^2} \int_0^\infty S_{C,C}\, dk,
\]

where, following the notation of Washburn et al. (1996), \(C_0 A\) is the slope of the linearized conductivity–temperature relation. When salinity effects cannot be ignored, the Washburn et al. (1996) technique provides a correction factor \(E\) that relates \(\chi_C\) to \(\chi_T\):

\[
\chi_T = \frac{\chi_C}{E}.
\]

Five factors determine the relative contribution of temperature and salinity to observed conductivity gradient spectra: 1) the local \(T–S\) relation, 2) the spatial response function of the conductivity probe, 3) the degree of \(T–S\) correlation at high wavenumbers, 4) the forms of temperature and salinity spectra, and 5) the
turbulent kinetic energy (TKE) dissipation rate. The \( T-S \) relation and conductivity probe response strongly affect the conductivity spectra, but these factors are well constrained. The local \( T-S \) relation is determined from the observed CTD profiles. The response of the SBE7 conductivity sensor is modeled as a single-pole spatial filter with a cutoff wavenumber of 100 cycles per meter (e.g., Washburn et al. 1996). Accounting for \( T-S \) correlation, spectral form and TKE dissipation rate require assumptions to be made, but fortunately these factors do not strongly affect the conductivity spectra. We assume that the underlying temperature and salinity fluctuations have the Batchelor spectral form and that the TKE dissipation rate is relatively small, ranging from \( 10^{-10} \) to \( 10^{-8} \text{W kg}^{-1} \), which is consistent with direct measurements made from a different instrument in use during the field program (L. Padman 2013, personal communication). Washburn et al. (1996) showed that, within such a range of TKE dissipation rates, the total conductivity variance is not sensitive to the details of the underlying temperature and salinity spectra. The amount of \( T-S \) correlation does have a modest effect on the total conductivity variance; however, in these observations, the amount of correlation at small scales is unknown.

Following previous work (Rehmann and Duda 2000; Duda and Rehmann 2002), bounds on this uncertainty can be provided by two limiting assumptions—that temperature and salinity are either perfectly correlated or perfectly uncorrelated. Here, an upper limit on the correction factor is made by taking a TKE dissipation rate of \( 10^{-8} \text{W kg}^{-1} \) and assuming perfect correlation between temperature and salinity, and a lower limit is made by taking the TKE dissipation rate to be \( 10^{-10} \text{W kg}^{-1} \) and assuming that temperature and salinity are uncorrelated. For this dataset, the upper and lower bounds result in a factor of 2 uncertainty in \( \chi_T \). Presented values are the average of the upper and lower limits. The minimum resolvable \( \chi_T \) is approximately \( 1 \times 10^{-10} \text{K}^2 \text{s}^{-1} \).

Thermal diffusivity was estimated from \( \chi_T \) using the method of Osborn and Cox (1972), which assumes that a local balance holds between the production and dissipation of turbulent temperature variance (TTV):

\[
-k_T = \frac{3\kappa_T}{2} \left( \frac{dT'/dz}{dT/dz} \right)^2 = \frac{1}{2} \frac{\chi_T}{(dT/dz)^2},
\]

where the molecular thermal diffusivity \( \kappa_T \) is set to a constant value of \( 1.4 \times 10^{-7} \text{m}^2 \text{s}^{-1} \).

The Osborn–Cox diffusivity estimate is determined by the ratio of the temperature gradient variance to the squared mean, or background, temperature gradient \( dT/dz \). In an episodically turbulent and vertically structured environment such as the Weddell Sea pycnocline, it is observationally difficult to characterize average values of these two quantities, especially with a sensor moving in the vertical direction. Large-scale vertical averaging does not resolve variability within the pycnocline associated with its exponential form or with embedded staircase features, and the temperature gradient inferred from a single profile at small vertical scales may not be representative of the background profile if turbulence is active. From a theoretical perspective, the Osborn–Cox diffusivity estimate is incomplete in regions where the TTV budget is not maintained locally (e.g., Davis 1994). For example, vertical transport of temperature variance can be significant in well-mixed areas adjacent to high-gradient areas (e.g., Shaw et al. 2001). In this case, Osborn–Cox is biased high because the numerator lacks transport convergence.

Example microconductivity profiles obtained during the first 4 h of D6 (Fig. 2) illustrate features of the weak but structured pycnocline observed in this study and challenges in applying the Osborn–Cox model. The profiles contain a continuous gradient layer, 5–10 m thick, immediately underlying the base of the surface mixed layer. The gradient layer overlies a series of interfaces and internal mixed layers that extends to about 60 m below the mixed layer base. The vertical scale of the internal mixed layers varies from 5 to 20 m. Turbulent patches are visible at scales of 1–5 m. The vertical structure varies rapidly in time and horizontal position, with layers merging and splitting throughout this 4-h-long example. The average of the density ratio over these profiles (Fig. 2b) has a uniform value of about 1.1 in the “core” of the staircases (5–27.5 m below the mixed layer base) and is larger in the gradient region above.

To best characterize the averaged quantities required in the Osborn–Cox model, Reynolds averaging was performed vertically over 5-m bins along a vertical coordinate that tracked the base of the mixed layer, as defined using the density profile-fitting algorithm, and temporally across profiles within 1-h long periods. So, the overline notation represents combined 5-m vertical averaging and profile ensemble averaging over 1-h periods. The 1-h interval is...
an effective compromise between achieving statistical stationarity for the turbulence estimates and resolving the spatiotemporal variability of the “mean” characteristics of the pycnocline, while the 5-m bin height resolves the vertical structure within the 40-m-thick pycnocline. CTD and ADCP data received the same averaging treatment, resulting in Reynolds averaged buoyancy frequency and shear. Shear estimates from the 8-m vertical resolution ADCP data were interpolated in time and space onto the midpoints of the 5-m bins of each downcast. There were occasional gaps in the ADCP data. Within each ensemble, if a particular depth bin had more than 60% ADCP drop outs (i.e., fewer than 7 5-min data points), that bin was excluded from further analysis. We required that each ensemble contain at least two high-quality CTD/LMP downcasts; 295 of 367 (80%) ensembles satisfied this criterion. High quality implies acceptable noise level and calibrations and readily identifiable pycnocline properties via the profile-fitting approach. Most of the ensembles comprised three or four high-quality profiles.

Despite our best efforts at 5-m and 1-h Reynolds averaging, we found that diffusivity and stability parameters and relationships between them are only robust when the pycnocline is considered in a bulk, or outer scale, perspective. For the vertical averaging necessary to compute bulk parameters, the top of pycnocline is defined as the depth of the surface layer base and the width of the pycnocline is taken as 40 m. Profile fitting yields an average e-folding length scale of about 20 m, so the pycnocline is about twice this scale. While the bulk approach is effective at characterizing the overall transport of heat across the pycnocline, it obviously averages over important aspects of the problem, such as the details of the diffusive layering staircases.

As the Froude number and density ratio are both ratios of background differences, the bulk versions of these quantities are naturally expressed as the ratios of these differences across the pycnocline, that is,

\[
Fr_b = \frac{\langle |d\mathbf{u}/dz| \rangle}{\langle \mathbf{N} \rangle}
\quad \text{and}
\]

\[
R_{\rho,b} = \frac{\beta \langle dS/dz \rangle}{\alpha \langle dT/dz \rangle},
\]

where the angular brackets indicate 40-m vertical averaging, and the subscript \(b\) indicates a bulk parameter. (These definitions and notation are analogous to those of the bulk Richardson number).

The choice of definition for pycnocline average diffusivity is more ambiguous, and we have considered two possibilities. The first is the 40-m pycnocline average of 5-m, 1-h \(k_T\):

\[
\langle k_T \rangle = \frac{1}{2} \left( \frac{\chi_T}{(dT/dz)^2} \right).
\]

The second possibility results from averaging \(\chi_T\) and \(dT/dz\) prior to forming the ratio

\[
k_{T,b} = \frac{1}{2} \langle \chi_T \rangle \langle dT/dz \rangle^2.
\]

If the heat flux across the pycnocline layer is approximately uniform, \(k_{T,b}\) (together with the average gradient across the pycnocline) provides an unbiased estimate of that flux. This version also has the benefit of representing a vertical integral of the TTV equation and so removes any errors associated with transport of TTV within the pycnocline (see above). In Part II, numerical results corroborate that heat fluxes calculated with diagnosed \(k_{T,b}\) are in near-perfect agreement with the average fluxes across the numerical domain. Overall, \(k_{T,b}\) is preferred over \(\langle k_T \rangle\) for use in the outer scaling approach in this application, and results are based on \(k_{T,b}\).
4. Results

a. Maud Rise area hydrography (Phase 1)

The regional survey provides an overview of the interaction between bathymetry and large-scale circulation and its effects on the stability of the Maud Rise area water column. Example profiles from the Ambient, Halo, and Taylor cap water masses (Fig. 3) and sections across Maud Rise (Fig. 4) capture the geographic variability in the static stability of the water column. Radial variability across the seamount is clearly visible in the northwest-to-southeast transect over the rise (Fig. 4, section A–B). Spatial variability in surface salinity is also highlighted by the color-coded symbols in Fig. 1.

Halo and warm pool water are distinguished by a shallow surface layer (50–75 m deep) and by deep water that is relatively warm (temperature maximum exceeding 1.0°C) and salty (average salinity about 34.7 from 0 to 100 m below the base of the surface layer; Fig. 3). Taylor cap deep water, by contrast, is cooler ($T_{\text{max}}$, 0.6°C), fresher ($S$, 34.67 psu), and is overlain by a deeper surface layer (greater than 100-m depth; Fig. 3). Outside of the Halo, in the Ambient water (first part of the A–B section in Fig. 4), the WDW has

![Figure 3](image-url)
properties very similar to those of the Taylor cap water. The Ambient water has the deepest surface layer (Fig. 3). The Halo was encountered in all radial transects, except the southeastern end of section A–B. Taylor cap water was encountered at water depths less than about 3500 m over the rise, including a broad area to the southwest of the summit, where most of the Phase 3 drifts took place (Fig. 1).

The radial gradient in surface layer salinity surrounding the seamount, from elevated salinity within the Taylor cap, largely determines the strength of pycnocline stratification in the region (Figs. 3b,c). In the Ambient water, surface salinity is less than 34.35 psu, while surface layer salinity in the Taylor cap is close to 34.45 psu. The resulting horizontal salinity gradient sets the salt and density differences across the pycnocline (Figs. 1 and 3c). Density difference across the pycnocline increases from a very small value of 0.025–0.050 kg m$^{-3}$ within the Taylor cap to a slightly more stable value of 0.15 kg m$^{-3}$ in the Ambient water. The density difference observed in the Taylor cap would be reduced to zero by only about 10 cm of sea ice growth. The density ratio in the pycnocline (Fig. 4d) also varies with the surface salinity, increasing from about 1.25 in the Taylor cap to about 2.25 in the Ambient water. The Taylor cap $R_p$ values are remarkably unstable. For example, the diffusive staircases above the Atlantic layer in the Arctic Ocean have $R_p$ in the range of about 4–6 (Timmermans et al. 2008).

In summary, Maud Rise topographic interactions result in a Taylor cap region with a very weakly stratified...
pycnocline that is highly susceptible to diffusive layering instability.

b. Pycnocline stability and diffusivity (Phases 2 and 3)

Sections of temperature and salinity recorded by the profiler during the 12 Phase 2 and 3 drifts included in the present analysis (Fig. 5) further illustrate the contrast between Ambient and Taylor cap stability observed in the Phase 1 survey. The depth of the base of the surface mixed layer varies as much as 50 m within the drifts (Fig. 5a), highlighting the usefulness of the mixed layer base tracking approach described above. Also shown in Fig. 5a is the estimate of the thickness of the pycnocline as represented by the \( e \)-folding scale of the profile fits. The median value of this scale is 17 m. In the latter portion of D13 and near the beginning of D12, the pycnocline is relatively broad and the \( e \)-folding scale exceeds 50 m. However, the density profile has a stronger linear component during these periods, the effect of
which is to make the e-folding scale less representative of pycnocline width. The sections in Figs. 4, 5, and 6 are presented with a depth scale relative to the depth of the mixed layer base.

That D13 took place in Ambient water is clear from the relatively fresh value of surface salinity and relatively large density difference across the pycnocline (Fig. 4d). D3, D4, D6, D7, D8, D9, D10, and D11 were all executed in the least stable water column found during the CTD survey, in the Taylor cap water to the southwest of the summit of Maud Rise. The conditions of these drifts are represented by the eastern end of the J–K leg of the CTD survey (Fig. 1), where the surface salinity also exceeded 34.5 psu (Fig. 4b). D1, D5, and D12 were executed in a horizontal-gradient “Transition” area between Taylor cap and Halo water masses, as evidenced by the intermediate values of surface salinity during these drifts. D5 also encountered a shallower mixed layer base and increased deep-water temperature and salinity. In the context provided by the Phase 1 survey, D5 occurred in the gradient region between the Halo water mass at point J and the low-stratification Taylor cap at point K of the CTD survey (Figs. 1 and 4b), where the surface layer was about 100 m deep. Based on these differences in surface salinity and stability, we group the drifts as follows: Ambient (D13), Transitional (D1, D5, and D12), and Taylor cap (D3, D4, D6, D7, D8, D9, D10, and D11). The transitional group includes D1, which was located near the summit of Maud Rise, and D5,
which was located very close to the eight Taylor cap drifts to the southwest.

For the southwest Taylor cap drifts, the maximum surface salinity is 34.51 psu during D11 (maximum values per drift exceeded 34.50 psu for all of the Taylor cap drifts). The corresponding density differences across the pycnocline were typically less than 0.02 kg m\(^{-3}\), and the corresponding density ratios were less than about 1.12 (smaller than captured in the CTD survey). In contrast, for D13, the surface salinity was about 34.34, the pycnocline density difference was about 4 times larger (0.085 kg m\(^{-3}\)), and the density ratio was almost twice as large (1.77). Several of the southwest Taylor cap drifts experienced subtle changes in surface salinity (e.g., D6, D7, and D12) associated with the horizontal gradient in surface salinity in this area associated with the transition to the Halo water type.

The combined profiler and ADCP dataset (Fig. 6) illustrates the susceptibility of the water column to shear-generated turbulence. As expected, water column shear was concentrated near the top of the pycnocline (within 20 m of the base of the surface layer), where the density gradients were strongest. The duration of the drifts was not long enough to calculate accurately the frequency content of the shear, but currents varied over 6–12-h intervals and were likely a superposition of internal tides and near-inertial motions. There was no clear geographical variability in shear. For example, shear magnitudes in the Ambient water (D13), away from the flanks of Maud Rise over the deep Weddell abyssal plain, were comparable to those observed in the Taylor cap waters. Peak shear values were as large as from 1 \(\times\) 10\(^{-3}\) to 2 \(\times\) 10\(^{-3}\) s\(^{-1}\) (Fig. 6a), but these values are small compared to the buoyancy frequency (cf. Fig. 6b) with the vast majority of 8-m scale Fr estimates below the critical value.

Mainly as a result of the horizontal near-surface salinity gradient discussed above, there was strong geographic variability in the buoyancy frequency within the pycnocline (Fig. 6b). Within the Ambient water D13 drift, the buoyancy frequency ranged from 4 \(\times\) 10\(^{-3}\) to 4.5 \(\times\) 10\(^{-3}\) s\(^{-1}\). For the Taylor cap drifts, the buoyancy frequency was typically within the range from 2 \(\times\) 10\(^{-3}\) to 2.5 \(\times\) 10\(^{-3}\) s\(^{-1}\).

Resulting bulk Froude numbers (Fig. 6c) varied from 0.1 to greater than 0.7. Within a few ensembles the shear was large enough to produce Fr\(_b\) values that approached 1, in the range 0.7–0.9. These ensembles, only five in total, all occurred during the Taylor cap drifts. However, this large-scale (40-m) shear likely distorts small-scale waves leading indirectly to turbulent production, as in the wave–wave interaction models of internal wave–induced mixing (e.g., Gregg 1989). Although the large-scale shear field was similar between drifts, the differences in stratification produced geographic differences in Fr\(_b\) between the Ambient and Taylor cap regions (Fig. 6c). The relatively strong pycnocline stratification of the Ambient water resulted in an average Fr\(_b\) value of 0.29 during D13, compared with average values of about 0.40 for the Taylor cap drifts.

Sections of \(\chi_T\) (Fig. 7a) illustrate variability in pycnocline mixing during the drift stations. As expected, \(\chi_T\) is the largest at the top of the pycnocline, where the large background temperature gradient amplifies turbulent temperature fluctuations (Fig. 7b). Within the pycnocline averaging interval, \(\chi_T\) varies between approximately 1 \(\times\) 10\(^{-9}\) and 1 \(\times\) 10\(^{-4}\) K\(^2\) s\(^{-1}\), above the 1 \(\times\) 10\(^{-10}\) K\(^2\) s\(^{-1}\) noise level of the LMP microconductivity measurement. The most striking feature of the microstructure observations is the drastic reduction in \(\chi_T\) within the Ambient water D13. During D13, the average value of \(\chi_T\) within the pycnocline was close to 2.9 \(\times\) 10\(^{-8}\) K\(^2\) s\(^{-1}\) while the average value for the least stable southwest drifts was close to 1.3 \(\times\) 10\(^{-7}\) K\(^2\) s\(^{-1}\). This difference is enhanced further (by the differences in the temperature gradient) in the calculated \(k_T\) values (Fig. 7c). The average values of \(k_T\) during D13 and the southwest Taylor cap drifts were 9.6 \(\times\) 10\(^{-6}\) and 9.8 \(\times\) 10\(^{-5}\) m\(^2\) s\(^{-1}\), respectively, a full order of magnitude difference. Note that the factor of 2 uncertainties introduced by the conductivity correction procedure described above are small compared to the observed regional variability. Within the drifts, there was only one case of clear transition in mixing rates and the stability parameters. About one-half of a day into D10, the surface salinity decreased moderately as the drift began to enter the transition region (Fig. 4d) and shear decreased (Fig. 6b). With these changes, there was a corresponding decrease in \(\chi_T\) and \(k_T\), with \(k_T\) decreasing from levels similar to the other Taylor cap drifts to a level of about 2.6 \(\times\) 10\(^{-5}\) m\(^2\) s\(^{-1}\). A final feature of note in the \(\chi_T\) sections is the occasional occurrence of elevated mixing levels above the mixed layer base, that is, within the surface mixing layer. Examples include most of D1 and the latter half of D12. We interpret these mixing events within the surface layer to be the signature of surface-forced turbulent entrainment. During D1, the wind forcing was strong. During D12 the vessel created an unusually large open water area as it was positioning in preparation for deploying the measurement equipment, and it is likely that subsequent refreezing of this area initiated free convection.

The observed variability in \(k_T\) leads to a corresponding variability in the diffusive heat flux \(F_{bd}\) across the pycnocline (Fig. 8). Heat fluxes in the least stable Taylor cap drifts have an average value of about 13.4 W m\(^{-2}\) in
contrast to an average of about 1.9 W m$^{-2}$ during the Ambient (D13) drift (Fig. 8a). In the limit of $R_{r,b}$ approaching one, the diffusive heat flux across the pycnocline exceeds 20 W m$^{-2}$ (Fig. 8b).

c. Parameter dependencies

The 12 drift stations (with D2 excluded, as described above) recorded variability in pycnocline-averaged diffusivity $k_{T,b}$ and the hypothesized significant stability parameters $F_{r,b}$ and $R_{p,b}$. The $F_r$–$R_p$ parameter space covered by the observations (Fig. 9) is largely composed of variation in $F_{r,b}$ within the low $R_{p,b}$ ensembles of the Taylor cap drifts and a smaller range of $F_{r,b}$ variation in the higher $R_{p,b}$ regime of the Ambient water. The band between these data point clusters is sparsely populated by observations from the three Transition drifts.

In an attempt to separate diffusive processes within the pycnocline from the effects of surface-forced entrainment, we imposed a criterion on $x_T$ near the bottom of the surface mixed layer (i.e., consistent with our interpretation above). If the average value of $x_T$ over the lower 40 m of the surface layer exceeded $1.25 \times 10^{-7}$ K s$^{-1}$, we assumed that surface forcing significantly affected the measured pycnocline diffusivities, and we excluded these ensembles from further analysis. These periods of elevated surface layer $x_T$ correspond to the surface forcing events described in the previous section and are clearly visible in D1 and D12 (Fig. 7a). Unfortunately, surface forcing influenced many of the Transition drifts (filled symbols in Fig. 9), which has a negative effect on the coverage of the parameter space. In total, 247 1-h ensembles were considered: 21 in the
Ambient water, 47 in the Transition regime, and 177 in the Taylor cap (open symbols in Fig. 9).

The Froude number alone is not capable of explaining the observed variability of $k_{T,b}$ (Fig. 10). For relatively weak shear ($F_{rb}$ less than about 0.35), there are two distinct groups of data points that are differentiated by density ratio. In this regime, ensembles with $R_{rb} > 1.5$ have diffusivities that are about one order of magnitude smaller ensembles with $R_{rb} < 1.5$. As $F_{rb}$ exceeds 0.35, the diffusivities of the “large $R_{rb}$” ensembles increase, approaching the values of the “small $R_{rb}$” ensembles. There is not a clear dependence of $k_{T,b}$ on $F_{rb}$ for the large $R_{rb}$ ensembles. We draw two conclusions from these features. First, $F_{rb}$ influences $k_{T,b}$ only after it exceeds a value of about 0.35. Second, below this $F_{rb}$ value, the observed variability in $k_{T,b}$ is due to physical processes other than internal wave shear.

Based on the above interpretation, considering only ensembles with $F_{rb} < 0.35$ (i.e., those for which there is no obvious $Fr$ dependence as described above) provides a separation of the effects of Froude number and density ratio on $k_{T,b}$. For these low shear cases, $k_{T,b}$ is strongly dependent on $R_{pb}$ (Fig. 11). This dependence, for example, covers the full range of observed variability in $k_{T,b}$ from about $1 \times 10^{-5}$ to $1 \times 10^{-4}$ m$^2$/s. The density ratio dependence is reasonably well described by a relationship of the form

$$k_{T,b} = k_0(1 - R_{pb}^{-1})^{-3/2},$$

with $k_0 = 3.9 \times 10^{-6}$ m$^2$/s. This functional dependence is further discussed in Part II.

For comparison, diffusivities based on the “4/3 flux law” are calculated following the procedure outlined by Kelley (1984), in which the temperature difference across individual staircase steps are related to the background gradients with a semiempirical model of layer thickness [see Kelley et al. (2003) for an overview]. Specifically, we start with Eq. (7a) of Kelley (1984):

$$k_{T,b} = C[\sigma(R_{pb} - 1)]^{-1/3} G^{4/3} k_T,$$

where $C = C(R_p)$ is the flux factor, $\sigma$ is Prandtl number for seawater, and $G = G(R_p)$ is a dimensionless layer
thickness. For the flux factor, we use the Kelley [1990, Eq. (4)] summary of available laboratory data. For layer thickness, we use the Kelley [1984, Eq. (9)] model. The observations are qualitatively similar to the 4/3 flux law predictions (Fig. 11). The largest quantitative difference occurs at small values of $R_{rb}$ ($R_{rb}$ less than about 1.2), where the 4/3 flux law predictions do not increase as rapidly as the observations.

5. Discussion

Weddell surface layer densification, and hence water column static stability, is primarily driven by brine rejection during winter sea ice growth. Although the ice cover is thin and the pycnocline is weak, the limited occurrence of open-ocean polynyas and deep convection indicates that the Weddell ocean/sea ice system is robust to a range of wintertime conditions including large heat loss to the atmosphere and severe storm forcing. The inherent robustness of the system is related to the fact that as pycnocline stratification weakens, heat contained in the pycnocline and underlying WDW is more readily transported to the surface layer, where it inhibits further ice growth through the thermal barrier mechanism (Martinson 1990).

The significance of the observed across-pycnocline heat fluxes (Fig. 8) on the static stability of the water column is illustrated by a consideration of the surface layer buoyancy budget. Following Martinson (1990), we use a 1D surface layer salinity budget, which is essentially equivalent to buoyancy for the near-freezing surface layer, as a framework for exploring the robustness of the ocean/sea ice system (Fig. 12). By assuming that the surface layer temperature is nearly steady and very close to its freezing temperature and then introducing the heat balance for the sea ice cover, the salt budget takes this form:

$$\frac{d(hS)}{dt} = \frac{(S - S_i)}{\rho_0 L_i} (F_a - F_h) + F_s,$$  \hspace{2cm} (7)

The terms on the right-hand side of Eq. (7) (blue arrows on the right of Fig. 12) are the salt fluxes that determine the evolution of the salinity $S$ averaged over the surface layer of depth $h$. The first term on the right represents the salt flux associated with brine rejection during growth of the sea ice cover. It is the resultant of the sea ice heat budget (red arrows on the left of Fig. 12), which is a competition between the heat loss to the atmosphere $F_a$ and the ocean heat flux, which results from entrainment at the top of the pycnocline and diffusion across the pycnocline. The factor $(S - S_i)/{(\rho_0 L_i)}$, containing the salinity difference between ice and ocean and ice density and latent heat of fusion, converts the resultant heat flux into a salt flux. The second term represents the direct effects on the salt budget of the entrainment and...
The diffusion of salt from the pycnocline. The entrainment fluxes are the result of incorporation of pycnocline water into the surface layer during surface-forced boundary layer growth. The diffusive fluxes are the result of transport from the deep water to the surface layer by internal mixing mechanisms within the pycnocline, such as the internal wave shear and double-diffusive convection characterized in the previous section.

The winter evolution of the Weddell ice cover indicates that pycnocline transports are a significant component of the surface layer buoyancy budget. Rapid early winter ice growth is typically followed by a period of slow ice growth once the cover has attained a thickness of about 0.6 m (e.g., Wadhams et al. 1987). According to the 1D ice heat balance (Fig. 12, left), heat transport from the pycnocline and deep water must be nearly capable of balancing the heat lost to the atmosphere (about 35 W m\(^{-2}\) averaged over the winter season) to significantly reduce the ice growth as observed.

The present observations indicate that diffusive heat fluxes across the pycnocline are an important component of this negative feedback. As the water column approaches neutral stability and the density ratio approaches unity, our results indicate that the diffusive heat fluxes alone are large enough to balance the heat loss to the atmosphere. This negative feedback is quantified and illustrated with an idealized simulation of the Taylor cap surface layer using Eq. (7) and the diffusivity laws for heat and salt obtained from the numerical results of Part II (Eqs. (13) and (15)). We assume that the surface layer thickness is steady at 120 m. The initial condition for surface layer salinity is 34.7 psu. WDW is represented by a thick underlying layer that is essentially fixed at 34.7 psu and 0.5°C. Fluxes across the pycnocline are driven by property differences across a layer 40 m thick, with the Part II diffusivity parameterizations (entrainment fluxes are ignored in this simple model). The equation for surface layer salinity is numerically integrated in time with an imposed heat loss of 30 W m\(^{-2}\) (Fig. 13).

Initially, the bulk density ratio is approximately equal to two. Pycnocline heat fluxes associated with this state are small in comparison to heat loss to the atmosphere and so ice grows at an approximately constant rate, which is forced by a constant rate of increase in surface layer salinity. Eventually, at about day 60 in the simulation, the bulk density ratio has decreases to a value of about 1.2. At this point, the diffusive fluxes across the pycnocline increase rapidly until by about day 80 when they are approximately in balance with the atmospheric heat loss, arresting the salinization of the surface layer. After this point, the system remains in a steady state with a density ratio equal to 1.1, surface salinity equal to 34.55 psu, and density difference across the pycnocline of 0.02 kg m\(^{-3}\), all quite consistent with the late winter conditions observed in the Maud Rise Taylor cap water.

As Martinson (1990) demonstrated, an important, and perhaps somewhat counterintuitive, property of the ice-covered Weddell surface salinity budget is that heat transport from the pycnocline to the surface layer has...
a larger effect on surface salinity and buoyancy than salt transport from the pycnocline. This effect is quantified in the model, where the salt flux driven by diffusive heat flux is initially 10 times greater than the diffusive salt flux, and increases to more than 100 times greater in the final steady state (Fig. 13c). Note that if diffusivities are set to the constant level $k_0$, the water column becomes statically unstable by day 80 of the simulation (Fig. 13d).

6. Summary and conclusions

As part of MaudNESS, an expedition to the eastern Weddell Sea was undertaken to study the stability of the marginally stable water column in this area in the austral winter of 2005. A regional CTD survey in the vicinity of the Maud Rise seamount delineated the boundaries between water masses associated with flow around the seamount and identified areas most susceptible to overturning. A downstream region (southwest of the summit) of the Taylor column that forms over the seamount was the least stable, with a potential density difference across the pycnocline less than 0.018 kg m$^{-3}$. The survey was followed by a series of 13 drift stations in which intensive water column measurements were made to investigate how vertical turbulent transports affected the evolution of water column stability. During these drifts, more than 1300 profiles of temperature, conductivity, and fast-response microconductivity were obtained with a CTD and microstructure profiler. The drift stations were mostly executed in the least stable Taylor cap area,
but four of the drifts were executed in relatively stable areas, more radially distant from the Taylor cap. The dependence of pycnocline diffusivity on the Froude number Fr (turbulence generated by internal wave shear) and density ratio $R_p$ (turbulence generated by double diffusion and possibly diapycnal cabbeling) is investigated. Observed $k_T$-variability cannot be explained by Fr alone. Instead, there is a strong dependence on $R_p$, with an order of magnitude increase in $k_T$ between the ambient water column that is unaffected by flow around Maud Rise and the very weakly stratified Taylor cap water over Maud Rise. In terms of water column stability, diffusive heat flux across the pycnocline inhibits winter ice growth and densification of the surface layer. The observed $R_p$ dependence of $k_T$ thus provides a strong, nonlinear negative feedback on the winter evolution of stability of the Maud Rise area water column that enables the system to maintain a consistently thin ice cover.

By themselves, the present observations are not capable of providing insight into the relative significance of the double-diffusive and cabbeling mechanisms in contributing to the strong dependence of diffusivity on the density ratio nor are the observations able to provide any guidance on the magnitudes and dependencies of salt flux in the pycnocline. These questions are taken up in Part II. Future research will investigate details of the instabilities on finer scales within the pycnocline and the conditions and processes that are required to overcome the intrinsic robustness of the weak Weddell Sea pycnocline that has been described in this paper.

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