Observational based evaluation of air-sea gas fluxes and turbulence in the surface ocean boundary layer

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Observational Based Evaluation of Air-Sea Gas Fluxes and Turbulence in the Surface Ocean Boundary Layer

A Dissertation Submitted in Accordance with the Requirements for the Degree of Doctor of Philosophy in the College of Science

by

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Abstract

Turbulence within the ocean surface boundary layer (OSBL) is an important quantity for many processes as it mixes the ocean and transports various ocean quantities such as pollutants, heat, and dissolved gases. However, direct observations of the dissipation rate of turbulent kinetic energy $\epsilon$ under open ocean conditions are limited. Consequently, our understanding on how to model turbulence and its related processes is constrained.

Open ocean measurements from the Air-Sea Interaction Profiler (ASIP) from five cruises are combined with ship-based meteorological information, direct measurements of air-sea gas fluxes, and wave data from dedicated runs of the ECWAM wave model. This comprehensive data set allowed for an evaluation of commonly applied approaches to scale profiles of $\epsilon$, as well as to formulate a scaling relationship. During daytime conditions a relationship based on the friction velocity and wave age describes the observations best. During conditions when convection dominates over wind and wave-induced turbulence the scaling considers buoyancy forcing as additional source for turbulence.

This data was also used to quantify the so-called small-eddy model under open-ocean conditions. This theoretical model relates air-sea gas transfer directly to turbulence, rather than often used empirical wind speed-based parameterisations. It can be shown that the agreement between the model and observations can be improved when using a variable Schmidt number exponent in the model, rather than a constant value of $1/2$.

Further analysis of a single deployment of ASIP in the Labrador Sea presents a unique situation where a stably stratified diurnally warmed OSBL is accompanied by a mixing event, which is most plausibly explained by a breaking internal wave. These results manifest the importance of observations in the upper ocean for understanding processes for ocean-atmosphere exchange.
Declarations

The work of this thesis is based on research carried out in the Air-Sea Physics Lab, School of Physics, NUI Galway. No part of this thesis has been submitted elsewhere for any other degree or qualification. This thesis reports my own work, unless referenced differently in the text.
Dedication

Dedicated to my family,
who always provides a double safety net

Das Wasser ist ein freundliches Element für den, der damit bekannt ist und es zu behandeln weiß.
Johann Wolfgang von Goethe, Die Wahlverwandtschaften, 1809
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This thesis was written in $\LaTeX$. 

Leonie Tabea Esters
Galway, December 2017
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1 Introduction and Motivation

The ocean and the atmosphere are closely linked to each other due to exchanges of heat, energy, mass, and momentum. These interaction processes control the weather and global climate.

By covering 70% of the Earth’s surface, the oceans provide a significant carbon sink for the rising concentration of atmospheric carbon dioxide (CO$_2$). Since the industrial revolution, the global CO$_2$ emissions are constantly increasing, which drives climate change. This increase in CO$_2$ emissions causes a proportional increase in the atmospheric CO$_2$ concentration (Fig. 1.1a). Figure 1.1b highlights the critical role of the oceans within the global carbon cycle, and shows that the air-sea CO$_2$ exchange as a key player. The efficiency of this air-sea gas exchange is driven by the level of turbulence within the ocean surface boundary layer (OSBL); when the OSBL is turbulent, gases can exchange faster (e.g., MacIntyre et al., 1995; Tokoro et al., 2008). In order to improve the gas flux estimations shown in Fig. 1.1b and to increase our knowledge about the oceans’ role, and how it might change, within the carbon cycle, it is important to fully understand surface-ocean turbulence.

However, instead of describing the gas exchange processes directly using turbulence information, it is still common practice to rely on empirical wind speed-based parameterisations. This can induce uncertainties within local and global predictions of air-sea exchange rates of CO$_2$ and other greenhouse gases. The small-eddy model (SEM) offers promising results for a physically-based parameterisation including turbulence directly. This model has been proven under various conditions in rivers, lakes, estuaries, coastal oceans, and the model-world Biosphere 2 (Zappa et al., 2007; Tokoro et al., 2008; Vachon et al., 2010; Wang et al., 2015; Gälkfeldt et al., 2013; Asher and Pankow, 1986; Moog and Jirka, 1999). Inclusion of such turbulence-based descriptions of the air-sea gas transfer into climate models has the potential to improve the predictions of the global carbon cycle and potential feedback mechanisms.

The OSBL is highly turbulent with enhanced production of turbulent
Introduction and Motivation

Figure 1.1: (a) Time series of the average atmospheric CO₂ concentration [ppm]; deseasonalised (blue) and the mean seasonal cycle (pink). (b) Schematic representation of the overall perturbation of the global carbon cycle caused by anthropogenic activities, averaged globally for the decade 2007-2016. Both figures are reprinted from Le Quéré et al. (2017).

kinetic energy (TKE). Turbulence plays a crucial role in ocean dynamics on various temporal and spatial scales. It mixes the oceans and is important for the dispersion of pollutants as well as for the transport of water mass characteristics, such as heat, salt, and dissolved gases. This mixing controls the ocean stratification, which itself is an important quantity for the oceans surface diurnal warming cycle. During the day, enhanced solar radiation heats the oceans surface layer. Under high-stratified ocean conditions this solar heating can form a well-defined diurnal warm layer, which suppresses mixing in the OSBL. Diurnal warming can increase the surface heat flux by the order of 10 W m⁻² (Fairall et al., 1996a) and lead to sea surface temperature amplitudes that reach up to 5 °C (e.g. Stramma et al., 1986; Flament et al., 1994; Fairall et al., 1996a; Soloviev and Lukas, 1997; Ward, 2006; Gentemann et al., 2008). Turbulence can erode the well-stratified warm layer, therefore mixes the heat deeper in to the ocean. Hence, understanding the driving mechanism of ocean turbulence is essential to fully understand those heat fluxes.

Several mechanisms are responsible for the generation of turbulence in the ocean. The upper ocean is bounded on top by the air-sea interface. At this interface, turbulence is generated due to the oceans interaction with the atmosphere. The interaction includes the exchange of density
through heat and freshwater fluxes, and the transfer of momentum through wind stress. Cooling of the upper ocean due to evaporation and longwave radiation leads to convective mixing. Surface heating on the other hand reduces the density and thus suppresses near surface turbulence. Waves, and in particular wave breaking form a further source of TKE in the top meters of the ocean (Gemmrich and Farmer, 2004). Besides breaking, these waves can additionally enhance ocean turbulence through the formation of Langmuir turbulence (Belcher et al., 2012). The enhanced turbulence close to the sea surface mixes the momentum down through the water column thus determines the shape of the near-surface current profiles.

However, measuring turbulence in the ocean is not straightforward. Measurements can be performed by tracking a tracer (e.g. Ledwell et al., 2011) or by observing microstructure fluctuations in temperature, conductivity, and shear (e.g. Lueck et al., 2002). However, all of these observations have one issue in common: they are limited in space and time. For this reason parameterisations of ocean turbulence are essential in order to describe the above-mentioned turbulence-driven processes properly.

This thesis focuses on direct open-ocean observations of the dissipation rate of TKE $\epsilon$ gained from the Air-Sea Interaction Profiler (ASIP). ASIP is a fully autonomous profiler measuring $\epsilon$ up to the air-sea interface, which makes it unique. The data set, which is applied in this thesis, consists of ASIP deployments during five cruises in different ocean basins. This thesis uses this comprehensive data set with the aim to improve the understanding of surface ocean turbulence and its related processes; in particular air-sea gas exchange and diurnal warming within the OSBL. To pursue this aim the following research question were covered:

1. Is the turbulence-based small-eddy model feasible to describe air-sea gas exchange in the open-ocean?

2. How can the measured turbulence profiles be best scaled with meteorological variables?

3. How can a mixing event within the OSBL occur simultaneously to strong diurnal warming, which stratifies the layer?

The outline of this thesis is as follows: Chapter 2 gives an overview on the theoretical background and the available literature being relevant
for this thesis. Chapter 3 introduces the data collection as well as the processing, and gives an overview of the field experiments. Chapter 4 presents a physically-based parametrisation of air-sea gas exchange. The work is published in the Journal of Geophysical Research (Esters et al., 2017). Chapter 5 evaluates commonly-applied scaling approaches for $\epsilon$ based on direct open-ocean measurements. This work is accepted in the Journal of Geophysical as Esters et al. (2018). Chapter 6 discusses a diurnal warming event observed in the Labrador Sea, which is accompanied by an internal wave. In Chapter 7 conclusions are drawn from the results of this thesis and some outlook for future work is given.
2 Theory and Literature Review

This chapter summarises the available literature, which is relevant to this thesis. Section 2.1 describes the basic concepts of turbulence in the ocean. In Section 2.2, common concepts to scale turbulence in the upper ocean are presented. These concepts intend to overcome difficulties in observing ocean turbulence directly. Scaling upper ocean turbulence is, for example, important for air-sea gas exchange. The basic concepts of air-sea gas exchange and its linkage to turbulence are presented in Section 2.3. The last two sections of this chapter describe processes that affect turbulence in the OSBL, namely, diurnal warming in Section 2.4 and internal waves in Section 2.5.

2.1 Upper Ocean Turbulence

First of all, it is important to highlight that turbulence is a characteristic of a flow, but not of a fluid; therefore the Gulf Stream can be turbulent, but a specific lake cannot. Turbulence occurs on many different spatial and temporal scales, from large ocean circulations down to microscale turbulence. On all of these different scales turbulence is important for transporting, thereby, mixing various properties of the fluid. Mixing is greatly increased by turbulence relative to molecular action alone. Turbulence increases the surface area between two adjacent fluids by stretching and stirring a fluid. Thus, turbulence increases the area in which diffusion can take place.

Despite its importance, it is difficult to describe turbulence, as it is not a property of a fluid, but rather a property of its state of motion. Therefore, it is often the case, that turbulence is described by its characteristics. Turbulent flows are highly random with its motion being unpredictable in their speed and direction. The speed at a point continuously changes ‘randomly’ in magnitude and direction. Hence, knowing the velocity at a specific time does not allow the prediction of the velocity a short time later. In addition,
turbulent flows are highly rotational and consist of three dimensional vorticity. Thereby, turbulent flows are flow regimes that stand in contrast to laminar flows (Fig 2.1).

To overcome the unpredictability of turbulent flows, a fundamental idea in turbulence analysis is the Reynolds decomposition, which describes the turbulent motion through statistics. If the assumption of a statistically stationary flow is fulfilled, the velocity of this flow $u$ can be split into a time-averaged value $\overline{u}$ and a zero-mean fluctuating part $u'$:

$$u = \overline{u} + u'.$$  \hspace{1cm} (2.1)

### 2.1.1 Turbulent Kinetic Energy

The ‘strength’ of turbulence in an ocean flow is represented by the turbulent kinetic energy (TKE). The TKE is the mean kinetic energy per unit mass associated with eddies in a turbulent flow. The idea of TKE is similar to the mean kinetic energy equation, but instead of focusing on mean velocities $\overline{u}_i$ the turbulent velocities $u'_i$ are taken into account:

$$E = \frac{1}{2}(\overline{u'^2} + \overline{v'^2} + \overline{w'^2}) = \frac{1}{2}\overline{u'^2}. \hspace{1cm} (2.2)$$

where $E$ is the TKE and $u'_i = (u, v, w)$ is the velocity in direction $x_i = (x, y, z)$. This equation gives a measure of the intensity of tur-
bulence. Since turbulence may change in time the TKE budget \( \frac{\partial E}{\partial t} \) is more interesting. This budget is obtained by starting from the Navier-Stokes Equations for an incompressible fluid, as:

\[
\frac{\partial u_i}{\partial x_i} = 0 \quad \text{(continuity)} \tag{2.3}
\]

and

\[
\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = \frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j^2} \quad \text{(momentum)}, \tag{2.4}
\]

where \( t \) is the time, \( \rho \) the water density, \( p \) the pressure, and \( \nu \) the molecular viscosity.

The Reynolds Decomposition is applied to Eq (2.4) for the velocity field \( u_i \) and pressure \( p \), and the resulting equation is time averaged to yield the mean momentum equation. This is then subtracted from the total Navier-Stokes Equation (2.4), to derive an equation for the fluctuation part of velocity \( u'_i \). This equation of the fluctuation on velocity is multiplied by \( u'_i \) to yield \( \mathcal{E} = \frac{1}{2} u'^2_i \). Averaging and rearranging leads to the following formula (a comprehensive and detailed derivation for this TKE budget is given in Kundu and Cohen (2001), even though basic work on turbulence was done earlier and dates back to the work of Richardson (1922) and Kolmogorov (1941a,b)):

\[
\frac{D\mathcal{E}}{Dt} = \frac{\partial \mathcal{E}}{\partial t} + u_j \frac{\partial \mathcal{E}}{\partial x_j} = - \frac{\partial}{\partial x_j} \left( \frac{1}{\rho_0} p' u'_i + u'_j \mathcal{E} - 2 \nu u'_i s'_{ij} \right) \quad \text{total rate of change in TKE}
\]

\[
- u'_i u'_j \frac{\partial u_i}{\partial x_j} - \mathcal{B}_o u'
\quad \text{shear production term} \quad \text{buoyancy production}
\]

\[
- 2 \nu s'_{ij} s'_{ij}
\quad \text{viscous dissipation} \quad \epsilon
\]

(2.5)

with \( s'_{ij} = \frac{1}{2} ( \frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} ) \) being the strain rate tensor, \( \rho_0 \) being a reference water density, and \( b_o \) being the buoyancy.

The fourth term on the right hand side of this TKE budget (viscous
dissipation) is the dissipation rate $\epsilon$, which describes the loss of TKE due to viscous forces. These viscous losses occur at the very small scale, where viscous drag forces convert velocity fluctuation to heat.

### 2.1.2 Dissipation Rate of Turbulent Kinetic Energy

Turbulence in the ocean is often described by $\epsilon$, which under a steady-state solution balances the shear production and buoyancy flux (Osborn, 1980):

$$
\epsilon = -\bar{u}'\bar{w}' \frac{\partial \overline{\mu}}{\partial z} - \overline{\nu'_c w'},
$$

(2.6)

where $z$ is the depth, $\overline{\mu}$ is the mean velocity and $\bar{u}'\bar{w}' = u'^2$ with $u_*$ being the water-side friction velocity, related to the Reynolds stress $\tau = \rho u'_w w'$.

In the TKE budget (Eq (2.5)) $\epsilon$ is given by:

$$
\epsilon = 2 \nu s_{ij} s_{ij},
$$

(2.7)

To simplify this expression of $\epsilon$, and to formulate it in a way that is measurable, ocean turbulence at dissipation scales are commonly assumed to be isotropic ($\bar{u'^2} = \bar{v'^2} = \bar{w'^2}$). Isotropy states that the properties of turbulence at each point are independent of the direction and the mean velocity is zero: $\overline{u_i} = 0$. Under this assumption, $\epsilon$ can be reduced to:

$$
\epsilon = \frac{15}{2} \nu \left( \frac{\partial u'}{\partial z} \right)^2 = 15 \nu \left( \frac{\partial u'}{\partial x} \right)^2,
$$

(2.8)

with $\partial u'/\partial z$ being any of the 6 shear components of the fluctuation (e.g. $\partial v'/\partial x$) and $\partial u'/\partial x$ being any of the 3 rates of strain. This equation describes the rate of the kinetic energy cascade across the entire inertial subrange.

### 2.1.3 Turbulence Spectrum – Energy Cascade

The concept of the TKE cascade was first proposed by Richardson (1922), who said that there exists large energy-containing eddies, which are deformed and stretched, and thus break into smaller and smaller eddies (Fig. 2.2). Injected energy is transported from large eddy scales, without any energy loss, to much smaller scales. At these smaller scales, the energy can be
dissipated to heat by the prevailing viscosity. Imaging these different eddies, turbulence can be described as a superimposition of many different sized eddies. To focus on the energy contained by different eddies, the problem is often viewed from a spectral perspective. The relative strength of these different eddies defines the turbulent spectrum. Thus, the wavenumber distribution can be related to the eddy size and the rate of their dissipation (Fig. 2.3). A theoretical form of the turbulence spectrum was hypothesised by Kolmogorov (1941a,b). The form of the spectrum only depends on the wavenumber $\ell$ and the rate at which energy is transferred from larger scales to smaller scales and thus at which rate it is dissipated: $S = S(\ell, \epsilon, \nu)$.

Three subranges are defined for this energy cascade as shown in Fig. 2.3. The forcing range is where the lowest wavenumbers are (largest eddies). This is the point at which the energy is injected by the given forcing. The dissipation range is the range at largest wavenumbers, where the energy dissipation overcomes the transfer and the cascade stops. It is associated with the Kolmogorov wavenumber,

$$\ell_k = \left(\frac{\nu^3}{\epsilon}\right)^{1/4},$$

which is the scale at which viscous dissipation dampens out the velocity fluctuations. Therefore, eddies at this length scale are directly affected by viscosity. The wavenumber range, that is large compared to the energy-
containing range and small compared to the dissipation range, is the inertial subrange. For wavenumbers $\ell << 1/\ell_k$, the velocity fluctuations are not dampened by viscosity. In this range, the velocity fluctuations only depend on $\epsilon$ and the wavenumber itself: $S = S(\ell, \epsilon)$. The level of $\epsilon$ equals the flow of kinetic energy from the energy containing scales towards the dissipating scales.

Assuming isotropic turbulence in the inertial subrange, the Kolmogorov spectrum is given by a universal form that only depends on $\epsilon$ as $S_k(\ell) = C \epsilon^{2/3} \ell^{-5/3}$, where $C \sim 0.53$, for ‘high enough’ Reynolds numbers, is the Kolmogorov constant (Sreenivasan, 1995).

From Equation 2.8, one can derive that in isotropic turbulence, $\epsilon$ is the integral of the shear spectrum, as:

$$\epsilon = \frac{15}{2} \nu \int_0^\infty S_s(\ell) d\ell, \quad (2.10)$$

where $S_s$ is the spectrum of the shear, $\partial u'/\partial z$, the velocity spectrum $S(\ell)$ is transformed into its gradient spectrum. This can be achieved by multiplying the quadratic wavenumber $\ell$ as $\ell^2 S(\ell)$ (the wavenumber needs to be in rad m$^{-1}$). Thus, the shear spectrum $\partial u'/\partial z$ has a $\ell^{1/3}$ dependency in the initial subrange.

![Figure 2.3: Schematic energy spectrum of the turbulent velocity cascade with $S(\ell)$ being the spectral density and $\ell$ being the wavenumber. The kinetic energy generated at large scale cascades through the inertial subrange down to the Kolmogorov scale, where viscous forces dissipate into heat.](image-url)
2.2 Scaling of Upper Ocean Turbulence

It is challenging to obtain a full image of the prevailing turbulence field, since turbulence is variable both in space and time. Nevertheless, understanding the structure of the OSBL requires understanding of turbulent mixing. Due to the difficulties regarding the observations of oceanic turbulence, attempts to parameterise profiles of $\epsilon$ within the OSBL have been proposed (e.g. Lombardo and Gregg (1989), Terray et al. (1996), Huang and Qiao (2010), and Belcher et al. (2012)). These scaling attempts are more complicated at the ocean surface than at the ocean floor due to the presence of surface waves. Thus, additional physical processes have to be considered.

In the OSBL, turbulence is generated due to the ocean’s interaction with the atmosphere by exchange of heat and freshwater fluxes, and the transfer of momentum through wind stress. Additionally, waves and wave breaking form a source of turbulence in the uppermost meters of the ocean (Gemmrich and Farmer, 2004). These surface waves can cause Langmuir circulation, which further modifies the upper ocean turbulence characteristics (Belcher et al., 2012). In addition, breaking of internal waves at the pycnocline (Thorpe, 2007; Wain et al., 2015) and submesoscale processes, including the onset of gravitational and symmetric instabilities resulting from steady winds blowing over ocean fronts can cause turbulence in the OSBL (Thomas and Taylor, 2010; D’Asaro et al., 2011).

2.2.1 The Law of the Wall (LOW)

The simplest description of the upper-ocean boundary layer is that of a shear driven wall layer. In the absence of waves and its related processes, the ocean surface could be seen as a flat, rigid ‘wall’, beneath which a purely shear-driven boundary layer evolves (Lorke and Peeters, 2006). Winds produce a constant stress on top of the layer forming the shear in the layer to be given by:

$$\frac{\partial \bar{u}}{\partial z} = \frac{u_*}{\kappa|z|},$$  \hspace{1cm} (2.11)

where $\kappa \approx 0.41$ is the von Kármán constant. Neglecting the buoyancy term in Eq (2.6) and expressing the shear through Eq (2.11), leads to $\epsilon$
being proportional to $z^{-1}$ (decaying away from the surface). This scaling is well-known as the ‘Law of the wall’ (LOW):

$$\epsilon_{\text{LOW}}(z) = \frac{u_*^3}{\kappa |z|}. \quad (2.12)$$

This balance between $\epsilon$ and the work of the Reynolds stress against the vertical, mean current shear has been found in many studies (Dillon et al., 1981; Oakey and Elliott, 1982; Soloviev et al., 1988; Lombardo and Gregg, 1989). The LOW describes the shear-driven turbulence only. Convection, which is driven by the heat loss at the ocean surface, provides an additional source of turbulence. By arguing that both wind stress and convection enhance $\epsilon$ Lombardo and Gregg (1989), hereafter LG89, added the buoyancy flux at the surface $B_0$ to the LOW scaling argument. They found that $\epsilon$ measured in the Pacific during the Patches Experiment (PATCHEX) was well described by the similarity scaling, as:

$$\epsilon_{\text{LG89}} = 0.87 \cdot (1.76 \epsilon_{\text{LOW}} + 0.58 B_0), \quad (2.13)$$

with $B_0 = \frac{Q_\rho}{c_{pw}}$ following Brainerd and Gregg (1993), where $Q_\rho = \alpha_\rho \frac{Q_{\text{net}}}{c_{pw}} + \beta_\rho \frac{S_0 Q_{\text{lat}}}{(1 - S_0)L_e}$ is the surface density flux, $Q_{\text{net}}$ the net heat flux at the surface, which is the difference between the net longwave radiation $LW_{\text{net}}$, sensible $Q_{\text{sen}}$, latent heat fluxes $Q_{\text{lat}}$, and the net shortwave radiation $SW_{\text{net}}$, $\alpha_\rho$ and $\beta_\rho$ are the thermal expansion and saline contraction coefficient respectively, $c_{pw}$ the specific heat of water at constant pressure, $L_e$ is the latent heat of evaporation, and $S_0$ is the surface salinity. The buoyancy flux is defined positive into the ocean.

In a situation of pure convection, without any momentum flux, turbulence is driven solely by the buoyancy flux. In this case, $\epsilon$ is assumed to be uniform in the entire mixing layer (Shay and Gregg, 1986; Peters et al., 1988).

The assumption that the ocean surface is a shear-driven wall layer is overly simplistic, as the presence of waves creates more complex dynamics. Observations of $\epsilon$, which are 1-2 orders of magnitude higher than expected from the LOW scaling were found at the air-sea interface (Kitaigorodskii et al., 1983; Agrawal et al., 1992; Anis and Moum, 1995; Terray et al., 1996; Drennan et al., 1996; Greenan et al., 2001; Soloviev and Lukas, 2003; Gemmrich and Farmer, 2004; Feddersen et al., 2007). This enhanced turbulence is explained by the presence of breaking waves and their influence on a shallow layer with
a depth of the order of the significant wave height $H_s$ (Terray et al., 1996).

### 2.2.2 Wind-Wave-Induced Turbulence

To account for wave breaking at the ocean surface the energy input from the wind to the waves $F$ can be determined. In their turbulent closure model, Craig and Banner (1994) parameterised $F$ as $F = \alpha u^3$ measured in water-side quantities with $\alpha$ being a constant. Craig and Banner (1994) found that the TKE flux is relatively insensitive to sea state and $\alpha \approx 100$ for wave ages from very young wind seas to fully developed seas. To introduce turbulence injected from the waves themselves rather than the wind alone, Gemmrich et al. (1994) introduced an effective wave speed $c$. This $c$ corresponds to the speed of the waves transferring the most energy to the ocean. By arguing that the wind stress is transferred to the ocean on particular scales, they define $F = cu^2$. Gemmrich et al. (1994) determined $c$ to be dominated by the short wind waves and found $c \approx 1$ m s$^{-1}$. These formulations of $F$ are evaluated by Thomson et al. (2016) using a comprehensive data set gained from several Surface Wave Instrument with Tracking (SWIFTs) in the North Pacific.

To account for waves in scaling $\epsilon$ with depth, Terray et al. (1996), hereafter T96, considered both expressions of $F$ and applied it to $\epsilon$ data collected in Lake Ontario. They divided the vertical decay structure of $\epsilon$ under breaking waves into three depth-dependent regions. Directly beneath the water surface down to a ‘breaking depth’ $z_b = 0.6 H_s$, with $H_s$ being the significant wave height, there is a layer which is directly influenced by wave breaking. In this ‘breaking layer’, $\epsilon$ is assumed to be constant and an order of magnitude larger than predicted by the LOW. The energy of this ‘breaking layer’ is dissipated downward to a ‘transition depth’, $z_t = 0.3 H_s \frac{u^2}{u_{sa}}$, where $u_{sa}$ is the air-side friction velocity. The air-side and water-side friction velocities are related via the law of momentum conservation via $u_{sa}^2 \rho_a = u_s^2 \rho$ with $\rho_a$ and $\rho$ being the air-side and water-side densities, respectively. Within the ‘transition layer’ $\epsilon$ behaves as:

$$\frac{\epsilon H_s}{F} = 0.3 \left( \frac{|z|}{H_s} \right)^b,$$

where $b = -2$ in T96.
Substituting $F = \alpha u^3$ into Eq (2.14), leads to

$$\frac{\epsilon H_s}{u_s^3} = 0.3\alpha \left( \frac{|z|}{H_s} \right)^b.$$  

(2.15)

Using the data from T96 and Drennan et al. (1996), Wang and Huang (2004) formulated $\alpha$ as a function of the wave age $c_p/u_s$:

$$\alpha = \begin{cases} 
0.5 \left( \frac{c_p}{u_s} \right) \left( \frac{\rho_w}{\rho_a} \right)^{1/2} & \text{for } c_p/u_s \leq 11 \\
12 \left( \frac{c_p}{u_s} \right)^{-1/3} \left( \frac{\rho_w}{\rho_a} \right)^{1/2} & \text{for } c_p/u_s > 11,
\end{cases}$$

(2.16)

where $c_p$ is the wave speed and $\alpha$ increases for waves younger than 11 but decreases for older ones.

T96 found that below the ‘transition layer’ local shear production dominates and $\epsilon$ follows the behaviour of a shear-driven flow, proportional to $z^{-1}$:

$$\epsilon_{T96}(z) = \begin{cases} 
0.3 \left( \frac{u_s}{u_s} \right)^2 \left( \frac{z_b}{H_s} \right)^{-2} & \text{above } z_b \\
0.3 \left( \frac{u_s}{u_s} \right)^2 \left( \frac{|z|}{H_s} \right)^{-2} & \text{between } z_b \text{ and } z_t \\
\left( \frac{u_s}{\kappa |z|} \right)^2 & \text{below } z_t
\end{cases}$$

(2.17)

This scaling suggested by T96 has been supported by several studies under different environmental conditions (Drennan et al., 1996; Greenan et al., 2001; Feddersen et al., 2007; Jones and Monismith, 2008; Gerbi et al., 2009; Shuiqing and Dongliang, 2016). Drennan et al. (1996) argued that $H_s$ should be calculated from the wind sea part of the wave spectrum only, under the assumption that swell does not break.

**Wave-Turbulence-Interaction**

Using a vertically rising profiler in the Pacific Ocean, Anis and Moum (1995) observed $\epsilon$ profiles which decayed exponentially with depth. They attributed the enhanced values of $\epsilon$ to breaking waves and wave-turbulence interactions. Huang and Qiao (2010), hereafter HQ10, neglected the buoyancy term in Eq (2.6) and expressed the mean flow by the Stokes drift $u_s$. The Stokes drift is a net drift in the down-wave direction caused by the open (non-circular) orbital particle motion in the wave field (Stokes, 1847).
HQ10 used the Stokes drift expression for a monochromatic wave:

\[ u_s = u_{s0} e^{2\ell z}, \]  

(2.18)

where \( u_{s0} \) is the magnitude at the ocean surface, which is \( u_{s0} = c_p (a\ell)^2 \), where \( a \) is the wave amplitude, such that \( u_s \) can be determined from the wave spectrum. HQ10 use the vertical shear to express a corresponding dissipation rate as:

\[ \epsilon_{HQ10}(z) = a_l u_s^2 \frac{\partial u_s}{\partial z}, \]  

(2.19)

where \( a_l \) is a dimensionless constant associated with the surface waves. This constant was determined through data regression by HQ10 using the data of Anis and Moum (1995) as:

\[ a_l = 3.75 \beta \pi \sqrt{\frac{H_s}{\lambda}}, \]  

(2.20)

where \( \lambda \) is the dominant wavelength and \( \beta \) is an empirical constant between 0 and 1. The values of \( \beta \) were determined by fitting the equation to various \( \epsilon \) measurements of Anis and Moum (1995).

Using Eq (2.18) to describe the Stokes drift, Eq (2.19) can be rewritten as:

\[ \epsilon_{HQ10}(z) = 2 a_l u_s^2 u_{s0} \ell e^{-2\ell z}. \]  

(2.21)

Alternatively, the Stokes drift in Eq (2.18) can be calculated separately for the windsea and swell part of the wave spectrum. Sutherland et al. (2013) showed that the performance of the scaling suggested by HQ10 could be improved when scaling profiles of \( \epsilon \) as the sum of both separately determined expressions.

It should be noted that for small \( \ell |z| \ll 1 \), Eq (2.18) results in

\[ \frac{\partial u_s}{\partial z} \propto \frac{1}{1 + 2\ell |z| + 2(\ell z)^2}, \]  

(2.22)

hence the HQ10 parametrisation should fall somewhere between the LOW and the scaling expression of T96, depending on the average wavelength.

Compared to the Stokes drift profile for a monochromatic wave Breivik
et al. (2016) proposed a new approximation for the Stokes drift velocity based on the exact solution for the Phillips (1958) spectrum, which has a much stronger gradient near the ocean surface. The shear of the Stokes drift velocity determined for the Phillips spectrum is:

\[
\frac{\partial u_s}{\partial z} = \alpha_p \sqrt{-\frac{2\pi g}{z}} \text{erfc}(\sqrt{-2\ell z}),
\]

where \(\alpha_p = 0.0083\) is the Phillips’ parameter and \(\text{erfc}\) is the complementary error function, which is defined for an arbitrary \(x\) as \(\text{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2} \, dt\).

### 2.2.3 Combinations of Wind, Wave, and Buoyancy Mixing

In order to determine the depth of the OSBL in global climate models and to include surface-wave processes that force Langmuir turbulence, Belcher et al. (2012), hereafter B12, took wind, buoyancy, and waves as sources for ocean turbulence into account. Each of the three mechanisms produces a distinct type of turbulence with its own scaling laws. B12 formulates \(\epsilon\) as a linear combination of these generation mechanisms at a depth of \(h/2\), where \(h\) is the mixed layer depth (MLD),

\[
\epsilon_{B12}(z/h = 0.5) = 2 \left(1 - e^{-0.5\sqrt{\text{La}_t}}\right) \frac{u_s^2}{h} + 0.22 \frac{u_{sL}^3}{h} + 0.3 \frac{w_s^3}{h},
\]

where \(w_s = (B_0h)^{1/3}\) is the scaling velocity for buoyancy-forced turbulence and only defined for positive \(B_0\), \(\text{La}_t^2 = \frac{w_s}{u_s}\) is the turbulent Langmuir number, which expresses the ratio of turbulence production due to wind- and wave forcing (McWilliams et al., 1997), and \(u_{sL} = (u_s^2 u_0)^{1/3}\). This scaling approach applies under uniform and steady conditions.

Sutherland et al. (2014a) showed that the most appropriate length scale for \(h\) was the mixing layer depth (XLD), which provided better results than the widely used MLD. The MLD describes the integration of all past mixing events, and is commonly determined as the layer of homogenous density. The XLD, in comparison, is the depth of the ocean surface layer of current active mixing. It is defined as the depth at which \(\epsilon\) falls to a level of \(\epsilon = 10^{-9} \, \text{m}^2 \, \text{s}^{-3}\) (Brainerd and Gregg, 1995; Sutherland et al., 2014b). The depth of the XLD is referred to as \(h_{\epsilon}\) in the following. The XLD and MLD are approximately the same under steady-state conditions, but differ under varying conditions.
2.3 Gas Exchange at the Air-Sea Interface

2.3.1 Principles

Air-sea gas exchange occurs through a thin interface layer between the ocean and the atmosphere. The concentration gradient across this layer determines the gas flux between both systems. The magnitude and direction of the gas flux $F_g$ at the interface are typically determined by the air-sea difference in the partial pressure of a particular gas $\Delta P$ and by the transfer velocity $K$. The transfer velocity describes the efficiency in the transport process using the following equation:

$$F_g = K \cdot s_g \cdot \Delta P,$$

(2.25)

where $K$ is the total gas transfer velocity, and $s$ is the solubility of a gas, which can be determined from sea surface temperature and salinity (Weiss, 1974; Wanninkhof et al., 2009). High precision field measurements of $\Delta P$ are readily available (e.g. Bakker et al., 2016; Watson et al., 2009; Lana et al., 2011), but direct measurements of $F_g$ are more challenging, and $K$ is frequently parameterised as a function of wind speed.

$K$ combines the effects of processes at the air as well as the water side of the air-sea interface. The inverses of the transfer velocities are the gas transfer resistances. The air-side and water-side resistances can be added to obtain the total resistance:

$$\frac{1}{K} = \frac{1}{k_a} + \frac{1}{k_w},$$

(2.26)

where $k_a$ and $k_w$ denote the air-side and the water-side gas transfer velocity expressed in the same units (typically of the water side gas transfer velocity).

Sparingly soluble gases such as CO$_2$ and DMS are water-side limited and mostly $k_a \gg k_w$; therefore $K \approx k_w$. In the following the water-side gas transfer velocity is referred to as $k$.

2.3.2 Wind Speed-Based Parameterisations

The most commonly used parameterisations of $k$ are based on functions of wind speed normalised to 10 m height: $k = f(u_{10N})$ (Liss and Merlivat,
Wind speed is a readily available parameter from both in-situ and satellite observations and directly or indirectly influences most of the physical processes controlling air-sea gas exchange. However, the most commonly used parameterisations are empirical fits to observations of $k$ and do not rely on the underlying physics of the exchange process. Wanninkhof (1992) used the global bomb $^{14}$C data and combined it with global averaged wind speeds to which he scaled a quadratic relationship $k = f(u_{10})$. This and further global quadratic relations feature a zero intercept (Nightingale et al., 2000; Sweeney et al., 2007), which leads to the assumption of zero gas exchange at low wind speeds. It is known however, that buoyancy effects, chemical enhancement, surface waves, and micro breaking events force gas exchange to occur even at low wind speeds (e.g. Sutherland and Melville, 2015; Wang and Liao, 2016). McGillis et al. (2001, 2004) accounted for these effects by adding a constant value of $k$ to wind speed-based parameterisations. Additionally, bubble entrainment and breaking waves at high wind speeds lead McGillis et al. (2001) to propose a cubic instead of quadratic wind speed dependence of $k$.

The empirical wind speed-based relations allow for approximate estimates of $k$, but they do not incorporate the complexity of the physics at the air-sea interface. Therefore, a physically-based parametrisation is desirable. The National Oceanic and Atmospheric Administration/Coupled-Ocean Atmospheric Response Experiment (NOAA/COARE) air-sea gas transfer algorithm (Fairall et al., 2000), which is based on the COARE Bulk Flux Algorithm (Fairall et al., 1996b) with additional implication of the surface renewal theory (Soloviev and Schlüssel, 1994) incorporates physical mechanisms of gas transfer to calculate $k$ from readily available input variables.

### 2.3.3 Relation of Gas Exchange to Ocean Near-Surface Turbulence

On the water-side, the exchange of gas across the air-sea interface is determined by the interplay of molecular and turbulent transport processes immediately below the interface. These fluxes are eventually limited by molecular diffusion across the diffusive boundary layer. By reducing the thickness of the diffusive boundary layer, random occurrence of turbulent
eddie intensify the gas transfer velocity $k$. 

Parameterising $k$ directly with $\epsilon$ offers an opportunity to fulfil the requirement of a physically-based parametrisation, as turbulence is the major physical mechanism that controls $k$ (e.g. Wanninkhof et al., 2009). Lamont and Scott (1970) derived a direct relation between $k$ and surface $\epsilon_0$ using the surface renewal theory (Higbie, 1935; Danckwerts, 1951). This theory describes periodic events of small eddies disturbing the sea surface with water from below (small-eddy model – SEM). Following Lamont and Scott (1970), $k$ can be parametrised by:

$$k = A \text{Sc}^{-n}(\epsilon_0 \nu)^{1/4}, \quad (2.27)$$

where $A$ is a proportionality constant, $\text{Sc} = \nu/D$ is the Schmidt number, which is defined as the ratio of $\nu$ to molecular diffusivity of the trace gas in water $D$, and $n$ is the Schmidt number exponent. Lamont and Scott (1970) formulated Eq (2.27) with a Schmidt number exponent of $n = \frac{1}{2}$ by predicting the time scales in the surface renewal gas/liquid transport model. For flat surfaces, which behave hydrodynamically analogous to solid/liquid interfaces, a Schmidt number exponent of $n = \frac{2}{3}$ is assumed (Davies, 1972). Flat surfaces can exist for open ocean conditions under either very low-wind conditions or in the presence of surface films at low to medium wind speeds. In reality, the sea surface might be partially covered with surfactants and waves might occur in different stages. Thus, $n$ can be assumed to vary between $\frac{1}{2}$ for a wavy, surfactant-free surface and $\frac{2}{3}$ for a flat surface depending on the conditions (Deacon, 1977; Jähne et al., 1987).

Studies in the field (Zappa et al., 2007; Tokoro et al., 2008; Vachon et al., 2010; Wang et al., 2015; Gällfalk et al., 2013) and in laboratories (Asher and Pankow, 1986; Moog and Jirka, 1999) have shown the SEM to hold well in various conditions. Measurements of $k$ and $\epsilon$ have been carried out in rivers, lakes, estuaries, coastal oceans, and the model-world Biosphere 2, under a wide range of forcings from wind, tides, and rain (Gällfalk et al., 2013; Zappa et al., 2007; Tokoro et al., 2008; Vachon et al., 2010; Wang et al., 2015). The instrumental setup varied for the different studies, and $\epsilon$ was measured at various depths below the surface. This causes the studies to observe different proportionalities within the SEM, represented in $A$. No investigations have been carried out in the open ocean relating $k$ to $\epsilon$. 

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2.3.4 Schmidt Number and Schmidt Number Exponent

The Schmidt number is a dimensionless number, named after Ernst Heinrich Wilhelm Schmidt, representing the ratio of the kinematic viscosity $\nu$ to the mass diffusivity $D$:

$$Sc = \frac{\nu}{D}. \quad (2.28)$$

In contrast to the low $Sc$ in the air, water-sided $Sc$ are much larger because of the low gas diffusivity $D$ in water.

The Schmidt number can be related to $k$ as follows. Fick’s law of diffusion, which states that the flux density $J$ of a tracer being forced by molecular diffusion is proportional to the concentration gradient. This law can be extended to also account for turbulent transport:

$$J = -(D + K_C) \frac{\partial C}{\partial z}, \quad (2.29)$$

where $D$ and $K_C$ are the molecular and turbulent diffusion coefficients, respectively. In case of stationary and homogeneity, where no chemical sources or sinks exist, $J$ points in the vertical and is constant. Integration of Eq (2.29) yields:

$$R = \frac{C(z_\gamma) - C(0)}{J} = \int_0^{z_\gamma} \frac{1}{D + K_C(z)} dz, \quad (2.30)$$

where $R$ is the resistance, which is equal to $1/k$. The profile of $K_C$ close to the air-sea interface depends on the sea surface conditions. For a smooth solid wall, $K_C(z)$ can be described by the Reichhardt approach (Reichardt, 1951). This approach describes $K_C(z)$ as $K_C \propto z^3$ close to the surface and changes to a linear relation at larger depth. For a free and wavy surface, the turbulent diffusivity increases with the distance squared ($K_C \propto z^2$) (Jähne, 2009). Integrating Eq (2.30) using these descriptions of $K_C(z)$ yields the gas transfer velocity $k$ proportional to the Schmidt number:

$$k \propto \begin{cases} Sc^{-2/3} & \text{for a smooth surface} \\ Sc^{-1/2} & \text{for a wavy surface} \end{cases}, \quad (2.31)$$

where $n = \frac{1}{2}$ and $n = \frac{2}{3}$ give the theoretical limits of the Schmidt number.
exponent $n$ for a film-covered smooth and a completely wavy ocean surface, respectively (Deacon, 1977; Jähne et al., 1987). Using the dual-tracer method, the change from $n = \frac{2}{3}$ for a film-covered surface to $n = \frac{1}{2}$ for a wave-covered surface was verified in tank experiments (Jähne et al., 1985, 1987). For a Schmidt number of 660, this leads to an increase of $k$ by a factor of 3.

As it is difficult to measure $n$ in the field, most studies that concentrate on the relation between $\epsilon$ and $k$ assume $n = \frac{1}{2}$ (Zappa et al., 2007; Tokoro et al., 2008; Vachon et al., 2010; Gålfalk et al., 2013; Wang et al., 2015). None of the empirical gas transfer models consider the transition of $n$. Even though the exact shape of the transition from $n = \frac{2}{3}$ to $n = \frac{1}{2}$ is not known, laboratory studies indicate this transition to occur smoothly. The transition has been described as a function of mean square slope (total variance of the sea surface slope), the friction velocity, and wind speed (Krall, 2013; Richter and Jähne, 2011; Jähne and Haußecker, 1998). Krall (2013) used the Aeolotron circular flume at the University of Heidelberg to investigate the transition of $n$ based on $u_*$ in the presence of surfactants (Fig. 2.4 with $u_*$ transferred to $u_{10}$). For each of the three surfactant conditions (clean surface; medium surfactant coverage with 0.052 µmol/l Triton; and high surfactant coverage with 0.26 µmol/l Triton), they found different relations of $n = f(u_*)$. For a clean water surface, $n = \frac{2}{3}$ is reached for the lowest $u_*$ and the transition towards $n = \frac{1}{2}$ is the smoothest. For higher surfactant
coverage, the relation becomes steeper and the onset is shifted to higher \( u_* \) values. The friction velocity \( u_* \) and wind speed \( u_{10} \) are closely related and can be determined from each other using the TOGA-COARE model.

### 2.4 Diurnal Warming

Solar radiation is a major determinant of the Earth’s climate and influences the Earth’s global and local energy budget. The amount of radiation incident at a particular site of the Earth experiences diurnal and seasonal variations. This diurnal cycle of solar radiation directly affects the sea surface temperature SST. As SST and surface salinity affect the concentration of aqueous \( \text{CO}_2 \) (and other gases) through their effect on solubility (Woolf et al., 2016), knowledge about it’s diurnal variability is essential for correct estimates of the air-sea gas exchange (Webster et al., 1996; Bellenger and Duvel, 2009; Ward et al., 2004).

#### 2.4.1 Diurnal Warm Layer

During the night, heat loss at the ocean surface causes convection, which deepens the MLD gradually down to depths in the order of 100 m. During the day, incoming solar radiation heats the ocean surface layer, with the net surface heat flux being defined as:

\[
Q_{\text{net}} = SW_{\text{net}} - Q_{\text{lat}} - Q_{\text{sen}} - LW_{\text{net}},
\]

where \( Q_{\text{lat}} \) is the latent heat flux, \( Q_{\text{sen}} \) is the sensible heat flux, \( SW_{\text{net}} \) is the shortwave radiation, and \( LW_{\text{net}} \) is the net longwave radiation. If the downwelling radiation is strong enough, the skies are clear, and wind speeds are low (< 5m/s) (Soloviev and Lukas, 1997; Eastwood et al., 2011), vertical mixing at the ocean surface and downward dissipation of heat is restricted. This causes the solar heating to create a distinct, stably stratified warm layer (e.g. Price et al., 1986; Sverdrup et al., 1942; Flament et al., 1994; Merchant et al., 2008; Brainerd and Gregg, 1993). The thickness of this warm layer depends on the prevailing vertical turbulent mixing and is observed from orders of a few centimetres (very low winds) to meters (e.g. Fairall et al., 1996a; Soloviev and Lukas, 1997). Beneath the warm layer,
the diurnal thermocline links the higher temperatures at the surface with the so-called foundation temperature below as shown in Fig. 2.5 (where the foundation temperature is shown as SST\textsubscript{fnd}). The foundation temperature is the minimum of the day’s temperature close to local midnight and thus corresponds to temperatures at minimum insolation. The diurnal warming amplitude is the difference between maximum SST and the foundation temperature. This amplitude can reach values of more than 6 °C (Gentemann \textit{et al.}, 2008), though in general, is of the order of several 0.1 °C (Kawai and Wada, 2007; Merchant \textit{et al.}, 2008; Stuart-Menteth \textit{et al.}, 2003; Kennedy \textit{et al.}, 2007). Stable stratification in this layer inhibits heat and momentum input within the diurnal warm layer from mixing into the MLD below.

In higher-wind conditions, however the surface ocean gets mixed, which causes the magnitude of the diurnal warm layer and density stratification to decrease (Gentemann \textit{et al.}, 2003). Furthermore, the wind mixies the solar heating into the ocean to reach greater depths (Price \textit{et al.}, 1986). In even stronger wind conditions, no warm layer will evolve at the ocean surface as the stronger turbulence levels prevent any thermal stratification from occurring. Therefore, the diurnal warming of the surface ocean and the evolution of a diurnal warm layer depends on prevailing wind conditions, as

![Figure 2.5: Schematic diagram showing idealised vertical temperature deviations from the foundation temperature, SST\textsubscript{fnd}, during (a) nighttime and (b) daytime conditions (reprinted from Donlon and the GHRSST-PP Science Team, 2005).](image-url)
Diurnal warming events with moderate diurnal SST amplitudes (∼2 °C) are observed to have an horizontal extension in $O$ (60 km) (Merchant et al., 2008). As the magnitude of the diurnal-warming event increases, the horizontal length scale decreases.

### 2.4.2 Local Coverage

The characteristics of the diurnal cycle vary in different regions and for different seasons. Several studies have examined diurnal surface warming in specific regions. Diurnal warming events in warmer seas are well studied by in-situ and satellite observations (e.g. Kudrayavtsev and Soloviev, 1990; Webster et al., 1996; Soloviev and Lukas, 1997; Clayson and Weitlich, 2005; Kawai et al., 2006; Clayson and Weitlich, 2007; Stuart-Menteth et al., 2003). These studies focus on areas where the diurnal SST amplitudes are particularly high, which are mainly found in low and mid-latitudes. The largest diurnal temperature differences are found in the western Pacific warm pool, the summer-hemisphere sub-tropics, and the Indian Ocean (Kennedy et al., 2007).

Variations in the diurnal SST within the tropical Pacific are investigated profoundly, which are for example attributed to the Tropical Ocean Global Atmosphere (TOGA) COARE project (e.g. Soloviev and Lukas, 1997). In other parts of the Pacific several studies have focused on diurnal warming events (e.g. Price et al., 1986). Further areas of high interest are the marginal seas around Japan, where large diurnal SST variations are frequently found (Kawai and Kawamura, 2000, 2002) or the mid-latitudes such as the North Sea (e.g. Gentemann et al., 2008; Merchant et al., 2008).

As in-situ observations are either temporal or spatial limited, or both, they mainly focus on the investigation of diurnal surface warming events in certain regions. Operational satellite SST observations starting in the 1980s, began to explore the variation in the diurnal SST with increased spatial coverage (Gentemann et al., 2003; Stuart-Menteth et al., 2003). Therefore, satellite observations provide the opportunity to determine the horizontal scales and distribution of diurnal warming events. In addition, they allow for global studies of diurnal warming including high latitudes (Stuart-Menteth et al., 2003; Kennedy et al., 2007; Kawai and Wada, 2007; Eastwood et al., 2011). However, the disadvantage of these satellite measurements is that...
they can only provide single snapshots in time. This complicates to study
the temporal evolution of diurnal cycles. Furthermore, they cannot provide
information of subsurface temperature profiles.

There are neither many in-situ nor satellite studies that have focused on
diurnal warming in high latitudes (Eastwood et al., 2011). The difficulties for
such studies in the Arctic are based on challenges for SST satellite retrievals
due to sea ice conditions and high cloud coverage. Nevertheless, diurnal
warming cycles which reach SST amplitudes of several degrees are observed
in the Greenland Sea, the Norwegian Sea, the Barent Sea, and the Kara Sea
during summer up to 80 °N (Eastwood et al., 2011). This under-sampling
of diurnal cycles in the Arctic is critical as the Northern Seas are crucial
for the discussion about climate change. In this region dense water masses
are formed by deep convection, which drives the meridional overturning
circulation.

2.5 Internal Waves

Internal waves may be most prominent due to their reputation of causing
the so-called dead-water phenomenon (e.g. Mercier et al., 2011). The
phenomenon, which was experienced by F. Nansen (Nansen, 1897) and later
explained by V. W. Ekman describes the situation, when a boat travelling
on a two-density-layer ocean experiences an additional drag due to internal
waves being generated at the interface between both layers, while the ocean
surface stays wave-free.

Internal waves occur in a density-stratified ocean because of gravitational
restoring forces acting on a vertical density perturbation. The larger the
ocean’s density gradient, the higher its perturbation frequency. The formed
internal waves propagate along density disturbances with wavelengths that
are much larger than those of surface gravity waves, as in the case of internal
waves, the restoring force is buoyancy rather than gravity.

An important parameter associated with internal waves is the buoyancy
frequency \( N(z) \), known as the Brunt-Väisälä frequency (Brunt, 1927). This
frequency is determined by the ratio of the restoring forces trying to return
the perturbed water parcel to its equilibrium density position (in the case
of internal waves being proportional to the vertical density gradient), to
the inertial forces (in the case of the internal waves are proportional to the density itself).

A small water parcel with density $\rho_p$ is displaced vertically upwards from an environment with a density $\rho = \rho(z)$ to a depth level of $z + z'$ (Fig. 2.6). At this new environment, the parcel will feel an additional gravitational force and its motion will be controlled by:

$$\rho_p V a_n = \rho(z) V g - \rho(z + z') V g$$

$$\rho_p \frac{\partial^2 z'}{\partial t^2} = -g(\rho(z) - \rho(z + z')),$$

(2.33)

where $V$ is the volume of the water parcel and $a_n = \frac{\partial^2 z'}{\partial t^2}$ the acceleration. Using a linear approximation to $\rho(z + z') - \rho(z) = \frac{\partial \rho(z)}{\partial z} z'$ leads to:

$$\frac{\partial^2 z'}{\partial t^2} = -\frac{g}{\rho_p} \frac{\partial \rho(z)}{\partial z} z'.$$

(2.34)

Therefore, $\frac{g}{\rho_p} \frac{\partial \rho(z)}{\partial z} z'$ is the upward acceleration of the parcel. If $\frac{\partial \rho}{\partial z} > 0$, density is upwardly increasing, acceleration is positive, and the parcel will move further upwards. This situation describes an unstable stratification, where small disturbances can grow. If $\frac{\partial \rho}{\partial z} < 0$, density is downwardly decreasing, stratification is stable, and the motion following an upward displacement of a small water parcel is oscillatory with the buoyancy frequency:

Figure 2.6: Schematic of a water parcel, which is vertically displaced from its environment (depth $z$) to a depth $z + z'$. 
\[ N = \sqrt{\frac{g}{\rho_p} \frac{\partial \rho(z)}{\partial z}}, \]  

(2.35)

where, \( N \) characterises the local density stratification. The larger \( N \) is, the more stable the water column is and internal waves can exist only in stable conditions.

### 2.5.1 Internal Wave Breaking

Internal waves can propagate thousands of kilometres through the ocean and eventually overturn and break (Ray and Mitchum, 1996). This breaking can take place in various different ways. Slopes, for example, are an important topographic feature for internal wave breaking (Cacchione et al., 2002; Legg and Adcroft, 2003; Martini et al., 2013). In addition, shear instabilities triggered by the shear flows induced through the internal waves themselves, or convectively unstable wave cores can lead to the breaking of internal waves, as well as instabilities in the bottom boundary layer (summarised in a review paper by Lamb, 2014).

During the breaking process energy is dissipated. The energy related turbulent mixing affect circulation, heat transport, nutrient distribution, and biological activity (Gregg, 1987). These breaking processes and the associated enhancement in \( \epsilon \) usually occur on sub-grid scales in regional and global ocean models. Accurate parametrisation and knowledge of internal wave breaking processes is thus important.

### 2.5.2 Internal Wave Breaking in the Upper Ocean

Internal waves can exist in the upper ocean away from any topographic features. Here, they can play an important role in mixing processes that occur through the pycnocline (Barton et al., 2001; Dewey et al., 1999). However, well-resolved direct observations of breaking waves in the upper ocean are rare. Wain et al. (2015) observed a breaking internal wave using ASIP measurements of the OSBL from the Labrador Sea. This wave breaking was associated with levels of \( \epsilon \) that were increased by 2-3 orders of magnitude relative to background levels.

In the surface layer of the open ocean in the absence of slopes, tides, and
ocean bathymetry, internal waves can break based on small differences in density of two overlying layers through two types of instabilities. The first type are convective instabilities, which occur when the isopycnals between wave crests and troughs steepen (Fig. 2.7). At some stage, these isopycnals can assume a vertical position. This results in a situation where denser water overlays lighter water and thus causes local density overturning (Bouruet-Aubertot et al., 2001; Koudella and Staquet, 2006; Sutherland, 2001). The second type are shear instabilities often referred to as Kelvin-Helmholtz instabilities, which occur when a disturbance in the shear of an internal wave grows.

Enhanced values of $\epsilon$ are observed for both types of instabilities, which, however show different pattern (Moum et al., 2003; Wain et al., 2015; Zhang and Alford, 2015). Convective instabilities are associated with elevated $\epsilon$ distributed throughout the wave core (Fig. 2.8b). Shear instabilities are associated with elevated dissipation concentrated at the sheared interface itself (Fig. 2.8a) (Zhang and Alford, 2015). The differentiation between both types of instabilities is not always clear: when the fluid velocity within the internal wave increases with increasing wave steepness, the shear between the two density layers increases simultaneously. Therefore, both a convective instability and a shear instability are likely to occur simultaneously. By studying over 318 internal waves, Zhang and Alford (2015) found that shear instabilities are more common and usually provide more mixing per wave. Focusing on the instabilities of breaking internal waves, the Richardson number $Ri$ is an important non-dimensional number:

$$Ri = \frac{N^2}{(du/dz)^2}; \quad (2.36)$$
with the shear $du/dz$ being the gradient of the horizontal current component $u(z)$. Following Thorpe (2007), the Miles-Howard theorem (Miles, 1961; Howard, 1961) states, that instabilities in a steady, inviscid, non-diffusive, two-dimensional, parallel horizontal flow can only be generated when $Ri < 0.25$. The flow field is considered to be stable if $Ri$ is larger than this threshold for all depths levels of the flow. However, if $Ri$ is smaller than a quarter the flow does not necessarily contain any instabilities. Therefore, for some density and velocity conditions instabilities may only occur at $Ri$ smaller than a quarter.

The Miles-Howard theorem is only valid in the afore-mentioned very specific flow conditions and thus only for steady flows. To relate it to internal waves, one has to assume that the flow field produced by the internal waves varies relatively slowly with time. The time that it takes for disturbances to grow is very small, relative to the wave period of the internal wave. In non-steady flow conditions caused by the internal waves, the $Ri$ at which small disturbances start to grow must be substantially less than the threshold value of $1/4$, of the equivalent steady flow.

Internal waves produce shear, locally reducing the $Ri$ and occasionally leading to instability or wave breaking (as described by Troy and Koseff, 2005). This wave breaking can create local patches of turbulence. Fringer and Street (2003) use the $Ri$ within a wave to determine the initial instability of an internal wave breaking process for waves propagating along a finite-thickness interface between two density layers. They use results from numerical

Figure 2.8: Schematic description of shear (a) and convective (b) instabilities in internal waves (reprinted from Zhang and Alford, 2015)
simulations to show that the type of instability depends on the thickness of the interface relative to the wavelength of the respective internal wave. To distinguish between convective and shear instabilities, they determine the critical breaking steepness \( \ell a_c \), where \( a_c \) is the critical wave amplitude, as a function of the interface thickness of the waves \( \ell \delta \), where \( \delta \) is a measure of the interface thickness. This \( \delta \) is defined by Troy and Koseff (2005) as a measure of the 99% density interface thickness.

As a result, Fringer and Street (2003) found that the initial instabilities of breaking internal waves for \( \ell \delta \leq 2.33 \) is based on shear. For internal waves with \( 0.31 < \ell \delta < 0.56 \), the Kelvin-Helmholtz instabilities grow without being impeded by the internal wave itself and do not induce a convective instability. Internal waves propagating along a thicker interface (shorter waves with \( 0.56 < \ell \delta < 2.33 \)) develop more energetic Kelvin-Helmholtz billows. In this case the billows reduce the phase speed of the wave and lead to a convective instability (a mixed shear-convective instability). When the interface thickness is too large, Kelvin-Helmholtz billows do not form and the instability is purely convective. Troy and Koseff (2005) completed the \( \ell \delta \) range covered by Fringer and Street (2003) for low-\( \ell \delta \) with \( 0 < \ell \delta < 0.3 \). For these internal waves, they found that wave breaking occurs due to shear instabilities. This wave breaking starts at a critical wave steepness which depends on the wavenumber and the amplitude of the wave \( a \) as \( \ell a \approx \sqrt{2 \ell \delta} \).

In cases of low resolved shear measurements, the determination of a relevant Ri may be complicated and cannot be used as a predictor for the generation of shear instabilities. For this situation, Zhang and Alford (2015) use the non-dimensional Froude number (\( Fr= u/c_p \)) to distinguish between shear and convective instabilities. A \( Fr \) smaller than unity predicts non-convective shear instabilities and a \( Fr \) larger than unity predicts convective instabilities (Fig. 2.8b).
3 Data Acquisition and Observations

This chapter describes the data included in the analysis of this thesis. In addition, the chapter presents how this data was measured and processed.

The field campaigns are presented in Sec. 3.1. As this thesis focuses on turbulence measurements gained with the Air-Sea Interaction Profiler (ASIP), the processing of these upper-ocean measurements is described in detail in Sec. 3.2. Section 3.3 describes the data acquisition of the gas transfer velocity, which is essential for the analysis in Chapter 4. Section 3.4 presents measured and modelled wave information, that are important for the $\epsilon$ scaling in Chapter 5. The modelled wave data is compared to actual wave measurements in Sec. 3.4.1.

3.1 Field Observations

The analysis of this thesis includes data conducted during six research campaigns (see a summary in Tab. 3.1 and their position in Fig. 3.1). ASIP was deployed during five of these cruises, which allows the inclusion of turbulence measurements into the analysis*. The $\epsilon$ data from these five cruises is shown in Fig. 3.2f. The total data is shown as a time series based on the cumulative time during which ASIP was profiling. In addition, the meteorological and wave conditions are presented that were conducted at the same time of the ASIP profiles. The different cruises are separated by blue vertical lines (the respective deployments of ASIP by grey vertical lines) and their background colour.

The atmospheric parameters that are considered in this thesis consist of

*The author of this thesis participated in one of the presented field campaigns, namely the NICE cruise. There she learnt how to deploy ASIP under open ocean conditions.
Data Acquisition and Observations

Table 3.1: Presented field campaigns with name of the campaign, date, the ship, and the number of ASIP deployments during the campaign as well as the overall number of ASIP profiles per cruise.

<table>
<thead>
<tr>
<th>Campaign</th>
<th>Date</th>
<th>Ship</th>
<th>Deployments</th>
<th>Profiles</th>
</tr>
</thead>
<tbody>
<tr>
<td>Labrador</td>
<td>May 2010</td>
<td>CCGS Hudson</td>
<td>5</td>
<td>192</td>
</tr>
<tr>
<td>Knorr11</td>
<td>Jun-Jul 2011</td>
<td>RV Knorr</td>
<td>4</td>
<td>283</td>
</tr>
<tr>
<td>SOAP</td>
<td>Feb-Mar 2012</td>
<td>RV Tangaroa</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>STRASSE</td>
<td>Aug 2012</td>
<td>RV Thalassa</td>
<td>7</td>
<td>528</td>
</tr>
<tr>
<td>MIDAS</td>
<td>Apr 2013</td>
<td>RV Sarmiento</td>
<td>5</td>
<td>676</td>
</tr>
<tr>
<td>NICE</td>
<td>Sep 2014</td>
<td>RV Hakon Mosby</td>
<td>4</td>
<td>188</td>
</tr>
</tbody>
</table>

Wind, friction velocity, and insolation measurements. Direct measurements of the air-side friction velocity $u_a^*$ were only carried out during the Knorr11, the SOAP, and MIDAS campaign. The water-side friction velocity $u_*$ can be determined from $u_a^*$ via the law of momentum conservation ($u_a^* \rho_a = u_*^2 \rho$ with $\rho_a$ and $\rho$ being the air and water densities, respectively). For this reason, direct measurements of $u_*$ are used only in Chapter 4’s analysis, which focuses exclusively on data from the Knorr11 and SOAP campaign. The analysis in Chapter 5 considers a more extensive data set, which includes data from cruises (Labrador and NICE) during which measurements of $u_*$ and insolation were omitted. To account for this missing information, $u_*$ is calculated from wind speed measurements using the COARE algorithm (Edson et al., 2013; Fairall et al., 1996a, 2003). The missing information on the insolation are essential to determine the buoyancy flux, which is provided by the European Centre for Medium-Range Weather Forecasts (ECMWF) model.

3.1.1 Labrador Sea

The Canadian Coast Guard ship CCGS Hudson cruise took place in the Labrador Sea in May 2010 (Fig 3.1). The cruise was conducted as part of the springtime hydrographic section across the Labrador Sea, which is annually performed since 1990 by the Bedford Institute of Oceanography (Wain et al., 2015; Yashayaev and Loder, 2016). The aim of this cruise was to investigate
Figure 3.1: (a) Map showing the position of all the cruises from which data is used in this thesis. Maps showing the cruise tracks (red) and the ASIP deployments (orange circles) for (b) the Labrador cruise with the pink circle showing the ASIP deployment that it discussed in detail in Chapter 6, (c) Knorr11, (d) SOAP, (e) NICE, (f) STRASSE, and (g) MIDAS with the cyan circle showing the WHOI mooring.
Figure 3.2: Time series of the boundary conditions with cumulative hours of ASIP deployments on the x-axis. The different cruises are separated by their background colours and the different deployments by vertical lines. (a) Modelled (red) and measured mean period $T_m$ and inverse wave age $A_{iw}$ (black). (b) Surface buoyancy flux $B_0$ (red) and surface heat flux $Q_0$ (black). (c) Significant wave height $H_s$ for the full wave spectrum from wave observations (green) and from the ECWAM wave model (red) and the wind-sea part of the wave spectrum $H_s^{ws}$ (black). (d) The measured (black) and modelled (red) wind speed time series and the grey interface mixed layer depth $h_{\epsilon}$ calculated from the measured wave height $H_\epsilon$ and the friction velocity $u_\ast$ calculated from the COARE algorithm. (e) The modelled (red) and measured (green) water-side friction velocity $u_\ast$ and the eddy covariance determined from the measured friction velocity $u_\ast$ and the surface Stokes drift velocity $u_s$ (grey), and the buoyancy velocity $w_B$ (black). (f) Levels of TKE dissipation $\epsilon$ with overlaid mixing layer depth $h_{\epsilon}$ (red).
the thin freshwater cap, which spans over the entire Labrador Sea basin, shortly after the deepest convection period in March (Lilly et al., 1999). To observe this freshwater lens at the ocean surface, ASIP was deployed five times descending down to 100 m depth gaining a total of 192 profiles.

Unfortunately, there was no wave measurement conducted during this cruise and the ship based meteorological measurements are not quality controlled; therefore they do not provide a high degree of certainty.

### 3.1.2 Knorr11

The Knorr11 field campaign took place in the North Atlantic aboard the US-American RV Knorr. The cruise started at Woods Hole, USA on June 24, 2011 and returned to its starting point on July 18, 2011 (Fig. 3.1c). The cruise was focused on conducting high quality DMS and CO$_2$ flux measurements. To fulfil this, the cruise track followed the region of high biological activity in the North Atlantic. These air-sea flux and gradient measurements for DMS and CO$_2$ as well as measurements of mean meteorological parameters and wave information were performed continuously for the duration of the cruise$^\dagger$. ASIP was deployed not continuously, but for four times. These deployments of ASIP combine 283 profiles.

### 3.1.3 SOAP

The Surface Ocean Aerosol Production Study (SOAP) was carried out in February-March 2012, east of New Zealand aboard the RV Tangaroa (Fig. 3.1d). Similarly to the Knorr11 cruise, sampling was performed in highly productive algal blooms. The main objective of the campaign was to study the influence of marine biology on aerosol production. During the SOAP cruise, ASIP was not deployed; therefore no information on ocean turbulence was recorded. In this thesis the observations of the DMS and CO$_2$ gas fluxes conducted during the SOAP cruise$^\dagger$ are used in Chapter 4 to compare them to the gas exchange analysis preformed for the Knorr11 cruise.

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$^\dagger$Measurements of the gas fluxes, the eddy-covariance $u_{*,a}$, and the 3-D wind speed were conducted and processed by Dr. Sebastian Landwehr, Prof. Eric Saltzman, Prof. Scott Miller, Dr. Tom Bell, and Dr. Brian Ward
Figure 3.3: Significant wave height ($H_s$), wind speed ($U_{10}$), water-side friction velocity ($u^*$), measured $CO_2$, $KCO_3$, and $K_DMS$ time series of the Knorr11 cruise. The grey shaded areas show the period of ASIP deployments.
3.1.4 STRASSE

The Sub-Tropical Atlantic Surface Salinity Experiment (STRASSE) took place from August 21 to September 9, 2012 as part of the Salinity Processes in the Upper-ocean Regional Study (SPURS-I) campaign (Sutherland et al., 2016; Reverdin et al., 2015; Sutherland et al., 2014b). The campaign investigated the high-salinity region of the North Atlantic subtropical gyre. The cruise track and the position of seven deployments of ASIP resulting in a total of 528 profiles are shown in Fig. 3.1f.

3.1.5 MIDAS

As 2nd leg of SPURS-I, the MIDAS cruise was carried out in the region of the North Atlantic Salinity Maximum aboard the RV Sarmiento de Gamboa to map the salinity structure of the upper ocean (Landwehr et al., 2015). The ship departed Las Palmas, Gran Canaria on the 16th of March 2013 and reached the Azores on the 17th of April (Fig. 3.1g). The majority of the cruise was spent within the salinity maximum of the tropical North Atlantic.

High-quality meteorological and wave information was available for the whole duration of the cruise, from a mooring at 24.5°N, 38°W deployed by the Woods Hole Oceanographic Institution (WHOI). However, the ships’ wind measurements are considered more representative of the conditions that ASIP experienced. These wind speeds are corrected for flow distortion using the mooring as reference. The corrected wind speeds were in agreement with onboard eddy covariance momentum fluxes ($u^*_{a}$). ASIP was deployed on five occasions of up to two days in a row, resulting in 676 $\epsilon$ profiles. During this campaign, ASIP was programmed to descend down to a maximum depth of 30 to 40 m. The mooring displays that the seasonal MLD was below 100 m; therefore out of ASIP’s operational range. However, the diurnal MLD and the XLD were within ASIP’s operational range for half of the cruise. For these deployments it was found that the depth of the daily MLD $h$, defined as a density difference of $\Delta\sigma = 0.03 kg m^{-3}$ from 2.5 m depth (de Boyer Montégut et al., 2004) agreed best with the above defined $h_{\epsilon}$. This definition for $h$ was applied on the observations from the mooring. The obtained $h$ from the mooring was then used as a reference for $h_{\epsilon}$ in the cases of missing information of the actual $h_{\epsilon}$ sampled by ASIP.
3.1.6 NICE

The 10-day long campaign NICE (on thiN ICE) studied the role of mixing for heat and biogeochemical budgets of the Arctic Ocean (Fig. 3.1e). The cruise was conducted from the RV Hakon Mosby in September 2014, leaving and returning to Longyearbyen, Svalbard. During this time, ASIP was successfully deployed on 4 occasion gaining a total of 188 samples. Mean meteorological parameters were provided from the ship’s weather station.

3.2 Upper Ocean Measurements

The Air-Sea Interaction Profiler (ASIP) is an autonomous, upwardly rising, microstructure profiler (Ward et al., 2014). It was developed to study the uppermost metres of the ocean. This region is often under-sampled by conventional instruments, as for example ship-mounted CTDs. These instruments commonly discard the upper 5–10 m of the ocean due to contamination from the ship’s wake (e.g. Oakey and Elliott, 1982; Brainerd and Gregg, 1993; and LG89). Autonomous profilers such as ARGO floats and sea gliders circumvent the problem of the ship wake (Rudnick, 2016; Wolk et al., 2009). However, to prevent their pumped conductivity sensor sucking in air, most ARGO floats stop sampling at a few meters below the ocean surface (Anderson and Riser, 2014). Being fully autonomous allows ASIP to get around the problem of ship-induced noise. Therefore, ASIP is able to provide data in an undisturbed environment from a maximum depth of 100 m up to the air-sea interface. By doing so, ASIP, which is built to focus on small-scale processes, is equipped with different microstructure sensors including temperature, conductivity, and two orthogonal mounted airfoil shear probes. This thesis focuses on upper-ocean turbulences, thus, the main interest lies in the shear measurements. These shear measurements allow estimations of the prevailing level of $\epsilon$ with a vertical resolution of approximately 0.5 m as for example used in Sutherland et al. (2013) and described in the following.

Even though ocean turbulence is described by $\epsilon$, it is not measured directly. Rather shear measurements are used to determine $\epsilon$. This shear information involves the measurements of microstructure velocity fluctuations. There
Figure 3.4: Schematic showing the three basic steps to determine the turbulent signal in form of the dissipation rate of turbulent kinetic energy $\epsilon$ from measurements of small-scale velocity fluctuations.

are three steps involved to reach from the measured velocity fluctuations to $\epsilon$ (Fig. 3.4):

1. Measuring the velocity fluctuations $\frac{\partial u'}{\partial t}$

2. Transforming them into a shear signal $\frac{\partial u'}{\partial z}$

3. Calculating the shear spectrum to determine $\epsilon$ as its integral.

There exists different approaches to measure velocity fluctuations and shear determination from it. Previously, hot-wire methods were the most common tool. They consist of a heated wire, whose resistance depends on the rate at which passing eddies would cool it down. This cooling can be related to the actual speed of the eddies. The main problem of this approach is that the heated wire is sensitive to temperature changes of surrounding water. This can cause immense errors in the determination of the prevailing velocity (Lueck and Osborn, 1980; Gargett, 1978).

Overcoming these temperature induced limitations, piezo-electric airfoil shear probes, as mounted on ASIP and described by Oakey and Elliott (1982); Osborn (1980); Lueck et al. (2002) and Macoun and Lueck (2004) were introduced. These probes were originally designed for atmospheric purposes and applied to the ocean for the first time in 1972 (Osborn, 1974).

The principle idea of airfoil shear probes is to measure velocity fluctuations via a piezo-ceramic beam that can deform as a result of eddies. This piezo-ceramic beam is mounted in a water-proof bullet-shaped rubber housing (Fig. 3.5). This housing is mounted on the head of a profiler like ASIP. While moving with the profiler, the airfoil shear probes measure velocity $u$ fluctuations in the cross-stream direction of ASIP’s ascent. When the
cross-stream flow reaches the sensor, it bends the piezo-ceramic beam. This bending creates a voltage $E_p$ that is proportional to $u$ times the velocity of the profiler $w_A$:

$$E_p = w_A u s,$$  \hspace{1cm} (3.1)

where $s$ is the sensitivity of the airfoil shear probe and can be determined by calibration. This Equation (3.1) allows one to determine the actual velocity fluctuation $\partial u / \partial t$ from the measured voltage.

However, the main interest lies on the small scale shear, $\partial u' / \partial z$. Therefore, the velocity fluctuations have to be converted from a 'time series' into a 'space series'. To relate these spatial and temporal characteristics of turbulence, the ‘Taylor Frozen Field Hypothesis’ is applied (Taylor, 1938). This hypothesis demands that a turbulent flow is measured at the same speed than it evolves. Thus, the turbulent eddies are sampled faster than they evolve in time. This implies that any spatial changes of the turbulent field are the same as its temporal changes. Thus, time and distance can be interchanged as:

$$f(t) \rightarrow f(z = w_A t).$$  \hspace{1cm} (3.2)

Any temporal changes of a turbulent quantity can then be converted using an along-path gradient:

$$\frac{\partial}{\partial t} = w_A \frac{\partial}{\partial z}$$  \hspace{1cm} (3.3)
as:
\[
\frac{\partial u'}{\partial z} w_A = \frac{\partial u'}{\partial t} .
\] (3.4)

Using the ‘Taylors Frozen Hypothesis’, the sensed voltage \( E_p \) can be related to the spatial shear, as:
\[
\frac{\partial u'}{\partial z} = \frac{1}{w_A} \frac{\partial u'}{\partial t} = \frac{dE_p/(sw_A)}{dt} \frac{1}{w_A} = \frac{dE_p}{dt} \frac{1}{sw_A^2} .
\] (3.5)

This assumption holds only if the relative turbulence intensity is small when compared to the mean flow \((u'/u << 1\) where \(u\) is the mean flow velocity and \(u\) the eddy velocity) and if ASIP moves sufficiently fast and with a constant velocity \(w_A\) through the turbulent flow. The constant \(w_A\), which is determined by ASIPs pressure signal is not always the case. This can lead to errors in shear estimations. The favoured rise velocity is \(0.5\) m s\(^{-1}\), which is a compromise between the request to move fast enough to fulfil the ‘Taylors Frozen Field Hypothesis’ and slow enough for the resolution of the sensor (and thus the spatial resolution of the final \(\epsilon\) estimates). While profiling, \(w_A\) remains relatively constant. However, it varies when ASIP enters the wave affected boundary layer around the uppermost 10 m as discussed in Ward et al. (2014).

ASIP is equipped with two Rockland SPM-38 airfoil shear probes, which are mounted on its head orthogonal to each other. This mounting allows one to measure vertical gradients of each component of the horizontal flow, \(\frac{\partial u'}{\partial z}\) and \(\frac{\partial v'}{\partial z}\). In isotropic turbulence both components should be statistically independent and thus, can increase the confidence in the resulting \(\epsilon\).

In a final step, the determined shear information is used to predict \(\epsilon\). Following Eq (2.10), the shear spectrum is calculated to determine \(\epsilon\) via its integration in wavenumber space. The shear spectrum is calculated for 1024-point segments corresponding to 1 second or about 0.5 m bins of data, using the pwelch method with a Hanning window. These segments are moved along the profile with an overlap of 512 points, which corresponds to around 0.25 m (Sutherland et al., 2013). For each of the segments ASIP’s rise velocity \(w_A\) and the kinematic viscosity are set to a constant mean value. A despiking algorithm and band-pass filter are applied to the shear signal to remove low and high frequency vibrations outside the desired frequency range.
The obtained shear spectrum is corrected for errors induced by the size of the shear probe. When measuring with an airfoil shear probe, eddies of comparable size to the width of the probe are averaged out. This averaging is often referred to as spatial averaging (Macoun and Lueck, 2004). Spatial averaging underestimates the shear spectrum at small scales and thus high wavenumbers (as shown in Fig. 3.6). This effect can cause a significantly underestimated prediction of $\epsilon$. Oakey and Elliott (1982) suggested the airfoil shear probes responds in the form of a single-pole low-pass filter, with

$$H(\ell) = \frac{1}{1 + (\ell/\ell_{cs})^2}, \tag{3.6}$$

where $\ell$ is the wavenumber and $\ell_{cs}$ is the cut-off wavenumber of the shear probe ($\ell_{cs} = 50 \text{ cpm}$). The obtained shear spectrum is corrected for this effect of spatial averaging by multiplication of $H(\ell)$. This correction allows one to resolve the shear spectrum to wavenumbers that could not be resolved due to the size of the shear probe. This enables the use of airfoil shear probes even in highly turbulent regions, where the peak of the shear spectrum is
shifted to higher wavenumbers (shown in Fig. 3.8).

To estimate $\epsilon$ the shear spectrum is integrated in an iterative way with the aim to resolve $\epsilon$ from the smallest wavenumbers up to the Kolmogorov wavenumber $\ell_k$ (Eq 2.9) (Moum et al., 1995). This is achieved by increasing the upper integral boundary and thus $\epsilon$ for each iteration. To estimate the magnitude of $\ell_k$, an initial guess of $\epsilon = \epsilon_i$ is important, as $\ell_k$ depends on $\epsilon$ (Eq (2.9)).

Figure 3.7: Example dimensional shear spectrum $S_d(\ell)$ showing the stepwise procedure of determining a final estimate of $\epsilon$. The original shear spectrum observed from ASIP (blue), the same spectrum linearly interpolated in log-space and corrected for the spatial averaging of the airfoil shear probe (green), and the determined Nasmyth spectrum (red) are shown. The grey area gives the interpolation range for the initial guess of $\epsilon = \epsilon_i$. This range is expanded iteratively, which is shown for the first iteration by the blue area and $\epsilon_1$. The final Kolmogorov wavenumber $\ell_k$ is indicated by the red vertical dashed line. The red area gives the range over which the final $\epsilon = \epsilon_f$ is integrated. Cover of the full wavenumber range is reached by extrapolation using the theoretical Nasmyth spectrum.

In order to gain the initial guess, the spectrum is integrated between a minimal wavenumber $\ell_{\text{min}}$ of 5 cpm and a maximal wavenumber $\ell_{\text{max}}$ of 6 cpm and $\epsilon$ is estimated from Eq (2.10). Thus, in reality the integral limits are not 0 and $\infty$, but rather $\ell_{\text{min}}$ and $\ell_{\text{max}}$:

$$\epsilon = \frac{15}{2} \nu \int_{\ell_{\text{min}}}^{\ell_{\text{max}}} S_S(l) dl.$$

(Eq 3.7)
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Figure 3.8: The dimensional Nasmyth spectrum for various levels of $\epsilon$, which are labelled on each graph. The spectra are calculated for a kinematic viscosity $\nu$ of $10^{-6}$ m$^2$s$^{-1}$.

Once a first guess of $\epsilon$ is calculated, a first guess of $\ell_k$ can be determined. This process is repeated by increasing $\ell_{\text{max}}$ in Eq (3.7) using steps of 2 cpm (or 3 cpm, 5 cpm, 10 cpm depending on the estimated level of $\epsilon$, the smaller $\epsilon$ the finer the step size). The aim is to reach $\ell_{\text{max}} = \ell_k$, with $\ell_k$ changing for each iteration, and thus refining the $\epsilon$ estimate.

There are three different criteria to finish the iteration process. The first one is when $\ell_{\text{max}}$ reaches a value of $\ell_k$. The second criteria is when $\ell_{\text{max}}$ reaches a value higher than a pre-defined wavenumber of 350 cpm. In this case $\ell_{\text{max}}$ is set equal to 350 cpm. The third criterion is when the iteration process has looped 50 times. If any of these criteria is reached, the iteration process stops and $\epsilon$ is predicted for the given wavenumber range.

The measured shear spectrum does not resolve the full wavenumber range. In order to include the unresolved wavenumber range, the spectrum is extrapolated to higher and lower wavenumbers using the Nasmyth spectrum. The Nasmyth spectrum is an empirical shear spectrum for distinct wavenumbers (Oakey and Elliott, 1982), which was later fit with a model by Wolk et al. (2002). The shape of the Nasmyth spectrum depends only on $\epsilon$ and $\nu$ and is considered to describe the universal shape of a shear spectrum for isotropic
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stationary turbulence:

\[ S(\ell) = \frac{8.05(\ell/\ell_k)^{1/3}}{1 + (20.6(\ell/\ell_k))^{3.715}}. \quad (3.8) \]

The estimates of the area beyond the theoretical spectra, in the wavenumber ranges that are unresolvable by the measured spectrum, are added to the estimates of \( \epsilon \) obtained from the iteration process. This yields a final prediction of \( \epsilon = \epsilon_f \) as shown in Fig. 3.7.

The benefits of the described integral method to obtain \( \epsilon \) is its robustness, even when the wavenumber range is not completely resolved by the measurements. Instead of estimating \( \epsilon \) from the shear spectrum it can be directly derived from the spatial-domain (in contrast to the wavenumber domain) (Yamazaki and Lueck, 1990; Johnson et al., 1994). This method is much more sensitive to noise infiltrations. Therefore, it is essential to derive a ‘clean’, low-pass filtered, and despiked signal. The filtered shear signal is then directly converted using the middle part of Eq (2.8).

The \( \epsilon \) data in this thesis was calculated using the presented integral method due to the higher noise resistance. This was achieved for the two mounted shear probes separately. The separated estimates of \( \epsilon \) were averaged. For further analysis the bottom most 10 m of each profile were rejected, as they are often contaminated by noise introduced through ASIP’s thrusters†.

3.3 Gas Fluxes

The eddy covariance system consisted of two sonic anemometers (Campbell CSAT3), measuring the 3-dimensional wind speed, and two inertial motion sensors (Systron Donner Motion Pack II) that recorded the platform motion. In order to minimise the effect on air-flow distortion the covariance system was mounted on the bow mast of the Knorr at a height of about 13.6 m above the mean water level. O’Sullivan et al. (2015) provides a detailed study of the effects of air-flow distortion on the measurements on the RV Knorr. The data set was restricted to measurements where the apparent relative wind direction was less than 90° from the bow for both CO\(_2\) and DMS.

†The data was provided by Dr. Graig Sutherland and Dr. Brian Ward and reprocessed for the analysis of this thesis.
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Air sampling inlets were mounted between the two anemometers at the same height and provided two closed chamber gas analyser systems, which are described in detail in Miller et al. (2010) and Bell et al. (2013), for CO₂ and DMS, respectively. These publications also provide descriptions of the measurements of the air-sea concentration gradients of CO₂ and DMS. The CO₂ and DMS concentration in seawater was continuously measured using equilibrator systems (Miller et al., 2010; Bell et al., 2013; Saltzman et al., 2009). In these systems air was equilibrated with uncontaminated surface sea water from the ship’s bow pumping system, and passed through a gas analyser.

The apparent wind speed was corrected for platform motion and mean tilt of the air-flow as described in Landwehr et al. (2015). The wind speed was then used to calculate the air-side friction velocity \( u_{*a} = \sqrt{(w'u')^2 + (w'v')^2} \), where \( u, v, w \) are the along wind and the horizontal and vertical cross wind components of the wind vector with \( u', v', w' \) representing the derivation of the mean in the respective wind components: \( u = \overline{u} + u' \), with \( \overline{u} \) referring to the mean velocity.

The gas fluxes \( F_{\text{DMS}} \) and \( F_{\text{CO₂}} \) were calculated as covariances of the vertical wind speed component \( w \) and the gas mixing ratios: \( F_x = \rho_a w'x' \), where \( \rho_a \) is the dry air density.

The 10 minute-averaged gas flux and concentration gradient measurements were used to obtain the total gas transfer velocity \( K \) via Eq (2.25). In the case of CO₂ and DMS \( K \) approximates the water-side transfer velocity \( k \) adequately. In order to account for the influence of the sea surface temperature and salinity the transfer velocities were normalised to a Schmidt number of 660, which corresponds to CO₂ in seawater at 20 °C:

\[
k_{660} = k \cdot \left( \frac{660}{\text{Sc}_x} \right)^{-n},
\]

where \( \text{Sc}_x \) refers to the Schmidt number at the in-situ seawater temperature and salinity for either DMS or CO₂. In the following, the normalised gas transfer velocities \( k_{660} \) are referred to as \( k_{\text{DMS}} \) and \( k_{\text{CO₂}} \) for DMS and CO₂, respectively.
### 3.4 Wave Data

Wave measurements were carried out onboard the ship using an ultrasonic altimeter mounted at the bow of the Knorr (*Christensen et al.*, 2013). To correct for ship motion, the altimeter was combined with an accelerometer. The wave observations consist of the full 1D-wave spectra, which allows for the calculations of the significant wave height $H_s$ and mean wave periods $T_m$ (based on different moments of the wave spectrum as described below). In addition to the wave measurements onboard the Knorr, there were wave measurements performed at the mooring deployed during the MIDAS campaign. The mooring provided high-quality wave information of $H_s$ and the average period $T_{m2}$.

Model wave data is obtained from runs of the ECMWF stand alone ECWAM wave model, cycle 43R1 (*ECMWF*, 2016) with an hourly output using a global 11 km grid, with a spectral resolution of 36 directions (10 degree resolution) and 36 frequencies (lowest frequency 0.035 Hz). For the different cruises, the wind forcing and the sea ice cover are taken from ECMWF operational analysis, available every 6 hours, with a resolution of 16 km. No wave data was assimilated and the runs were done without any surface ocean current information. For each run, a warm-up period of 10 days was used. The atmospheric data was obtained from ERA-Interim (*Dee et al.*, 2011), using the short range forecasts 3 hourly interval (forecast steps 3, 6, 9, and 12) in order to get the different fluxes. The Stokes drift was calculated from the full 2D-wave spectra and all integrations were performed by extending the discretised spectra with a $f^{-5}$ tail.

The significant wave height $H_s$ (Parameter 229) can be determined from the sea surface elevation $\zeta$ as $H_s = 4 \text{ std}(\zeta)$, which is similar to $H_s = 4 \sqrt{m_0}$, where $m_0$ is the zeroth moment of the wave spectrum. The spectral moments are gained by integrating the wave spectrum:

$$m_p = \int_0^\infty S_f(f) f^p \, df,$$

with $S_f(f)$ being the spectral density, and $f$ the frequencies.

---

§These wave measurements were conducted and processed by Dr. Kai Christensen.
¶The model was run by Dr. Øyvind Breivik and Dr. Jean Bidlot and the output data was provided for the analysis in Chapter 5. In addition, it was used to overcome a shortage in ship observations for the Labrador cruise in Chapter 6.
Mean wave periods can be defined based on moments of different orders. The mean period $T_{m0} = \frac{m_{-1}}{m_0}$ (ECWAM Parameter 232), which is also known as the energy mean wave period, is based on the moment of order $-1$. The mean wave period $T_{m1} = \frac{m_0}{m_1}$ (ECWAM Parameter 220), which is the reciprocal of the mean frequency, is based on the first moment. The $T_{m1}$ is used to estimate the magnitude of Stokes drift transport. The mean wave period based on the second moment $T_{m2} = \sqrt{m_0/m_2}$ (ECWAM Parameter 221) approximates the time domain zero-upcrossing wave period $T_0$. The zero-upcrossing period is the wave period that is determined from observations of the sea surface elevation.

### 3.4.1 Wave Model Validation

In order to validate the modelled wave information for its use in the analysis of this thesis, the data is compared to the actual wave observations. Therefore, the modelled information from the runs of the ECMWF stand alone ECWAM wave model are compared to the observations based on measured 1D-wave spectra from the Knorr11 and MIDAS cruise. These variables comprise the significant wave height $H_s$, the mean wave periods based on different spectral moments of the wave spectrum ($T_{m1}$, $T_{m2}$, and $T_{m0}$), and the wind speed $u_{10}$.

The superimposing of long and far-travelled swell waves with locally generated and relatively shorter wind waves often presents a complex wave field. In many air-sea interaction studies the wind-sea part of the wave spectrum is of major interest. Drennan et al. (1996) and T96 show that $H_s$ from only the wind-sea should be used to describe profiles of $\epsilon$. Therefore, the wave spectrum has to be separated properly.

Section 3.4.1 focuses on wave parameters derived from the full wave spectrum for the Knorr11 and MIDAS campaign. In Sec. 3.4.1 the wave information from the separated wave spectra are compared for the Knorr11 campaign. The wave model separates the wind and swell part based on the 3D-spectrum (height and direction), whereas the observations only provide 1D-spectra; therefore different separation mechanism are considered.
**Full Wave Spectrum**

Figure 3.9 shows the different mean wave periods ($T_{m0}$, $T_{m1}$, and $T_{m2}$) and $H_s$ extracted for the Knorr11 and MIDAS cruise. The modelled time series are interpolated spatially to match the location of the ship. The figure highlights that the modelled wave periods follow the same pattern. They differ, however in their magnitudes, with $T_{m0}$ reaching the highest values and $T_{m2}$ the lowest.

The measured mean wave periods ($T_{m1}$ only for Knorr11, and $T_{m2}$ for Knorr11 and MIDAS), and $H_s$ are compared to the modelled wave information for the Knorr11 and MIDAS campaigns. Following Christensen *et al.* (2013) only time periods when the ship was on station were investigated for the Knorr11 cruise (Fig. 3.9 – periods of dark colour). For the MIDAS cruise, time periods when the ship was in a 100 km range to the buoy were considered. In addition to the wave information, the modelled and measured $u_{10}$ from the ship’s mast are compared for both campaigns. These observations are compared for both complete cruises.

For both cruises, the modelled times series of $u_{10}$, $T_{m1}$, and $H_s$ capture the general behaviour of the measured parameters (Fig. 3.9). For the first days of the Knorr11 cruise, from the 24th of June to the 8th of July, the modelled $u_{10}$ tends to under-predict the observed $u_{10}$. This under prediction is particularly pronounced whenever the wind speed lies in a range between 5 and 10 m s$^{-1}$ (Fig. 3.9e). For the last days, when the wind picks up, the model predicts the measured $u_{10}$ much more precisely. The discrepancy of the modelled and measured $u_{10}$ in the range between 5 and 10 m s$^{-1}$ becomes more visible in Fig. 3.10c. The figure shows that the cumulative probabilities of the modelled and measured $u_{10}$ for the Knorr11 cruise generally follow the same shape. However, they clearly deviate in the wind speed range of 5 to 10 m s$^{-1}$. The model’s underestimation of $u_{10}$ relative to the observations in this wind speed range causes an overall underestimation of the modelled $u_{10}$ by 0.52 m s$^{-1}$.

For the MIDAS cruise, the magnitude of the modelled $u_{10}$ is precise for the period from 23th till 31st of March, when the wind stays below 5 m s$^{-1}$. Later, $u_{10}$ increases and reaches magnitudes between 5 and 10 m s$^{-1}$. In this time, the modelled $u_{10}$ tends to over-predict the measured one. This is opposite to what was found for the Knorr11.

Combining the data from both cruises shows a distinct separation between
Figure 3.9: Time series of (a) the modelled (dashed lines) and observed (solid lines) mean periods $T_m$ for the Knorr11 cruise with the modelled $T_{m1}$ in blue, $T_{m2}$ in grey, $T_{m01}$ in black, and observed $T_{m1}$ in red, $T_{z0}$ in yellow, $T_{m2}$ in green and (b) similar for the MIDAS cruise. (c) The modelled (dashed blue line) and observed (solid red line) significant wave height $H_s$ for the Knorr11 cruise and (d) the MIDAS cruise. (e) The modelled (blue dashed line) and observed (solid red line) wind speed $u_{10}$ for the Knorr11 cruise and (f) the MIDAS cruise, where the yellow line indicates $u_{10}$ observed from the ship and the red line observed from a near-by buoy. The higher shadings indicate periods in which either the ship is in motion (Knorr11) or the ship is further than 100 km away from the mooring (MIDAS).
Figure 3.10: The occurrence of observed (red) and modelled (black) [%] (a) of the mean periods ($T_m$), (b) the significant wave height $H_s$ and (c) the wind speed $u_{10}$, and (d-f) similar for the cumulative probability. The dashed lines represent the data from the Knorr11 cruise, the dotted lines for the MIDAS cruise and the solid lines the combined data of both cruises. For the Knorr11 cruise the $T_m$ based on the first moment ($T_{m1}$) is added in (a) and (d) as dark red (observations) and grey (model) dashed lines.
the peak percentage occurrence in the 5-10 m s\(^{-1}\) wind speed range, where the model shows highest occurrence at 9 m s\(^{-1}\) and the observations at 7 m s\(^{-1}\). Compared to the MIDAS cruise alone, the cumulative probability of the combined data set merges at wind speeds above 11 m s\(^{-1}\). This is caused by the higher \(u_{10}\) from the Knorr11 cruise. The higher over-prediction of the model performance for the MIDAS cruise causes the model to over-predict the combined \(u_{10}\) by 0.37 m s\(^{-1}\) (Fig. 3.11c).

The modelled \(H_s\) for both cruises stays in general in the same range of magnitudes for the model and the observations. More specifically, the under-prediction of the modelled \(u_{10}\) during Knorr11 causes a constant under-estimation of the measured \(H_s\), which is most distinct when the measured \(H_s\) peaks. For example, the modelled \(H_s\) under-predicts the measured \(H_s\) by 1.5 m when it peaks on the 3rd of July. The tendency of the model to predict lower \(H_s\) is additionally shown in the percentage occurrence (Fig. 3.10b). Figure 3.10b shows that both lines have a clear peak that differs by 0.5 m. For the MIDAS cruise the differences between modelled and measured \(H_s\) are less distinct. Both peaks of the percentage occurrence in Fig. 3.10b occur at the same \(H_s\) of 2.8 m and reach similar levels of percentage. For the overall comparison (Knorr11 and MIDAS combined) the occurrence peaks are widened due to each cruise peaking at different \(H_s\). However, the shape of both the modelled and measured occurrence curves are similar. The similarities are highlighted in the high correlation coefficients of 0.97 for the Knorr11 and 0.91 for the MIDAS cruise (in Fig. 3.11c and Table 3.2).

The time series plot in Fig. 3.9a for the mean periods \(T_m\) includes the periods determined from different definitions of \(T_m\) (\(T_{m1}\), \(T_{m2}\), and \(T_{m0}\)). The measured \(T_{m1}\) and \(T_{m2}\) from the Knorr11 are much closer to each other than the ones predicted by the model (Fig. 3.9a). Thereby, all the measured \(T_m\) fall closest to the modelled \(T_{m1}\). This explains the higher offset between the modelled and measured \(T_{m2}\) (0.68 s underestimation by the model) relative to the one between both \(T_{m1}\) (0.4 s underestimation by the model). Besides the constant offset, both the modelled \(T_{m1}\) and \(T_{m2}\) describe the occurrence of the measured \(T_{m1}\) and \(T_{m2}\) well with all the values falling in a range of 4 s (Fig. 3.10a). For the MIDAS campaign the measured \(T_{m2}\) falls between the predicted \(T_{m1}\) and \(T_{m2}\). During the MIDAS campaign larger wave periods are observed than during the Knorr11 campaign. This broader range of periods is well covered by the model with a general underestimation of 0.63 s.

The similar offsets for the Knorr11 and MIDAS cruise between the modelled
Figure 3.11: (a) Modelled mean waveperiods based on the second $T_{m2}$, and (b) first moment $T_{m1}$ for the Knorr11 campaign, (c) significant wave height $H_s$ and (d) wind speeds $u_{10}$ versus measured ones. The red data was conducted during the Knorr11 cruise and the green data during the MIDAS cruise. The dashed grey line shows the one to one relation and the coloured solid lines the offset values for the respective data sets.
Table 3.2: Determined offset and correlation coefficient (R) between the observed and measured wind and wave parameters. A negative offset describes an under-prediction by the model. The approach of Sahleé et al. (2012) was applied to separate the wave spectrum.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Offset</th>
<th>R</th>
</tr>
</thead>
<tbody>
<tr>
<td>Knorr11</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$H_s$</td>
<td>-0.40 m</td>
<td>0.97</td>
</tr>
<tr>
<td>$u_{10}$</td>
<td>-0.52 m s$^{-1}$</td>
<td>0.90</td>
</tr>
<tr>
<td>$T_{m1}$</td>
<td>-0.40 m</td>
<td>0.74</td>
</tr>
<tr>
<td>$T_{m2}$</td>
<td>-0.68 m</td>
<td>0.59</td>
</tr>
<tr>
<td>$H_{w}^{\text{wind}}$</td>
<td>-0.10 m</td>
<td>0.97</td>
</tr>
<tr>
<td>$H_{s}^{\text{swell}}$</td>
<td>-0.48 m</td>
<td>0.26</td>
</tr>
<tr>
<td>$T_{w}^{\text{wind}}$</td>
<td>-0.25 s</td>
<td>0.95</td>
</tr>
<tr>
<td>$T_{s}^{\text{swell}}$</td>
<td>-0.73 s</td>
<td>0.84</td>
</tr>
<tr>
<td>MIDAS</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$H_s$</td>
<td>0.06 m</td>
<td>0.91</td>
</tr>
<tr>
<td>$u_{10}$</td>
<td>1.22 m s$^{-1}$</td>
<td>0.90</td>
</tr>
<tr>
<td>$T_{m2}$</td>
<td>-0.63 m</td>
<td>0.88</td>
</tr>
<tr>
<td>Combined (Knorr11 and MIDAS)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$H_s$</td>
<td>-0.07 m</td>
<td>0.87</td>
</tr>
<tr>
<td>$u_{10}$</td>
<td>0.37 m s$^{-1}$</td>
<td>0.85</td>
</tr>
<tr>
<td>$T_{m2}$</td>
<td>-0.64 m</td>
<td>0.91</td>
</tr>
</tbody>
</table>

and measured $T_{m2}$ cause an offset of 0.64 s for the combined data set. The combined data set consists of the lower $T_{m2}$ from the Knorr11 cruise and higher ones from the MIDAS cruise. Thus, it covers a large range of periods. This is well represented by the model with a correlation coefficient of 0.91 (Fig. 3.11a and Tab. 3.2).

**Wind-and Swell Separation**

Several methods have been presented using directional wave spectra to determine frequencies, which separate wind and swell waves (Gerling, 1992; Hanson and Phillips, 2001; Portilla et al., 2009). In the ECWAM re-analysis the wind-sea part of the wave spectrum is defined as the spectral components that are influenced by wind forcing when $1.2 \times 28(u_{*}/c_{p})\cos(\theta - \Phi) > 1$, where $c_{p}$ is the phase speed, $\theta$ the wave direction, and $\Phi$ the wind direction. However, in case of the Knorr11 cruise only 1D-wave spectra were obtained, without information of the wave direction. The same is the case for many ocean buoys. Therefore, studies aimed to gain methods for the wave partitioning from 1D-spectra (Hwang et al., 2012; Wang and Hwang,
Figure 3.12: Time series of (a) the significant wave height for the swell part $H^s_{\text{swell}}$, and (b) for the wind-sea part of the wave spectrum $H^s_{\text{wind}}$, as well as (c) the mean period based on the swell $T^s_{m_1}$ and (d) wind-sea part $T^w_{m_1}$. The blue dashed lines show the model predictions, in comparison to the measurements based on a separation at a fixed frequency of 0.1 Hz (red), of 0.2 Hz (cyan), the approach proposed by Wang and Hwang (2001) (WH01 in black), by Hwang et al. (2012) (H12 in yellow) and by Sahleć et al. (2012) (S12 in pink).
Sahleé et al. (2012) define a separation frequency $f_s$ for individual 1D-wave spectra, as:

$$f_{ss12} = \frac{g}{2\pi 1.2 u_{10}}.$$  \hfill (3.11)

In order to overcome the dependence on variables other than the wave information alone, methods that do not rely on external information have been proposed (e.g. Wang and Hwang, 2001; Hwang et al., 2012). The wave steepness method follows the basic idea that mainly short waves contribute to the steepness. The contribution of the swell components is almost negligible because of their long wavelengths. As a result, the peak of the wave steepness function is very close to the peak of the wind sea portion of the spectrum. The wave steepness function is defined as the ratio of $H_s$ to the wavelength $L$ integrated from a given frequency to the maximum frequency of the wave spectrum, as:

$$\xi(f) = \frac{H_s(f)}{L(f)} = \frac{2\pi H_s(f)}{gT_{m2}^2(f)} = \frac{8\pi m_2(f)}{g\sqrt{m_0(f)}},$$  \hfill (3.12)

with $L = gT_{m2}^2/2\pi$ (deep-water dispersion relation). The peak frequency $f_p$ of $\xi(f)$ is then related to the separation frequency of wind sea and swell. Wang and Hwang (2001) found an empirical relation between $u_{10}$ and $f_p$, which they apply to gain a separation frequency $f_{sw01}$ without the need to use $u_{10}$:

$$f_{sw01} = 4.112 f_p^{1.746}.$$  \hfill (3.13)

A further separation frequency was defined by Hwang et al. (2012) via least-square fitting as:

$$f_{sh12} = 24.2084 f_{m1}^3 - 9.2021 f_{m1}^2 + 1.8906 f_{m1} - 0.04286,$$  \hfill (3.14)

where $f_{m1}$ is the peak frequency of the spectrum integration function $I_1(f) = \frac{m_1(f)}{\sqrt{m_{-1}(f)}}$ (the spectral moment $m_p$ of the wave spectrum are defined in Chapter 3.4).

Figure 3.12 shows $H_s$ and $T_{m1}$ calculated from the separated parts of the wave spectra, based on the introduced separation approaches, in comparison
Figure 3.13: (a) Modelled significant wave height for the swell part of the wave spectrum $H_{swell}$ versus measured one, and (b) for the wind-sea part of the wave spectrum $H_{wind}$, as well as (d) the mean period based on the swell $T_{m1}^{swell}$ and (d) wind-sea part $T_{m1}^{wind}$ of the wave spectrum. The data based on the different separation approaches is shown in different colours: for a fixed frequency of 0.1 Hz (red), 0.2 Hz (cyan), the approach proposed by Wang and Hwang (2001) (WH01 in black), by Hwang et al. (2012) (H12 in yellow) and by Sahleé et al. (2012) (S12 in pink). The black line shows the one to one relation. The offset and correlation coefficient (R) between the modelled and measured variables are provided according to the colour code.
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to the model predictions. In addition to the described separation methods, partitioning based on constant cutoff frequencies are performed. These frequencies are chosen as 0.1 Hz based on the suggested default frequency in the Simulating WAves Nearshore (SWAN) model and 0.2 Hz. The time series in Fig. 3.12 can be divided into two periods: the first one when the Knorr was on station for the first four times (24/Jul until 09/Jul). During this time \( u_{10} \) was relatively low in a range between 5 and 10 m s\(^{-1} \). The second one covers the last station (from 09/Jul onwards) when the wind picked up and \( u_{10} \) reached values of up to 18 m s\(^{-1} \).

For the first period the height of the swell waves \( H_{swell}^s \) is more dominant than the one of the wind waves \( H_{wind}^s \). This changes in the second period, when the wind induces energy locally into the frequencies representing the wind sea. Therefore, \( H_{wind}^s \) increases while \( H_{swell}^s \) stays in a similar range of magnitudes than in the first period.

Overall, \( f_{ss12} \), which depends on the wind input, is the only frequency which seems to be capable to separate the wave spectrum for both the low wind and the high wind situations in accordance with the model output. This separation approach matches the model prediction of \( H_s \) for the wind sea nearly perfectly with a correlation coefficient of 0.97 (Fig. 3.13a). The approach does a worse performance for the swell with a correlation coefficient of 0.26. This correlation coefficient, however is sill much higher than for the other separation methods (all predict a negative correlation as shown in Fig. 3.13b).

The \( H_{swell}^s \) determined from both the \( f_{swH01} \) and \( f_{sh12} \) over-predict the modelled ones clearly with more energy assigned to the wind-sea part of the spectrum and less in the swell. Oppositely, the \( H_{swell}^s \) under-predicts the modelled one. This swaps for the second period, when the wind increases. Both methods assign most of the additional energy to the swell rather than the wind sea.

During the first low-wind period the constant \( f_s \) of 0.1 Hz assigns energy from the swell to the wind sea. This results in an over-prediction of \( H_{wind}^s \) and an under-prediction of \( H_{wind}^s \) compared to the model. The higher \( f_s \) of 0.2 Hz shows the opposite behaviour during the same time. During the second period, the higher \( f_s \) assigns most of the additional wind energy to the swell part of the spectrum similar as discussed for \( f_{swH01} \) and \( f_{sh12} \). This effect is less pronounced for \( f_s \) of 0.1 Hz.

The good performance of \( f_{ss12} \) in separating the wave spectrum according
to the modelled separation, is additionally demonstrated in the comparison of $T_{m1}$ based on the different parts of the wave spectrum. The $T_{swell}^{S1}$ determined based on $f_{S12}$ slightly (less than 1 s) under-predicts the $T_{swell}^{S1}$ for the first low-wind period. For the second high-wind period this $T_{swell}^{S1}$ over-predicts it by up to 4 s. This energy is missing in the wind-sea part and causes an under-prediction for the modelled $T_{wind}^{S1}$. All the other methods to separate the spectrum cause a constant over prediction of the modelled $T_{wind}^{S1}$. 


4 Parameterising Air-Sea Gas Transfer Velocity with Dissipation

Preface

This chapter is an adapted version of the article:


The primary goal of Esters et al. (2017) was to validate the theoretical small-eddy model (SEM), which scales the gas transfer velocity with ocean surface turbulence, using direct open-ocean measurements of $\epsilon$. This has only been done previously for laboratories, lakes, and coastal regions.

The right to share and adapt this work is freely available under the Creative Commons Attribution 3.0 License. The data analysis, the interpretation and synthesis of results, the production of figures, and the writing were done exclusively by the author of this thesis. Dr. B. Ward contributed by supervising, assisting, and reviewing the work. Dr. S. Landwehr provided the CO$_2$ data, which he collected with the eddy covariance flux setup provided by Dr. S. Miller. Dr. T. Bell provided the DMS data and Dr. G. Sutherland was in charge of conducting the $\epsilon$ data during the Knorr11 cruise. Dr. E. Saltzman and Dr. K.-H. Christensen assisted and reviewed the publication.
As said in the preface, this chapter combines surface values of $\epsilon$ from four ASIP deployments during the Knorr11 cruise (283 samples in total) with the values of $k$ derived from direct DMS and CO$_2$ flux and air-sea concentration difference measurements. The Knorr11 is the only campaign with information on both $\epsilon$ and $k$. These measurements are used to validate the applicability of the SEM. This model has been validated in laboratories, lakes, estuaries, and coastal areas (Zappa et al., 2007; Tokoro et al., 2008; Vachon et al., 2010; Wang et al., 2015; Gålfalk et al., 2013), but never in the open-ocean.

Section 4.1 defines a variable Schmidt number exponent $n$ depending on the sea state. In Sec. 4.2 the SEM is evaluated with the measurements from the Knorr11 cruise. These findings are applied to the SOAP cruise in Sec. 4.3 and compared to commonly used wind speed based-parameterisations in Sec. 4.2. Investigations on the proportionality constant are presented in Sec. 4.4. Section 4.5 summarises the results of this chapter and presents conclusions.

4.1 Schmidt Number Exponent

In order to determine the Schmidt number exponent $n$ as a function of $u_*$, representing the sea state, the least-square method was used in Eq (2.27). The SEM in Eq (2.27) describes the physical mechanism occurring at the air-sea interface. However, the $\epsilon$ measurements closest to the interface $\epsilon_{05}$ are determined for a depth of 0.5 m. Therefore, they had to be extrapolated closer to the interface. This extrapolation is formalised using the LOW and T96 scaling approaches.

The LOW reproduces the shape of the measured $\epsilon$ profiles during the Knorr11 cruise relatively well, but overestimates the observed values of $\epsilon$ within the mixing layer for the majority of ASIP profiles (Fig. 4.1). Through a detailed analysis of $\epsilon$ measured during the Knorr11 cruise, Sutherland et al. (2013) found that the LOW predicts $\epsilon$ within an order of magnitude, but with a tendency to overestimate the observed $\epsilon$.

The observations of reduced $\epsilon$ may be caused by the presence of surfactants at the ocean surface damping turbulence, as the Knorr11 campaign experienced high levels of phytoplankton blooms (Bell et al., 2013). To
Figure 4.1: Dissipation profiles, which are averaged over all ASIP deployments, with their 95% confidence interval (black), and the respective averaged LOW profile (blue) and T96 profiles (green) and their 95% confidence intervals. The LOW is fitted to the measurements (multiplied offset of 0.394) and extrapolated to the thickness of the viscous sublayer – the resulting profile is shown in red. The same is done with the T96 scaling (orange). The circles give the averaged values at each normalised depth level – normalised to the mixing layer depth ($h_\epsilon$).

determine the offset between the observed and scaled profiles, measured $\epsilon$ profiles of ASIP were averaged over 200-minute time intervals (typically an average of 7 $\epsilon$ profiles) and normalised with the LOW ($\epsilon/\epsilon_{LOW}$) within the mixing layer ($\epsilon_{LOW} = 0.394 \pm 0.0729 \cdot \epsilon_{LOW}$).

In order to determine $\epsilon$ immediately below the air-sea interface, the scaled profiles $\epsilon_{LOW}$ are extrapolated to the thickness of the viscous sublayer, so that $z = z_\nu$ in Eq (2.12) following Lorke and Peeters (2006). This thickness is a function of wind speed (Ward and Donelan, 2006; Ward, 2007) and is inversely proportional to the friction velocity (Wu, 1971; Chriss and Caldwell, 1984):

$$ z_\nu = 11 \frac{\nu}{u_*} \quad (4.1) $$
This allows for the formulation of an \( \epsilon_{0,\text{LOW}} \) at the depth of the viscous sublayer, as \( \epsilon_{0,\text{LOW}} = 0.394 \left[ \pm 0.0729 \right] \frac{u^4}{u_{*}^2} \), where the found offset is applied.

When applying the same offset to the scaled \( \epsilon_{T96} \) profiles (Fig. 4.1), those profiles underestimate the measured \( \epsilon \) close to the surface. The extrapolated values of \( \epsilon_{T96} = 0.3282 \left[ \pm 0.0607 \right] \frac{u^4}{u_{*}^2} \) at the thickness of the viscous sublayer are consistently smaller than those modelled by the LOW and are often even smaller than the measured \( \epsilon \) values at 0.5 m depth.

The extrapolated values of \( \epsilon_{0,\text{LOW}} \) at \( z_{\nu} \) assuming the LOW are used to find the best fit for \( n = f(u_{*}) \) using Eq (2.27). These \( \epsilon_{0,\text{LOW}} \) do not rely on the actually measured \( \epsilon \) but on \( u_{*} \) based on in-situ momentum flux measurements, which allows for taking all combined measurements of \( k \) and \( u_{*} \) from the Knorr11 and the SOAP cruises into account. The best fits are determined with respect to the best combination in the proportionality coefficient \( A \) and \( n = f(u_{*}) \) in the SEM. This was performed separately for \( k_{\text{DMS}} \) and \( k_{\text{CO}_2} \). Following this assumption, a function \( n = -0.22 \cdot \log_{10}(u_{*}) + 0.13 \) is determined based on \( k_{\text{DMS}} \), which is associated with an \( A = 0.20 \). A similar fit was determined based on the \( k_{\text{CO}_2} \) observations. As the fit based on observations of \( k_{\text{DMS}} \) describes the relation between \( k \) and the SEM better (RMSD = \( \pm 7.18 \) cm hr\(^{-1}\)) than the one based on observations of \( k_{\text{CO}_2} \) (RMSD = \( \pm 9.03 \) cm hr\(^{-1}\)), in the following this fit is chosen to describe the transition of \( n \) for both gases.
When calculating $n = f(u_*)$ from the observations during Knorr11 and SOAP using the least-squares method, a function that follows closest the medium surfactant case of Krall (2013) is found (Fig. 4.2). It is reasonable to assume that there have been biological surfactants present, given the high levels of chlorophyll observed during the Knorr11 cruise (Bell et al., 2013).

### 4.2 Small-Eddy Model

The SEM for measured surface $\epsilon$ data (surface refers to the upper 0.5 m of the ocean: $\epsilon_{05}$), averaged over 200 min intervals, describes 46% of the variability in $k_{DMS}$, when applying constant $n = \frac{1}{2}$, as it was assumed by previous studies (e.g. Zappa et al., 2007) (Fig. 4.3a in grey). The performance of the SEM can be significantly improved, when applying a variable $n = f(u_*)$, which then describes 80% of the variability in $k_{DMS}$ (Fig. 4.3a in color).

The measured $k_{CO_2}$ is much more variable than the $k_{DMS}$, especially for lower wind speeds. This high variability leads to a lower correlation, where the weighted coefficient of determination is, $R^2_w = 0.72$ for a variable $n = f(u_*)$ and $R^2_w = 0.27$ for $n = \frac{1}{2}$. The weighted correlation coefficient is given by $R^2_w = 1 - \frac{\sum_i (y_i-x_i)^2}{\sum_i (y_i-\bar{y})^2}$ and takes the relative error $\sigma_i$ of each data point $i$ into account, where $y$ and $x$ are the observed and predicted data respectively.

These determination coefficients were gained for relation based on $\epsilon$ measured in the uppermost 0.5 m of the ocean. However, the SEM is defined for an $\epsilon_0$ measured directly at the air-sea interface. To account for this, the measured profiles of $\epsilon$ are extrapolated to the viscous sublayer, using the LOW and the T96 scaling (Fig. 4.1).

Expressing $\epsilon_0$ with the LOW scaling approach as $\epsilon_{0,LOW}$ at the depth of the viscous sublayer, allows Eq (2.27) to be rewritten as:

$$k = A \ u_* \ \text{Sc}^{-n} \left( \frac{0.394 \ [\pm \ 0.0729]}{11 \ \kappa} \right)^{1/4},$$

which is a function of $u_*$ rather than $\epsilon$. Therefore, scaling $\epsilon$ with the LOW allows to directly compare the SEM with the commonly used wind speed based-parameterisations (over the open ocean wind speed and $u_*$ are closely related as shown by Edson et al. (2013)). For this analysis the TOGA
COARE model is used to relate $u_*$ to $u_{10}$.

Figure 4.3: Measured (a) $k_{\text{DMS}}$ and (b) $k_{\text{CO}_2}$ versus the prediction of the SEM based on measured $\epsilon$ taken within the uppermost 0.5 m of the ocean averaged over 200-min intervals in log-log space. The colour code represents $n = f(u_*)$, the errors bars show the std-error. The grey data in the background represents the same calculations based on a constant Schmidt number exponent of $n = \frac{1}{2}$ (Note that applying $n = f(u_*)$ shifts the data points parallel to the x-axis). The dashed line shows the 1:1 relation between measured $k$ and the SEM. The proportionality coefficient $A$ is determined using a weighted least-squares method and the $R^2_w$ values is weighted with the relative errors of the averaged measurements. For the analysis all temporal bins, which hold only one data point and those with a standard deviation higher than 8 times the averaged standard deviation were excluded.

The air-sea gas transfer parameterisation in Eq (4.2) only includes $u_*$ as a determining parameter. As this formulation is based on the LOW, it is only valid in-situations in which no waves are present, so that the prevailing turbulence is purely shear induced. To take surface waves into account, $\epsilon_0$ in Eq (2.27) can be expressed with $\epsilon_{0_{T96}}$ providing:

$$k = A \frac{(0.3282 \pm 0.0607) u_*^2 c \rho \nu}{H_s \rho} \left( \frac{A \text{Sc}^{-n}}{\text{cm hr}^{-1}} \right)^{1/4}. \quad (4.3)$$

Figure 4.4 shows the same setup as Fig. 4.3 with $\epsilon$ extrapolated to $z_\nu$ (Eq (4.2)). The SEM holds well for this extrapolated data for both $k_{\text{DMS}}$ ($R^2_{w,\text{LOW}} = 0.85$ and $R^2_{w,T96} = 0.78$) and $k_{\text{CO}_2}$ ($R^2_{w,\text{LOW}} = 0.69$ and $R^2_{w,T96} = 0.67$) based on the LOW and the wave induced turbulence T96 scaling; all for a variable $n$. These $R^2_w$ values are close to the ones determined for the analysis based on the measured $\epsilon_{05}$ in Fig. 4.3 (an increase of 6 % and decrease
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Figure 4.4: Same as in Fig. 4.3, except with $\epsilon$ extrapolated to the surface using LOW scaling based on the measured $u_*$ values (coloured data points) and using the T96 scaling (black diamonds).

of 3 % for $R_{w,LOW}$ and $R_{w,T96}$ respectively for $k_{DMS}$ and a decrease of 4 % and 7 % for $R_{w,LOW}$ and $R_{w,T96}$ respectively for $k_{CO_2}$). This indicates that both the LOW and the T96 scaling are appropriate methods for parameterising $k$.

4.3 Relating the Gas Transfer Velocity to Modelled Dissipation Estimates

Figure 4.5 shows the prediction of the SEM based on $\epsilon_{0,LOW}$ (Eq (4.2)) and $\epsilon_{0,T96}$ the scaled wave induced turbulence (Eq (4.3)) for the complete Knorr11 data set including the periods for which ASIP was not deployed (Fig. 3.3). For both scaling approaches it shows a linear relation for $k_{DMS}$ at low and medium wind speeds (Fig. 4.5a). Only at high wind speeds, which correspond to the last station of the Knorr11 cruise, $k_{DMS}$ significantly deviates from this linear relation, which has been discussed by Bell et al. (2013). They speculate that variations in surfactants and/or wind/wave interactions are causing this deviation. When excluding this last station from the analysis, the SEM explains 94% of the variability based on the LOW and 91% based on the T96 scaling in $k_{DMS}$. Therefore, the SEM explains a large part of the variability in $k_{DMS}$ for low and medium wind speeds.

For high wind speeds, there exists no direct measurements of $\epsilon$ during
the Knorr11 cruise, because the recovery of ASIP after the storm failed. A reduction in ϵ during these high wind speeds could explain the discrepancy between the predicted and the measured \( k_{\text{DMS}} \). The SEM successfully predicted \( k_{\text{CO}_2} \) at high wind speeds (Fig. 4.5b). The different behaviour of \( k_{\text{DMS}} \) and \( k_{\text{CO}_2} \) in high winds could be explained by a reduction in ϵ with a simultaneous increase in bubble-mediated transfer, which is expected to be relevant for \( \text{CO}_2 \) but not for DMS (Bell, 2015; Gemmrich, 2012). Figure 4.5b shows the same analysis for \( k_{\text{CO}_2} \) for which the SEM explains 27% and 25% of the variability based on the LOW and T96 scaling, respectively. Highest variability of the measured \( k_{\text{CO}_2} \) occurs at low wind speeds.

The prediction of the SEM based on different ϵ scaling approaches (excluding and including surface waves) yield similar strong results for \( k_{\text{DMS}} \) and \( k_{\text{CO}_2} \) with the T96 scaling explaining nearly as much of the variability as the LOW.

Having consistent measurements of \( u_* \), \( k_{\text{DMS}} \), and \( k_{\text{CO}_2} \), the same analysis based on \( \epsilon_{0,\text{LOW}} \) is applied to \( k \) measured in the Pacific during the SOAP cruise. Taking the same relations determined for the North Atlantic and applying them on the \( k_{\text{DMS}} \) and \( k_{\text{CO}_2} \) measurements in the Pacific explains 76% of the variability for \( k_{\text{DMS}} \) and 98% for \( k_{\text{CO}_2} \) (Fig. 4.6).

When inserting the proportionality coefficients \( A_{0,\text{LOW}} \) found for \( \epsilon_{0,\text{LOW}} \) in the North Atlantic (Fig. 4.5) and for the Pacific (Fig. 4.6) into Eq (4.2), \( k \)
can be parameterised by:

\[ k_{CO_2} = 0.224 \pm 0.06 \, u_\ast \cdot Sc^{-0.13-0.22 \cdot \log_{10}(u_\ast)} \]

(with \( A = 0.39 \pm 0.02 \) for Knorr11 and \( A = 0.43 \pm 0.06 \) for SOAP)

(4.4)

\[ k_{DMS} = 0.137 \pm 0.04 \, u_\ast \cdot Sc^{-0.13-0.22 \cdot \log_{10}(u_\ast)} \]

(with \( A = 0.26 \pm 0.04 \) for Knorr11 and \( A = 0.24 \pm 0.02 \) for SOAP).

(4.5)

Using the LOW to determine these parameterisations assumes the ocean to be purely shear driven; therefore ignoring any wave enhanced turbulence near the surface. Different scaling approaches, which suggest a deviation from the LOW with \( \epsilon \) being proportional to \( z^{-2} \) to \( z^{-4} \) (Garrett, 1989; Craig and Banner, 1994; Terray et al., 1996; Sutherland and Melville, 2015), change the magnitude of the extrapolated \( \epsilon_0 \) and thus the proportionality coefficient \( A \). However, for T96 it is shown that the performance of the SEM is not changed significantly. When inserting the proportionality coefficients \( A \) for \( \epsilon_{0T96} \) in the North Atlantic (Fig. 4.5 and Eq (4.3)), \( k \) can be parameterised
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by:

\[ k_{CO_2} = 0.89 \pm 0.20 \cdot Sc^{-n} \left( \frac{u^2 \tau \rho_a \nu}{H_s \rho_w} \right)^{1/4} \]  
\[ (\text{with } A = 1.18 \pm 0.05 \text{ for Knorr11}) \quad (4.6) \]

\[ k_{DMS} = 0.51 \pm 0.13 \cdot Sc^{-n} \left( \frac{u^2 \tau \rho_a \nu}{H_s \rho_w} \right)^{1/4} \]  
\[ (\text{with } A = 0.68 \pm 0.05 \text{ for Knorr11}) \quad (4.7) \]

Neither of the scaling attempts perfectly describes the measured \( \epsilon \) profiles during Knorr11. The profiles modelled by T96 over-predict the magnitude of the measured \( \epsilon \) profiles even further than the LOW (Fig. 4.1). To overcome this over-prediction, an offset was applied. At the depth of the viscous sublayer, above the ‘breaking’ depth \( z_b \), the uniform \( \epsilon_{T96} \) falls below the values predicted by the LOW. Further investigations on scaling \( \epsilon \) close to the air-sea interface are desirable to accurately describe \( \epsilon_0 \). This scaling could be used to extrapolate \( \epsilon \) in the SEM to \( z_v \). This would permit to obtain a more accurate and more universally applicable parameterisation of \( k \).

The performance of both, in this chapter applied, \( \epsilon \) scaling approaches were equally feasible within the SEM (similar \( R^2_w \) values for both scaling approaches in Fig. 4.4). The LOW, which is only applicable when no waves occur, offers a straightforward opportunity to compare the commonly used empirical wind speed parameterisations with the SEM using Eq (4.4) and Eq (4.5) (Fig. 4.7). It is worthwhile to address this attempt as wave measurements are be necessary for the T96 scaling, which are not achievable for every measurement campaign. Note that the wave measurements during the Knorr11 campaign provided only 1D-wave spectra. This does not allow to account for the full complexity of the wave field, e.g., alignment of swell and wind sea or directional spread of the wave spectrum.
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![Graph showing gas transfer velocity parameterisations](image)

Figure 4.7: A selection of wind speed-based (dashed lines) and friction velocity (dashed-dotted lines) gas transfer velocity parameterisations are compared to the turbulence-based parameterisation determined in this study (solid lines) for $k_{\text{DMS}}$ (green) and $k_{\text{CO}_2}$ (red). These lines do not implicate any direct measurements but are based on idealised water-side friction velocity $u^*$ using the $k = f(u^*)$ relations determined in this study in Eq (4.4) and Eq (4.5). The range (shaded area) of these relations is caused by the different proportionality coefficients $A$ for the North Atlantic and the Pacific. Note that $u^*$ and $u_{10}$ are not related linearly with each other.

The function derived for $k_{\text{CO}_2}$ based on the LOW falls between the estimates of Wanninkhof (1992) and Sweeney et al. (2007) (Fig. 4.7). The latter parameterisation is an update of the first based on a revision of the C$^{14}$ data. The here determined function for $k_{\text{DMS}}$ based on the LOW lies in the lower range of the conventional wind-based parameterisations and is in the range of the results of the COARE model for DMS.

For a completely smooth water surface ($n = \frac{2}{3}$), Deacon (1977) derived $k$ based on $u^*$ using the turbulent diffusion model (Table 4.1). This model can be interpreted as a lower boundary for the wind driven gas transfer. Our $k = f(u^*)$ relation results in higher values of $k$ for both gases and comes close to Deacon’s theoretical relation only for the lowest wind speeds (Fig. 4.7). Krall (2013) empirically fitted an upper boundary to their measurements for surfactant-free conditions using $n = \frac{1}{2}$. The here determined $k_{\text{DMS}}$ relation based on the LOW falls within these boundaries showing the transition from a completely smooth to wavy ocean surface. The here found relation for $k_{\text{CO}_2}$ exceeds the empirical upper boundary of Krall (2013).
Table 4.1: Wind speed $u_{10}$ and friction velocity $u_*$ based parameterisations used in Fig. 4.7 for comparison to the relation determined in this study.

<table>
<thead>
<tr>
<th>Parameterisation</th>
<th>Equation</th>
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</thead>
<tbody>
<tr>
<td>Wanninkhof (1992)</td>
<td>$k_{660} = 0.31 , u_{10}^2$</td>
</tr>
<tr>
<td>Wanninkhof and McGillis (1999)</td>
<td>$k_{660} = 0.0283 , u_{10}^3$</td>
</tr>
<tr>
<td>Nightingale et al. (2000)</td>
<td>$k_{600} = 0.222 , u_{10}^2 + 0.333 , u_{10}$</td>
</tr>
<tr>
<td>McGillis et al. (2001)</td>
<td>$k_{600} = 3.3 + 0.026 , u_{10}^3$</td>
</tr>
<tr>
<td>Sweeney et al. (2007)</td>
<td>$k_{660} = 0.27 , u_{10}^2$</td>
</tr>
<tr>
<td>Deacon (1977)</td>
<td>$k = 0.0826 \cdot S c^{-2/3} u_*$</td>
</tr>
<tr>
<td>Lorke and Peeters (2006)</td>
<td>$k = 0.1111 \cdot S c^{-1/2} u_*$</td>
</tr>
<tr>
<td>Krall (2013)</td>
<td>$k = 0.1493 \cdot S c^{-1/2} u_*$</td>
</tr>
<tr>
<td>This study for CO$_2$</td>
<td>$k = 0.224 , \pm , 0.06 \cdot S c^{-n} u_*$</td>
</tr>
<tr>
<td>This study for DMS</td>
<td>$k = 0.137 , \pm , 0.04 \cdot S c^{-n} u_*$</td>
</tr>
<tr>
<td></td>
<td>where $n , = , 0.13 - 0.22 \cdot \log_{10}(u_*)$</td>
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</tbody>
</table>

### 4.4 Proportionality Coefficient $A$

The proportionality between both sides of the SEM (Eq (2.27)) is expressed by the coefficient $A$, which is determined through data regression. At the measurement depth of 0.5 m, $A$ is determined to be $0.70 \, \pm \, 0.07$ for $k_{DMS}$ when using a variable $n = f(u_*)$. When using $n = \frac{1}{2}$ for $k_{DMS}$, $A$ is determined to be $0.37 \, \pm \, 0.07$, which is similar to the values found in a wide range of field studies by Zappa et al. (2007) ($A = 0.419 \, \pm \, 0.130$) and also for large lakes ($A = 0.44 \, \pm \, 0.01$) as well as for small lakes ($A = 0.39 \, \pm \, 0.02$) observed by Vachon et al. (2010). Thus, the proportionality for $k_{DMS}$ between both sides of the SEM found in the open ocean, is similar to the ones found in previous studies when using the same assumptions (summarised values of $A$ in Table 4.2). Note however, that most of these studies are based on CO$_2$ measurements.

As the measured $k_{CO_2}$ are greater than the measured $k_{DMS}$, the values of $A$ have to be proportionally higher for $k_{DMS}$. The differences in the values between $k_{CO_2}$ and $k_{DMS}$ might be driven by wave/bubble effects. Breaking waves and bubbles are suggested to enhance the transfer of lower-solubility gases like CO$_2$ relative to higher-solubility gases like DMS. The coefficient $A$ based on a constant $n$ for $k_{CO_2}$ is lower ($A = 0.73 \, \pm \, 0.06$) than for a variable $n = f(u_*)$ ($A = 1.46 \, \pm \, 0.27$). These values of $A$ are significantly lower.
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Table 4.2: Proportionality coefficients, z measurement depth, and the used Schmidt number exponent n found in the literature and determined in this study.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Proportionality</th>
<th>Exponent</th>
<th>Measurements</th>
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<tbody>
<tr>
<td>CH4</td>
<td>z</td>
<td>0.42</td>
<td>隧道小波浪 (2013)</td>
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<td>Zappa et al. (2007)</td>
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<td>Gålfalk et al. (2013)</td>
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<td>Wang et al. (2015)</td>
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<td>- large lakes</td>
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<td>- small lakes</td>
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<td>Vachon et al. (2008)</td>
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<td>Zappa et al. (2007)</td>
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<td>- large lakes</td>
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<td>- small lakes</td>
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<td>Zappa et al. (2007)</td>
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Figure 4.8: The proportionality coefficient $A$ versus $\epsilon$ on $k_{\text{DMS}}$ (for $n = f(u_*)$ in red and $n = \frac{1}{2}$ in blue) and $k_{\text{CO}_2}$ (for $n = f(u_*)$ in orange and $n = \frac{1}{2}$ in green) based on ASIP measurements during the Knorr11 cruise. The circles give the relation calculated for 0.5 m depth intervals of the measured $\epsilon$ profiles and the lines show the best fitted functions. The relations found for the viscous sublayer for both the LOW scaling ($z_{\nu,\text{LOW}}$) and the T96 scaling ($z_{\nu,T96}$) as well as the uppermost 0.5 m are highlighted. The Knorr11 data is shown together with data from the literature.

higher than those found in the literature.

As pointed out before, the T96 scaling with applied offset predicts lower values of $\epsilon_0$ than the LOW. The different magnitudes of $\epsilon_0$ from both scaling approaches are reflected in different values of the constant $A_0$, which has to balance the different $\epsilon_0$ (Fig. 4.3). The values of $A_{0,T96}$ are higher than the $A_{0,\text{LOW}}$ for both $k_{\text{DMS}}$ ($A_{0,T96} = 0.67 \pm 0.05$ and $A_{0,\text{LOW}} = 0.26 \pm 0.03$) and $k_{\text{CO}_2}$ ($A_{0,T96} = 1.21 \pm 0.30$ and $A_{0,\text{LOW}} = 0.46 \pm 0.14$).

For the extrapolated $\epsilon_{0,\text{LOW}}$, $A_{0,\text{LOW}}$ was pre-determined for $k_{\text{DMS}}$ to be $A_0 = 0.20$, when using the least-square fitting to assess $n = f(u_*)$ (Section 4.1). This approach was based on the complete Knorr11 and SOAP data. As the extrapolated $\epsilon_{0,\text{LOW}}$ based on the ASIP measurements only shows a small segment of this complete data in relatively low wind speeds, it is not surprising, that $A_{0,\text{LOW}} = 0.26 \pm 0.03$ does not agree perfectly with this pre-determined value.

When taking the complete Knorr11 data into account, $A_0$ changes within the range of error for the SEM based on both the LOW and the T96
Parameterising Air-Sea Gas Transfer Velocity with Dissipation

approaches, from $A_{0_{\text{LOW}}} = 0.46 [\pm 0.14]$ and $A_{0_{\text{T96}}} = 1.21 [\pm 0.30]$ for the extrapolated ASIP $\epsilon_0$ to $A_{0_{\text{LOW}}} = 0.39 [\pm 0.02]$ and $A_{0_{\text{T96}}} = 1.18 [\pm 0.05]$ for the complete Knorr11 data for $k_{\text{CO}_2}$ and from $A_{0_{\text{LOW}}} = 0.26 [\pm 0.03]$ and $A_{0_{\text{T96}}} = 0.67 [\pm 0.05]$ the extrapolated ASIP $\epsilon_0$ to $A_{0_{\text{LOW}}} = 0.26 [\pm 0.04]$ and $A_{0_{\text{T96}}} = 0.68 [\pm 0.05]$ the complete Knorr11 data for $k_{\text{DMS}}$. The values obtained for $A$ in the Pacific based on the LOW scaling are for both gases the same (within the range of error) than found in the North Atlantic.

The most significant difference between the SEM based on the measured $\epsilon$ at a depth of 0.5 m and the one based on the extrapolated $\epsilon_0$ is the change in the proportionality constant $A$, which has to balance the change of $\epsilon$ towards the air-sea interface. For the LOW the extrapolated $\epsilon_{0_{\text{LOW}}}$ are higher than those measured at 0.5 m depth. Therefore, $A$ has to decrease towards the surface. The offset T96 scaling predicts extrapolated values of $\epsilon_{0_{\text{T96}}}$ that are similar to those measured at 0.5 m depth. Thus, $A_0$ has to stay in the same range than $A$ found in 0.5 m depth. The values of $A$ found for the extrapolated ASIP $\epsilon_{0_{\text{LOW}}}$ show lower values ($A_{0_{\text{LOW}}} = 0.12 [\pm 0.02]$ for $k_{\text{DMS}}$ and $A_{0_{\text{LOW}}} = 0.25 [\pm 0.04]$ for $k_{\text{CO}_2}$ for constant $n = \frac{1}{2}$) than for $\epsilon$ measured at 0.5 m. These values of $A_{0_{\text{LOW}}}$ for the commonly used $n = \frac{1}{2}$ are closer to those observed by Wang et al. (2015) (0.08 $\leq A \leq 0.34$), measured at 0.25 cm depth, than the $A$ found for the same setting within the uppermost 0.5 m. This highlights the depth dependency of $A$, which makes a comparison with previous studies more difficult since for each study $\epsilon$ was measured at different depths. The ASIP profiles provide $\epsilon$ measurements covering a wide range of water depths. This offers the great opportunity to investigate the depth dependency of the proportionality ‘constant’ $A$. The same analysis, which was carried out for the uppermost 0.5 m, is implemented for depth intervals of 0.5 m. The values for $A$ in these depth intervals are presented against the prevailing turbulence in Fig. 4.8.

The coefficient $A$ balances the $k - \epsilon$ relation and consequently follows the strong depth dependency of $\epsilon$. However, for the comparison of the here presented results to previously published values of $A$, it is clearer to use $A$ based on $\epsilon = f(z)$. This approach offers the ability to relate $A$ and $\epsilon$ without information about the depth (Fig. 4.8). When ignoring the measurement depth and only concentrating on the prevailing turbulence, $A$ can be formulated as $A = \beta_\epsilon \epsilon^{\gamma_\epsilon}$ with $\beta_\epsilon$ and $\gamma_\epsilon$ listed in Table 4.3. This function gives a range of values for $A$ based on measurements of $\epsilon$ at different levels of turbulences. A known value of $\epsilon$ defines the proportionality
Table 4.3: Determined coefficients to describe the dependency of the proportionality coefficient $A$ of the SEM on $\epsilon$: $A = \beta_\epsilon \epsilon^{\gamma_\epsilon}$

<table>
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<th></th>
<th>$\beta_\epsilon$</th>
<th>$\gamma_\epsilon$</th>
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</thead>
<tbody>
<tr>
<td>$k_{CO_2}$ and $n = \frac{1}{2}$</td>
<td>-0.211</td>
<td>0.052</td>
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<td>$k_{CO_2}$ and $n = f(u_*)$</td>
<td>-0.229</td>
<td>0.080</td>
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<tr>
<td>$k_{DMS}$ and $n = \frac{1}{2}$</td>
<td>-0.267</td>
<td>0.011</td>
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<tr>
<td>$k_{DMS}$ and $n = f(u_*)$</td>
<td>-0.269</td>
<td>0.023</td>
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</table>

Table 4.4: Same as Table 4.3 but for $A$ as a function of depth using a normalised $u_*$ to 0.01 m s$^{-1}$: $A = \beta_z z^{\gamma_z}$

<table>
<thead>
<tr>
<th></th>
<th>$\beta_z$</th>
<th>$\gamma_z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_{CO_2}$ and $n = \frac{1}{2}$</td>
<td>0.272</td>
<td>0.897</td>
</tr>
<tr>
<td>$k_{CO_2}$ and $n = f(u_*)$</td>
<td>0.300</td>
<td>1.735</td>
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<tr>
<td>$k_{DMS}$ and $n = \frac{1}{2}$</td>
<td>0.146</td>
<td>0.495</td>
</tr>
<tr>
<td>$k_{DMS}$ and $n = f(u_*)$</td>
<td>0.145</td>
<td>1.089</td>
</tr>
</tbody>
</table>

coefficient $A$ in the SEM.

When comparing these functions to the literature (where $n = \frac{1}{2}$), good agreement for both $k_{DMS}$ and $k_{CO_2}$ is found. As the functions fit well with the $A - \epsilon$ relations found in estuaries and coastal oceans they offer a good opportunity to predict $A = f(\epsilon(z))$. The values of $A$ for $n = f(u_*)$ are, as expected, higher than those found in the literature.

In order to avoid using $\epsilon$ as a proxy for the depth dependency of $A$, the measured $u_*$ was normalised to 0.01 m s$^{-1}$, which leads to $A = f(z, u_{*\text{norm}})$. Thus, one can formulate a depth dependency of $A = \beta_z z^{\gamma_z}$ with $\beta_z$ and $\gamma_z$ listed in Table 4.4.

### 4.5 Summary

Various studies on gas exchange across the air-sea interface have verified the dissipation rate of turbulent kinetic energy $\epsilon$ to be a good predictor for $k$ using the small-eddy model (SEM) (*Lorke and Peeters*, 2006; *Asher and Pankow*, 1986; *Moog and Jirka*, 1999; *Zappa et al.*, 2007; *Tokoro et al.*, 2011).
2008; Vachon et al., 2010). These studies include a variety of methods and techniques ranging from theoretical approaches, laboratory studies, and field campaigns in lakes, coastal areas and estuaries. In this chapter, eddy covariance DMS and CO$_2$ gas transfer measurements and observations from the Air-Sea Interaction Profiler (ASIP) have been used to confirm that this theoretical model performs well for $\epsilon$ measured at 0.5 m depth in the open-ocean.

It was shown that the performance of the SEM can be significantly improved by using a varying Schmidt number exponent $n$, which is determined as a function of $u_*$, instead of the frequently used constant of $n = \frac{1}{2}$. When applying the same assumption that $n = \frac{1}{2}$, as in former studies, the SEM explains 46 % of the variability in $k_{\text{DMS}}$ and 27 % of the variability in $k_{\text{CO}_2}$. Applying $n = f(u_*)$ improves the predictability of the SEM to 80 % for $k_{\text{DMS}}$ and 72 % for $k_{\text{CO}_2}$. This $n = f(u_*)$ changes the SEM in a similar way to the approach of Wang et al. (2015), who scale the proportionality coefficient with $A \propto \log(\epsilon)$. In both cases, the expression is shifted towards lower values for low $\epsilon$ and towards higher values for high $\epsilon$.

The two cases of ‘no waves’ (law of the wall – LOW) and ‘wave induced turbulences’ (scaling proposed by T96) have been tested to extrapolate the measurements of $\epsilon$ to the viscous sublayer $z_\nu$. For both cases, it was found that the presented basic analysis holds well, but with different set of model constants. The SEM based on both scaling approaches yields good results for both gases ($R^2_w_{\text{LOW}} = 0.85$ and $R^2_w_{\text{T96}} = 0.78$ for $k_{\text{DMS}}$ and $R^2_w_{\text{LOW}} = 0.69$ and $R^2_w_{\text{T96}} = 0.67$ for $k_{\text{CO}_2}$). The main difference between the scaling approaches is the different profile behaviour. When fitting the modelled $\epsilon$ profiles to the measured ones, the uniform values of $\epsilon_{\text{T96}}$ in the ‘breaking layer’, tend to model lower values of $\epsilon_0$ for the viscous sublayer than the LOW. These differences towards the LOW in the magnitude of extrapolated $\epsilon_0$ are reflected in the difference in the proportionality coefficient $A$ for the SEM based on the different $\epsilon$ scaling approaches. The coefficient $A$ is determined for a certain $\epsilon$-$k$ relation according to the SEM. Moving away from the surface, $A$ has to increase, because $\epsilon$ decreases, in order to obtain the same $k$.

Reliable wave measurements are not conducted during every field experiment. Therefore, the feasible results of the SEM based on the LOW are promising. Using the LOW to model $\epsilon_0$ enables the simplification of the SEM and a physically-based parameterisation that solely depends on
the water side friction velocity \( u_\ast \) in Eq (4.4) and Eq (4.5). This relation, which holds not only in the North Atlantic but also in the Pacific Ocean, allows for a validation of the commonly used wind speed parameterisation, where the LOW provides a good enough parameterisation. At that, the here presented relation follows closest the parameterisation of Sweeney et al. (2007). Measuring \( \epsilon_0 \) directly at the air-sea interface is complicated and none of the proposed scaling approaches could scale the \( \epsilon \) profiles during Knorr11 perfectly. Therefore, the usage of parameterisations based on \( u_\ast \) measurements appears to be a reliable alternative for low to intermediate wind speeds.

For the SEM, there exists a range of different values of proportionality coefficients \( A \) in literature. These different values of \( A \) are based on measurements at various depths and feature a broad range of magnitudes for \( \epsilon \). The profiling ability of ASIP was exploited to evaluate the dependency of \( A \) on \( \epsilon \), which makes a comparison between the different studies possible. The determined functions of \( A = f(\epsilon) \) cover the published values of \( A \) from Zappa et al. (2007); Wang et al. (2015); Tokoro et al. (2008); Vachon et al. (2010). Normalising \( u_\ast \) to 0.01 m s\(^{-1}\) allowed to formulate an applicable \( A - z \) relation (Table 4.4), which mirrors \( A \) to be a function of measurement depth. This function could help to overcome the uncertainty in \( A \) which has limited the application of the SEM to estimate \( k \).
5 Turbulence Scaling
Comparisons in the Ocean Surface Boundary Layer

Preface

This chapter is an adapted version of a paper currently under review:


The primary goal of Esters et al. (2018) was to compare commonly used approaches to scale $\epsilon$ with ASIP’s direct open-ocean turbulence measurements conducted during the Labrador, Knorr11, MIDAS, STRASSE, and NICE campaign.

The right to share and adapt this work is freely available under the Creative Commons Attribution 3.0 License. The data analysis, the interpretation and synthesis of results, the production of figures and the writing were done exclusively by the author of this thesis.

Dr. B. Ward contributed by supervising, assisting, and reviewing the work. Dr. Ø. Breivik and Dr. J.-R. Bidlot run the ECWAM model, extracted the output variables according to the ship tracks, and provided the modelled data. They also contributed with discussions to the analysis. Dr. G. Sutherland was in charge of ASIP for all the campaigns except the NICE campaign and provided the turbulence data for those. Dr. S. Landwehr provided the wind measurements for the Knorr11, MIDAS, and STRASSE campaign. Dr. K. H. Christensen provided the measured wave information, for the Knorr11 cruise and helped in reviewing the publication. A. ten Doeschate assisted and reviewed the publication.
This chapter uses data from all the presented cruises with available $\epsilon$ measurements (the Labrador, Knorr11, MIDAS, STRASSE, and NICE campaign) to evaluate commonly applied $\epsilon$ scaling approaches: LOW, T96, HQ10, LG89, and B12 scalings. These scaling approaches cover wind, waves, and buoyancy forcing as sources for turbulence in the OSBL. To account for these boundary conditions when scaling ASIP’s $\epsilon$ profiles, the measured $u_{10}$ for all cruises but the Labrador Sea (for which it is replaced by the predicted $u_{10}$ from the ECMWF) is considered. To be consistent for all five cruises, the $u_{10}$ measurements are used to calculate $u^*$ based on the COARE algorithm. Measured buoyancy fluxes are included when they exist, but replaced by the predictions of the ECMWF when they are missing. Hourly wave information are gained from dedicated integrations of the ECMWF stand-alone ECWAM wave model proving an unprecedented opportunity to evaluate and compare scaling assumptions and theories with direct open ocean measurements.

This chapter focuses on applying this integrated set of meteorological data, wave information, and $\epsilon$ observations in the ocean mixing layer to assess the $\epsilon$ profiles, their slopes with depth, and the coefficient $\alpha$ scaling the wind input to surface waves as a function of the wave age. The conclusions are used to predict an own empirical scaling relationship.

Section 5.1 focuses on shear and surface waves as the main driver for near-surface turbulence, where the LOW and the ‘constant-dissipation layer’ scalings (suggested by T96) are compared, as well as turbulence-wave interaction and $\epsilon$ induced by Stokes drift shear as proposed by HQ10. Section 5.2 discusses scaling approaches that consider buoyancy forcing as the generating mechanism for turbulence. Finally, these results are discussed in Sec. 5.4 and a summary is given in Sec. 5.5.

### 5.1 Wind-Wave-Induced Turbulence

Figure 5.1 shows the hourly averaged observations of $\epsilon$, which were scaled using Eq (2.15) and $H_{sw}$ calculated from the wind sea part of the spectrum (T96; *Drennan et al.* (1996)). The ‘breaking depth’ $z_b$ and the averaged ‘transition depth’ $\overline{z_t}$ ($\pm$ its standard deviation) are indicated in Fig. 5.1. Following T96 the depth is normalised with $H_{sw}$, whose magnitudes are
Figure 5.1: (a) Vertical distribution of the measured $\epsilon$ normalised with the ratio of the significant wave height based on the wind-sea part of the wave spectrum $H_{sw}$ to the cubic water-side friction velocity $u_{sw}^3$ versus the normalised depth $z/H_{sw}$ for the full 70-min time averaged data. The data is divided into subsets according to the inverse wave age $A_{iw} = u^*/a_c$: (b) For $0.03 < A_{iw} < 0.035$, (c) $0.035 < A_{iw} < 0.04$, (d) $0.04 < A_{iw} < 0.045$, (e) $0.045 < A_{iw} < 0.05$, (f) $0.05 < A_{iw} < 0.055$, (g) $0.055 < A_{iw} < 0.06$, (h) $0.06 < A_{iw} < 0.065$. The colour bar gives the range of $A_{iw}$. The dashed horizontal lines show the ‘breaking depth’ $z_b$, the mean transition depth $z_t$ (with its standard deviation as vertical thick black lines), and the mean mixing layer depth $h_\epsilon$ as green dashed line. Linear regressions through the data are performed for all the data above the $h_\epsilon$ (red) and above $z_t$ as suggested by T96 (dashed in blue). For reference the T96 scaling is plotted in black and the LOW scaling in grey.

shown in Fig. 3.2.

The coefficient $\alpha$ based on $F$ in water-side quantities and the exponent $b$ in Eq (2.15) were determined for the depth range above $z_t$ and separately for the range above $h_\epsilon$ using a linear regression. As shown in Fig. 5.1a, the best fit through the observations above $z_t$ is obtained with $\alpha = 8.07$ and $b = -1.29$, where $|z|^{-b}$ describes the depth dependency of the $\epsilon$ profiles (summarised in Table 5.1). This depth dependency of $\epsilon$ is closer to the actual wall layer dependency of $|z|^{-1}$ than to the dependency proposed by T96 of $|z|^{-2}$. It is concluded that the observed magnitude and depth dependency of $\epsilon$ profiles indicate that the LOW follows our measurements more closely than the scaling proposed by T96.

As it is suggested that $\epsilon$ is enhanced in the presence of breaking waves,
relative to the LOW, potential differences between non-breaking and breaking wave conditions should be investigated. With this intention, the data set is divided into ensembles, based on the ambient wind speed: \( u_{10} < 4 \text{ m s}^{-1} \) and \( u_{10} > 8.5 \text{ m s}^{-1} \) (Fig. 5.2). Wind speed is here used as a proxy for the fraction of breaking waves. No wave breaking is expected to occur at wind speeds below \( 4 \text{ m s}^{-1} \). The threshold of \( 8.5 \text{ m s}^{-1} \) was chosen because it lies in the range of wind speeds for which whitecapping parameterisations start to diverge (Fig. 3 in Scanlon and Ward (2016)). Figure 5.2 shows that for both the low and higher wind speeds, the depth dependency of the observed \( \epsilon \) follow closer to the classical wall layer scaling of \( |z|^{-1} \) than a suggested \( |z|^{-2} \) \((|z|^{-1.14} \text{ above } h_e \text{ and } |z|^{-1.34} \text{ above } z_t \text{ for low wind speeds and } |z|^{-1.12} \text{ above } h_e \text{ and } |z|^{-1.20} \text{ above } z_t \text{ for higher wind speeds})\). However, the data used within this thesis was mostly collected in situations of lower wind situations; therefore, not many wave breaking events are expected. Hence, there could still be regimes of higher dissipation under larger waves than observed in this study. T96 collected their data in wind conditions of 7 to 16 m s\(^{-1}\), which includes less low wind conditions but similar maximum wind speeds as observed in this study.

The data distribution of the scaled \( \epsilon \) measurements in Fig. 5.1a spans over two orders of magnitude above \( z_t \). This range in magnitudes could be explained by the wave energy parameter \( \alpha \) being a function of wave age. Dividing the data set into subsets based on the inverse wave age \( A_{iw} = \frac{u_{10}}{c_p} \) (Fig. 5.1b - 5.1f) and determining \( \alpha \) and \( b \) for each of these
subsets using a linear regression as before, shows a clear dependency of $\alpha$ on $A_{iw}$: $\alpha = 26 - (388 \, A_{iw})$ above $z_t$ and $\alpha = 24 - (361 \, A_{iw})$ above $h_\epsilon$ (Fig. 5.3). These functions are valid for $A_{iw}$ between 0.03 and 0.065. For the presented range, these functions describe the values of $\alpha$ well, with determination coefficients of $R^2 = 0.96$ and $R^2 = 0.97$ for depth levels above $z_t$ and above $h_\epsilon$, respectively. Here, the coefficient of determination, $R^2$ (the square of Pearson’s linear correlation coefficient), is weighted by the uncertainties in $\alpha$. The 95% confidence interval of $\alpha$ is determined from a linear regression based on Eq (2.15). All the values for $\alpha$ and $b$ are summarised in Table 5.1.

In contrast to $\alpha$, the exponent $b$ does not depend on $A_{iw}$ and stays constant as $b = -1.27 [\pm 0.087]$ (above the $z_t$) and $b = -1.20 [\pm 0.127]$ (above the $h_\epsilon$) for the whole range of sea states. The determined coefficient for $b$ and the relation between $\alpha$ and $A_{iw}$, which are summarised in Tab. 5.1, allow us to formulate a refined scaling approach based on Eq (2.15):

$$\epsilon_{wind}(z) = (7.2 - 108.3 \, A_{iw}) \left( \frac{u^3_{*sw}}{H_{sw}} \right) \left( \frac{z}{H_{sw}} \right)^{-1.15} \quad (5.1)$$

in this case determined for the range above $h_\epsilon$.  

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**Figure 5.3:** The value for $\alpha$ in Eq (2.15) determined through the linear regressions in Figure 5.1 as a function of the inverse wave age $A_{iw} = u_{*s}/c_p$. The regression for the $\epsilon$ data above the mixing layer depth $h_\epsilon$ is given by $\alpha = 24 - 361 \, A_{iw}$ (red) and above the ‘transition depth’ $z_t$ by $\alpha = 26 - 388 \, A_{iw}$ (blue). The error bars give the 95% confidence level of $\alpha$ and the horizontal dashed lines show the value of $\alpha$ determined from the full data set.
Table 5.1: Values of the exponent $b$ and coefficient $\alpha$ in Eq (2.15) determined via linear regression through the measurements above the $h_\epsilon$ and above $z_t$, for the full data, the data separated into subsets according to their inverse wave age $A_{iw}$ as in Fig. 5.1, $\alpha$ as a function of $A_{iw}$ as in Fig. 5.3 and separated into low and high wind speeds as in Fig. 5.2.

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<td><strong>All</strong></td>
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<tr>
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</tr>
<tr>
<td>$b$</td>
<td>-1.20 [± 0.127]</td>
<td>-1.27 [± 0.087]</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>26 - 388 $A_{iw}$</td>
<td>24 - 361 $A_{iw}$</td>
</tr>
<tr>
<td>$R^2$</td>
<td>0.86</td>
<td>0.98</td>
</tr>
<tr>
<td><strong>Wind speed subsets</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$0 \text{ m s}^{-1} &lt; u_{10} &lt; 4 \text{ m s}^{-1}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$b$</td>
<td>-1.14</td>
<td>-1.34</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>17.48</td>
<td>31.91</td>
</tr>
<tr>
<td>$R^2$</td>
<td>0.86</td>
<td>0.98</td>
</tr>
<tr>
<td>$u_{10} &gt; 8.5 \text{ m s}^{-1}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$b$</td>
<td>-1.12</td>
<td>-1.20</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>2.73</td>
<td>2.97</td>
</tr>
<tr>
<td>$R^2$</td>
<td>0.68</td>
<td>0.73</td>
</tr>
</tbody>
</table>

HQ10 modelled the effect of wave-induced turbulence on $\epsilon$ with Eq (2.19). The presented observations here were normalised with the scaling approach proposed by HQ10 based on separated wind and swell seas (Figs. 5.4a and 5.4b), respectively, as well as the sum of both (Fig. 5.4c). The HQ10 wind sea scaling (Fig. 5.4a) underestimates the presented observations close to the sea surface above a depth corresponding to $H_s$, but describes the observations better below (albeit with a scatter two orders of magnitude). The most appropriate value for $\beta$ (Eq (2.20)) is determined to be 1.53 (Tab. 5.2). The normalised data based on the swell (Fig. 5.4b) deviates considerably from the observed $\epsilon$, with highest underestimation below $H_s$ (several orders of magnitude).
magnitudes). The sum of both the wind and swell part of the spectrum (Fig. 5.4c) describes the observed $\epsilon$ better than the separated sea states. The determined $\beta = 0.97$ (Tab. 5.2) agrees with HQ10 who suggested that $\beta \leq 1.0$. However, there remains significant scatter which is a function of the surface Stokes drift velocity $u_{s0}$ (see the colour coding in Fig. 5.4).

Figure 5.4: Vertical distribution of the measured $\epsilon$ normalised with the scaling proposed by HQ10 ($\epsilon_{HQ10}$) versus the normalised depth $z/h$ for the full 200-min time averaged data. (a) For the wind sea part of the wave spectrum. (b) Swell part of the wave spectrum. (c) Modelled $\epsilon$ from both parts added together with Stokes drift shear for a monochromatic wave as suggested by HQ10. (d) The same is calculated for the Stokes shear profile based on the Phillips approximation. The colour bar indicates the surface Stokes velocity $u_{s0}$. The horizontal green dashed line represents the mixing layer depth $h_\epsilon$ and the horizontal black dashed line represents the mean of the significant wave height $H_s$ (with its standard deviation as thick vertical black line). The vertical red line gives the average through the data and is expressed by $\beta$ in Eq (2.20).

The surface Stokes drift is sensitive to errors in the wind field, but not more so than other wave parameters. By comparison, $H_s$ is proportional to the square root of the zeroth moment $m_0$ of the wave spectrum, and is more sensitive to errors in the swell representation. The surface Stokes drift is more directly related to the wind sea spectrum since it is heavily weighted towards the higher frequencies of the spectrum, which respond quickly to changes in the wind field. It is found that the analysed wind field is generally in good agreement with the observations from the cruises for which wind measurements exist (see Fig 3.2d).

The values of higher Stokes drift shear at the surface from the Phillips approximation relative to the ones for a monochromatic wave, give higher estimates for $\epsilon$ (Eq (2.19)). This is reflected in a lower value of $\beta = 0.21$ (Fig. 5.4d) compared to the HQ10 scaling for monochromatic waves (Fig. 5.4c), where $\beta = 0.97$ (Table 5.2). For the approach based on the
Table 5.2: Values of the factor $\beta$ in Eq (2.20) indicated as red vertical lines in Fig. 5.4 and the respective root mean square error (RMSE) determined for the HQ10 scaling in the same figure.

<table>
<thead>
<tr>
<th></th>
<th>$\beta$</th>
<th>RMSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monochromatic wave</td>
<td>1.53</td>
<td>4.09</td>
</tr>
<tr>
<td>Wind sea part</td>
<td>158.17</td>
<td>47.15</td>
</tr>
<tr>
<td>Swell part</td>
<td>0.97</td>
<td>3.79</td>
</tr>
<tr>
<td>Both parts added</td>
<td>0.21</td>
<td>3.26</td>
</tr>
</tbody>
</table>

monochromatic wave, most of the variability among the different parameterisations can be explained by $u_{s0}$. For lower $u_{s0}$ ($u_{s0} < 0.06 \text{ m s}^{-1}$) the scaled profiles underestimate the measured ones and vice versa for higher $u_{s0}$ as these surface values directly influence the values of the modelled $\epsilon$ in Eq (2.19). Using the Phillips approximation results in less variability (root mean square error (RMSE) of 3.26 compared to 3.79 for the monochromatic wave), especially closer to the surface, and the parameterisations for periods of lower and higher $u_{s0}$ fall closer together than based on the conventionally proposed approach (Fig. 5.4d). Applying $\beta = 0.21$ in Eq (2.20) and using the Stokes drift shear from the Phillips approximation (Eq (2.23)) allows for a reformulation of the HQ10’s scaling (Eq (2.19)) as:

$$
\epsilon_{\text{wave,}}(z) = 0.79 \pi \sqrt{\frac{H_s}{\lambda}} u^2_s \alpha_p \sqrt{-\frac{2\pi g}{z}} \text{erfc}(\sqrt{-2\ell z}).
$$

(5.2)

### 5.2 Buoyancy-Induced Turbulence

To identify periods during which convective forcing dominates over wind-wave forcing, the ratio of $h_\epsilon$ to the Langmuir stability length $L_L = u^2_s u_{s0}/B_0$, where a positive $B_0$ describes destabalising periods, is used (B12, Sutherland et al. 2014a). The threshold for a dominant convective forcing is considered to be unity ($h_\epsilon/L_L = 1$ for $h_\epsilon$ defined as being positive), so that in cases of $h_\epsilon/L_L > 1$, buoyancy forcing is considered as important.

Figure 5.5a shows the measured $\epsilon$ normalised with the LOW ($\tilde{\epsilon}_{\text{LOW}} = \epsilon/\epsilon_{\text{LOW}}$) for both the wind-wave dominated regime ($h_\epsilon/L_L < 1$) and the
Figure 5.5: Vertical distribution of measured $\epsilon$ for destabilising periods of positive surface buoyancy flux $B_0 > 0$ normalised with: (a) LOW; (b) $B_0$; (c) a combination of both. The data is divided into periods during which convection is important ($h_c/L_L > 1$) in red and during which convection is less important ($h_c/L_L < 1$) in green. The mean values are indicated by the vertical lines for periods during which convection is important (red) and convection is less important (green). The blue line shows the value suggested by LG89. These mean values are used to determine the normalisation in (c). The horizontal dashed green line indicates the $h_c/\epsilon/L_L$ and the dashed black line shows the mean significant wave height $H_s$ with the thick vertical black lines being its standard deviations. The circled data indicate situations during which $u_{10}$ is higher than 8.5 m s$^{-1}$.

convective regime ($h_c/L_L > 1$). The near uniformity of $\bar{\epsilon}_{LOW}$ ($\bar{\epsilon}_{LOW} = 0.90$) of the wind-wave dominated regime indicates that when convection is minor, $\epsilon$ approximately follows the LOW scaling (Fig. 5.5a). The observed $\epsilon$ during periods of strong convection is better scaled by including $B_0$ (Fig. 5.5b).

At depths below $H_s$, the $\epsilon$ measured for the convective regime normalised by $B_0$ ($\bar{\epsilon}_{B_0} = \epsilon/\epsilon_{B_0}$) stays relatively uniform over depth. This is typical as convectively forced turbulence has not been found to display a significant depth dependency (LG89, Callaghan et al. 2014). The higher values of $\bar{\epsilon}_{B_0}$ near the surface could be explained by the presence of shear.

Table 5.3: Values of the factors $\bar{\epsilon}_{LOW}$, $\bar{\epsilon}_{B_0}$, and their combination $\bar{\epsilon}_{B_0} \cdot B_0 + \bar{\epsilon}_{LOW} \cdot \epsilon_{LOW}$ in Fig. 5.5 and shown by the vertical lines in the same figure.

<table>
<thead>
<tr>
<th>$h_c/L_L$</th>
<th>$\bar{\epsilon}_{LOW}$</th>
<th>$\bar{\epsilon}_{B_0}$</th>
<th>$\bar{\epsilon}<em>{B_0} \cdot B_0 + \bar{\epsilon}</em>{LOW} \cdot \epsilon_{LOW}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$h_c/L_L &lt; 1$</td>
<td>0.9</td>
<td>–</td>
<td>1.00</td>
</tr>
<tr>
<td>$h_c/L_L &gt; 1$</td>
<td>–</td>
<td>0.91</td>
<td>0.63</td>
</tr>
<tr>
<td>LG89</td>
<td>1.76</td>
<td>0.58</td>
<td>0.87</td>
</tr>
</tbody>
</table>
In order to yield a refined formulation, $\epsilon_{\text{buoyancy}*}$, to describe the observed $\epsilon$ in a similar form to LG89, the averaged values of $\bar{\epsilon}_{\text{LOW}}$ and $\bar{\epsilon}_{B_0}$ are applied as scaling coefficients (summarised in Tab. 5.3). In periods where the wind-wave forcing dominates, $\epsilon_{\text{buoyancy}*}$ is given by the averaged $\bar{\epsilon}_{\text{LOW}}$. In this case a value of 0.90 of $\bar{\epsilon}_{\text{LOW}}$ scales the observed $\epsilon$ best. To account for the additional buoyancy effect when convection is dominant, the similarity scaling for those periods is a linear combination of the LOW and $B_0$. Thus, $\epsilon_{\text{buoyancy}*}$ is extended by the averaged $\bar{\epsilon}_{B_0}$ of 0.91 times the prevailing $B_0$:

$$
\epsilon_{\text{buoyancy}*}(z) = \begin{cases} 
0.90 \cdot \epsilon_{\text{LOW}} & \text{for } h_{\epsilon}/L_L < 1 \\
0.63 \cdot (0.90 \cdot \epsilon_{\text{LOW}} + 0.91 \cdot B_0) & \text{for } h_{\epsilon}/L_L > 1.
\end{cases}
$$

(5.3)

Following LG89, this formulation of $\epsilon_{\text{buoyancy}*}$ is used in order to describe the full turbulence field during conditions of positive $B_0$ and represents the turbulence induced by shear and convection. Figure 5.5c shows that the extended similarity scaling reduces the variability relative to the ones based on wind or buoyancy only.

In conditions when convection dominates over wind-wave forcing ($h_{\epsilon}/L_L > 1$ red in Fig. 5.5c), $\epsilon$ is well scaled with scale factors of $u_*$ and $B_0$. Even most of the observations of $\epsilon$ during situations in which wave breaking is expected to occur, which are indicated by black circles in Fig. 5.5c, fall in the midst of the normalised data. Highest bias with up to more than an order of magnitude is found for periods during which convection is less important ($h_{\epsilon}/L_L < 1$ shown in green in Fig. 5.5c). This suggests that wind and buoyancy alone do not explain all the turbulence for these periods and wave-induced turbulence might contribute. The outlying profile in Fig. 5.5c left of the mean normalised $\epsilon$, which was taken during wave-breaking conditions, falls into a period during which wind-wave forcing dominates over convection. This data was taken during the NICE cruise when $u_{10}$, $u_*$, and $H_s$ increased, $B_0$ reached minimal negative values, and thus wind-wave-induced turbulence is suggested to be important. In comparison to the scaling in Fig. 5.5c, the $\epsilon$ profile is well described by the regression line in Fig 5.2c, which additionally considers wave information in form of the significant wave height $H_s$. In this figure all the high wind speed data falls within the cluster.

The scaling approach suggested by B12 in Eq (2.24) formulates a linear combination of $\epsilon$ from the three processes (i.e. shear, Stokes drift, and buoy-
Figure 5.6: The upper panels show the regime diagram for mixing in the OSBL as introduced by B12 for the Labrador cruise in orange (a), the Knorr11 cruise in blue (b), the STRASSE cruise in green (c), the MIDAS cruise in red (d), and the NICE cruise in black (e). The thick solid black lines divide the diagram into regions where the single forcing produce more than 90% of the total $\epsilon$. As the regime diagram is only defined for periods of $B_0 > 0$, the lower panel (f) shows the remaining data as a function of the turbulent Langmuir number $La_t$ to fall between wave- and wind dominated turbulence. During the NICE campaign all data falls in the $B_0 > 0$. 
Figure 5.7: The surface Stokes velocity $u_{s0}$ determined from the ECWAM wave model versus the water-side friction velocity $u_*$ determined from the measured $u_{10}$ using the COARE algorithm. The red line indicates the linear fit through the data, which is given by $u_{s0} = 12.04 u_*$.

Figure 5.7: The surface Stokes velocity $u_{s0}$ determined from the ECWAM wave model versus the water-side friction velocity $u_*$ determined from the measured $u_{10}$ using the COARE algorithm. The red line indicates the linear fit through the data, which is given by $u_{s0} = 12.04 u_*$. The time series of $u_*$, estimated from the measured $u_{10}$ by the COARE algorithm, and $u_{s0}$, determined from the ECWAM model, is suggestive of a linear relationship between both velocity scales (Fig. 3.2a). It is well known that the relationship between the wind sea part of the spectrum and its Stokes drift is close to linear (see Kenyon 1969; Ardhuin et al. 2009, and Li et al. 2017). This relationship is applied for regimes of constant $La_t$ as shown in the regime diagram in Fig. 5.6. A constant $La_t$ predicts no variation within the composition of the dominant wind-wave turbulence generation processes over the periods of ASIP’s deployments.

A linear regression $u_{s0} = -5.5 \cdot 10^{-4} + 12.75 u_*$ explains 67% of the variability between $u_*$ and $u_{s0}$ (Fig. 5.7). The slope is very close to the value 12 found by Gargett and Grosch (2014) for cases in which Langmuir circulation dominates the turbulence forcing. Also, this slope agrees with a slope of $\approx 11–12$ by Kitaigorodskii et al. (1983) as well as a derived slope between 9.2 and 13.8 from the Pierson-Moskowitz (PM) spectrum by Li and Garrett (1993). Forcing the described linear regression between the water-side friction velocity $u_*$ and $u_{s0}$ to pass through the origin, changes
The relation to:

$$u_{s0} = 12.04 \, u_*$$, \hspace{0.5cm} (5.4)

which does not significantly reduce the statistics as the coefficient of determination is still $R^2 = 0.67$.

Considering this linear relation between $u_{s0}$ and $u_*$ allows for the substitution of $u_{s0}$ in Eq (2.24) with Eq (5.4) as:

$$\epsilon_{B12} = (2 - 2e^{-0.5\sqrt{1/12.04}} + 2.65) \frac{u_*^3}{h} + 0.3B_0.$$ \hspace{0.5cm} (5.5)

By setting $La_t$ to a constant in this equation, the scaled turbulence is forced to have its origin in a specific wind-wave regime as discussed above. This means that no distinction between a Langmuir or wind-dominated regime exists, but rather $u_{s0}$ is greater than the wind stress by a constant factor.

The formulation in Eq (5.5) of the scaling suggested by B12 has the same form as that suggested by LG89 (Eq (2.13)). Both scalings overestimate the observed $\epsilon$ profiles (Fig. 5.8). The $\epsilon_{bouyancy_*}$ describes these observations.
with a RMSE of 2.50 compared to 3.11 for the B12 scaling from Eq (5.5) and compared to 3.25 for the LG89 scaling.

5.3 Evaluation of Coefficients and Scaling Relationships

The coefficients for \( \alpha, b, \beta, \overline{\epsilon}_{\text{LOW}}, \) and \( \overline{\epsilon}_{B_0} \) as summarised in Tab. 5.4 were extracted for the whole data set (i.e. the data from all five cruises for which \( \epsilon \) data exists). To determine the optimal scaling, these coefficients are compared to the ones gained from the same analysis based on training data sets. The training data sets consist of four of the five cruises with respectively one (the testing data set) being withheld from each run. This procedure results in five sets of coefficients summarised in Tab. 5.4.

The RMSE of these tests is highest for the \( \epsilon_{\text{wave}} \) scaling (with the respective coefficients) for the Labrador and the Knorr11 cruise for negative \( B_0 \) conditions. Also, the \( \epsilon_{\text{wind}} \) scaling for negative \( B_0 \) and the \( \epsilon_{\text{wave}} \) for positive \( B_0 \) (with the respective coefficients) for those cruises show clearly higher RMSE in comparison to the other testing data sets. Both of these cruises were located along the Canadian continental shelf.

For both the Knorr11 and Labrador cruise the \( \epsilon_{\text{wave}} \) consistently over-predicts the measured \( \epsilon \) by more than 3 orders of magnitude. This suggests that the waves induced by the Stokes shear affect the growth of turbulence less in the shelf areas than in the other sites of the Atlantic. Already the regime diagram in Figure 5.6 indicated this as the data of those both cruises reaches least far into the wave regime during negative \( B_0 \) conditions. Therefore, other processes are expected to cause the prevailing turbulence. In the case of the Knorr11 cruise this might be wind. The \( \epsilon_{\text{wind}} \) (with the \( \alpha \) and \( b \) from Tab. 5.4) under-predicts the measured \( \epsilon \) for periods of negative \( B_0 \), but describes them within one order of magnitude for positive \( B_0 \) conditions.

The overall RMSE (averaged) is lowest for the \( \epsilon_{\text{wind}} \) scaling for positive \( B_0 \) conditions with RMSE = 7.07. For these conditions only the scalings based on wind-wave-induced turbulence are compared. The \( \epsilon_{\text{wind}} \) and the \( \epsilon_{\text{buoyancy}} \), scaling collapse to the measured \( \epsilon \) of the respective training data sets within an order of magnitude as shown in Fig. 5.9. Thereby, the \( \epsilon_{\text{buoyancy}} \) describes...
Table 5.4: Values of the coefficients $\alpha$, $\beta$, $\tilde{\epsilon}$, $\tilde{\epsilon}_B$, and $\tilde{\epsilon}_B \times B_0 + \tilde{\epsilon}_L \times \tilde{\epsilon}_L$ from the five training data sets with the name referring to the respective testing data set of each analysis, the averaged coefficients of these runs, and the coefficients gained from the analysis using the whole data set (including data from the five here presented cruises). The root mean square error (RMSE) refers to the tests of the gained coefficients on the testing data sets and the RMSE for the averaged data refers to the median of the single RMSEs.

<table>
<thead>
<tr>
<th></th>
<th>Labrador Knorr</th>
<th>STRASSE</th>
<th>MIDAS</th>
<th>NICE</th>
<th>Averaged</th>
<th>Whole data</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$ (above $z_t$)</td>
<td>26 - 395</td>
<td>26 - 388</td>
<td>24 - 362</td>
<td>28 - 425</td>
<td>25 - 363</td>
<td>25.8 - 392</td>
</tr>
<tr>
<td>$\beta$ (above $h_\epsilon$)</td>
<td>-1.30 - 0.068</td>
<td>-1.29 - 0.193</td>
<td>-1.15 - 0.183</td>
<td>-1.15 - 0.193</td>
<td>-1.29 - 0.193</td>
<td>-1.15 - 0.193</td>
</tr>
<tr>
<td>$\tilde{\epsilon}_L$</td>
<td>0.90 - 0.126</td>
<td>0.90 - 0.195</td>
<td>0.60 - 0.195</td>
<td>0.82 - 0.195</td>
<td>0.91 - 0.195</td>
<td>0.91 - 0.195</td>
</tr>
<tr>
<td>$\tilde{\epsilon}_B$</td>
<td>0.91 - 0.195</td>
<td>0.90 - 0.195</td>
<td>0.60 - 0.195</td>
<td>0.89 - 0.195</td>
<td>0.90 - 0.195</td>
<td>0.90 - 0.195</td>
</tr>
</tbody>
</table>

RMSE $\epsilon_{\text{wind}}$ ($B_0 < 0$) | 208.92 | 66.74 | 2.23 | 9.87 | -38.31 |
RMSE $\epsilon_{\text{wind}}$ ($B_0 > 0$) | -10.20 | 2.90 | 6.79 | 7.35 | 7.07 |
RMSE $\epsilon_{\text{wave}}$ ($B_0 < 0$) | 543.71 | 318.62 | 5.08 | 6.49 | -162.56 |
RMSE $\epsilon_{\text{wave}}$ ($B_0 > 0$) | -46.04 | 6.37 | 4.98 | 16.90 | 11.64 |
RMSE $\epsilon_{\text{buoyancy}}$ ($B_0 > 0$) | -14.68 | 7.03 | 3.08 | 9.54 | 8.29 |
Figure 5.9: Bin-averaged vertical distribution of the measured $\epsilon$ normalised with the improved wind-wave based scaling $\epsilon_{\text{wind}}$ (green); wave-based $\epsilon_{\text{wave}}$ (blue); buoyancy-based $\epsilon_{\text{buoyancy}}$ (red). The profiles are averaged over the five respective profiles from the ‘testing’ analysis and the symbols indicate the mean values for periods of (a) negative surface buoyancy flux $B_0$; (b) positive $B_0$; (c) all data.

The magnitudes of the measured $\epsilon$ better than the other scalings for $B_0 > 0$ conditions, where $\epsilon_{\text{buoyancy}} = 1.18 \pm 2.339$ is closest to unity (Fig. 5.9b). For $B_0 < 0$ conditions, $\epsilon_{\text{wind}} = 0.85 \pm 3.089$ is closest to unity (Fig. 5.9a). The $\epsilon_{\text{buoyancy}}$ scaling describes the behaviour of the here presented data best for conditions when convection dominates over wind-wave induced turbulence ($h_\epsilon/L_L < 1$). This is represented by the relatively higher RMSEs for the Knorr11 cruise (RMSE = 14.68 in Tab. 5.4). For this cruise most of the data is spread in the wind-wave domain during positive $B_0$ conditions, and thus convection is considered to be less important (Fig. 5.6b).

The performance of these scaling approaches seems suitable even though not all possible sources of turbulence in the OSBL are included. For example, internal waves (breaking or non-breaking) enhance the observed turbulence by redistributing energy vertically or by releasing energy when they actually break. Additionally, submesoscale processes and inertial shear are further sources of turbulence that are expected to enhance $\epsilon$ relative to the introduced scaling approaches.

The averaged coefficients from the analysis on all training data sets are similar (within their range of error) to those found for the whole data set, which gives confidence in the coefficients determined through the analysis of this study. Excluding the coefficients gained from the two training data sets with the highest RMSE (Labrador and Knorr11) yields similar values for the coefficients of $\alpha, b, \beta, \epsilon_{\text{LOW}},$ and $\epsilon_{B_0}$. 
Table 5.5: Mean [± standard deviation] and root mean square error (RMSE) of the $\epsilon$ observations from the testing data sets normalised by the different scaling assumptions as determined in Fig. 5.9 using the coefficients from the respective training data sets for daytime ($B_0 < 0$) and nighttime conditions ($B_0 > 0$) as well as for all the data.

<table>
<thead>
<tr>
<th></th>
<th>$\epsilon_{\text{wind}}$</th>
<th></th>
<th>$\epsilon_{\text{wave}}$</th>
<th></th>
<th>$\epsilon_{\text{buoyancy}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>mean ± std</td>
<td>RMSE</td>
<td>mean ± std</td>
<td>RMSE</td>
<td>mean ± std</td>
</tr>
<tr>
<td>$B_0 &lt; 0$</td>
<td>0.85 [± 3.080]</td>
<td>38.31</td>
<td>0.49 [± 2.926]</td>
<td>142.56</td>
<td>–</td>
</tr>
<tr>
<td>all data</td>
<td>1.24 [± 3.060]</td>
<td>7.35</td>
<td>0.87 [± 4.033]</td>
<td>16.90</td>
<td>–</td>
</tr>
</tbody>
</table>

5.4 Discussion

The observations presented here support a depth dependency of $\epsilon$ described by $b = -1.29$ above $z_t$. This is less than that proposed by T96 ($b = -2$), which was supported by observations in Lake Michigan (Wang and Liao, 2016), in the Pacific Ocean at depths below approximately one $H_s$ (Sutherland and Melville, 2015), and in the laboratory (Siddiqui and Loewen, 2007) at depths below 0.4 $H_s$. For measurements in coastal waters of the South China Sea, Shuiqing and Dongliang (2016) find an even more gentle slope with $b = -2.11$. Feddersen et al. (2007) show a slightly smaller decay rate of $b = -1.9$ in nearshore regions, which still is higher than the $b$ found in the presented study. The studies that are referred to are summarised with their measurement technique and depth in Tab. 5.6.

Greenan et al. (2001) found that the T96 scaling holds for the case in which the swell can be easily separated. However, for open-ocean conditions in the presence of more complex sea states the T96 scaling does not hold. In these situations, where wind sea and swell interact, $\epsilon$ seems to decay rather with $|z|^{-1}$ than with $|z|^{-2}$. T96 measured in Lake Ontario with young seas in the absence of swell. The T96 scaling was confirmed in the open ocean by Drennan et al. (1996) but most of the cases were under wind sea conditions. Similarly, Gemmrich (2010) observed $\epsilon$ profiles that decayed with $|z|^{-1}$ in a depth range between $\approx 2H_s$ and $\approx 0.3H_s$. Only above $\approx 0.3H_s$ they found a layer where $\epsilon$ was enhanced with respect to the profile decaying with $|z|^{-1}$. Thomson et al. (2016) found values for $b$ that fall between the depth dependency of the LOW and T96 as $-1.56 [\pm 0.03]$ for a fixed reference frame at depth shallower than $z/H_s = 10^{-1}$.

Near the surface, above $z_b = 0.6H_s$, the T96 scaling predicts a layer of
Table 5.6: Studies cited in this chapter listing the location of experiments, number of $\epsilon$ measurements, the measurement technique, and respective depth range.

<table>
<thead>
<tr>
<th>Location</th>
<th>Number of $\epsilon$ estimates</th>
<th>Measurement technique</th>
<th>Depth range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lombardo and Gregg (1989)</td>
<td>North Pacific Ocean</td>
<td>Advanced Microstructure Profiler (AMP)</td>
<td>$\approx$ 5 m to 300 m</td>
</tr>
<tr>
<td>Anis and Moum (1995)</td>
<td>Off the Oregon coast</td>
<td>Vertical profiler Chameleon</td>
<td>0.5 m to 120 m</td>
</tr>
<tr>
<td>Terray et al. (1996)</td>
<td>Lake Ontario</td>
<td>Three types of current meters</td>
<td>0.153 m to 2.153 m</td>
</tr>
<tr>
<td>Greenan et al. (2001)</td>
<td>Scotian Shelf</td>
<td>Acoustic travel-time current meters (Minilab SD-12)</td>
<td>2 m</td>
</tr>
<tr>
<td>Terray et al. (1996)</td>
<td>Lake Ontario</td>
<td>Vertical profiler Chameleon</td>
<td>5 m to sea bed</td>
</tr>
<tr>
<td>Greenan et al. (2001)</td>
<td>Quasi-horizontal profiler (EPSONDE-Glider)</td>
<td>Digital particle image velocimetry (PIV)</td>
<td>1 to 25 mm</td>
</tr>
<tr>
<td>Drennan et al. (1996)</td>
<td>Off Maryland Coast</td>
<td>Three ADVs</td>
<td>0.56 m, 1.32 m, 1.86 m above the bed (water depth 2.3 m)</td>
</tr>
<tr>
<td>Siddiqui and Loewen (2007)</td>
<td>Wind-wave flume</td>
<td>Tethered free-fall vertical profiler (EPSONDE2)</td>
<td>0.15 m, 0.5 m, 1.5 m, 2 m above bed (water depth 2.5 m)</td>
</tr>
<tr>
<td>Jones and Monismith (2008)</td>
<td>Grizzly Bay in San Francisco Bay</td>
<td>Four Acoustic Doppler velocimeter (ADVs)</td>
<td>0.06 to 7</td>
</tr>
<tr>
<td>Huang and Qiao (2010)</td>
<td>Pacific Ocean</td>
<td>Array of acoustic Doppler profiler (subsurface)</td>
<td>0 m</td>
</tr>
<tr>
<td>Sutherland and Melville (2015)</td>
<td>Coastal waters of South China Sea</td>
<td>Stereo IR particle image velocimetry (surface)</td>
<td>4 m to 6 m</td>
</tr>
<tr>
<td>Shuiqing and Dongliang (2016)</td>
<td>North Pacific (30°N, 145°W)</td>
<td>SWIFTs</td>
<td>0 to 0.5 m</td>
</tr>
<tr>
<td>Thomson et al. (2016)</td>
<td>Lake Michigan</td>
<td>Free-floating PIV (FP IV)</td>
<td>0 to 15 cm</td>
</tr>
</tbody>
</table>
constant dissipation. However, this is not supported by the here presented 1867 open-ocean profiles of $\epsilon$. Soloviev and Lukas (2003) and Gemmrich and Farmer (1999, 2004) question the feasibility of scaling a ‘breaking layer’ with $H_s$ using wave-following observations. T96 never actually observed this layer of constant $\epsilon$ as their sensors were located below wave troughs from a fixed tower-based system. In fact, they determined this depth by assuming that the integrated water column dissipation would equal the energy input of the wind. The ‘breaking layer’ would then be the depth at which half of the wind energy input has dissipated. Some studies find shallower depth levels for this ‘breaking depth’ e.g. $z_b = 0.4 H_s$ (Jones and Monismith, 2008; Siddiqui and Loewen, 2007; Wang and Liao, 2016), $z_b = 0.25 H_s$ (Young and Babanin, 2006) and $z_b = 0.01 H_s$ (Thomson et al., 2016, for a wave-following reference frame). However, these studies observe $\epsilon$ closer to the surface than $\epsilon$ could be determined from ASIP measurements.

In the wave age range covered by T96, $\alpha$-values between 90 and 250 were found, where $\alpha$ is determined from the water-side normalised TKE flux from the wind to the waves $F$. The highest values of $\alpha$ were found at levels of $A_{iw}$ around 0.0667. These values were confirmed by Feddersen et al. (2007) ($\alpha = 250$) and Gerbi et al. (2009) ($\alpha = 168$), which are larger than used in the modelling study of Craig and Banner (1994). Other observational studies within the same wave age regime find slightly smaller values of $\alpha$, e.g. Jones and Monismith (2008), $\alpha = 54 \pm 6$. This lower $\alpha$ is explained by a more limited conversion of the wind energy to wave breaking.

This study finds smaller values of $\alpha$ than Jones and Monismith (2008), and significantly smaller (one order of magnitude) than those found by T96. These low values of $\alpha$ are related to the lower levels of $\epsilon$ found here, see (2.15). The $\pi_m$ in the ECWAM (see ECMWF 2016; Breivik et al. 2015 for details on the calculation of $\alpha$ in ECWAM) lies in the range of 143.74 $\pm$ 112.70 with low-wind outliers being removed. A different behaviour of the relationship between $\alpha$ and $A_{iw}$ was found compared to T96’s parameterisation from Wang and Huang (2004): here, a consistent decrease for $\alpha$ with $A_{iw}$ was found even for $A_{iw}$ that are below 0.0833. In a similar way Shuiqing and Dongliang (2016) observed a decrease of $\alpha$ with $A_{iw}$ and found higher values of $\alpha$ when using their complete data set; when focusing only on young seas with $A_{iw}$ above 0.0286, $\alpha$ was lower. However, their values of $\alpha = 1700$ (full data) and $\alpha = 230$ (young seas) are still higher than the ones here. Similar to the results presented here, Fig. 6 of Thomson et al. (2016) suggests a
decrease in $\tau$ with inverse wave age, defined as $u_{10}/c_p$, for young seas ($c_p/u_{10}$ smaller than 2, which corresponds to $A_{iw} \sim 0.0148$). They show that the assumption of a constant $\tau$ is supported by histograms showing $\tau$ centring around 2 m s$^{-1}$. This $\tau$ is related to $\alpha$ as $\tau = \alpha u_\ast$. When applying an average $u_\ast = 0.0066$ m s$^{-1}$ for the here presented data, $\tau$ of 2 m s$^{-1}$ corresponds to an $\alpha$ of 303.

Determining $\epsilon$ from ASIP’s shear measurements, does not allow for estimates of $\epsilon$ closer than 0.25 m to the air-sea interface. This is a limitation for studies on the air-sea gas exchange as highlighted in Esters et al. (2017). Other instruments, such as SWIFTs (Thomson, 2012) measure $\epsilon$ acoustically up to the air-sea interface. These buoys resolve the upper 0.6 m with a 5-min temporal resolution and, therefore, yield higher-resolution time series of $\epsilon$. However, these buoys do not allow for any assertion of $\epsilon$ deeper than 1 m. Therefore, a combination of the advantages of both types of instruments would be desirable: ASIP’s ability to gain turbulence information down to the XLD and SWIFTs ability to gain high spatial and temporal resolution $\epsilon$ directly at the air-sea interface.

The data analysed in the preceding sections was conducted at different locations within the Atlantic Ocean. Different sources of turbulence could be expected in the tropics (STRASSE and MIDAS), the Canadian continental shelf region (Labrador and Knorr11), and the Arctic region (NICE). The regime diagram introduced by B12 shows regions where a single forcing (wind, waves, or buoyancy) produces the majority of the total $\epsilon$. The upper panels in Figure 5.6a-e cover periods of positive $B_0$. As the diagram is not defined for negative $B_0$, those periods are shown in the lowest panel (Fig. 5.6) as a single function of $L_\alpha$. Most of the data is cluttered in the regime range where no single forcing is expected to explain the total of the prevailing turbulence. Some of the $\epsilon$ data from the MIDAS cruise is mainly driven by buoyancy effects. This explains the $\epsilon_{buoyancy}$ to scale the observed $\epsilon$ profiles well during periods of positive $B_0$, in particular for this cruise. Only data gained in the Arctic during the NICE cruise is expected to be mainly driven by wave effects. The data from the STRASSE cruise covers the smallest range of $L_\alpha$ and is most constrained to the wave region, in particular for negative $B_0$. The data from the other tropical cruise (MIDAS) covers a much wider range of $L_\alpha$. Additional turbulence sources, not considered in the B12 regime diagram, include internal waves that might break along the continental shelves, as well as submesoscale processes, and
inertial shear, which could occur at these sites; therefore, shape the local turbulence characteristics differently.

5.5 Summary

Parameterising turbulence in the OSBL is of great importance as observations of turbulence in the ocean are still limited. Microstructure measurements of $\epsilon$ from five cruises in different parts of the Atlantic Ocean have been presented. ASIP took $\epsilon$ profiles from the mixing layer depth all the way up to the sea surface; a significant advantage over traditional microstructure profilers. The observations were used to evaluate and improve existing parameterisations of $\epsilon$, summarised as follows:

1. T96 proposed wind and wave forcing to model profiles of $\epsilon$. They divided the ocean near-surface region into three different layers. The here presented data does not support the idea of different layers. In addition, the presented open-ocean measurements do not show the existence of a ‘breaking layer’ near the ocean surface as proposed by T96. Instead, the depth dependency of the observed $\epsilon$ follows a decay of $|z|^{-1.15}$, which is closer to the slope of the traditional LOW ($|z|^{-1}$) than to the ‘transition layer’ as suggested by T96 with $|z|^{-2}$.

2. Wave-turbulence interaction as a mechanism for ocean turbulence generation was proposed by HQ10. They used the Stokes shear profile of a monochromatic wave to model profiles of $\epsilon$. Here, the scaling is found to improve when used with the Stokes shear profile based on the Phillips approximation as suggested by Breivik et al. (2016).

3. A linear relationship of $u_*$ with the surface Stokes drift velocity $u_{s0}$ allowed for the substitution of $u_*$ for $u_{s0}$ in the scaling of B12. This permitted for a direct comparison between the scaling suggested by B12 and the similarity scaling proposed by LG89. Both approaches consider a destabilising buoyancy forcing, and therefore could be applied under conditions of surface cooling.

4. During daytime conditions of negative buoyancy flux, the observation
are best described by a scaling relationship:

\[ \epsilon(z) = (7.2 - 108.3 A_{iw}) \left( \frac{u^3}{H_{sw}} \right) \left( \frac{z}{H_{sw}} \right)^{-1.15}, \]  

(5.6)

which considers the inverse wave age \( A_{iw} \) and the friction velocity \( u_* \).

5. In conditions when convection dominates over wind-wave forcing with \( h_c/L_L > 1 \), the observations are best described by:

\[ \epsilon(z) = 0.63 \times \left( 0.90 \times \frac{u^3}{\kappa |z|} + 0.91 \ B_0 \right). \]  

(5.7)
6 Mixing Event During Stratified Conditions

This chapter presents two distinctive features observed during a deployment of ASIP in the Labrador Sea. Both of the features are linked to turbulence in the OSBL. The first is a diurnal warming event, which increases the surface water temperature by more than 1 °C. To the best of the authors’ knowledge this is the northernmost directly observed diurnal warming event. Therefore, the observations offer insights into air-sea heat fluxes gained from such events within the Arctic. The second feature is a descending of the water column by around 20 m at the time of maximal warming, when a stable stratification of the water column is expected. The most prominent explanation to cause this sinking, is the breaking of an internal wave. Internal wave breaking is a source for turbulence within the ocean. Therefore, studying the characteristics can increase the knowledge of turbulence sources within the surface layer of the Arctic Ocean.

Section 6.1 describes the observations and in Sec. 6.2 the diurnal warming event is analysed. Section 6.3 discusses possible processes causing the mixing event occurring at the same time of maximal diurnal warming. In order to explain the observation, four different hypotheses are evaluated, namely turbulent mixing caused by the influence of warm rain at the ocean surface in Sec. 6.3.1, by the influence of evaporation due to the diurnal surface warming in Sec. 6.3.2, advection in Sec. 6.3.3, as well as the breaking of an internal wave in Sec. 6.3.4. Section 6.4 summarises the chapter.
Figure 6.1: (a) Modelled surface buoyancy- and heat fluxes [W m$^{-2}$ s$^{-1}$], (b) temperature at different depth (modelled and observed) [$^\circ$C], (c) modelled evaporation [equivalent m], total precipitation [m], and cloud coverage [0 to 1], (d) and wind speed $u_{10}$ (modelled and observed) and significant wave height $H_s$ [m]. The green area indicates the time of the ASIP deployment.
6.1 Observations

ASIP was deployed on the 23rd of May 2010 in the Labrador Sea at 55.3 °N, 53.9 °W (marked by the pink star on the map in Fig. 3.1). The data set consists of 50 profiles sampled every 7-minutes. The acquisition of meteorological data conducted during the Labrador cruise was restricted to $u_{10}$. Using the re-analysis data from the ECMWF allowed to expand the meteorological information beyond the ASIP deployment (Fig. 6.1).

The temperature evolution in Fig. 6.2a (more detailed for the upper 30 m in Fig. 6.3a) shows strong diurnal warming in the Labrador Sea. The warming starts around 10:00 LST (local solar time) and is strongest at 15:00 LST with the surface temperature reaching amplitudes of 1.5 °C relative to the foundation temperature. Such high-surface temperatures can only be reached due to strong insolation and low-wind speed. The formed diurnal warm layer is constrained to the uppermost metres of the ocean. Once it is evolved at 12:00 LST, it determines the XLD. Before this, the XLD reaches down to 10 m.

The sub-skin temperature $T_{\text{subskin}}$ measured by ASIP shows a stronger increase than the modelled SST with up to 1.7 °C difference between both. This highlights that despite the high performance of the model, it is not capable to resolve a fine-scale warming event (maximal surface temperatures only stay for one hour). Therefore, direct in-situ observations like those from ASIP are significant to describe such warming events; thus, to understand the air-sea heat fluxes and mixing behaviour.
Mixing Event During Stratified Conditions

Figure 6.2: (a) Temperature $T$ [$^\circ$C], (b) salinity $S$, (c) density $\sigma$ [kg m$^{-2}$], (d) the dissipation rate $\epsilon$ [m$^2$ s$^{-3}$], (e) Brunt-Väisälä frequency $N$ [cph], and (f) PAR [W m$^{-2}$] distribution during the presented ASIP deployment in the Labrador Sea. The black line in each plot shows the XLD, the green line the depth of the diurnal warm layer determined in this study, and the grey line the depth of a maximal $N_{max}$. The temperature, dissipation rate, density, and salinity are shown in more detail for the upper 30 m in Fig. 6.3.
Mixing Event During Stratified Conditions

Figure 6.3: Same as Fig. 6.2 zoomed in on the uppermost 30 m of the ocean to focus on the diurnal warming event, for (a) temperature $T$ [$^\circ$C] with the red rectangle highlighting the discussed mixing event, (b) the dissipation rate $\epsilon$ [$m^2 s^{-3}$] with overlaid isolines of the Brunt-Väisälä frequency $N$ and the red rectangle highlighting the discussed elevated levels of $\epsilon$, (c) density $\sigma$ [$kg m^{-3}$] (d), salinity $S$. The black line in each plot show the XLD, the green line in each plot show the XTLD, the green line in each plot show the XTLD, and the red rectangle highlighting the discussed elevated levels of $\epsilon$. The black line in each plot show the XLD, the green line in each plot show the XTLD, and the dark blue line the depth of the maximal Brunt-Väisälä frequency $N_{max}$. 

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A strong warming event as observed was only possible due to cloud-free conditions. Those conditions are predicted by the ECMWF for the time of ASIPs deployment (Fig. 6.1). The predictions, however, show an increase in the cloud coverage up to 90-100% for the times before and after the deployment. The high cloud coverage predicted by the ECMWF for the times before and after the ASIP deployment, is also visible in satellite images. Figure 6.4 shows the SST from MODIS-Aqua (Moderate-resolution Imaging Spectroradiometre) at the time of the ASIP deployment (12:43 LST). The noticeable white areas are regions with bad data due to clouds. Higher latitudes are more prominent for cloud formation. Beesley and Moritz (1999) showed that the Arctic is covered by clouds for 80% of the year. This underlines, how highly localised the observed diurnal warming event was. Even though the satellite data was gained while ASIP was deployed, the data at ASIPs deployment site is discarded due to clouds. There is only one pixel of available data close to this deployment site (in the zoomed in plot in Fig. 6.4). The pixel represents an area of 1 km$^2$ and thus highlights the limited size of cloud-free area that are necessary to promote diurnal warming. This illustrates that warming events are often under-sampled, because these small cloud-free areas are not considered. Thus, the air-sea heat flux might be underestimated in the Arctic.

Another noticeable feature is the presence of a cold water layer with temperatures of 1.5 °C at depths of around 10 to 40 m. The cold-water layer shows wavelike characteristics with amplitudes of around 6 m. The wavelike movement coincides with the depth of the maximal values of the Brunt-Väisälä frequency $N_{max}$. This suggests an internal wave traveling along the pycnocline between the two layers (shown in Fig. 6.2e in cph with the grey line being the depth of $N_{max}$). At 15:00 LST when the diurnal SST amplitude reaches its maximum, the water column abruptly descends by around 20 m, which is most dominant in the cold water layer in Fig. 6.2a. This descent is similarly reflected in the density and salinity distribution (Fig. 6.2b and Fig. 6.2c). After less than an hour the water column relaxes back to similar levels of stratification as observed before 15:00 LST.

At the beginning of the deployment low-salinity water ($S < 33.9$) reaching from the surface down to 20 m, is visible in Fig. 6.2b. This fresh water might be the result of a rain event that (according to the ECMWF model) occurred in advance of the ASIP deployment (green line in Fig 6.1c).
6.2 Diurnal Warming Event

The ASIP deployment does not cover a full diurnal cycle, but only its daytime period. Between 9:00 and 11:30 LST there is still a well mixed isothermal layer observed over the top 10 m of the ocean. From 10:00 LST onwards the surface warms, until it reaches a maximum of 3.7 °C at 13:30 LST. These elevated temperature values remain for nearly 2 hours.

The strong diurnal warming can be explained by the high absorption of solar radiation. The underwater spectral irradiance was measured on ASIP in form of the photosynthetically available radiation (PAR), which is visible light (400 to 700 nm). The vertical PAR distribution is a direct response to the incident solar irradiance entering at the sea surface and its attenuation with depth. This distribution follows an exponential decay with depth, which depends on the water turbidity. In general around half the solar irradiance is absorbed in the top 1 m of the ocean (e.g. Kara et al.,
ASIP measures PAR in units of $\mu\text{mol s}^{-1}\text{m}^{-2}$. This is expressed in W m$^{-2}$ via multiplication with the Avogadro’s number of $6.022 \times 10^{17}$ representing the number of molecules in one mole to reach units of quanta. To get from quanta to energy, it has to be divided by their ratio, which is given for a wide range of conditions by Morel and Smith (1974) as $2.77 \times 10^{18}$.

At the surface of the ocean, the maximal PAR signal is observed just after local noon and reaches 350 W m$^{-2}$, with averaged values over the whole deployment being $230 \pm 60$ W m$^{-2}$. The ECMWF model’s surface solar radiation predicts maximal values of 780 W m$^{-2}$ during the time of noon (Fig. 6.1). This discrepancy can be explained by the fact that PAR only describes the visible range and thus a portion of the full solar spectrum. PAR accounts for 43% to 50% of the solar irradiance at the sea surface (e.g. Rochford et al., 2001). The increase in solar radiance during the day, is visible in the increase of PAR and its depth penetration (Fig. 6.2f).

The surface warming forms a stably stratified diurnal warm layer, which is confined to the uppermost few metres of the ocean (Fig. 6.2a). The depth of the diurnal warm layer $z_{WL}$ is defined with a threshold temperature, and follows a fixed isotherm (e.g. Matthews et al., 2014). ASIP’s deployment period does not allow for the choice of a foundation temperature that occurred before sunrise (as described in Sec. 2.4.1). For the purpose of further analysis, the temperature of the well-mixed isothermal surface layer before the onset of the warming, is considered as the foundation temperature. This temperature is found to be 2.11 °C. The depth of the diurnal warm layer is then determined as:

$$z_{WL} = z(T = 2.11).$$

(6.1)

In cases that this isotherm is deeper than 10 m the depth is set to zero (which means that the warm layer is not yet evolved). This diurnal warm layer deepens within an hour from the start of its formation to 2.5 m depth (Fig. 6.5a). It remains approximately at this depth (within 0.5 m) until shortly before 15:00 LST, when it deepens further to 3.8 m. This additional deepening coincides with an increased wind peak, as discussed later.

Within the diurnal warm layer temperature is not uniformly distributed due to the ocean’s stratification. For consistency, the temperature closest to the air-sea interface that is measured by ASIP, is in the following referred
Figure 6.5: Time series of (a) the ship-based wind speed $u_{10}$ [m s$^{-1}$] (blue) and the depth of the diurnal warm layer $z_{wl}$ [m] (orange), (b) temperature amplitudes with respect to the foundation temperature of 2.11 °C (shown as horizontal dashed line) $\Delta T$ [°C] at depth levels of 1 m, 2 m, 3 m, 4 m, and 5 m. The same colour coding is used for the respective (c) salinity and (d) density.
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to as $T_{\text{subskin}}$. This $T_{\text{subskin}}$ reaches maximal amplitudes at 13:30 LST and stays constant for 1.5 h. Up to the point of $T_{\text{subskin}}$ reaching maximal amplitudes, the temperature at 1 m depth $T_{1m}$ increases gradually in accordance with the increase of $T_{\text{subskin}}$. This increase occurs with a delay to the increase in $T_{\text{subskin}}$. Therefore, $T_{1m}$ remains 0.4 to 0.9 °C colder than $T_{\text{subskin}}$ highlighting the prevailing stratification (Fig. 6.5b). At 14:45 LST $T_{1m}$ increases within 15 min by 1.1 °C and reaches similar levels than the maximal $T_{\text{subskin}}$. A similar strong temperature increase of 0.9 °C is observed at 2 m depth. Figure 6.5b shows that smaller but still distinguishable warming is seen down to 4 m depth. At all depth levels the strong warming only stays for around 20 min. At 15:15 LST the temperatures at all depth levels decrease again, also with the decrease in $T_{\text{subskin}}$. At the same time, the ship measures peak in $u_{10}$ by 6 m s$^{-1}$ (Fig. 6.5a). This peak in $u_{10}$ lasts for less than an hour. The ship measurements are not quality controlled, which leads to an inestimable uncertainty on the gained data. Therefore, it is not absolutely certain that this wind gust describes reality. However, the existence of a gust would be a logical cause for the observed mixing of the warming signal to deeper depth. Additionally, wind mixing would explain the deepening of the $z_{WL}$ and XLD by 1 m as well as the increase of $\epsilon$ within the mixing layer (Fig. 6.5a). The occurrence of the wind burst can further explain the drop in $T_{\text{subskin}}$ observed after 15:15 h LST (Fig. 6.5b).

A wind burst causing the mixing of the surface warming signal to deeper depth is in accordance with Stuart-Menteth et al. (2005), who found that diurnal warm layers are highly sensitive to wind fluctuations. They show that depending on the degree of stratification, an increase in $u_{10}$ of only 1 m s$^{-1}$ is enough to break down surface stratification. Additionally, they show that a sudden wind burst, at the time of maximal SST, mixes the water within the top metre deeper into the ocean. This mixing causes a reduction in temperature as observed during the here presented warming event.

From 250 diurnal cycles in the Arabian Sea observed with a mooring located at 61.5 °E and 15.5 °N for one year, Stuart-Menteth et al. (2005) classified four main categories of diurnal warming events depending on the wind and insolation conditions. They classify the evolution of $T_{\text{subskin}}$ and $T_{1m}$. In their Fig. 7 (here in Fig. 6.6) they show an example diurnal temperature shape responding to a fairly constant wind condition with wind speeds below 3 m s$^{-1}$ (reproduced together with the data of this study in
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Fig. 6.6). Stuart-Menteth et al. (2005) classify this situation as category 1b. In this case, stratification builds up in the uppermost metre of the ocean, which causes $T_{1m}$ and $T_{subskin}$ to develop different amplitudes. The $\Delta T_{subskin}$ can reach over 4-5 °C, while the $\Delta T_{1m}$ is unlikely to exceed 2 °C. For $T_{subskin}$ the peak would typically occur around 16:00 - 17:00 LST assuming the wind remains low.

This category 1b of Stuart-Menteth et al. (2005) provides most similarities to the warming event observed here, at least until 14:00 LST (Fig. 6.6). In this time range both the ship-measured and ECMWF-modelled $u_{10}$ are fairly constant. The modelled $u_{10}$ stays constantly below 5 m s$^{-1}$. The ship-based $u_{10}$ stays around 2 m s$^{-1}$ and increases to 4 m s$^{-1}$ for two hours at local noon. These $u_{10}$ are slightly higher than the suggested threshold of 3 m s$^{-1}$ for category 1b in Stuart-Menteth et al. (2005). Similar to their category 1b, the here observed $T_{subskin}$ increases gradually during the day and the ocean stratifies. This results in an increase of both $T_{1m}$ and $T_{subskin}$, but with different magnitudes. The difference at times of maximal temperature amplitudes is 1 °C, which is lower than found in Stuart-Menteth et al. (2005). In general, the magnitudes of the presented warming event are lower than in their observations with $\Delta T_{subskin}$ reaching 1.5 °C compared to 4-5 °C and $\Delta T_{1m}$ reaching 0.5 °C compared to 2 °C. These differences are most likely explained by the temporal and spatial mismatches of the observations. These mismatches reflect the differences in the insolation at the observational site.

Shortwave radiation depends on the time of the year as well as on the location. More radiation reaches the equator than the poles, and it is highest during local summer time. This makes it complicated to compare different diurnal warming events to each other. Commonly reported $\Delta T$ range from less than 0.2 °C at high-wind speeds (Soloviev and Lukas, 1997; Prytherch et al., 2013) up to 3 to 4 °C under lighter winds and clear skies (Bruce and Firing, 1974; Price et al., 1986; Soloviev and Lukas, 1997; Stramma et al., 1986; Prytherch et al., 2013). Even larger values of $\Delta T$ have been found up to 5 °C (Ward, 2006; Flament et al., 1994). The largest diurnal temperature differences can be found in the Pacific warm pool, the summer-hemisphere sub-tropics and the Indian Ocean (Kennedy et al., 2007). However, none of these observed diurnal-warming events occurred as far north as the here presented case. With maximal $\Delta T_{subskin}$ of 1.5 °C at $u_{10}$ between 2 and 5 m s$^{-1}$ falls very well into the range of previous observations. Still, it has to be kept in mind that not all of the observations are referred to the $T_{subskin}$
Figure 6.6: Time series of temperature amplitudes with respect to the foundation temperature $\Delta T \,[^\circ C]$ at sub-skin level (black) and 1-m depth (red). The dashed lines show the data of Stuart-Menteth et al. (2005) from their Fig. 7 (category 1b) for an exemplary diurnal temperature shape and the solid lines show the data from this study.

but rather some depth level below it, which implies additional complexity in generalising reported observations.

The diurnal warming does not only cause changes in the surface ocean temperatures, but also in its salinity, and consequently in its density. In general, the sea surface salinity SSS within the diurnal warm layer increases during the deployment. This increase occurs from a SSS of 33.80 before 10:30 LST to 33.85 at 10:30 LST (Fig. 6.5c). This increase could be explained by ASIP leaving the above-mentioned freshwater lenses. Similarly, the lenses could have been advected and been replaced with surrounding saltier water. From 10:30 LST onwards the increase in salinity occurs more gradually with a mean increase of 0.06 within the diurnal warm layer throughout the warming period. The mixing that was discussed for the temperature evolution is similarly observed for salinity. Therefore, at 14:45 LST the fresher surface waters mix further down. This shows that diurnal warming events are not only significant for the local heat but also the salinity, and thus buoyancy flux.

At low temperatures, changes in density are mainly driven by changes in salinity as shown in Fig. 6.7. The lower $S_{\text{subskin}}$ and higher $T_{\text{subskin}}$ causes
the subskin density $\sigma_{\text{subskin}}$ ($\sigma = \rho - 1000$) to decrease from 27.03 kg m$^{-3}$ at 10:30 LST to 26.87 kg m$^{-3}$ at 13:30 LST. The increase in $S_{\text{subskin}}$ at 14:00 LST with constantly high $T_{\text{subskin}}$ causes the $\sigma_{\text{subskin}}$ to stabilise at 26.95 kg m$^{-3}$ for an hour. A distinctive stratification forms at the direct surface of the ocean.

6.3 Mixing Event

At the same time of maximal $T_{\text{subskin}}$ at 15:00 LST, the water column mixes down by around 20 m (Fig. 6.3). This descending starts at 14:45 LST stays for around 30 min and relaxes back to the stratification that prevailed beforehand. It is well known that an increase in temperature decreases density. Consequently, the observed surface warming results in a stabilisation of the water column. In the observed case, however the water column is destabilised.

6.3.1 Warm Rain

The main question is, why does the surface water get lighter but nevertheless sinks down? Warm rain at the surface would induce warm and fresh, thus light, water into the ocean. At the same time, rain would induce turbulent mixing that could trigger the observed descending. However, the ECMWF model does not predict any rain during the mixing event. Even though there is no direct rain information available, the strong diurnal temperature amplitudes suggest that at least relatively clear skies must have dominated during ASIP’s deployment.

6.3.2 Evaporation

Instead of lighter water being mechanically mixed into the water column, heavier water at the surface could cause convection, and thus lead to a collapse of the water column. SSS is primarily controlled by the balance between evaporation and precipitation (Boutin and Martin, 2006; Boutin et al., 2014; Soloviev and Lukas, 1996; Saunders, 1967; Soloviev and Lukas, 1997). At high latitudes, the interplay between sea-ice melting and sea-water freezing can create additional effects on the prevailing SSS.
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Precipitation is a freshwater source at the sea surface, and thus reduces the ocean’s salinity. This induced freshwater reduces the ocean’s density and leads to ocean stratification (Soloviev and Lukas, 1996). Diurnal warming that persists for many hours can lead to evaporation (i.e., the latent heat flux). Evaporation removes water from the sea surface via water vapour and the salt remains, which increases the ocean’s salinity. This positive salinity anomaly increases the ocean’s density. As even slightly denser water sinks below less dense water, this process can cause convective mixing. The dense water sinks down to a depth at which it reaches equilibrium density. However, if the temperature gradient is large enough, the decrease in density due to the increase in temperature will counter salinity-based increase in density. In this case, a stable, positive salinity anomaly at the surface can form. This effect is greater in colder regions, as in cold waters, changes in temperature have higher effects on changes in density, than changes in salinity as shown in Fig. 6.7.

For a surface-water parcel with a given SSS the depth of equilibrium density is at the surface. However, when the salinity increases the depth of equilibrium density will be deeper. The depth is determined as the depth closest to the surface with a density equal to the one of the surface parcel.
Figure 6.8 shows the depth to which a surface water parcel sinks if a specific salinity $\text{SSS}_{\text{add}}$ was added to the surface salinity. The figure suggests that the surface salinity has to increase by around 0.4 for a surface parcel to sink down approximately 20 m.

During the observed warming event, however, the salinity within the diurnal warm layer increases by less than 0.1 (Fig. 6.5c). Beyond that, it is implausible that after the convection took place the water column would re-stratify within less than 30 min.

### 6.3.3 3-Dimensional Phenomena

Excluding air-sea exchange processes as a trigger for the observed mixing event draws the attention to a water mass input by advection. An advected water mass could change the observed stratification. Temperature-salinity (T-S) diagrams were analysed to determine the present water masses. Figure 6.9 shows the 10 cm averaged T-S diagrams from ASIP. All profiles from the deployment follow a similar shape. Differences exist only at lower depths (dark blue), where the formation of the diurnal warm layer creates an additional warm-water mass. In addition, the freshwater lenses before the onset of the diurnal warming can be identified as the fresher water with similar temperature characteristics than the surrounding profiles at depths below 20 m. However, Fig. 6.9 does not show any additional water mass being advected to the site. The black profile measured during the time of
the mixing event shows the same signature as all other profiles. The profile sinks down but does not change its shape. Therefore, water mass advection as a source for changes in the stratification or convection is excluded to force the mixing event.

Figure 6.9: Temperature-salinity diagrams for all 10 cm averaged ASIP profiles. The colour coding gives the depth levels and the black data represents the profile at times of the mixing event. The green contours in the background give the determined density $\sigma$ levels.

6.3.4 Internal Wave Breaking

Figure 6.2 shows a wavelike displacement of the pycnocline between the surface layer and the cold water layer below. It clearly indicates an internal wave propagating along the pycnocline. The frequency of the wave is $1.28 \pm 0.338$ cph, which corresponds to a period of $49 \pm 11.1$ min. The amplitude is $5.8 \pm 1.11$ m determined from the vertical displacements of the pycnocline. At 14:30 LST, just before the water column mixes down, this displacement is associated with a patch of elevated $\epsilon$, which is shown in Fig. 6.3b. This elevated $\epsilon$ at 10 m depth reaches values of $10^{-7.4}$ m$^2$s$^{-3}$ and stands out from the surrounding levels of $\epsilon$ of around $10^{-9}$ m$^2$s$^{-3}$. The patch is well separated by an over 5 m thick layer from the mixing layer.
Mixing Event During Stratified Conditions

(marked by the black line in Fig. 6.3). As the high $\epsilon$ patch occurs at times of maximal diurnal temperatures, the XLD mainly follows the $z_{wl}$ and is constrained to the surface.

Similar observations were made during an earlier deployment of ASIP during the same cruise in the Labrador Sea. Wain et al. (2015) describe those intensively and relate the enhanced levels of $\epsilon$ to internal wave breaking. Such a breaking of the internal wave could explain the observed mixing event herein. It is therefore seen as most plausible hypothesis to explain the downward movement of the water column.

Combined with the observation of Wain et al. (2015) this makes two internal wave breaking events during the same cruise in the Labrador Sea. This density of breaking events suggests that it is most probable that more of its kind take place, but remain unnoticed. Therefore, it is of high interest to study the wave breaking in detail as it’s induced energy is a potential source for turbulence. This source of turbulence might be important in the Arctic; yet underpredicted.

Following Wain et al. (2015), the wave speed and wavelength are determined using two different approaches. The first one uses eigenfunctions of the vertical distribution of the isopycnal and determines their matching mode. To do so, the wave equation for the vertical velocity is used with varying $N(z)$ and boundary conditions of $w = 0$ at $z = 0$ and at $z = -h$. The boundary conditions lead to an eigenvalue problem for the vertical wavenumber, which has only solutions for the particular wavenumbers. The eigenvalues matching the boundary conditions were calculated for the density profiles determined from ship-based full-depth CTD casts. The first five eigenmodes of the CTD casts closest to the time of the ASIP deployment (06:03 LST and 17:27 LST) are shown in Figure 6.10. In both cases the fifth mode provides an extremum closest to the depth of the observed internal wave. For the earlier CTD cast the depth of this extremum was at 32 m and for the later one at 27 m. The resulting wave speed is $0.21 \text{ m s}^{-1}$ for the earlier CTD cast and $0.19 \text{ m s}^{-1}$ for the later one. In addition, the horizontal wavenumber $\ell$ for each profile was determined as $\ell = \omega/c$ using the observed wave frequency of $\omega = 1.28 \pm 0.338 \text{ cph}$. This yields a $\ell$ of 0.0112 rad m$^{-1}$ and a horizontal wavelength of 562.5 m.

The second approach to determine the wave speed and wavelength assumes the applicability of the shallow-water approximation. Thus, assuming that the layer above the internal wave is shallow and the layer below is infinitely
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Figure 6.10: The upper 500 m of the vertical structure functions for the first five vertical modes. The functions are determined for two full-depth CTD casts at 06:03 LST (solid lines) and at 17:27 LST (dashed lines). The bold lines represent the fifth mode, which has its shallowest extremum closest to the depth of the internal wave.

depth. In this case, the wavelength is much longer than the depth of the surface layer. This assumption yields a description of the wave speed $c_p = \sqrt{g' H}$, where $H$ is the depth of the surface layer, $g' = \frac{\Delta \rho}{\rho_0} g$ the reduced gravity, $\Delta \rho$ the density change over the interface, and $\rho_0$ a reference density of 1027 kg m$^{-3}$. Here, $H$ was chosen as the average depth of the layer above the main pycnocline from all the presented ASIP profiles and determined to be 15.3 ± 2.9 m. The $\Delta \rho$ was determined as the density difference between the density above and below the pycnocline, from which $g'$ was calculated as 0.0024 m s$^{-2}$. Using $H$ and $g'$, $c_p$ was determined to be 0.19 ± 0.036 m s$^{-1}$. Both different approaches, to determine $c$ yield similar estimates. This internal wave is slower than the one observed by Wain et al. (2015).

The evolution of the internal wave is not only observed in the temperature and density distribution, but also in PAR. The wavelike evolution in PAR is out of phase with the internal wave. The correlation between the propagation
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of the internal wave (shown as depth of $N_{\text{max}}$ in Fig. 6.11) and the evolution of the isolines of the PAR signal only occurs below the depth levels of the internal wave. There is no wavelike characteristics found in the PAR isolines above the depth of $N_{\text{max}}$, represented by the 30 W m$^{-2}$ and 20 W m$^{-2}$ isolines in Fig. 6.11b.

For further correlation analysis, the PAR isolines are de-trended from the general diurnal signal by subtracting a signal filtered at 1.5 h. The depth of $N_{\text{max}}$ is subtracted by its own mean and shown in Fig. 6.11b. The clear anti-correlation between the propagation of the internal wave and the light evolution below it ($R = -0.74$ for the 5 W m$^{-2}$ isoline) suggests the incoming light to be refracted at the surface of the internal wave. This is supported by the fact, that any distinct correlation between the light and $N_{\text{max}}$ is found above the wave (correlation coefficient of -0.33 for the 30 W m$^{-2}$ isoline). Therefore, it is suggested that light is a suitable variable to detect internal waves in the ocean.

In order to evaluate the hypothesis of a breaking internal wave to cause the descending of the water column, possible breaking mechanisms are investigated. Fringer and Street (2003) showed that a critical wave steepness, to cause convective instabilities, depends on a non-dimensional thickness of the interface $\delta \ell$. Here, $\delta$ is the thickness of the layer of the internal wave, $\delta = 15$ m. From this thickness, the amplitude of $5.8 \pm 1.11$ m and $\ell = 0.0122$ rad m$^{-1}$, $a\ell$ can be determined to be 0.065 and $\delta \ell$ to be 0.17. In their numerical simulations, Fringer and Street (2003) found convective instabilities for values of $\delta \ell$ greater than 2.33 and $a\ell$ greater than 1. As the observed values of $a\ell$ and $\delta \ell$ are significantly smaller than those found by Fringer and Street (2003), convective instabilities are not likely to cause the internal wave to break.

For smaller values of $\delta \ell$ than 2.33 Fringer and Street (2003) found shear instabilities to cause the internal wave to break. However, they did not investigate values of $\delta \ell$ smaller than 0.31. To complete the studies for longer waves, Troy and Koseff (2005) focused on waves with smaller $\delta \ell$. They found that waves break at a critical wave steepness of $a\ell_{\text{crit}} = \sqrt{2 \delta \ell}$. For the given internal wave this calculated $a\ell_{\text{crit}}$ is 0.58. Thus, $a\ell_{\text{crit}}$ is an order of magnitude larger than the determined $a\ell$. This means that the observed internal wave is too shallow to break without shear from other sources. This is similar to the observations in Wain et al. (2015).
Figure 6.11: Time series of the (a) 100 W m$^{-2}$ PAR isoline together with the time series of the depth $N_{max}$ [cph] in black, (b) the 5 W m$^{-2}$ (red), 10 W m$^{-2}$ (purple), 20 W m$^{-2}$ (blue), and 30 W m$^{-2}$ (green) PAR isoline together with the time series of the depth $N_{max}$ [cph] in black. (c) The same time series for 5 W m$^{-2}$ (red) and 30 W m$^{-2}$ (green) for PAR as well as $N_{max}$ are de-trended with the correlation coefficients (R) between them listed according to the colour code.
Even though, Wain et al. (2015) could not clearly identify the breaking mechanism due to observational limitations, they concluded that interaction with background shear could lead to the observed wave breaking. A source for this background shear might be the observed wind burst that occurred simultaneous to the maximal SST amplitudes. This would explain the simultaneous appearance of this maximal warming and the descending of the water column.

6.4 Summary

A strong diurnal warming event was observed in the Labrador Sea at 55.3 °N. To the best of the authors’ knowledge, this is the northernmost directly observed event of its kind. High-cloud coverage in the Arctic normally prevents the formation of strong warming events in this region. Satellite imagery highlighted the high-cloud coverage and emphasised the observed warming event to be highly localised. This highly localised characteristic of the warming event suggests that despite the high-cloud coverage, more than commonly expected diurnal warming events exist in the Arctic. As the observed diurnal warming heats the surface ocean by up to 1.5 °C, such warming events could have a higher influence on the heat input in the Arctic than usually assumed. Wind-induced mixing can transport the heat deeper into the ocean. This highlights diurnal warming as a potentially-underestimated heat source in the Arctic.

In addition to the diurnal warming, an internal wave with a frequency of 1.28 ± 0.38 cph and amplitude of 5.8 ± 1.11 m was observed. This internal wave travelled along the main pycnocline between around 10 m and 25 m depth. The pycnocline separates a warmer surface layer from a colder water layer below.

At times of the largest SST amplitudes, the internal wave breaks. This internal wave breaking is seen as the most likely source to explain an observed descending of the water column by 20 m. Combining these findings with those of Wain et al. (2015), two breaking internal waves have been observed on the same cruise in the Labrador Sea during which ASIP was deployed for around 8 hours. Both of the breaking events took place within the upper 100 m of the ocean. This shows a high density of breaking events
and suggests a high probability of even more such events, which remain unnoticed, occurring in the region of the Labrador Sea. As the breaking of an internal wave releases energy and causes turbulent mixing, these events are a potentially-underestimated source for turbulence in the upper Arctic Ocean.
7 Conclusions and Future Work

The main aim of this thesis was to improve the understanding of surface ocean turbulence and its related processes. These processes included air-sea gas exchange and diurnal warming within the ocean surface boundary layer (OSBL). The analysis was performed using a comprehensive data set of open-ocean observations of the dissipation rate of turbulent kinetic energy $\epsilon$, eddy covariance measurements of dimethyl sulphite (DMS) and carbon dioxide (CO$_2$), ship-based, as well as modelled wind, insolation and wave information.

To follow this aim three research question were posed:

Is the turbulence-based small-eddy model feasible to describe air-sea gas exchange in the open-ocean?

The air-sea gas exchange is commonly described using wind measurements. Various empirical parameterisations exist for this purpose. However, physically viewed, it is turbulence that drives the gas exchange. The wind speed is only used as a proxy for the prevailing oceanic turbulence. The small-eddy model (SEM) physically describes this gas exchange and relates it to turbulence directly at the air-sea interface. This thesis could show for the first time that the SEM holds well in open-ocean conditions. In addition, the thesis showed that the SEM’s performance can be significantly improved using a Schmidt number exponent $n$ as a function of the friction velocity $u_*$, rather than assuming a constant $n = \frac{1}{2}$ following previous studies.

How can the measured turbulence profiles be best scaled with meteorological variables?

Measurements of turbulence profiles in the oceans are difficult to conduct, in particular close to the air-sea interface. These constraints lead to several different attempts to scale profiles of the dissipation rate $\epsilon$ based on easier accessible variables. Several scaling approaches including wind, wave, and buoyancy forcing as sources for turbulence within the OSBL were evaluated.
Conclusions and Future Work

The thesis showed, that during daytime conditions a scaling considering the inverse wave age and $u_*$ describes the open-ocean observations best. In addition, the thesis showed that during conditions when convection dominates over wind and wave forcing, buoyancy should additionally be considered. The performance of the scaling approaches seems suitable even though not all possible sources of turbulence in the OSBL are included.

**How can a mixing event within the OSBL occur simultaneously to strong diurnal warming, which stratifies the layer?**

A strongly localised diurnal warming event in the Labrador Sea has been analysed in this thesis using data from ASIP. This event, which heats the surface water by more than 1 °C, is the northernmost directly observed of its kind. The observations show that despite the high-cloud coverage in the Arctic, localised warming events can occur. Underestimating their existence might cause an underestimation of the heat input into the Arctic Ocean. At the time of maximal warming, when a stable stratification is expected, the water column mixes down by around 20 m. After half an hour of mixing, the stratification relaxes back to its original levels. The thesis describes the breaking of an internal wave as the most likely process causing this mixing. It cannot be verified that there is any connection between the breaking internal wave and the surface stratification. The observation of two breaking internal waves during the same cruise suggest a high probability of more breaking events, which occur unnoticed. As the breaking of an internal wave generates turbulent mixing, these breaking events might imply a significant (and underestimated) source for turbulence in the Arctic OSBL.

**Future Work**

This thesis highlighted the importance of complete data, which is interlinked in several ways. Predictions of air-sea gas exchange rely on the knowledge of turbulence directly at the air-sea interface. Turbulence and its description rely on accurate wind, wave, and meteorological information. Additionally, observations of the ocean’s temperature and salinity are crucial to describe the diurnal warming and mixing events, as observed in the Labrador Sea. Therefore, this thesis might be considered as an appeal for future field campaigns aiming for various different direct and quality-controlled measurements.

In this sense, future work should include field campaigns gaining all the
above mentioned information to evaluate the determined gas exchange and turbulence parameterisations, in particular in higher wind speed regimes. This thesis was restricted to low and medium wind speeds. As it is known that research cruises are not only expensive but also time-consuming, it is important to promote the interaction between the ocean observational and modelling communities.

Scientifically, future work should address the implication of the here presented turbulence-based description of the air-sea gas exchange velocity for climate predictions. Until now, climate models use wind-speed based parameterisations to represent the exchange velocity. An open question is, how an implementation of the small-eddy model into climate models would change the estimations of the oceans’ global and local carbon uptake; and how it would affect the global carbon cycle.

It is worth to mention that the approaches to scale $\epsilon$ as found in literature (Terray et al., 1996; Lombardo and Gregg, 1989; Belcher et al., 2012; Huang and Qiao, 2010) are based on different observational methods to determine $\epsilon$; reaching from profiling techniques to fixed platforms. It would be of scientific interest to directly compare those methods in a controlled environment. Such a setting could demonstrate to which level, differences in the scaling approaches stem from potential differences in the measured $\epsilon$ gained from the different observational methods. Consequently, such a study could highlight the level of potential uncertainties in the methods used to determine $\epsilon$ in the ocean.
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Figure: Vertical distribution of the measured $\epsilon$ normalised with the LOW ($\epsilon_{LOW}$) versus the normalised depth $z/h_c$. The data from the different cruises is coloured in different shades of green. As it suits the time of the year, the ‘data-tree’ was accordingly decorated.