Chapter 1

Introduction

In 1984, three pioneering studies (Knox and McElroy, 1984; Sarmiento and Toggweiler, 1984; Siegenthaler and Wenk, 1984) suggested that the polar oceans have played the most critical role for regulating carbon dioxide (CO₂) concentrations in the Earth's atmosphere over the past thousands of years, prior to any human influence. Ever since, the climate research community has built overwhelming evidence that this connection between the atmospheric CO₂ concentrations and polar oceans stems from the Southern Ocean (Toggweiler, 1999; Sigman et al., 2010). The rationale behind this hypothesis is that this region acts as the major pathway for deep ocean waters to rise to the surface (Talley, 2013), fueling the surface ocean with large amounts of dissolved carbon and nutrients (Marinov et al., 2006). These upwelled waters provide a natural source of CO₂ to the atmosphere (Gruber et al., 2009) and nutrients for the global marine biological production (Sarmiento et al., 2004). However, it is not just this upwelling of deep waters in this region that is important for the climate system, but also the subduction of newly formed water masses that ventilate most of the interior ocean (Ganachaud and Wunsch, 2000; DeVries and Primeau, 2011). This subduction process buffers perturbations that occur in the surface climate, such as human-induced climate change (IPCC, 2013), by taking up anthropogenic CO₂ (Sarmiento et al., 1998; Caldeira and Duffy, 2000; Sabine et al., 2004; Gruber et al., 2009) and heat (Gille, 2002; Levitus et al., 2012; Purkey and Johnson, 2013; Frölicher et al., 2015; Morrison et al., 2015) from the atmosphere. Due to these profound influences on the global carbon cycle and the surface energy balance, the upwelling and subduction of waters in the Southern Ocean are thought to be key elements to understand past, current, and future changes of the global climate.

In this chapter, I will describe the link between changes in the global carbon cycle and Earth's surface climate (section 1.1), followed by a discussion of the role of ocean circulation in altering both the carbon cycle and the surface energy balance (section 1.2). Then, I will describe why the ocean circulation and density stratification in the Southern Ocean might be critically linked to surface freshwater fluxes (section 1.3) and why this system might be very sensitive to changes in global climate (section 1.4). Finally, I will formulate my objectives (section 1.5), and outline the chapters of this thesis (section 1.6).

1.1 Atmospheric carbon dioxide & the global surface climate

The Earth's surface temperature is tightly coupled to the atmospheric CO_2 concentration (Pierrehumbert, 2011). This relation stems from the absorption of long-wave radiation by atmospheric CO_2 , which is the second most important greenhouse gas—next to atmospheric water vapor. Using Stefan-Boltzmann's law for a black body, one finds that the natural atmospheric greenhouse effect rises the Earth's mean surface temperature by roughly 33° C and that roughly one third of this effect can be attributed to atmospheric CO_2 (Sarmiento and Gruber, 2006), making the Earth a habitable planet. Therefore, the anthropogenic perturbation and natural variations of the atmospheric CO_2 concentration can strongly alter the global surface climate, as I will briefly describe in this section.

1.1.1 Anthropogenic perturbation

Through fossil fuel burning and land-use change, human activity has increased the atmospheric CO_2 concentrations since pre-industrial times (Figure 1.1) to a current mean level of about 403 ppm (June, 2016, after removing the seasonal cycle; http://www.esrl.noaa.gov/gmd/ccgg/trends/global.html). Small air bubbles trapped in the East-Antarctic ice sheet show that such high atmospheric CO_2 concentrations have not occurred over at least the last 800,000 years (EPICA



Figure 1.1 Changes in the global carbon cycle 1850–2014: The black curve shows the increase in atmospheric CO_2 concentration. The colored curves show the atmospheric CO_2 concentration equivalent if there were only anthropogenic sources but no sinks (red) and if there was no ocean sink (blue). The land sink is indicated in light green and the ocean sink in light blue shading. The land sink is computed from the residual after subtracting the ocean and atmosphere from the total emissions. Data stems from the Global Carbon Budget (Le Quéré et al., 2015) and from the observed atmospheric CO_2 concentration after 1980 (Dlugokencky & Tans, NOAA/ESRL, www. esrl.noaa.gov/gmd/ccgg/trends, Ballantyne et al., 2012).

community members et al., 2004; IPCC, 2013). The current atmospheric CO_2 concentration is about 44% higher compared to the pre-industrial level (about 280 ppm, Figure 1.1) and this increase led to an increase of the radiative forcing, dominating the observed temperature rise of about 0.85° C over the past 130 years (Hansen et al., 2010; IPCC, 2013). Earth System Models (ESMs) suggest that even if anthropogenic atmospheric CO_2 emissions would stall, warming could continue over centuries (Frölicher et al., 2014). However, the atmospheric growth rate of CO_2 has been accelerating over recent decades, reaching an average growth of about 2.1 ppm per year over the past decade (Le Quéré et al., 2015).

Figure 1.2a illustrates that the actual anthropogenic emissions of CO_2 are considerably larger than the growth rate of atmospheric CO_2 . In fact, the anthropogenic emissions of about 10 Pg of carbon per year over the last decade (Le Quéré et al., 2015) have been stronger than any reconstructed natural carbon release rate to the atmosphere over the past 66 million years (Figure 1.2a;



Figure 1.2 Sources and sinks of anthropogenic carbon 1959–2014: (a) Anthropogenic carbon emissions from fossil fuel burning (red) and land use change (orange) from the global carbon budget (Le Quéré et al., 2015). The estimate of the natural emissions during the Palaeocene-Eocene Thermal Maximum is given as a comparison (PETM; Zeebe et al., 2016). (b) Land (green; residual) and ocean sinks (blue; multi-model mean) for anthropogenic carbon from the Global Carbon Budget (Le Quéré et al., 2015). The dased line shows an observation based estimate from Landschützer et al. (2015a) for the global ocean sink (corrected as described by Landschützer et al. (2014b) to obtain the anthropogenic contribution) and the dash-dotted line the Southern Ocean sink (Landschützer et al., 2015b, scaled according to the global correction).

Zeebe et al., 2016). The current release rate is about one order of magnitude higher than estimates for the Palaeocene-Eocene Thermal Maximum (PETM; Zeebe et al., 2016)—a strong warming period which is often compared to the current global warming (Zachos et al., 2001). Thus, the an-thropogenic perturbation forces the Earth's carbon cycle into unprecedented rapid changes. The carbon cycle responds with a rapid increase of the uptake of carbon by the land and the ocean, which took up about 60% of the emitted carbon between 1850 and 2014 (Figure 1.1; Sabine et al., 2004; Le Quéré et al., 2015). Without these sinks, the atmospheric CO₂ concentration would have reached 550 ppm in 2014 (Figure 1.1).

About 30% of the anthropogenic emission since pre-industrial times were taken up by the ocean, and another 30% by the land (Figure 1.1; Sabine et al., 2004; Le Quéré et al., 2015). Both the strength of the anthropogenic sources as well as the overall strength of the sinks have been gradually increasing (Figure 1.2; Khatiwala et al., 2009). However, in contrast to the anthropogenic sources, the sinks reveal large variability over time with periods of stronger and weaker uptake (Le Quéré et al., 2009). These variations result from variations in the surface climate. In particular, the land sink undergoes large interannual variability, which is largely driven by El Niño Southern Oscillation (ENSO; Zeng et al., 2005). The multi-model mean of the ocean sink from the Global Carbon Budget (Le Quéré et al., 2015) exhibits much less variability. However, new observationally constrained estimates show that also the ocean sink undergoes large variability on decadal time scales (Landschützer et al., 2015b,a), especially in the Southern Ocean (Figure 1.2b), which dominates the overall global uptake of anthropogenic CO₂ from the atmosphere (see section 1.3; see also Mikaloff Fletcher et al., 2006; Gruber et al., 2009; Khatiwala et al., 2009). Thus, variations in the global surface climate can alter the rate at which anthropogenic CO₂ is taken up by the ocean and land.

Global models suggest that in the long-term the link between climatic changes and the global carbon cycle induces a positive feedback, which accelerates the projected global warming over the 21st century and beyond (Cox et al., 2000; Friedlingstein et al., 2001, 2006). This feedback is induced by a reduction of the efficiency at which both the land and the ocean take up anthropogenic CO₂ as the climate is warming. In particular, the projected future uptake of anthropogenic carbon by the land decreases; eventually turning the land into a carbon source (Cao and Woodward, 1998; Stocker et al., 2013). This change in the land sink results in the ocean becoming the dominant sink in the long-term (Cox et al., 2000; Randerson et al., 2015). However, the ocean sink will probably also weaken over time, which is mostly a result of positive feedbacks from ocean acidification, surface ocean warming, and changes in mixing and transport (see section 1.2; Manabe and Stouffer, 1993; Sarmiento et al., 1995; Sarmiento and Le Quéré, 1996; Sarmiento et al., 1998; Joos et al., 1999; Gruber, 2011; Stocker, 2015). These feedbacks between the carbon sinks and global climate have been identified as a key challenge in climate research in order to understand the dissipation of anthropogenic carbon perturbations in the climate system and to make reliable estimates of future climatic changes (IPCC, 2013; Ilyina and Friedlingstein, 2016).

1.1.2 Natural fluctuations

While the above considerations are concerned with the addition of anthropogenic CO₂ to the atmosphere that drives an increase of the global surface temperature, Earth's history shows that, conversely, variations in surface temperature can also drive changes in the atmospheric CO₂ concentration. This relation becomes evident from synchronously varying atmospheric CO₂ (EPICA community members et al., 2004; Lüthi et al., 2008) and Antarctic surface temperatures over the last glacial cycles (Figure 1.3; Petit et al., 1999; EPICA community members et al., 2004; Jouzel et al., 2007; Parrenin et al., 2013). The coincidence of these variations with the Earth's orbital eccentricity suggests that the solar radiation received by the Earth surface paces these variations (Hays et al., 1976), even though this causal link has been debated (Saltzman et al., 1984; Wunsch and Ferrari, 2004; Huybers and Wunsch, 2005). In any case, changes in direct solar forcing would be largely insufficient to change the surface temperature by the reconstructed amplitude (Imbrie et al., 1993). Thus, most of the observed amplitude must result from internal feedbacks in the climate system (Köhler et al., 2010).



Figure 1.3 Glacial-interglacial variations of atmospheric CO_2 and temperature: The blue line shows the variations of atmospheric CO_2 over the past 800,000 years as measured in Antarctic ice cores (EPICA community members et al., 2004; Lüthi et al., 2008). The red line shows the Antarctic surface temperature anomalies with respect to the past 1,000 years that were inferred from deuterium in the ice cores (Petit et al., 1999; EPICA community members et al., 2004; Jouzel et al., 2007; Parrenin et al., 2013).

For a long time the theory prevailed that these changes are associated with the growth and decay of the northern hemisphere ice sheets that would lead, among other changes, to large changes in the surface albedo (Imbrie and Imbrie, 1980; Oerlemans, 1980; Abe-Ouchi et al., 2013). Shackleton (2000) challenged this perspective, arguing that the proxy for ice sheet volume, which is derived from the oxygen isotopic composition (δ^{18} O) of deep-sea sediments and ice cores, lags the proxies for the Antarctic surface temperatures, as well as the atmospheric CO₂ concentration and orbital eccentricity. As the latter three quantities appear to be in phase, he concludes that the amplitude of the glacial-interglacial variations could be explained by carbon-cycle feedbacks rather than northern hemisphere ice-sheet feedbacks. A more recent compilation of surface temperature proxies (Shakun et al., 2012) supports such a theory, because it shows that the global mean temperature lags both atmospheric CO_2 and Antarctic surface temperatures during the last deglaciation. This suggests a southern-hemisphere driven change in the carbon cycle as a predominant cause for the deglaciation. Yet, large uncertainties exist in both the magnitude and timing of all these proxy data sets, exacerbating arguments related to the phasing and location of these changes.

Results with a simplified model by Berger et al. (1993) suggest that a change in atmospheric CO_2 of 80 to 100 ppm during the last four glacial cycles (Figures 1.1 and 1.3; Petit et al., 1999) can only explain about one third of the temperature variation, when indirect effects such as the associated water vapor feedback are included. Current state-of-the-art ESMs suggest that this small response is probably an underestimation of the warming resulting from the CO_2 increase. Using the estimated long-term climate feedback parameter from these model simulations of about $0.8 \text{ W m}^{-2} \text{ K}^{-1}$ (Andrews et al., 2015), the equilibrium temperature change resulting from glacial-interglacial CO_2 variations and related indirect effects would be about 2.5° C. Such a simplified consideration thus suggests that more than half of the last deglacial global mean temperature rise (about 3.5° C; Shakun et al., 2012) could be related to the atmospheric CO_2 rise. However, the climate feedback parameter varies widely among different models and long-term responses from ice sheets are not included in these ESMs, leading to no conclusive answer on whether a southern hemisphere carbon-cycle feedback or a northern hemisphere ice-sheet feedback would trigger deglaciations.

Despite these contrasting views on the causes for the global temperature changes during glacial-interglacial changes, the ice core records clearly reveal that a warming of the climate system during deglaciations leads to a natural rise of atmospheric CO_2 , with strong positive feedbacks in the global climate system that amplified the global warming. This lesson from Earth's history leads to concerns that the anthropogenic induced climate change might be considerably amplified over many centuries not only due to the anthropogenic perturbation itself, as outlined in section 1.1.1, but also due to positive feedbacks with the natural carbon cycle. Consequently, it is an urgent matter to understand why the atmospheric CO_2 has been increasing at all during deglaciations in order to better understand the response of the natural carbon cycle to future changes in the surface temperature.

1.2 The importance of ocean circulation for global climate: A Southern Ocean perspective

The ocean circulation redistributes heat, carbon, and nutrients between low and high latitudes and between the surface and the deep ocean. Thereby, it regulates the regional and global surface climate. In this section, I will briefly discuss the influence of this circulation on the global carbon cycle and the surface energy balance from a perspective of both a natural system and the anthropogenic perturbation of this system. This discussion will elucidate the critical role played by the Southern Ocean in the climate system.

1.2.1 Global overturning circulation

The circulation of ocean waters on a global scale is driven by a modification of the seawater density through surface heat and freshwater fluxes as well as by surface winds. The densest and deepest waters of the global ocean are formed in high-latitudes, where a strong loss of buoyancy occurs; namely in the north Atlantic (North Atlantic Deep Water, NADW) and around the coast of the Antarctic continent (Antarctic Bottom Water, AABW). These water masses sink to the abyssal ocean and spread to lower latitudes. They are then brought back towards surface by upwelling in the Southern Ocean (Toggweiler and Samuels, 1995; Gnanadesikan, 1999; Marshall and Speer, 2012; Morrison et al., 2015) and vertical mixing in low latitudes (Munk, 1966; Munk and Wunsch, 1998; Ganachaud and Wunsch, 2000; Wunsch and Ferrari, 2004). A second major type of sub-surface water masses, namely Antarctic Intermediate Water (AAIW) and Subantarctic Mode Water (SAMW), is subducted to intermediate depth in sub-polar regions of the Southern Ocean, ventilating the global low-latitude thermocline. All these deep, intermediate, and surface waters are intertwined (Schmitz, 1995, Talley, 2013) to constitute a global-scale overturning circulation (Gordon, 1986a,b; Broecker, 1987, 1991; Lumpkin and Speer, 2007).

The dominant role of the Southern Ocean in this circulation manifests itself in the fraction of global water masses that is ventilated through the Southern Ocean. Up to 80% of subducted NADW and AABW re-surface through transport and mixing in the Southern Ocean (Talley, 2013). Watson et al. (2013) argue that roughly 20 to 30% of this upwelling is caused by cross-density (diapycnal) mixing and the remainder through isopycnal mixing and transport. However, not only the upwelling is dominated by the Southern Ocean, but also around 65% of global sub-surface waters originate from the surface waters of this region through the subduction of AABW, AAIW, and SAMW (DeVries and Primeau, 2011).

The return time scale for water parcels participating in the global overturning circulation is on the order of 1,000 years (Broecker and Peng, 1982). This time scale is largely governed by slow, counter-gradient, upward mixing of bottom waters in deep northern Pacific (Munk, 1966).

However, the time scales at which the global overturning circulation interacts with global climate is much shorter (Weaver et al., 1991; Delworth et al., 1993; Ganopolski and Rahmstorf, 2001; Cunningham et al., 2007; Park and Latif, 2008). This shorter time scale is owing to relatively faster variations in some upwelling and subduction processes, which are on the order of years to several decades for NADW (Weaver et al., 1991; Delworth et al., 1993; Cunningham et al., 2007) and AAIW/SAMW (Santoso and England, 2004; Naveira Garabato et al., 2009; Sallée et al., 2010a; Kwon, 2013) and possibly even centuries in the high-latitude Southern Ocean (incl. AABW formation; Latif et al., 2013; Martin et al., 2013). On these time scales the interaction of overturning circulation with the surface climate occurs through the meridional and vertical advection of heat, salt, and carbon and through related changes in the air-sea fluxes.

As the subduction of water masses in both hemispheres occurs on time scales equivalent to the anthropogenic perturbation, concerns have been raised that the upwelling and subduction in the higher latitudes might change in future (Stocker and Schmittner, 1997; Toggweiler and Russell, 2008; Meredith et al., 2012; Waugh, 2014), potentially altering the ability of the ocean to take up anthropogenic carbon and excess heat (Manabe and Stouffer, 1993; Sarmiento et al., 1998; Stocker, 2015). A major difference that exists between the subduction of water masses in the northern and southern hemisphere is that water masses subducted in the northern hemisphere stem from the surface waters of the low latitudes, whereas those subducted in the Southern Ocean have been upwelled from the deep ocean. Thus, the waters that are subducted in the Southern Ocean have not yet seen the anthropogenic perturbation and have a much larger potential to buffer this perturbation. The rate at which this buffering of variations in the surface climate by the Southern Ocean waters occurs depends on the rate of upwelling and subduction or the surface residence time of these waters (see section 1.3).

1.2.2 Ocean carbon pumps

The ocean contains 60 times more carbon than the atmosphere and most of this carbon is stored in the form of dissolved inorganic carbon (DIC) in the deep ocean (Sarmiento and Gruber, 2006). At the surface the concentration of DIC is about 15% lower than in the deep ocean. This gradient comes about mostly due to gravitational sinking of biologically produced matter out of the sunlit, euphotic layer (upper about 100 m) into deeper layers—a process referred to as export production. As illustrated in Figure 1.4 (following Heinze et al., 1991; IPCC, 2013), this biological pump can be split into processes associated with the export of particulate organic carbon (POC), the softtissue pump, and the export of biogenic calcium carbonate (CaCO₃), the carbonate or hard-tissue pump.

The soft-tissue pump is the major biological process that is responsible for the surface to the deep ocean gradient in DIC (Sarmiento and Gruber, 2006). It is driven by the formation of organic matter through photosynthesis by marine phytoplankton. During this process the phytoplankton

takes up dissolved carbon and nutrients from the seawater to build organic matter. The net biological uptake of CO_2 resulting from production and respiration by phytoplankton is referred to as net primary production (NPP). The total amount of NPP is limited by the availability of light and nutrients. Some phytoplankton and zooplankton species form calcareous shells that consist of mineral CaCO₃. Thereby they do not only extract DIC from the seawater but also lower the seawater alkalinity (Alk). The latter is defined through the excess of bases over acids. A lower Alk leads to a release of CO_2 to the atmosphere. Consequently, while the soft-tissue pump leads to a net uptake of CO_2 from the atmosphere, the carbonate pump leads to a net release to the atmosphere (Figure 1.4).

The organic detritus that sinks out of the surface layer is to a large extent remineralized by heterotrophic organisms at intermediate depth (Figure 1.4). Only a small fraction of the NPP sinks further into the deep ocean (Suess, 1980). Kwon et al. (2009) argue that the depth at which the bulk of the organic carbon is remineralized, the remineralization depth, significantly influences the atmospheric CO₂ levels, underpinning the importance of this sinking processes. The line of thought behind this relation is that the deeper the carbon sinks into the ocean, the longer is its return period to the surface (Primeau, 2005). If we consider an extreme condition where no carbon is exported to depth, i.e., in absence of a vertical DIC gradient, simplified model experiments show that the atmospheric CO_2 concentration could be roughly 150 ppm higher (Gruber and Sarmiento, 2002). Even though this case is unrealistically extreme, it demonstrates that a change in the vertical gradient could substantially alter the atmospheric CO_2 levels. The carbonate pump also leads to vertical DIC gradients, but plays a secondary role. One key difference of this mechanism to the soft-tissue pump is that CaCO₃ is dissolved much deeper in the water column and that a much larger fraction is buried in the sediment as compared to the particulate organic carbon. Thus, it becomes an important process on time scales longer than a few hundred years (Broecker, 1987; Sarmiento et al., 1988; Archer et al., 2000; Sigman and Boyle, 2000).

The major physical processes in the ocean that influence the carbon cycle are vertical transport and mixing of dissolved carbon and nutrients. They counteract vertical gradients induced by the carbon pumps through their tendency to restore a homogenous distribution of tracers in the ocean. Upwelling in the Southern Ocean returns nutrients to the surface (Marinov et al., 2006). However, not all nutrients are consumed in the Southern Ocean surface waters and are subducted again with AAIW and SAMW. These nutrient-rich waters then feed into the low-latitude thermocline waters, where they can be mixed to the surface and fuel biological production (Sarmiento et al., 2004). Model experiments show that about 75% of the total biological production in the low-latitudes (north of 30° S) can be explained by the provision of nutrients through the Southern Ocean, and if it were not for the ocean circulation, biological production in the global surface ocean would diminish (Sarmiento et al., 2004). Therefore, the return path of nutrients through the ocean circulation to the surface closes the major biogeochemical loop in the global ocean (bold white in Figure 1.4).



Figure 1.4 Cycling of carbon in the ocean: Physical and biological processes responsible for the vertical exchange of carbon between the deep and surface ocean (Heinze et al., 1991; IPCC, 2013). Soft-tissue pump: Photosynthetic production of organic matter, gravitational sinking, and heterotrophic remineralization of particulate organic carbon (POC). Carbonate pump: Biogenic formation of calcareous shells consisting of mineral calcium carbonate (CaCO₃), gravitational sinking, and dissolution. Physical processes: Vertical mixing and transport of dissolved inorganic carbon (DIC) and nutrients, as well as changes in solubility of carbon dioxide (CO_2) in seawater due to variations in temperature and salinity. All processes affect the air–sea gas exchange of CO_2 (green). In red: The major pathway of anthropogenic CO_2 into the ocean.

The mixing and transport of subsurface waters into the surface ocean bring not only nutrients but also DIC to the surface. This process counteracts the biologically produced vertical DIC gradient in the ocean. Thus, the vertical DIC gradient could either be altered by a change in mixing and transport or by biological productivity (Sarmiento et al., 1988). The sum of these two effects is often referred to as the efficiency of the biological pump (Sarmiento and Gruber, 2006). A very efficient biological pump occurs in the low latitudes due to the almost complete use of nutrients. The opposite, i.e., a low efficiency of the biological pump, occurs in high latitudes due to a reduced usage of nutrients (Gruber and Sarmiento, 2002). Since the production in low latitudes is largely nutrient-limited, the rate at which nutrients are provided through the high-latitudes ultimately determines the productivity in the global ocean (Sarmiento and Toggweiler, 1986). Thus, the high-latitudes provide the major control on the exchange of carbon between the atmosphere and the deep ocean either through changing the upwelling or changing the high-latitude productivity (Toggweiler, 1999; Sigman and Boyle, 2000). In a natural system, an increased vertical exchange in high-latitudes would lead to rise in atmospheric CO2 while a decrease would lower atmospheric CO₂ (Knox and McElroy, 1984; Sarmiento and Toggweiler, 1984; Siegenthaler and Wenk, 1984). Therefore, physical processes associated with ocean transport and mixing have a large potential to alter the atmospheric CO₂ concentration on time-scales of decades to several centuries.

A third mechanism that substantially alters the vertical DIC gradient is associated with the solubility of CO₂ in seawater depending on its temperature and salinity (Figure 1.4). Surface cooling or freshening lead to an uptake of CO₂ from the atmosphere and warming or salinification lead to the contrary. Thus, waters that are transported towards higher latitudes and cool take up carbon (Gruber et al., 2009). As these waters are the source for deep and bottom waters, the solubility pump acts together with the ocean circulation to remove DIC from the surface ocean, especially in the North Atlantic (Sarmiento and Gruber, 2006). In contrast, the waters that upwell in equatorial regions gain heat and thus lose carbon to the atmosphere as a result of the solubility pump (Gruber et al., 2009). For example, water masses that are subducted to the thermocline depth in the relatively cold Southern Ocean, i.e., AAIW and SAMW, are upwelled to the surface in the very warm equatorial regions leading to substantial release of carbon due to a lower solubility. These effects resulting from the solubility, especially in response to temperature changes, can be as large as effects resulting from the soft-tissue pump or transport and mixing of DIC to the surface. Consequently, in combination with surface ocean physical or biological processes, ocean transport and mixing can effectively remove DIC and also dissolved organic carbon from the surface ocean (Figure 1.4).

The sum of all physical and biogeochemical effects on the air–sea CO_2 flux as displayed in Figure 1.4 is referred to as gas-exchange pump (Sarmiento and Gruber, 2006). Often the single contributions of each pump strongly oppose each other leading to a small net gas-exchange. For example, in a natural system (without anthropogenic influence), the upwelling in the Southern Ocean leads to an over-saturation of the seawater partial pressure of CO_2 (p CO_2) with respect to the atmosphere and thus to an out-gassing of CO_2 from the surface ocean (Figure 1.4; Mikaloff Fletcher et al., 2007; Gruber et al., 2009). This effect is partly compensated by a change in solubility due to the surface cooling and freshening and by biological productivity (Takahashi et al., 2002; Wang and Moore, 2012; Dufour et al., 2013; Hauck et al., 2013). The latter two effects become stronger towards lower latitudes of the Southern Ocean, gradually changing the surface ocean from a net source to a net sink of CO_2 (Mikaloff Fletcher et al., 2007; Gruber et al., 2009; Takahashi et al., 2009). In a natural (i.e., unperturbed) system, carbon is released from the ocean to the atmosphere in the Southern Ocean and in equatorial regions and taken up by the ocean in mid-latitudes and high northern latitudes (Mikaloff Fletcher et al., 2007; Gruber et al., 2009).

The spatial and temporal variations of the air–sea exchange mainly depend on the variations of the surface ocean pCO_2 since CO_2 in the atmosphere is well-mixed and thus rather uniform. Yet, the ultimate flux not only depends on the pCO_2 gradient but is also determined by the gas transfer coefficient, which depends on the wind speed and sea-ice concentration (Wanninkhof and McGillis, 1999; Butterworth and Miller, 2016). In order for the surface ocean pCO_2 to equilibrate with the atmosphere, it takes about six months to one year depending on the wind speed and the thickness of the surface layer (Sarmiento and Gruber, 2006). Yet, on longer time scales than one year the gradient in pCO_2 , and thus the surface ocean pCO_2 , dominates variations in the surface

flux (Landschützer et al., 2015b). The human induced increase in atmospheric pCO₂ offsets the long-term balance between the ocean and the atmosphere, leading to an average under-saturation of the surface ocean pCO₂ with respect to the atmosphere, which is the primary driver for the invasion of anthropogenic CO₂ into the ocean (red in Figure 1.4; Gruber et al., 2004). Thus, the larger the increase in the atmospheric pCO₂ is, the larger is the uptake by the ocean.

In order to sustain the surface ocean under-saturation and the effectiveness of the ocean carbon uptake, the anthropogenic carbon needs to be removed from the ocean surface and exported into the ocean interior. Recently, Bopp et al. (2015) suggested that vertical mixing is the major pathway for anthropogenic CO_2 to be exported from the surface ocean at the base of the mixed layer-a process which accounts for about 65% of the total subduction in their model. These results are overall consistent with findings by Dufour et al. (2013), who argue that vertical mixing is the major component of the surface mixed layer carbon budget in the Southern Ocean. However, below the surface mixed layer vertical mixing rapidly decreases, which would inhibit the carbon to be subducted into deeper layers. Reconstructions of the invasion of anthropogenic carbon into the subsurface ocean suggest that transport (i.e., advection) with NADW, AAIW and SAMW provides a major pathway for anthropogenic carbon to intermediate depths (Sabine et al., 2004; Mikaloff Fletcher et al., 2006; Gruber et al., 2009; Khatiwala et al., 2013). Thus, both vertical mixing and transport are likely critical components for the ocean uptake of anthropogenic CO₂ (red in Figure 1.4). Due to inhibited gas exchange by sea ice and dilution with deep water, AABW contains comparably little anthropogenic carbon, despite large formation rates (Poisson and Chen, 1987).

As I described earlier (section 1.2.1), the typical time-scale for subduction of surface waters is of the order of several years to decades, whereas the time-scale associated with the gas-exchange is much shorter. Thus, the ocean transport and mixing is the rate limiting factor for anthropogenic carbon uptake (Sarmiento et al., 1992). Without these subduction mechanisms, the ocean carbon sink would saturate in the long-term and the rate of uptake would slow down. Global model simulations show that the deep ocean ventilation through mixing and transport is reduced in a warming climate. Broecker (1997), and Stocker and Schmittner (1997) suggest that a decrease in the overturning circulation in the North Atlantic with global warming reduces the anthropogenic CO_2 uptake and amplifies global warming. For the Southern Ocean, Manabe and Stouffer (1993) and Sarmiento et al. (1998) suggest that an increased vertical density stratification strongly reduces the subduction of anthropogenic CO_2 due to increased warming and surface freshening, acting as a positive feedback on global warming (see also section 1.4).

A change in ocean mixing and transport would not only affect the subduction of anthropogenic CO_2 but could also alter the upwelling of DIC-rich waters in the Southern Ocean and thus alter the natural carbon cycle (Le Quéré et al., 2007; Pérez et al., 2013). A decrease in upward mixing and transport with global warming due to increased stratification would thus lead to a decrease in natural surface DIC, allowing the ocean to take up more CO_2 from the atmosphere. Such a natural negative feedback on the upwelling could outweigh the positive feedback on the subduction rates, especially on shorter time scales of a few decades (Gruber et al., 2004). Because these two contrasting feedbacks associated with ocean mixing and transport are probably the strongest feedbacks between global warming and the carbon cycle in the long-term (Gruber et al., 2004) and their exact magnitude in projections with global climate models is still rather uncertain (Orr et al., 2001; Doney et al., 2004; Majkut et al., 2014; Kessler and Tjiputra, 2016), it is critical to better understand Southern Ocean circulation and stratification changes that are associated with a warming climate. Several other feedbacks may alter the long-term diminution of anthropogenic CO_2 in the ocean. An obvious positive feedback is related to a change in the solubility pump. The solubility of CO_2 in the surface ocean would decrease in a warming climate, leading to a reduction in the uptake. Other feedbacks include changes in the ocean chemistry and biology, which are discussed in detail by Gruber et al. (2004).

1.2.3 Ocean heat uptake

Due to its high heat capacity, the ocean buffers short-term fluctuations in the surface temperature and acts as an important regulator for the surface climate. Through the ocean circulation it redistributes the heat around the globe (Talley, 2003)-sometimes also in unexpected ways. The largest ocean heat gain occurs in the tropics, where the surface receives the largest amount of radiation, and the largest heat loss occurs in the high latitudes. However, surprisingly most of the heat is lost from the surface ocean in the high-latitude northern hemisphere (Ganachaud and Wunsch, 2000; Stammer et al., 2004), even though a much larger surface ocean area is exposed to the colder atmosphere in the southern hemisphere high-latitudes. This paradox can be explained through the ocean circulation. The heat that is gained in the tropics is mostly transport northward with the surface ocean currents (MacDonald and Wunsch, 1996; Ganachaud and Wunsch, 2000; Trenberth et al., 2001). After losing a large amount of heat to the atmosphere, NADW sinks in the north Atlantic and is transported southward at depth. On its way, it diffuses some of the heat in the deep ocean. In the Southern Ocean these water masses surface south of the Polar Front (PF), where surface temperatures are substantially colder than the temperature of NADW. Thus, a portion of the heat that these water masses originally gained in the tropics is also lost in the Southern Ocean surface waters. However, this heat has not been transported to the high-latitude Southern Ocean directly by surface waters, but by taking a detour through the North Atlantic and the deep ocean.

In the Southern Ocean, a fraction of the upwelled waters experiences a very large heat loss close to the Antarctic coast where the surface water is exposed to a very cold atmosphere in open water areas in the sea ice, called coastal polynyas. This heat loss leads to the formation of the densest and deepest water mass globally: the AABW (Jacobs et al., 1985; Orsi et al., 1999; Jacobs, 2004). Even though the rate of heat loss in the Antarctic coastal polynyas is very high, the

surface area through which the heat loss occurs is rather small. In the other high-latitude areas, heat exchange is largely inhibited by the presence of sea ice, which acts as an isolating layer between the ocean and the atmosphere (Maykut and Untersteiner, 1971). Thus, the total amount of heat lost to the atmosphere is much larger when transforming the warm surface waters from low latitudes to NADW then when transforming NADW to AABW. Another fraction of the upwelled deep waters in the Southern Ocean is transported northward. At first, they lose heat to the atmosphere becomes warmer than the ocean surface towards lower latitudes. Until they are subducted as AAIW and SAMW, these waters take up a substantial amount of heat and transport it to intermediate depths. In consequence, apart from the tropical regions, this region of AAIW and SAMW subduction is the second most important region for surface ocean heat gain (Stammer et al., 2003, 2004).

Changes in this heat redistribution through changes in ocean circulation could critically affect the global climate especially in the northern hemisphere where the largest meridional heat transport occurs. For example, it has been suggested that changes in the Atlantic Meridional Overturning Circulation (AMOC) are responsible for several abrupt changes in the northern hemisphere surface temperatures (Clark et al., 2002; Rahmstorf, 2002). Similarly, a slowdown of the AMOC with global warming could actually lead to reduced sub-polar cooling in the northern hemisphere (Rahmstorf et al., 2015).

While changes in the meridional heat transport affect the regional climate, the vertical transport of heat into the deep ocean can effectively delay the man-made surface warming globally. About 90% of the excess heat in the Earth's climate system since the 1950s went into heating the ocean (Levitus et al., 2001, 2012). Roemmich et al. (2012) suggest that even before that time the ocean took up excess heat at a similar rate. Thus, without this heat uptake through the ocean the global surface warming would have been substantially larger (Stocker, 2015). This uptake of heat by the global ocean has been increasing in concert with the global surface temperatures with about half of the total uptake occurring over the last two decades (Gleckler et al., 2016).

Similarly to the invasion of the anthropogenic CO_2 into the sub-surface ocean (section 1.1), the heat enters the ocean through the subduction of water masses from the surface. This subduction of heat seems to be dominated by the Southern Ocean (Durack et al., 2014; Roemmich et al., 2015; Frölicher et al., 2015; Cummins et al., 2016). Global climate models suggest that about 75% of the total global heat uptake since pre-industrial time occurred in this region (Frölicher et al., 2015). This uptake is largely driven by a subduction and northward transport of the heat by AAIW and SAMW (Cummins et al., 2016; Morrison et al., 2016). However, models also show a very large spread of the rate and patterns of subduction, which is a major concern for reducing uncertainties in projected future global warming (Boé et al., 2009; Cheng et al., 2016; Frölicher et al., 2015). Changes have not only occurred in relation to the subduction of AAIW and SAMW, but also the abyssal Southern Ocean (AABW) shows a long-term warming over recent decades (Purkey and Johnson, 2013). Overall, a potential future change in subduction of excess heat in

the Southern Ocean through changes in mixing and transport could critically accelerate or delay global warming in the future. Consequently, it is an urgent matter to reduce the uncertainty in projections with global climate models by understanding the mechanisms that lead to changes in mixing, transport, and air–sea fluxes.

1.3 Upwelling & subduction in the Southern Ocean

In the discussion on the role of ocean circulation for the ocean carbon and heat uptake in section 1.2, I illustrated the major importance of the upwelling and subduction for long-term changes in the climate system, both from a perspective of natural variability and the anthropogenic perturbation of the climate system. I also highlighted that most of the global ocean is ventilated through the Southern Ocean. Assuming that this ventilation happens mostly through the surface waters (upper 100 m) in an area south of a region somewhere between the SAF and STF (Figure 1.5), one obtains a residence time of about 3 to 6 years (using a total formation rate of all water masses of about 40 Sverdrup (Sv) = $40 \cdot 10^6 \text{ m}^3 \text{ s}^{-1}$ (Talley, 2013)). However, much of the upwelling and subduction is not uniform but much more localized, e.g., to the region of Drake Passage, and depends on surface mixing and advection processes (Sallée et al., 2010a). A potentially smaller surface area through which ventilation typically occurs would imply a much shorter residence time that might even be less than a year (Viglione and Thompson, 2016). During this time, the water masses exchange heat, freshwater, and dissolved constituents with the atmosphere, the sea ice, and the land ice. The signature that is imprinted by this exchange is then carried to the subsurface (Iudicone et al., 2011). I will discuss the processes leading to this enormous turn-over rate in the Southern Ocean in section 1.3.1 and the special role of surface freshwater fluxes that are the focus of my thesis in section 1.3.2.

1.3.1 Circulation & water masses

The Southern Ocean connects the three major global ocean basins, namely the Pacific, Atlantic, and Indian Ocean (Figure 1.5). The exchange rate between the Pacific and the Atlantic through the Southern Ocean (Drake Passage) amounts to a net eastward transport of about 140 Sv (Meredith et al., 2011b; Naveira Garabato et al., 2014; Koenig et al., 2014) and the one between the Indian Ocean and the Pacific (south of Australia) to about 150 Sv (Ganachaud and Wunsch, 2000; Naveira Garabato et al., 2014). This vast inter-basin exchange opposes a very weak exchange north of the Southern Ocean of about 10 Sv in the Indonesian Throughflow and about 1 Sv through the Bering Strait (Ganachaud and Wunsch, 2000; Stammer et al., 2003).

The strong and deep-reaching eastward transport of water in the Southern Ocean is represented by the Antarctic Circumpolar Current (ACC), which consists of several filaments of peak transport (Sokolov and Rintoul, 2009a, see Figure 1.5). These jets are associated with frontal regions of strong across-flow gradients in ocean properties, particularly in temperature, that are traditionally divided into the southern ACC front, the Polar Front (PF), and the Subantarctic Front (SAF; Orsi et al., 1995; Rintoul and Naveira Garabato, 2013). The dynamics of this current are rather complex and differ from other ocean currents. Its zonal transport is mainly set up by a meridional density gradient that is induced by Ekman divergence in the south of the ACC and the surface buoyancy forcing (Olbers et al., 2004; Hogg, 2010). The resulting horizontal density gradient at each geopotential level leads to a geostrophic flow to the east. The direct eastward momentum forcing by the wind only plays a minor role. Standing and transient eddies transfer the zonal momentum to the ocean floor, where it is thought to be compensated by bottom form stress. These mesoscale eddies form from baroclinic instabilities of the zonal flow and act not only to transfer momentum to depth but also to exchange heat and tracers in a meridional direction across the frontal region and the ACC (Dufour et al., 2015; Frenger et al., 2015), which shield the high-latitude and thus the deep ocean from the low-latitude surface ocean. This meridional exchange and thus the dynamics of the ACC are closely linked to the meridional overturning circulation in the Southern Ocean. Yet, the total ACC transport seems not to be very sensitive to changes in the surface wind stress as well as to changes in the eddy field (Meredith et al., 2004; Böning et al., 2008), as the energy of an increased momentum flux almost entirely propagates to the mesoscale rather than increasing the mean flow; a process which is known as eddy saturation (Hallberg and Gnanadesikan, 2006; Meredith and Hogg, 2006; Meredith et al., 2012).

The isopycnal surfaces in the Southern Ocean ascend towards the pole (Figure 1.5). This ascent results from a combination of surface wind and buoyancy forcing (Rintoul and Naveira Garabato, 2013). Strong westerly winds drive water masses to the north at the surface through Ekman transport, leading to a divergence south of the maximum wind stress and to a convergence north of the maximum wind stress. The surface divergence south of the PF leads to upwelling of waters from below and lifts the isopycnal surfaces (Toggweiler and Samuels, 1993; Döös and Webb, 1994; Toggweiler and Samuels, 1995; Gnanadesikan, 1999). The northward Ekman transport to the north is balanced by a southward transport in the deep ocean. By analyzing hydrographic data from the Southern Ocean, Sverdrup (1933) and Deacon (1937) already noticed the existence of such a wind-driven upper circulation cell. More recently, surface buoyancy forcing was found to critically contribute to this overturning circulation as well (Speer et al., 2000; Marshall and Radko, 2003; Olbers et al., 2004; Morrison et al., 2011). As the upwelled waters are transported to lower latitudes at the surface, buoyancy is gained due to a net surface warming and freshening, making these waters lighter. This meridional gradient in the buoyancy forcing results in a meridional density gradient in the ocean, which is reflected by the upward tilt of the isopycnal surface from north to south. Model simulations show that a substantial fraction of the upper overturning cell can be attributed to this buoyancy gain (Olbers et al., 2004; Morrison et al., 2011). While the surface momentum and buoyancy forcing act to steepen the isopycnals, the eddy field that results from the baroclinic instabilities flattens them through a net southward transport of heat and thus density. This eddy-induced transport counter-acts the mean wind- and buoyancy-driven transport, resulting in residual overturning circulation with a more complex vertical structure (Karsten et al., 2002; Marshall and Radko, 2003; Marshall and Speer, 2012). While most of the mean transport occurs at the surface and in the deep ocean, the eddy-induced transport acts at the surface and intermediate depth. Therefore, in contrast to the ACC transport, it has been shown that the magnitude and structure of the meridional overturning circulation is sensitive to changes in the wind stress and the eddy field (Meredith et al., 2012).

Close to the Antarctic coast, strong easterly winds drive the westward transport of the Antarctic Coastal Current (Fahrbach et al., 1992; Schröder and Fahrbach, 1999; Dong et al., 2016, blue in Figure 1.5). The peak transport occurs at the continental shelf break and is associated with strong gradients in temperature and tracers, referred to as the Antarctic Slope Front (Jacobs, 1991). The easterly winds also drive an onshore surface Ekman transport and a subsurface eddy-induced transport of warmer deep waters onto the continental shelf (Ito and Marshall, 2008; Stewart and Thompson, 2013; Thompson et al., 2014). The waters that are upwelled to the Antarctic Surface Waters (AASW) and transported southward onto the continental shelf lose buoyancy through cooling making these waters much denser. After a complex modification of the water masses along the Antarctic coast, which involves interaction with the sea ice, land ice, and atmosphere (Orsi et al., 1999, 2002; Jacobs, 2004; Snow et al., 2016), these dense shelf waters mix with NADW and CDW and flow northward following the ocean floor as AABW. This return flow compensates for the onshore convergence created by the combined southward Ekman and eddy transport above. This overturning circulation forms the lower circulation cell in the Southern Ocean, which is responsible for ventilating large parts of the abyssal global ocean.

In a zonal mean, upwelling and subduction form together a double-celled meridional overturning circulation in the Southern Ocean (Gordon, 1986b; Sloyan and Rintoul, 2001b; Lumpkin and Speer, 2007; Marshall and Speer, 2012, see Figure 1.5). The upper cell is associated with a buoyancy gain and the lower cell with a buoyancy loss with respect to the upwelled water masses (Speer et al., 2000). The ratio between the amount of the upwelled water that enters the upper cell to feed the low latitude thermocline versus the amount that enters the lower cell to be subducted to the abyssal ocean essentially depends on the processes acting on the Southern Ocean surface waters south of the SAF, i.e. in the Polar Frontal Zone and the Antarctic Zone. In the interior ocean within the Southern Ocean and at lower latitudes the upper and lower circulation cells are eventually connected through diapycnal mixing processes between AABW and NADW in the Atlantic and between AABW and CDW in the Pacific and Indian Ocean (Gordon, 1986b; Talley, 2013). Gordon (1986b) estimated that the lower and upper cells are associated with an overturning of about 30 Sv and 20 Sv, respectively. These estimates broadly agree with newer, more confined estimates by Talley (2013), who estimates a net AABW formation of about 29 Sv and a net AAIW and SAMW formation of about 13 Sv. Estimates in literature range between 12 Sv and 21 Sv for the transformation from upwelling waters to AAIW and SAMW and between 10 Sv to 50 Sv for the transformation of NADW and CDW to AABW (Rintoul and Naveira Garabato, 2013, and references therein). Part of the large uncertainty associated with the lower cell stems from the uncertainty in the rate of mixing and entrainment of NADW and CDW into AABW (Rintoul and Naveira Garabato, 2013).

The meridional overturning circulation arising from the zonal mean consists in reality of large circumpolar variations of upwelling and subduction. AABW is predominantly formed in



Figure 1.5 Southern Ocean circulation, water masses, and stratification: The top shows the main fronts (STF: Subtropical front, SAF: Subantarctic Front, PF: Polar Front, SACCF: Southern ACC Front; white; Orsi et al., 1995), the Antarctic Circumpolar Current (ACC; red), the Antarctic Coastal Current (blue), the winter sea-ice extent (September; gray), and ocean velocity (back-ground). The left cross-section shows the mean Atlantic conservative temperature and the right cross-section the mean Pacific absolute salinity (Ingleby and Huddleston, 2007). The white contours show the corresponding isopycnals (from top to bottom: $\sigma_0 = 25.8$, $\sigma_0 = 26.6$, $\sigma_0 = 27.4$, $\sigma_0 = 27.8$, $\gamma = 28.27$). The black arrows in the cross-sections schematically illustrate the overturning circulation and water masses (AABW: Antarctic Bottom Water, NADW: North Atlantic Deep Water, CDW: Circumpolar Deep Water, AAIW: Antarctic Intermediate Water, SAMW: Subantarctic Mode Water).

the high-latitude embayments of the Weddell and Ross Seas, and along the Adélie coast (Orsi et al., 1999; Jacobs, 2004; Williams et al., 2010), but other formation sides around the Antarctic continent have been identified as well (e.g. Ohshima et al., 2013). AABW forms from NADW and denser CDW classes, because they upwell further south than the lighter CDWs from the Pacific and Indian Ocean (Talley, 2013). NADW that enters the Southern Ocean in the Atlantic basin is not transported directly into the high-latitude Atlantic but is, instead, circulated around the Southern Ocean with the ACC until it surfaces close to the continental shelf (pers. comm. L. Talley and J. Sarmiento).

Lighter CDW, referred to as Upper Circumpolar Deep Water (UCDW), returns to the Southern Ocean from the Pacific and Indian Ocean and lies above the NADW and Lower Circumpolar Deep Water (LCDW). Therefore, it upwells further north, in the region between the seasonal seaice zone and the Polar Front. However, upwelling of UCDW into the AASW occurs not uniformly in time and space and depends on topographic features, eddy-induced mixing, local Ekman divergence, and surface mixed-layer processes (Morrison et al., 2011; Sallée et al., 2010a). Very little is currently known on the actual upwelling processes, magnitude, and variability. Large parts of the upwelled water masses are subducted again as AAIW, which forms south of the SAF, after being transformed by surface buoyancy fluxes during the northward transport. Strong mixing and cabbeling are important components of this AAIW formation process (Iudicone et al., 2008, 2011; Urakawa and Hasumi, 2012). It occurs predominately in the south-eastern Pacific and south-western Atlantic (England et al., 1993; Talley, 1996; Sloyan and Rintoul, 2001a; Saenko et al., 2003; Iudicone et al., 2007; Sallée et al., 2010a; Hartin et al., 2011). Thus, AAIW is imprinted by the buoyancy forcing further downstream in the South Pacific where the water masses considerably freshen, resulting in a pronounced salinity minimum at intermediate depth north of the SAF (England et al., 1993; Iudicone et al., 2007; Hartin et al., 2011). Another fraction of the the upwelled waters is transported across the SAF at the surface layers by northward Ekman transport. In this Subantarctic Zone between the Subtropical Front (STF) and the SAF, SAMW forms through a convergence of waters from the north (Subtropical waters) and south (Iudicone et al., 2008, 2011; Cerovečki and Mazloff, 2016). The subduction of SAMW occurs mostly over large parts of the Pacific sector and in the south-eastern Indian Ocean (Sallée et al., 2010a).

1.3.2 Stratification & surface freshwater fluxes

The close connection between the deep ocean and surface waters in the Southern Ocean arises mainly from the relatively low vertical density stratification. Whereas the low latitudes are strongly stratified by temperature (thermocline), surface cooling of the polar ocean induces statically unstable conditions. However, a strong supply of freshwater to this region counteracts the destabilizing temperature effects by lightening the Southern Ocean surface waters. As the polar ocean's temperature is close to the freezing point, the contribution of the vertical temperature structure to the density stratification is drastically reduced and the salinity structure dominates the surface ocean stratification. This effect is owing to a non-linear dependence of the seawater density on temperature and salinity (Haug et al., 1999; Sigman et al., 2004). A typical vertical profile in the high-latitude Southern Ocean (south of the Polar Front) is characterized by a very fresh surface layer that is warm in summer and cold in winter (upper 50 m to 100 m). As the cold winter temperatures destabilize the water column, the surface waters mix deeper. The resulting cold sub-surface temperature minimum that arises in the annual mean profile is referred to as Winter Water (WW). This layer is slightly more saline than the surface water but still fresher than the underlying deep water. Below the WW both salinity and temperature considerably increase

(halocline) as one enters the upwelling deep waters (Gordon and Huber, 1984, 1990; Gordon, 1991; Martinson, 1990, 1991). Thus, unlike most of the global ocean, the high-latitude Southern Ocean's vertical stability is dominated by the salinity profile and with a marginally stable density stratification.

Because the marginal stability of the Southern Ocean surface waters is driven by salinity, changes in surface freshwater fluxes might implicate crucial changes in its vertical stability and, consequently, its overturning circulation, mixed layer depth, and water masses. Therefore, I will focus on the buoyancy forcings induced by freshwater fluxes and their effects on stratification and overturning circulation in this thesis. Surface freshwater fluxes in the Southern Ocean consist of atmospheric freshwater fluxes from evaporation (E) and precipitation (P), glacial meltwater fluxes from the Antarctic continent that are induced either by under ice-shelf melting or by ice-berg calving, and freshwater fluxes from the formation, transport, and melting of sea ice. Additionally, freshwater in the ocean is redistributed through ocean circulation and mixing.

The net atmospheric flux (P-E) is a freshwater source for the ocean almost everywhere over the Southern Ocean as precipitation exceeds evaporation. It is generally high north of 60° S and decreases towards the continent. An exception, however, is the south-east Pacific where fluxes increase towards the coastal regions of the Bellingshausen and Amundsen Seas, specifically at the western coast of the Antarctic Peninsula (Tietäväinen and Vihma, 2008). This zonal asymmetry in the atmospheric freshwater flux is caused by a spiraling of the freshwater distribution from more northern latitudes in the western Atlantic towards more southern latitudes in the eastern Pacific. Papritz et al. (2014) show that this pattern stems from the strong precipitation that is associated with extra-tropical cyclones and fronts that move along a spiraling storm-track. Atmospheric freshwater supply is lowest in the southern Ross and Weddell Seas due to a large influence of dry and cold continental air-masses from Antarctica. As a consequence, from an ocean perspective, most coastal regions experience only a small buoyancy gain from atmospheric freshwater, and the positive buoyancy forcing in regions of the PF and further north is substantial. While the patterns of the atmospheric freshwater fluxes over the Southern Ocean are understood rather well, the exact magnitude of these fluxes is highly uncertain and varies strongly among different reanalysis products (Bromwich et al., 2011; Nicolas and Bromwich, 2011).

The overall net accumulation of freshwater over the Antarctic continent (about 2'600 Gt per year or 82 mSv; Lenaerts et al., 2016) is balanced by freshwater input into the Southern Ocean in coastal regions either through under ice shelf melt or calving of ice bergs (about 2'780 Gt per year or 88 mSv; Depoorter et al., 2013; Rignot et al., 2013). An imbalance exists between the total melting and the accumulation due to increased grounding line fluxes (Rignot et al., 2008; Shepherd et al., 2012) over recent decades. The largest basal ice-shelf melting fluxes are found along the coasts of the Bellingshausen and Amundsen Seas where the continental shelf is narrow and the relatively warm CDW intrudes on the shelf (Martinson and McKee, 2012; Cook et al., 2016). Only very little freshwater is added overall to the ocean by surface runoff, since temper-

atures are too cold at the ice-shelf surface. However, this process might be important locally or also on larger scales under a warming future climate. Roughly half of the total freshwater input from the ice sheet to the Southern Ocean occurs through ice-berg melting (Depoorter et al., 2013; Rignot et al., 2013). These icebergs are typically transported westward with the coastal current and only about 40% of them drift to lower latitudes (Silva et al., 2006). The combined effect of basal melting and iceberg melting provide a major source of freshwater to the coastal region affecting sea-ice and AABW formation (Hellmer, 2004; Martin and Adcroft, 2010; Stössel et al., 2015; Merino et al., 2016).

The seasonal cycle of melting and freezing of the surface ocean redistributes freshwater vertically in the sea-ice covered regions. In winter-time, the colder and more saline waters induced by the brine rejection are heavier and mix deeper in the water column than the fresher and warmer summer-time waters. In the course of several seasonal cycles this process can lead to a stable vertical salinity stratification (Martinson et al., 1981; Goosse and Zunz, 2014). Such a process was suggested to be an important contributor to the characteristic haloclines in both the northern (Aagaard et al., 1981; Aagaard and Carmack, 1989) and southern high latitudes (Martinson et al., 1981; Fahrbach et al., 1994; Goosse et al., 1999; Goosse and Zunz, 2014), yet observational evidence is sparse. A first attempt to derive basin-wide freshwater fluxes from sea ice to the ocean is provided by Tamura et al. (2011), using atmospheric re-analysis data. They conclude that the sea-ice fluxes might exceed regionally the atmospheric flux by one order of magnitude and that, in coastal regions, it is slightly larger than the glacial melt water flux. However, a lack of observational data to constrain these products as well as their methodology induce a very large uncertainty. More recently, Abernathey et al. (2016) also suggest such a dominance of the sea-ice freshwater fluxes in the surface freshwater balance by assimilating ocean observational data with an ocean circulation model.

Sea ice in the Southern Ocean is very dynamic and a strong drift of the thin seasonal sea ice occurs all around the Antarctic continent as a response to the southerly and easterly winds, and ocean currents. Along East Antarctica and the southern coast of the Bellingshausen and Amundsen Seas, easterly winds drive the sea ice along the continent with a small on-shore component due to the Ekman drift. In the Weddell and Ross Seas, however, it is exported northward due to southerly winds and the cyclonicity of the gyres (Emery et al., 1997; Haumann, 2011). It forms in the coastal polynya regions affecting AABW formation by brine rejection (Jacobs et al., 1985; Zwally et al., 1985; Toggweiler and Samuels, 1995; Duffy and Caldeira, 1997; Duffy et al., 1999). After being transported to the north, it melts along the ice edge adding freshwater to the surface ocean. This freshwater redistribution could considerably affect the stratification and upwelling north of the continental shelf, as well as the occurrence of open ocean convection (Gordon and Taylor, 1975; Martinson, 1991; Fahrbach et al., 1994; Timmermann et al., 2001). It is not only this local effect that might be important, but it might also considerably influence AAIW and SAMW through cross-frontal Ekman and eddy transport of freshwater (Rintoul and England, 2002). In fact, numerous modeling studies suggested that AAIW, SAMW and AABW could only be repre-

sented quasi-realistically in models if they included the meridional transport of sea ice (England, 1992; Saenko and Weaver, 2001; Saenko et al., 2002; Komuro and Hasumi, 2003; Santoso and England, 2004; Ogura, 2004; Kirkman and Bitz, 2011; Abernathey et al., 2016). However, in many current global climate models this process is not well represented (England, 1992; Uotila et al., 2014; Lecomte et al., 2016), providing a potential contribution to their large biases in the Southern Ocean water-mass structure (Downes et al., 2010, 2011; Heuzé et al., 2013, 2015; Sallée et al., 2013b).

The net freshwater input over the Southern Ocean is balanced by a northward export of freshwater by AAIW and SAMW, a southward salt flux with the mean circulation (Wijffels, 2001; Talley, 2008), and a southward eddy flux (Meijers et al., 2007). Actually, the largest global meridional freshwater transport by the ocean occurs between the Southern Ocean and the southern hemisphere subtropics (Stammer et al., 2004). Interestingly, this is opposite to the meridional heat transport that is dominated by the northern hemisphere (section 1.2.3). This large redistribution of the freshwater with the ocean circulation is represented by a large tongue of minimum salinity at intermediate depth, a key characteristic of AAIW and SAMW.

Multiple studies show that the freshwater fluxes and their partitioning are strongly variable in space and time. Timmermann et al. (2001) suggest that the sea-ice freshwater export from the south-western Weddell Sea is almost twice as large as the atmospheric flux and that it balances the inflow of freshwater from the atmosphere, glacial melt water, and oceanic advection. Using δ^{18} O and salinity, Jacobs et al. (1985) argue that these different freshwater components indeed tend to balance in the high-latitude embayments of the Ross and Weddell Seas. Meredith et al. (2013) use δ^{18} O and salinity measurements along the west coast of the Antarctic Peninsula and found that the net atmospheric and glacial waters are the dominant fluxes. In the open Southern Ocean north the sea-ice edge, Ren et al. (2011) make a first attempt to derive a freshwater budget for the mixed layer. They found that the sea-ice contribution is comparable to the ocean advection and atmospheric fluxes. In sum, all these studies suggest that the cryospheric freshwater fluxes from land or sea ice are critical to understand the freshwater balance of the Southern Ocean.

Each of the freshwater components is sensitive to changes in the surface climate. The net atmospheric freshwater flux to the Southern Ocean is expected to increase in a warming climate and decrease in a cooling climate (Trenberth et al., 2011; Durack et al., 2012; Knutti and Sedláček, 2013). Similarly, one expects glacial meltwater input to increase in a warming climate in the long-term due to increased basal melting and break-ups of ice shelves (Golledge et al., 2015). With sea ice this relation seems more difficult: a warming surface climate potentially reduces the amount of sea-ice formation and a retreat of the northern ice edge. This could lead to a reduction in both the vertical and horizontal salinity distribution in the ocean. The latter effect is complicated by the role of changes in surface winds in redistributing the sea ice around the Antarctic continent. Thus, there are probably compensating effects between the freshwater fluxes in a warming climate, with potentially increasing atmospheric and glacial freshwater fluxes and hypothetically decreasing

sea-ice freshwater fluxes. These effects could be additionally complicated by regional variations in the warming of the surface climate (see section 1.4.1).

To date, there is no consensus either on the total magnitude of the surface freshwater fluxes over the Southern Ocean, on the contribution of each freshwater flux component, or on their spatial and temporal variations (Speer et al., 2012; Bourassa et al., 2013). This gap of knowledge is mostly owing to sparse observations in this region, providing a major limitation to our understanding of Southern Ocean surface processes and hinders the improvement of current global climate models. The representation of the Southern Ocean water mass structure and circulation is very sensitive to the surface freshwater fluxes and the vertical mixing of freshwater (England, 1992; Timmermann and Beckmann, 2004; Kjellsson et al., 2015; Stössel et al., 2015). Gordon (2016) argues that in the near future advances in satellite-based estimates of the ocean sea-surface salinity will greatly improve our understanding of the magnitude and variability of freshwater fluxes. However, in order to distinguish the contributions of the different sources, other methods will be required.

1.4 Recent changes in the Southern Ocean

The previous sections of this chapter illustrated that upwelling and subduction in the Southern Ocean might change in response to changes in the surface forcing on time scales of decades to centuries, and even glacial cycles, with important implications for the global climate. Therefore, it is extremely important to better understand the response of the Southern Ocean to changes in the surface forcing. For this purpose, I will focus in this thesis on the most recent changes, as these changes are much better constrained by observations as opposed to simulations of the past and future with global climate models or past changes inferred from proxy data. This discussion will reveal that many of the observed changes in the Southern Ocean and Antarctica are rather surprising and puzzling in the context of a warming global climate. A better understanding of the processes at work over recent decades will then help to better constrain past and future changes, as I will outline at the end of this thesis (chapter 6). In this section, I will first describe recent changes in the Southern Ocean surface climate (1.4.1), which will be followed by a discussion on the impact of these changes on upwelling and subduction (1.4.2), and the carbon uptake (1.4.3).

1.4.1 Changes in the surface climate

One of the key features of changes in the Southern Ocean surface climate over recent decades are changes in the atmospheric circulation. These changes are reflected in a reconstructed long-term shift of the Southern Annular Mode (SAM) index to more positive phases (Marshall, 2003; Abram et al., 2014). The SAM is largely measure of meridional gradients in sea-level pressure and its recent increase thus reflects a strengthening of the zonal geostrophic winds close to the surface. Model simulations consistently suggest that such an intensification and a poleward shift of the westerly winds over the Southern Ocean is a response to stratospheric ozone depletion and greenhouse gas increase (Arblaster and Meehl, 2006; Son et al., 2008; Thompson et al., 2011; Lee and Feldstein, 2013).

While the SAM index provides a measure for zonal mean circulation changes in the atmosphere, it does not allow to study zonal variations and spatial patterns in circulation changes. However, atmospheric reanalysis suggests that these changes were asymmetric in a zonal direction (Turner et al., 2009; Bromwich et al., 2011; Haumann et al., 2014). This zonal asymmetry incorporates a significant deepening of the Amundsen Sea Low (ASL), which induced a southerly wind anomaly over the Ross and Amundsen Seas and a northerly wind anomaly in the Antarctic Peninsula region and the adjacent ocean, mostly over the Bellingshausen Sea. At the same time the deepening and expansion of the ASL induces a slight northward shift of the westerly winds in the Pacific sector, while they moved southward in the other sectors. The influence of the anthropogenic forcing on the observed ASL trend over recent decades has been debated. In climatological mean state the circulation around the Antarctic continent is not perfectly annular either with large interannual to decadal variations in the zonal symmetry. Sea-level pressure variations in the ASL region are associated with quasi-stationary, planetary wave-number 1 and 2 patterns (van Loon and Jenne, 1972; Carril and Navarra, 2001; Yuan and Martinson, 2001; Turner et al., 2016). Their variability is directly linked to changes in the tropical Pacific (Ding et al., 2011; Schneider et al., 2012b; Meehl et al., 2016) and Atlantic (Li et al., 2014; Simpkins et al., 2014). Thus, the observed long-term trend in the ASL could be related to multi-decadal variations in the tropical Pacific and Atlantic (Li et al., 2014; Meehl et al., 2016), especially in light of the prevailing La Niña conditions over the recent decade (Landschützer et al., 2015b). On the other hand, the long-term decrease of the surface pressure in the ASL region is also consistent with the anthropogenic forcing (Neff et al., 2008; Turner et al., 2009; Hosking et al., 2013; Haumann et al., 2014; Raphael et al., 2016, see chapter A for a more in-depth discussion).

Both the zonally symmetric (i.e., westerly wind) and asymmetric (i.e., primarily meridional wind) changes of the atmospheric circulation are considered the prime drivers of the observed changes in the Southern Ocean and Antarctic surface climate over recent decades. As I will describe in the remainder of this section, many of the observed changes can be linked to zonally asymmetric changes in the atmospheric circulation.

Despite global warming, much of the high-latitude Southern Ocean surface has cooled during the satellite era (since 1979), especially in the Pacific sector (Fan et al., 2014; Armour et al., 2016). A series of very recent studies (Ferreira et al., 2015; Armour et al., 2016; Kostov et al., 2016; Seviour et al., 2016) suggests that this cooling or delayed warming of the Southern Ocean surface is an initial response of the sea-surface temperature (SST) to an increase in westerly winds. It is proposed that these winds increase the northward transport of cold polar surface waters through Ekman transport (Thompson et al., 2011). Yet, several other potential explanations exist. One of them is that an increased surface ocean stratification that is observed over large regions in the high-latitudes (de Lavergne et al., 2014) could inhibit the mixing of warmer CDW into the surface layer and lead to a long-term cooling (Zhang, 2007; Bintanja et al., 2013; Goosse and Zunz, 2014; Pauling et al., 2016). Another potential explanation is that the zonally asymmetric circulation changes in the atmosphere lead to a more intense meridional exchange of heat between the cold Antarctic continent and the warmer air over the open Southern Ocean, which would effectively cool the open ocean region especially in the Pacific sector (Haumann, 2011; Papritz et al., 2015; Landschützer et al., 2015b; Raphael et al., 2016). In addition, an expansion or retreat of Antarctic sea ice in relation to changes in meridional winds induces positive ice-albedo and surface heat flux feedbacks that lead to anomalies in the SST (Haumann et al., 2014). In summary, the absence of recent decadal warming in large parts of the Southern Ocean surface has not yet been fully understood, which is also owing to problems in global climate models to reproduce these changes.

An absence of decadal warming has also been recorded over the Antarctic continent over the satellite era (Jones et al., 2016; Smith and Polvani, 2016) and even since pre-industrial times (Abram et al., 2016; Smith and Polvani, 2016). However, a significant warming occurred along the coastal regions of the Antarctic Peninsula, and the Bellingshausen and Amundsen Seas (Jacobs et al., 2012; Schmidtko et al., 2014). This warming probably results from an increased upwelling of CDW onto the continental shelf (Cook et al., 2016) leading to an accelerated melting of the ice shelves in this region (Pritchard et al., 2012; Paolo et al., 2015). The increased upwelling of CDW onto the shelf can be directly linked to an increasing alongshore (mostly easterly) winds in this region (Spence et al., 2014), which are in turn part of an increasing cyclonic atmospheric circulation in the ASL region.

Antarctic sea ice has been expanding moderately over the satellite era (Comiso and Nishio, 2008). This expansion is the result of multiple opposing regional trends, with an increasing seaice cover mostly in the Ross Sea and decreasing sea-ice cover in the Antarctic Peninsula region and the Bellingshausen and Amundsen Seas (Stammerjohn et al., 2008). These regional changes have been related to regional changes in the meridional winds, with stronger southerly winds pushing the sea-ice edge northward through increasing ice drift in the Ross Sea and stronger northerly winds in the Antarctic Peninsula region advecting warmer maritime air masses that melt the ice (Haumann, 2011; Holland and Kwok, 2012; Haumann et al., 2014). Thus, the observed sea-ice changes can be directly related to zonally asymmetric changes in the atmospheric circulation. The question whether or not these changes are a forced response or induced by multidecadal variability is directly linked to the question if the zonal asymmetry in the atmospheric circulation is a forced response (Turner et al., 2009; Haumann et al., 2014; Hobbs et al., 2016). Currently, it is not possible to confidently answer this question since not only the sign and pattern of the forced response but also the magnitude and pattern of the natural variability in global climate models disagree with the observed changes (Haumann et al., 2014) and observed changes seem to short to fully capture the natural variability of the system (Hobbs et al., 2016; Jones et al., 2016). While the regional sea-ice cover indeed undergoes large decadal variations that superimpose a long-term trend (Haumann, 2011), a recent review by Hobbs et al. (2016) suggests that regional trends over the satellite era in the Ross Sea exceed natural variability in all CMIP5 models in the warm season. This observation is confirmed by a most recent sea-ice reconstruction that suggests that the increase in the sea-ice cover in the Ross Sea is unprecedented over the past three centuries (Thomas and Abram, 2016). Thus, it is possible that there is an anthropogenic influence on the recent sea-ice changes around Antarctica (Haumann et al., 2014).

The changes in the cryosphere, that I described above, induced pronounced changes in the Southern Ocean freshwater balance. Large amounts of additional glacial meltwater entered the coastal ocean of the Amundsen Sea over the last two decades (Sutterley et al., 2014; Paolo et al., 2015), freshening the waters of the continental shelf in this region and in the Ross Sea (Jacobs et al., 2002; Jacobs and Giulivi, 2010). Also the sea-ice changes potentially induce large changes in the surface freshwater balance over large regions of the Southern Ocean coastal and open ocean. However, this contribution has not been adequately quantified yet. Changes in the third surface freshwater flux component, the atmospheric freshwater flux (P-E), are highly uncertain and most

reliable estimates from atmospheric reanalysis do not show significant changes in the atmospheric flux over the Southern Ocean (Bromwich et al., 2011; Nicolas and Bromwich, 2011). However, simulations with global climate models suggest a long-term increase of the excess precipitation over the Southern Ocean with global warming (Knutti and Sedláček, 2013), consistent with an observed decrease in surface salinity over recent decades (Durack et al., 2012).

De Lavergne et al. (2014) suggest that the increased freshening observed over much of the high-latitude Southern Ocean surface waters acted to increase the vertical density stratification. This would imply a reduction in vertical mixing. However, the increased wind-driven mixing, especially in the Polar Frontal Zone, could have acted to deepen the surface mixed layer (Sallée et al., 2010b). Global climate models have generally large biases in the surface mixed-layer depth and tend to simulate a shoaling that is associated with a surface warming (Sallée et al., 2013a).

1.4.2 Changes in ocean circulation & hydrography

In contrast to the surface ocean, much of the Southern Ocean subsurface waters have been warming over recent decades. This warming is most pronounced in the region of AAIW subduction (Gille, 2002; Böning et al., 2008; Schmidtko and Johnson, 2012), suggesting an increased heat uptake by AAIW that is expected with global warming (Cai et al., 2010; Armour et al., 2016). In contrast, some of the warming has also been related to a potential poleward shift of the ACC (Böning et al., 2008; Gille, 2008; Meijers et al., 2011). However, these shifts in the ACC can only explain parts of the subsurface warming in the Atlantic and Indian Ocean sectors, as there are strong regional variations similar to the atmospheric circulation changes (Sokolov and Rintoul, 2009b; Meijers et al., 2011). AAIW did not only warm, but it also significantly freshened over recent decades, with most of the freshening occurring in the Pacific sector (Wong et al., 1999; Böning et al., 2008; Helm et al., 2010; Schmidtko and Johnson, 2012). This freshening has been attributed to changes in the atmospheric freshwater flux, even though simulated changes by global climate models appear to be largely insufficient to explain the recent freshening of AAIW (Wong et al., 1999; Helm et al., 2010).

An additional contribution to the subsurface warming and freshening might be an increased subduction of AAIW and SAMW, even though such a contribution has been debated (Böning et al., 2008). Observational evidence for changes in subduction rates has been very difficult to obtain. Yet, using chlorofluorocarbon (CFC) and sulfur hexafluoride (SF6), Waugh et al. (2013) and Waugh (2014) suggest an increase in AAIW and SAMW subduction due to an increase in westerly winds. This finding is somewhat in conflict with the finding by Helm et al. (2011) that the dissolved oxygen content in AAIW decreased, which could mean that the subduction decreased. Thus, even though there is some evidence for changes in the overturning circulation, there is yet no consensus.

A warming and freshening is also present in the other major water mass that is subducted in the Southern Ocean, AABW (Jullion et al., 2013; Purkey and Johnson, 2013). The freshening of the AABW has been attributed to the increased glacial meltwater from the Antarctic continent that freshens the continental shelf waters (Jacobs et al., 2002; Jacobs and Giulivi, 2010; Purkey and Johnson, 2013; Nakayama et al., 2014). The source of the AABW warming has been less well understood. One potential contribution might be the increased advection of warmer CDW onto the shelf of the Bellingshausen and Amundsen Seas (Schmidtko et al., 2014; Spence et al., 2014). However, AABW is not formed in this region, but rather in the high-latitude embayments of the Weddell and Ross Seas. A more likely explanation is that AABW warming would be related to changes in the gyre circulation or changes in the subduction rates (Meredith et al., 2011a). Using CFCs and SF6, Purkey et al. (2016, Ocean Sciences Meeting) argue that AABW production in the Ross Sea might have decreased. Such a decrease in AABW subduction might occur due to an increased surface buoyancy from glacial meltwater (Williams et al., 2016).

While the potential of changes in Southern Ocean upwelling and subduction to modulate the global climate in the long-term is renowned (sections 1.2 and 1.3), the driving processes are less evident and have been a major incentive to explore the Southern Ocean. To date, two prevailing views on these driving processes exist: A number of studies (Toggweiler and Samuels, 1995; Toggweiler et al., 2006; Russell et al., 2006; Toggweiler and Russell, 2008; Anderson et al., 2009; Sigmond et al., 2011) put forward the theory that long-term changes in the vertical exchange are largely induced by the wind-driven overturning circulation. However, at the dawn of high-resolution ocean circulation models, the response of the overturning circulation to changes in the surface wind field was found to be somewhat less sensitive, i.e. a higher southward eddy transport compensates for at least part of the increased surface northward Ekman transport (Hallberg and Gnanadesikan, 2006; Farneti et al., 2010; Meredith et al., 2012). Indeed, more recent studies show that the eddy kinetic energy in the Southern Ocean increased with increasing winds over recent decades (Hogg et al., 2015; Patara et al., 2016). Such an increased eddy activity could potentially also increase the tracer transport through isopycnal mixing.

An alternative hypothesis is that the vertical mixing and transport in the Southern Ocean can be altered by changes in the vertical density stratification (Hasselmann, 1991; Manabe and Stouffer, 1993; Francois et al., 1997; Sarmiento et al., 1998; Sigman et al., 2004). More recently, this theory found support by conceptual considerations and simple models that the vertical exchange is sensitive to changes in the surface buoyancy fluxes, i.e., the alteration of the surface density through surface heat and freshwater fluxes (Watson and Naveira Garabato, 2006; Morrison et al., 2011; Ferrari et al., 2014; Watson et al., 2015; Sun et al., 2016). Since the density stratification in the Southern Ocean is set up by salinity (section 1.3.2), there are reasonable grounds to believe that surface freshwater fluxes might be a critical controlling factor of changes in upwelling and subduction in the Southern Ocean. Much of the discussion on the influence of changes in surface buoyancy forcing has so far been around past or future changes, but given the potential strong changes in the surface freshwater fluxes over recent decades (section 1.4.1), they might

have influenced changes in upwelling and subduction over recent decades.

1.4.3 Carbon uptake changes

Ultimately, I turn the discussion of changes in the Southern Ocean to changes in the carbon uptake. Due to the anthropogenic increase in atmospheric pCO_2 , the Southern Ocean turned from a net carbon source to a net carbon sink (Hoppema, 2004; Gruber et al., 2009) with seasonal outgassing of natural CO₂ that is overcompensated by a seasonal uptake of anthropogenic CO₂ (Hauck et al., 2013; Landschützer et al., 2014b). The subduction of CO₂ with AAIW and SAMW in the Southern Ocean is the most important sink for anthropogenic CO₂ in the global ocean (see Figure 1.1, and section 1.1.1). Multiple concerns have been raised that this sink could weaken with global warming and could have weakened already over recent decades.

One concern is that an acceleration of the upper overturning cell in response to increasing westerly winds could saturate the Southern Ocean carbon sink by upwelling more DIC-rich waters into the surface layer. This argument arose from inverse estimates and modeling studies that seemed to confirm a saturation of the carbon sink over past decades and the upcoming century due to winds (Le Quéré et al., 2007; Lovenduski et al., 2007, 2008; Lovenduski and Ito, 2009; Lenton et al., 2009, 2013; Hauck et al., 2013). Using a model of higher resolution, Dufour et al. (2013) argue that about one third of the outgassing from enhanced Ekman pumping is compensated by enhanced southward eddy transport. This value of eddy compensation might be even larger if one used an even higher resolution than 0.5° . They further argue that it is actually not only the response of the Ekman pumping that is important for enhanced outgassing under stronger winds but even more so the enhanced mixing at the base of the mixed layer.

Very recent observational studies show that contrary to expectations, the Southern Ocean carbon sink actually strengthened again over the last decade despite a continued strengthening of the westerly winds (Fay et al., 2014; Landschützer et al., 2015; Munro et al., 2015; Tagliabue and Arrigo, 2016). These studies illustrate that the Southern Ocean carbon sink is much more complex than previously thought. A first long-term observation-based estimate of surface CO_2 fluxes over the Southern Ocean by Landschützer et al. (2015b) shows that the carbon uptake undergoes a large decadal variability with an apparent saturation in the 1990s and a strengthening in the 2000s. They argue that this variability is induced by decadal changes in the zonal asymmetry of the atmospheric circulation, which is consistent with decadal variations found in other variables of the surface climate, such as temperature (Yuan and Yonekura, 2011; Yeo and Kim, 2015; Turner et al., 2016), ACC transport (Meredith et al., 2004, 2011b), and water-mass formation (Santoso and England, 2004; Naveira Garabato et al., 2009; Sallée et al., 2010a; Kwon, 2013). Yet another interesting observation in the longer-term record of surface CO_2 fluxes is that the Southern Ocean carbon sink did not saturate over the past 30 years but actually increased its strength according to what is expected from the increase of atmospheric pCO₂ alone (Landschützer et al., 2015b). This

raises the questions if other mechanisms are at work in the long-term that counter-act a potential saturation due to increasing winds.

Another factor that could alter the carbon uptake by the Southern Ocean is a changing stratification of the surface layer. Even before concerns regarding the effect of changes in winds were raised, simulations with global climate models led to the concern that an increased stratification due to a surface warming in the areas of the subduction could inhibit the uptake of anthropogenic CO_2 (Manabe and Stouffer, 1993; Sarmiento et al., 1998; Bernardello et al., 2014a,b). This reduction in the models occurs largely due to a stabilization of the surface mixed layer and an associated reduced mixing into the subsurface layers from where isopycnal transport could subduct the carbon into deeper layers, i.e. an isolation of the surface layer from the outcropping isopycnals (Caldeira and Duffy, 2000). This hypothesis is in stark contrast to the perception of changes in the natural carbon cycle between glacial–interglacial cycles. It is thought that a warming climate during deglaciations is associated with a decrease in stratification in the high-latitudes and that this decreased stratification actually leads to an increased release of CO_2 to the atmosphere rather than an increased uptake (Francois et al., 1997; Toggweiler, 1999; Sigman and Boyle, 2000; Watson and Naveira Garabato, 2006; Skinner et al., 2010).

The key difference between the two scenarios above is that the former is concerned with changes in the uptake of anthropogenic CO_2 from the atmosphere during the subduction process and the latter with the release of CO₂ to the atmosphere during the upwelling of DIC-rich waters. Consequently, the essential question is where and when an increase in stratification occurs and if the decrease in the outgassing or the decrease in the uptake dominates. Mikaloff Fletcher et al. (2007) and Matear and Lenton (2008) conclude that a reduction in outgassing of natural CO_2 would overwhelm the reduction in uptake of anthropogenic CO_2 leading to a net strengthening of the CO₂ uptake by the Southern Ocean under increased stratification. Nevertheless, before this question can be answered, one has to understand the factors that alter the stratification of the Southern Ocean (section 1.3.2) and how stratification changes alter the pathway of carbon into the Southern Ocean. An answer to this question seems even more pressing when considering that physical changes in the Southern Ocean were found to be very sensitive to the surface freshwater forcing (Hogg, 2010; Morrison et al., 2011; Kjellsson et al., 2015; Stössel et al., 2015) and that these physical changes induce the largest uncertainty in the present and future CO₂ uptake by the ocean, apart from the uncertainty in future emissions (Doney et al., 2004; Hewitt et al., 2016; Kessler and Tjiputra, 2016; Nevison et al., 2016).

1.5 Objectives & approach

After building the case that changes in surface freshwater fluxes might be critical in driving changes in Southern Ocean overturning and stratification and thus might cause changes in the global carbon cycle and surface energy balance, I will formulate the goals of this thesis in this section. The overarching goal of my thesis is to better understand the sensitivity of the Southern Ocean stratification, circulation, and carbon uptake to changes in the surface freshwater forcing with a focus on the effect of sea-ice changes.

- (1) Very little is known on the type and magnitude of freshwater fluxes in the Southern Ocean. While estimates exist for both the atmospheric freshwater fluxes and the glacial freshwater fluxes and their changes (sections 1.3.2 and 1.4.1), freshwater fluxes from sea ice to the ocean are largely unconstrained. I here intend to quantify surface freshwater fluxes associated with sea-ice formation, transport, and melting and their changes over recent decades. For this purpose, I will derive sea-ice–ocean freshwater fluxes from currently available satellite, in-situ, and reanalysis data and estimate their uncertainties.
- (2) The new sea-ice-ocean freshwater flux estimates will allow me to directly compare the individual surface freshwater flux components in the Southern Ocean. I will base the comparison on freshwater flux estimates from atmospheric reanalysis data and estimates of glacial meltwater. Despite potentially large remaining uncertainties, I aim to assess the relative contribution of the freshwater fluxes and their changes to the Southern Ocean salinity distribution. For this purpose, I will use both simple box model considerations and a regional ocean circulation model (ROMS).
- (3) The latter involves the goal to set up a model for the Southern Ocean that simulates presentday stratification and circulation as accurately as possible. Therefore, I will use a realistic geographic setting and constrain the model by the observation-based surface fluxes from the atmosphere, and from the sea and land ice.
- (4) While the response of the Southern Ocean to changes in the surface wind forcing has been extensively studied (section 1.4.2 and 1.3.1), its response to changes in surface freshwater fluxes has received less attention even though idealized model experiments (Morrison et al., 2011; Watson et al., 2015) and ocean proxy data (Adkins et al., 2002; Sigman et al., 2004) suggest a high sensitivity. This is mostly owing to previously unconstrained surface freshwater fluxes as well as poorly performing models. Using the advances from objectives 1 through 4, I will perform sensitivity experiments with the model to study the response of stratification, temperature, and circulation to changes in the freshwater forcing.
- (5) Finally, I will run the model coupled to a biogeochemistry-ecosystem-circulation (BEC) model, to better understand the response of the Southern Ocean carbon release and uptake

in response to changing surface freshwater fluxes and compare this response to the response to the surface wind changes.

I hypothesize that freshwater fluxes associated with sea-ice formation, transport, and melting are a key factor in redistributing salt in the Southern Ocean vertically and horizontally, and thereby establishing the characteristic halocline. An increase in the sea-ice fluxes would lead to an enhanced salt redistribution that strengthens the halocline. Enhanced sea-ice fluxes would result from either a surface cooling or enhanced offshore winds and vice versa. As the sea-ice forms around the Antarctic coast and melts a along the ice edge, an increased flux would make the lower circulation cell, i.e. AABW, saltier and the upper circulation cell, i.e. AAIW and SAMW, fresher. This process would not only strengthen the surface halocline, but it would also enhance the salinity gradient between the deep and the surface ocean. Therefore, the surface waters would decouple from the deep ocean due to a shoaling of the overturning circulation and a reduction of the mixing of deep water into the surface layer. Such a reduced mixing of deep waters into the surface layer would hypothetically lead to a surface cooling, subsurface warming in the open ocean, and an enhanced uptake of carbon by the Southern Ocean mainly through reduced outgassing. These hypotheses seem consistent with some of the observed changes over recent decades (section 1.4). Thus, sea-ice freshwater fluxes might have contributed to some of these changes. In terms of carbon fluxes, a recent increase in stratification might have acted to maintain an efficient uptake of anthropogenic carbon over recent decades despite increasing winds by suppressing the upwelling of carbon-rich deep waters.

1.6 Thesis structure

Apart from the introduction chapter, this thesis consists of four main chapters, a synthesis chapter, and an appendix:

Chapter 2 provides estimates of sea-ice freshwater fluxes due to ice formation, transport, and melting and their changes over the period 1982 through 2008. I provide an estimate of their contribution to the ocean salinity distribution in the Southern Ocean by using a simple box model. This chapter was published as:

Haumann, F. A., N. Gruber, M. Münnich, I. Frenger, S. Kern (2016): Sea-ice transport driving Southern Ocean salinity and its recent trends. *Nature*, 537(7618):89–92. doi:10.1038/nature19101.

Chapter 3 describes the regional ocean circulation model (ROMS) used for chapters 4 and 5 in detail. I will provide an overview on challenges that one faces and considerations to make when modeling the Southern Ocean. I will describe both the physical and biogeochemical components of the model, the model domain and topography, as well as the model forcing at the surface and lateral boundaries. Moreover, in this chapter, I will provide a discussion of the model initialization, spin-up, and drift and a detailed evaluation of the model's mean state using observational data. Parts of this chapter will be published in a condensed form as part of chapter 4.

Chapter 4 examines the impact of changes in surface freshwater fluxes on the Southern Ocean hydrography and circulation. I will perform sensitivity experiments with ROMS by perturbing the different surface freshwater flux components and compare the response to changes induced by the surface momentum fluxes. These perturbations will correspond in terms of their spatial pattern and magnitude to the recently observed changes. I will then assess the resulting changes in salinity, temperature, stratification, and overturning circulation. This will elucidate whether freshwater fluxes could be responsible for some of the observed changes in the Southern Ocean. I will specifically focus on the changes induced by sea-ice–ocean freshwater fluxes. This chapter is in preparation for *Journal of Climate*.

Chapter 5 explores the response of the Southern Ocean CO_2 uptake to the observation-based changes in sea-ice–ocean freshwater fluxes. I will contrast these changes in terms of spatial patterns, and magnitude with changes induced by the surface wind stress that have been the focus of many previous studies. Then, I will contextualize these model-based findings in the light of the recent observation-based estimates of CO_2 fluxes in the Southern Ocean to better understand the observed changes. This chapter is in preparation for a peer-reviewed journal.

Chapter 6 synthesizes the questions that are addressed in each chapter of the this thesis. I will summarize the main findings and conclusions and discuss the limitations arising from the approach. Then, I will relate my findings to the broader picture of the interaction between the ocean circulation, the carbon cycle, and the global climate. This involves implications for the future of the Southern Ocean carbon and heat uptake and for glacial–interglacial variations in

the climate. Finally, I will provide some recommendations for future research activities and for potential improvements in global climate models that could reduce the large uncertainty in their representation of Southern Ocean processes.

Appendix chapter A addresses the question whether the recently observed zonally asymmetric changes in the atmospheric circulation and Antarctic sea ice could be induced by human activity in the form of stratospheric ozone depletion and greenhouse gas increase or are simply a result of multi-decadal natural variations. This question directly relates to the question if the processes described in this thesis are of anthropogenic origin and if they can be expected to continue in future. This chapter was published as:

Haumann, F. A., D. Notz and H. Schmidt (2014): Anthropogenic influence on recent circulationdriven Antarctic sea-ice changes. *Geophysical Research Letters*, 41(23):8429–8437. doi: 10.1002/2014GL061659.

In the course of this thesis, I made additional and directly related contributions to the studies by Stössel et al. (2015) and Landschützer et al. (2015b) that are not included as chapters.