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Kev Points:

- CCSM4 accurately depicts the southeast Pacific as the main region of formation
- Formation rates for SAMW are underestimated in CCSM4 compared to observations
- Formation rates for AAIW are overestimated in CCSM4 compared to observations

Supporting Information:

- Readme
- Figure S1
- Figure S2

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Comparison of Subantarctic Mode Water and Antarctic Intermediate Water formation rates in the South Pacific between NCAR-CCSM4 and observations

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Abstract Average formation rates for Subantarctic Mode Water (SAMW) and Antarctic Intermediate Water (AAIW) in the South Pacific are calculated from the National Center for Atmospheric Research Community Climate System Model version 4 (NCAR-CCSM4), using chlorofluorocarbon inventories (CFC-12). When compared to observations, CCSM4 accurately simulates the southeast Pacific as the main formation region for SAMW and AAIW. Formation rates for SAMW in CCSM4 are 3.4 sverdrup (Sv), about half of the observational rate, due in part to shallow mixed layers, a thinner SAMW layer, and insufficient meridional transport. A formation rate of 8.1 Sv for AAIW in CCSM4 is higher than observations due to higher inventories in the southwest and central Pacific and surface concentrations within CCSM4. Also, a lack of data in the southwest Pacific may bias the observational rate low. This model-observation comparison is useful for understanding the uptake and transport of other gases, e.g., CO₂ by the model.

1. Introduction

Subantarctic Mode Water (SAMW) and Antarctic Intermediate Water (AAIW) are large volume, lower thermocline, and intermediate water masses that fill the Southern Hemisphere subtropical gyres. They ventilate the subtropical gyres with atmospheric gases and transfer climatically and biologically important properties such as heat, freshwater, nutrients, and oxygen into the interior ocean [Sallee et al., 2006; Talley, 2003; 2008; Toggweiler et al., 1991]. SAMW and AAIW are also responsible for a significant fraction of the uptake of anthropogenic CO₂ in the world's oceans [Mikaloff-Fletcher et al., 2006; Sabine et al., 2004]. Thus, variations in SAMW and AAIW formation have an important role in climate variability and change.

The focus of this study is to compare and asses the formation rates of SAMW and AAIW in the South Pacific, from the National Center for Atmospheric Research Community Climate System Model version 4 (NCAR-CCSM4) to formation rates calculated from ocean observations in *Hartin et al.* [2011] using chlorofluorocarbon inventories. Chlorofluorocarbons (CFC-11 and CFC-12) are conservative oceanic tracers that are used to evaluate circulation, water mass ages, and formation rates [e.g., *Fine*, 2011]. Importantly, CFCs provide an analogue to the physical processes of uptake and storage of carbon in the global ocean.

In a recent evaluation of CCSM4, Weijer et al. [2012] find that in all three sectors of the Southern Ocean to 30°S, model CFC-11 and CFC-12 concentrations in lower thermocline and intermediate waters are reduced compared with observations. In this study, we quantify SAMW and AAIW inventories and formation rates in the South Pacific in CCSM4 and investigate how they are influenced by biases in the model. SAMW formation rates are underestimated in CCSM4 when compared to observations, primarily due to shallow mixed layers, a thinner SAMW layer, and insufficient meridional transport. While AAIW formation rates are greater than observations in CCSM4, due to higher inventories and surface saturations in the central and southwest Pacific. Also, this study finds that a lack of observational data in the southwest Pacific may bias the observational rate low. This study helps us better understand the processes influencing SAMW and AAIW formation and document future needs for model improvement and observational data gaps.



2. Data

2.1. Ocean Observations

The observational data used in this study are the same data used in Hartin et al. [2011]. The data are from World Ocean Circulation Experiment (WOCE) collected in the 1990s, Climate Variability and Predictability (CLIVAR), now formally coordinated by Global Ocean Ship-Based Hydrographic Investigations Program (www.go-ship.org) collected in the 2000s, and data collected on board the R/V Knorr in austral winter 2005 in the southeast Pacific. All data are freely available at CLIVAR and Carbon Hydrographic Data Office (www.cchdo.ucsd.edu).

2.2. Model Description

The CCSM4 is a global coupled ocean, atmosphere, sea ice, and land surface general circulation climate model. The atmospheric model is the NCAR Community Atmospheric Model version 4 with 26 levels in the vertical and an approximate horizontal grid spacing of 1.25° × 0.9°. The ocean model is the NCAR implementation of the Parallel Ocean Program version 2 with 320 × 384 points and 60 vertical levels, with an approximate grid spacing of $1.11^{\circ} \times 0.54^{\circ}$ and finer resolution in the tropics [Danabasoglu et al., 2012]. The analyses presented in this paper focus on an ensemble of five twentieth century monthly integrations. These simulations were run from 1850 to 2005. Each ensemble was branched off at a different time from a preindustrial control. For more information on CCSM4 see Gent et al. [2011].

2.3. Defining SAMW and AAIW

The coldest, freshest, and densest variety of SAMW is formed in the southeast Pacific, just west of the Drake Passage [McCartney, 1977, 1982]. SAMW is found north of the Subantarctic Front (SAF), forming in deep winter mixed layers, usually >500 m [Holte et al., 2012]. SAMW is characterized by a minimum in potential vorticity, and high oxygen and CFC concentrations, occupying the lower thermocline of Southern Hemisphere oceans [Fine et al., 2001]. Within CCSM4, we define SAMW as the density layer in the 26.8–27.0 kg m⁻³ range, based on the density of the deepest winter mixed layer in the southeast Pacific and a minimum in potential vorticity (not shown). However, the mixed layer depth in the model is not as deep, and potential vorticity is not as low as in observations [Weijer et al., 2012]. AAIW forms equatorward of the Polar Front (PF) and subducts at the SAF, characterized by a salinity minimum [e.g., Hanawa and Talley, 2001; Sloyan and Rintoul, 2001]. In CCSM4, AAIW is defined in the 27.0–27.4 kg m⁻³ density range, based on the location of the salinity minimum and poleward of the deepest mixed layer. These model density surfaces correspond to similar density surfaces used to identify SAMW and AAIW in Hartin et al. [2011]. The small 0.6 kg m⁻³ density difference between observations reported in Hartin et al. [2011] and the model does not translate into a significant difference in thickness, inventories, or formation rates.

3. Methodology

3.1. CFC-12 Inventory Calculation

CFC-12 was chosen as the compound to use in this study because it continually increased in the atmosphere longer, compared with CFC-11. CFC-12 inventories are calculated for SAMW and AAIW using a technique described in earlier studies [LeBel et al., 2008; Orsi et al., 1999; Rhein et al., 2002; Smethie and Fine, 2001; Willey et al., 2004]. As in Hartin et al. [2011],

$$\mathsf{CFC}_{\mathsf{inv}} = \rho \Sigma_{ij}([\mathsf{CFC}](ij) \cdot A(ij) \cdot D(ij)) \tag{1}$$

where CFC_{inv} is the CFC-12 inventory (moles), ρ is the density of water (kg m⁻³), [CFC]_(ij) is the CFC-12 concentration (pmol kg^{-1}) at latitude (i) and longitude (j), $A_{(ij)}$ (m²) is the area of the corresponding grid box, and $D_{(ii)}$ (m) is the thickness of each water mass. The inventories are averaged over all five CCSM4 ensembles in the year 2005. They represent the average CFC accumulation in SAMW and AAIW, beginning primarily in the 1970s when the concentration of CFCs started increasing rapidly, to the year 2005. The year 2005 was chosen because Hartin et al. [2011] normalized the observations to a constant date of 1 January 2005 in order to give a quasi-synoptic inventory within these water masses. The inventories for SAMW (26.8–27.0 kg m⁻³) are calculated between the SAF and the equator and for AAIW (27.0–27.4 kg m⁻³) from PF to 20°N in CCSM4. The boundaries for both SAMW and AAIW extend from 150°E to 70°W. SAMW and AAIW in this work and in Hartin et al. [2011] are defined from their surface outcrop in the mixed layer, as this is where the water masses gain their characteristic properties, i.e., low potential vorticity and salinity

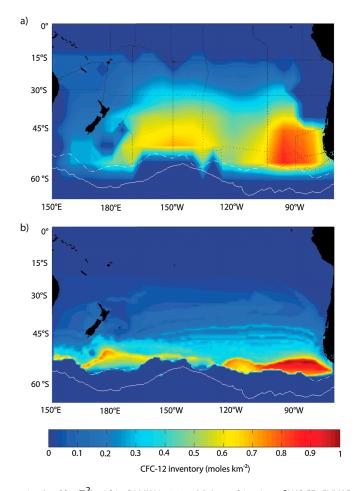


Figure 1. CFC-12 inventories (mol km⁻²) within SAMW in 2005. (a) A combination of WOCE, CLIVAR, and data collected in 2005 all corrected to a common collection date of 2005 (26.8–27.06 kg m⁻³); black dots show sample locations. Reprinted from Formation Rates of Subantarctic Mode Water and Antarctic Intermediate Water within the South Pacific, 58, C.A. Hartin, R.A. Fine, B.M. Sloyan, L.D. Talley, T.K. Chereskin, J. Happell, 524-534, Copyright [2013], with permission from Elsevier. (b) CCSM4 ensemble average $(26.8-27.0 \text{ kg m}^{-3})$. The poleward boundary for SAMW is the SAF (dashed white contour) and the PF (solid white contour), taken from Orsi et al. [1995].

minimum. SAF and PF locations are well simulated compared to the observations [Weijer et al., 2012]. Therefore, for the ease of comparison, we use the observational frontal locations from Orsi et al. [1995] as the southern boundaries for the inventory calculations.

3.2. Water Mass Formation Rate Calculation

CFC-12-based average water mass formation rates for SAMW and AAIW within the South Pacific over the major period of CFC-12 input from 1970 to 2005 are calculated based on methods from Hartin et al. [2011], Kieke et al. [2006], LeBel et al. [2008], and Smethie and Fine [2001]:

$$R = \frac{\mathsf{CFC}_{\mathsf{inv}}}{\rho \int_{t_0}^{t_n} [C_{\mathsf{s}}(t)^* \mathsf{sat}] \mathsf{d}t} \tag{2}$$

where $C_s(t)$ (pmol kg⁻¹) is the CFC-12 concentration at the formation region at equilibrium with the atmosphere for the years 1970 to 2005, and sat is the CFC-12 percent saturation at that location. When using this equation, the percent saturation at the time of formation and the formation rate are both assumed to be constant over the period of CFC-12 input. This method calculates an average formation rate over the years 1970-2005 using the inventory of CFC-12 sampled in 2005. Sources of variability in SAMW and AAIW formation rates in the South Pacific are the southern annular mode (SAM) and the El Niño-Southern Oscillation (ENSO). CCSM4 accurately captures the trend to more positive phases of SAM [Weijer et al., 2012]. Oceanic observations suggest up to 20% variability in AAIW due to the SAM [Roemmich et al., 2007]. Similarly,

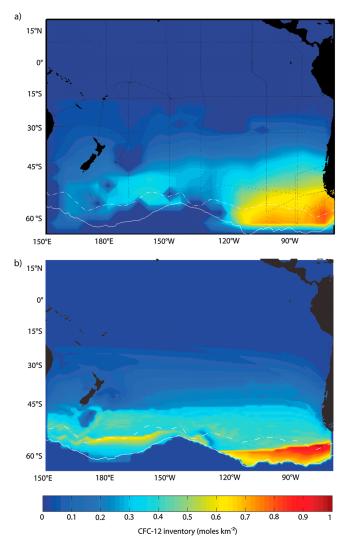


Figure 2. CFC-12 inventory (moles km⁻²) within AAIW for 2005. (a) A combination of WOCE, CLIVAR, and data collected in 2005 all corrected to a common collection date of 2005 (27.06–27.4 kg m⁻³); black dots show sample locations. Reprinted from Formation Rates of Subantarctic Mode Water and Antarctic Intermediate Water within the South Pacific, 58, C.A. Hartin, R.A. Fine, B.M. Sloyan, L.D. Talley, T.K. Chereskin, J. Happell, 524–534, Copyright [2013], with permission from Elsevier. (b) CCSM4 ensemble average $(27.0-27.4 \, \text{kg m}^{-3})$. The poleward boundary for AAIW is the PF (solid white contour) and the SAF (dashed white contour), taken from Orsi et al. [1995].

formation rates during this period may be variable. ENSO has been shown to significantly influence the properties of SAMW and AAIW in the South Pacific [Naveira Garabato et al., 2009]. In CCSM4, ENSO has similar variability as observations but a stronger amplitude [Weijer et al., 2012].

Percent saturations relative to the 2005 atmosphere are calculated after Warner and Weiss [1985] by comparing the model CFC-12 oceanic concentrations to the atmospheric concentrations from 2005. Model CFC-12 saturations within the mixed layer of SAMW in the South Pacific are 94% saturated with respect to the 2005 atmosphere, which compares well with the observed value of 95%. Poleward of the SAF in the model mixed layer at the 27.2 kg m⁻³ isopycnal, AAIW is 82% saturated relative to the 2005 atmosphere, which is lower than observations of 85%. Once AAIW subducts below the SAF, average model saturations decrease to 54%, below the observed value of 60%. It is this saturation of 54% that is used in the formation rate calculation.

4. Discussion

The CCSM4 CFC-12 inventories for both SAMW and AAIW simulate the maxima in the southeast Pacific as shown in the observations (Figures 1 and 2). In both the simulated SAMW and AAIW, CFC-12 inventory

Table 1. SAMW and AAIW Inventories, CFC-12 Saturations, and Formation Rates for Both Observations and Model ^a		
	Observations	Model
	SAMW	
Inventories	16×10 ⁶ mol	7.5×10 ⁶ mol
Saturations	95%	94%
Formation rates	$7.3 \pm 2.1 \text{Sv}$	3.4 Sv
	AAIW	
Inventories	8.7×10 ⁶ mol	11.9×10 ⁶ mol
Saturations (equatorward of SAF)	60%	54%
Saturations (poleward of SAF)	85%	82%
Formation rates	5.8 ± 1.7 Sv	8.1 Sv

^aObservations are from *Hartin et al*. [2011].

(>0.7 mol km⁻²) maxima are centered at 90°W and a secondary maxima (>0.5 mol km⁻²) centered at about 180° (Figures 1a and 2a). In the observations, these secondary maxima are present for SAMW and AAIW, although with lower inventories and centered farther eastward at 150°W for SAMW and closer to 170°W for AAIW. The CCSM4 inventory maps agree well with other studies that suggest the southeast Pacific as a major site of formation for SAMW and AAIW [Hartin et al., 2011; Iudicone et al., 2007; McCartney, 1982; Sallee et al., 2010; Sloyan and Rintoul, 2001].

The majority of the model CFC-12 inventory lies within the subtropical gyre and reaches nearly zero levels as SAMW and AAIW approach 30°S. There is a significant decrease in the model CFC-12 inventory equatorward of 50°S and 60°S for SAMW and AAIW, respectively. The simulated SAMW and AAIW are not transporting CFCs as far equatorward as observed. For example, for SAMW the 0.5 mol km⁻² contour in observations extends to approximately 35°S, while the 0.5 mol km⁻² contour in the model inventories only extends to approximately 45°S-50°S. This insufficient meridional transport of CFCs into the interior subtropical gyre has been shown to be closely related to the biases in the parameterization of lateral subgrid-scale mixing [Dutay et al., 2002].

4.1. Subantarctic Mode Water

Total CFC-12 inventories for SAMW from observations are 16×10^6 mol, which is significantly higher than 7.5×10^{6} mol within CCSM4 (Table 1). These inventories correspond to formation rates of 7.3 ± 2.1 sverdrup (Sv) for observations and 3.4 Sv for CCSM4. For this study, we use the observational formation rates of SAMW that are formed and circulate around the South Pacific. They do not include SAMW that has been transported out of the subtropical gyre [see Hartin et al., 2011]. The underestimation in the SAMW inventory and formation rate within the model is attributed to a combination of shallower than observed mixed layers and a thinner SAMW. In addition, Hartin et al. [2011] show that cold-core eddies are sites of SAMW formation in the South Pacific. However, as this is a 1.11° × 0.54° model, effects of eddies on CFC distribution are not simulated but instead parameterized using Gent and McWilliams [1990], and this may be another source of the model bias in the inventories and formation rates.

In order to verify the first attribute of shallow model mixed layers, the inventories (mol km⁻²) are divided by the mixed layer depth (m) to obtain a CFC-12 concentration in the mixed layer in mol km⁻³ (Figure S1). For the observations across the entire South Pacific, we used the Commonwealth Scientific and Industrial Research Organization Atlas of Regional Seas 2009 (CARS2009) [Ridgway et al., 2002] monthly mixed layer depth climatology and the monthly mean output of mixed layer depth from CCSM4. When comparing the observations and model output for SAMW (Figure S1), it is apparent that CFC-12 concentrations in the mixed layer along the SAF are similar, suggesting that a low bias in the simulated CFC inventories are in part explained by a shallow bias in the model mixed layer. The model-simulated winter mixed layer depth in these regions is approximately 150 m, which is significantly shallower than the average winter mixed layer depths of >250 m from CARS2009 climatology [Weijer et al., 2012] (see Sloyan and Kamenkovich [2007] for a similar conclusion for many AR4 climate models).

Model mixed layer depths, inventories, and formation rates are approximately half the values of observations. Therefore, we can conclude that if the mixed layer depths in the model were more realistic, then the inventories and formation rates would be closer to observations. A possible reason for the shallow bias within the CCSM4 mixed layer is due to the parameterization of the subgrid-scale mixing processes involved in mixed layer formation. These parameterizations used in the model tend to cause the mixed layer to be



shallower than observations, with the greatest effects seen in the high latitudes [Fox-Kemper et al., 2011]. The mixed layer depth can also be affected by wind forcing. However, even though in the Southern Hemisphere westerlies are significantly stronger in CCSM4 compared with observations [Danabasoglu et al., 2012], mixed layers are still underestimated. Wind variability can be an important factor in the formation of deep mixed layers [Kamenkovich, 2005].

In addition, weak vertical mixing within the mixed layers is noticeable in CCSM4 as higher potential vorticity at the base of the mixed layer, compared with observations [Weijer et al., 2012]. Along with shallower mixed layers, SAMW (26.8–27.0 kg m⁻³) in CCSM4 is thinner by up to 400 m in the subtropical gyre of the South Pacific (Figure S2a). Since the inventory calculation in equation (1) is dependent upon the thickness of the water mass, model inventories can be expected to be more realistic if the layer thickness of SAMW was more realistic. These lower SAMW inventories and formation rates in the model also imply weaker ventilation of the subtropical gyre with atmospheric gases in general.

4.2. Antarctic Intermediate Water

Total CFC-12 inventories for AAIW in observations are 8.7×10^6 mol and 11.9×10^6 mol in CCSM4. These inventories correspond to formation rates of 5.8 ± 1.7 Sv for observations of water formed and circulating within the South Pacific and 8.1 Sv for CCSM4. A closer inspection of the observational and model estimates offers a potential explanation for the differences which exceed the observational errors. The CCSM4 AAIW CFC-12 inventories are higher in the central and southwest Pacific, where there is a lack of ocean observations, between 150°E and 180°. In order to estimate the potential significance of a lack of data in the southwest Pacific, model-simulated data in southwest Pacific at all latitudes from 150°E to 180° were excluded from calculations and inventories were recalculated. This resulted in a substantially reduced inventory of 9.9×10^6 mol and a formation rate of 6.7 Sy, as compared with 11.9×10^6 mol and 8.1 Sy in the calculation with full model output. Since this is a region of significant gaps in data coverage, it remains unclear whether the differences between the observed and simulated inventories correspond to model biases in this region or are due to a lack of data resolution in observations. If the latter is true, the model may be simulating another primary region of AAIW formation, not shown in CFC observations. Indeed, Sallee et al. [2010] show the southwest and central Pacific as important subduction regions.

Surface and subsurface concentrations and inventories (0-500 m) reported in Weijer et al. [2012] in the model are higher than observations, particularly within the ACC and along AAIW outcrops. This overestimation in surface concentrations is likely due to a cold bias in CCSM4, poleward of 45°S, related to the bias in wind stress [Danabasoqlu et al., 2012] and insufficient meridional transport of CFCs into the interior as mentioned earlier. Colder temperatures and higher wind stress allow for a greater flux of CFCs into the surface waters, contributing to the overestimation of the total CFC-12 inventory in AAIW.

AAIW across the subtropical gyre is thinner by between 100 and 200 m in CCSM4 compared with observations. This thinner layer would bias the inventories and formation rates lower than observations (Figure S2b) as in the case with SAMW. However, the increased surface and southwest Pacific inventories have a greater effect on the total AAIW inventory and formation rate. Another striking feature of model simulations is the sharp meridional gradients in AAIW/SAMW inventories, which suggest that the meridional transport of CFC in CCSM4 is underestimated. This may be due to insufficient mixing by mesoscale eddies, which represent the main vehicle for the meridional transport across ACC. However, mesoscale eddies are parameterized in this coarse-resolution model.

5. Conclusions

Comparisons of CFC-12 inventories and formation rates of SAMW and AAIW from observations and model output are important for validating a model on time scales relevant for anthropogenic CO₂ uptake. CCSM4 accurately depicts the southeast Pacific as the main region of formation for SAMW and AAIW. Inventories and formation rates of SAMW in the South Pacific in CCSM4 are significantly less than observations, due to the shallow bias in the model mixed layer depths and a thinner SAMW throughout the South Pacific [e.g., Dutay et al., 2002; Sloyan and Kamenkovich, 2007; Danabasoglu et al., 2012]. The inventories and formation rates for AAIW in CCSM4 by contrast are higher than the observational estimates, primarily due to higher model inventories in the southwest Pacific and higher surface and subsurface concentrations along the outcropping region of AAIW. Causes for the latter biases are related to a combination of a cold bias in sea

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surface temperatures poleward of 45°S in CCSM4 and stronger wind stress [Danabasoglu et al., 2012]. There are also indications of insufficient meridional penetration of CFC in the near-surface layers, which may indicate parameterization of eddy-driven transport is underestimating the process. Furthermore, this study shows that when data from the southwest Pacific are not used in the model inventory calculations, it results in lower formation rates for AAIW. This suggests that a lack of CFC data from the southwest Pacific may bias the observational formation rates lower.

Differences in the modeled and observed CFC-12 concentrations, inventories, and formation rates emphasize the need for further model improvement in ocean-atmosphere exchange and upper ocean parameterizations. They highlight the need for more ocean observations, especially within the southwest Pacific. Given the CFC analogue with ocean carbon, this study of model data comparison further suggests that CO₂ uptake and sequestration may not be simulated accurately in CCSM4 and climate model that show similar model biases.

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