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2 **Global Meridional Overturning Circulation Estimation in a Multiscale Ensemble**  
3 **Filtering CDA System with Improved Atmosphere-Ocean Exchange Fluxes**

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18 **Key Points:**

- 19 • Multiscale ensemble coupled data assimilation (CDA) is used to reconstruct atmosphere  
20 and ocean mean meridional circulation structures.
- 21 • Global meridional overturning circulation (GMOC) estimation in multiscale CDA  
22 highlights balanced and coherent state estimation.
- 23 • More coherent ocean state estimation is critical for improving GMOC estimation with  
24 more ocean observations that represent richer scales.

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**Abstract**

Reconstruction of global meridional overturning circulation (GMOC) by combining Earth observing system with coupled climate models is crucial for climate analysis and prediction initialization. However, achieving balanced and coherent incorporation of data and model dynamics is challenging. Coupled data assimilation (CDA) addresses this by leveraging coupled model dynamics and observational information. Here with a biased twin experiment framework consisting of two coupled general circulation models (CGCMs) and a newly-developed multiscale ensemble filtering CDA algorithm, this study addresses important aspects of reconstructing GMOC. Subsequently, the CDA-reconstructed GMOC achieves error reduction over 34% (4.6 Sv out of 7.4 Sv in terms of mass transport) compared to free model simulation. The CDA data-incorporation improves atmosphere-to-ocean work and ocean-to-atmosphere heat fluxes by approximately 51% (5.7 out of 11.2 GW) and 32% (24 out of 75.6 TW) respectively, while improving 6% ( $3.6 \times 10^{-7}$  out of  $63.7 \times 10^{-7}$  W/kg) of diagnosed turbulence kinetic energy dissipation. Pivotal processes in GMOC estimation are examined. The residual circulation in the Antarctic Circumpolar Circulation system is reconstructed by CDA, resulting in a 34% error reduction (.14 out of .21  $\text{m}^2/\text{s}$ ). In the North Atlantic, CDA recovers the North Atlantic Deep Water index by 50% (159 out of 316 m). Historical GMOC estimation using real observations aligns well with climatology data but requiring further deep analyses. To improve the estimation in the future, the great light shall be darted on improving ocean estimation coherence by incorporating more types of observations that represent interactions of richer scales especially in retrieving tropical multiscale processes.

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**Plain Language Summary**

Ocean tracers such as heat, salt, and carbon are carried by the global meridional overturning circulation (GMOC), conveying between the Hemispheres. However due to sparse observations and imperfect ocean model, accurately understanding of GMOC is still challenging. Data assimilation, a method combining ocean models with real observations, could produce an accurate estimation of GMOC. Unfortunately, even in datasets produced by data assimilation procedures, the behavior of GMOC is quite different. This study introduces a new data assimilation approach that incorporates atmospheric and oceanic observations within a coupled Earth system model with the capability addressing multiscale and probabilistic nature of the data incorporation process. We demonstrate that, through a balanced and coherent data integration procedure, our new approach is able to retrieve the fundamental behavior of GMOC, which is crucial for understanding the global transport of heat, salt, carbon and nutrients.

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## 73 1 Introduction

74 The global meridional overturning circulation (GMOC) is often defined as the result  
75 obtained by zonal integration and vertical accumulation of meridional ocean volume transport in  
76 global ocean (*Wright and Stocker, 1991*). GMOC is a complex system primarily driven by  
77 multiscale and intensive air-sea interactions (*Danabasoglu et al., 1994; Macdonald and Wunsch,*  
78 *1996; Wright et al., 1998*). In the North Atlantic and Arctic Oceans, water masses at high latitudes  
79 are cooled and sink into the ocean abyss through deep convection (*Bjerknes, 1964; Shaffrey and*  
80 *Sutton, 2006; H Yang et al., 2013*). Concurrently, the Southern Ocean experiences wind-driven  
81 upwelling (*Price et al., 1987*), while in low-latitude regions, upwelling is usually induced by  
82 mixing processes (*Thompson, 1978*). The role of GMOC in transporting substantial heat  
83 northward in both hemispheres is important, contributing to the global redistribution of heat,  
84 freshwater, carbon, and nutrients (*H L Johnson et al., 2019*). It has been the subject of numerous  
85 studies due to its vital role in the climate system (*G C Johnson et al., 2021*). The importance of  
86 GMOC can extend to marine ecosystems, the carbon cycle, sea-level, and extreme weather (*Lee et*  
87 *al., 2023; R Zhang et al., 2019*).

88 Historically, hydrographic sections (observations of temperature and salinity by depth at  
89 certain transections) have been repeatedly used to estimate GMOC (*Ganachaud and Wunsch,*  
90 *2000; Lumpkin and Speer, 2003*). However, such estimation may be subject to large  
91 spatiotemporal sampling errors inherent in the one-time synoptic hydrographic sections (*Lee et al.,*  
92 *2019*). The establishment of sustained monitoring programs like RAPID-MOCHA (RAPID –  
93 Meridional Overturning Circulation and Heat flux Array) (*Cunningham et al., 2007*) and OSNAP  
94 (Overturning in the Subpolar North Atlantic Program) (*Lozier et al., 2017*) has facilitated the data  
95 to calculate volume transport along specific latitude transects. Utilizing data along with Argo  
96 (Array for Real-Time Geostrophic Oceanography) (*Wong et al., 2020*) and satellite altimeter  
97 records (*T Yang and Xu, 2015*), some observation-based estimations have enabled the estimation  
98 extending back to the beginning of the altimeter record in 1993 at specific latitude (*Mercier et al.,*  
99 *2015; Perez et al., 2018*). However, it is still an open question whether the estimated GMOC  
100 exhibits coherent variability across latitude or not (*Bingham et al., 2007*).

101 The coupled general circulation models (CGCMs) are often used to fill the gap between our  
102 physical understanding of oceanic processes and observation-based estimation (*Sugiura et al.,*  
103 *2008; S. Zhang et al., 2007*). However, models inevitably have shortcomings in their ability to  
104 represent the physics of nature. For example, in the coarse-resolution models (nominal  $1^\circ$  or  
105 coarser) current, which are known that simulated jet-like currents such as Kuroshio are broad and  
106 diffuse, and much weaker than the observation, sometimes even with erroneous location and  
107 vertical structure (*Ma et al., 2016*). For high-resolution model (nominal  $0.25^\circ$  or finer), some  
108 important processes like mixing are still unclear (*Hirschi et al., 2020*). Therefore, the GMOC  
109 variability in current CGCMs exhibits notable systematic biases and discrepancies (*Danabasoglu*  
110 *et al., 2014; Danabasoglu et al., 2016*).

111 Given the nature of sparse observations and inaccurate numerical models, data assimilation  
112 (DA) is a suitable tool to resolve the dilemma. DA combines prior information from imperfect  
113 models with incomplete observed data to obtain the best estimation of state evolution and its  
114 uncertainty (*Jazwinski, 2007*) of atmospheric and oceanic motions (*Carrassi et al., 2018*) as a  
115 stochastic dynamics system (*S. Zhang et al., 2020*). Although DA in ocean model (ODA) shows  
116 increased AMOC (Atlantic Meridional Overturning Circulation) time mean agreement in strength  
117 with the RAPID mean in multiple ODA analyses, less consistence exists in their spatial structure

118 and temporal variability (*Karspeck et al., 2017*). Such discrepancies imply that ocean reanalysis  
119 contains too much spurious variability in its climate (*Lu et al., 2020*). One of the main reasons for  
120 this disparity is the widespread inhomogeneous ocean observation network. Although Expendable  
121 bathythermograph (XBT) can provide heat content data in the upper 500 m since 1970s (*Cheng et*  
122 *al., 2018*), the comprehensive sampling of temperature and salinity down to 2000 m depth has only  
123 been made possible by the deployment of Argo profiling floats, which began in the mid-2000s  
124 (*Wong et al., 2020*). Consequently, most part of the ocean is unobserved below 2000 m. In ODA,  
125 the unconstrained ocean abyss can exert significant influence on the constrained regions (*Lu et al.,*  
126 *2020*). To relax this issue, *Lu et al. (2020)* implemented a climatological restoring scheme for deep  
127 ocean temperature and salinity within the ODA procedure, which is identified as a crucial strategy  
128 for reconstructing AMOC mean state and variability.

129 Coupled data assimilation (CDA) refers to perform DA in a coupled model framework  
130 (*Penny and Hamill, 2017; Sugiura et al., 2008; S. Zhang et al., 2007; S. Zhang et al., 2020*). This  
131 involves the joint execution of coupled model forecasts and state estimations, enabling each  
132 component of the model receives observational information from other components. Such an  
133 integrated approach facilitates the exchange of information across different model components,  
134 producing more balanced and coherent state estimation (*S. Zhang et al., 2020*). Specifically, as  
135 GMOC is the result of intense air-sea interaction, CDA therefore can be beneficial to the  
136 estimation of GMOC.

137 In this study, we first develop a new data assimilation (DA) algorithm within the coupled  
138 model framework, drawing inspiration from two key concepts: the optimal proposal density  
139 (*Evensen et al., 2022*) and the multi-timescale filtering algorithm (*Yu et al., 2019*) including the  
140 climatological restoring scheme. This algorithm is specifically designed to tend to improve both  
141 the accuracy of state estimation and physical balance and coherence within the coupled system.  
142 Given the challenge of distinguishing authentic changes in the climate system from spurious  
143 climate drift due to incorporation of data into a model, we first perform CDA in the  
144 twin-experiment framework. In the perspective of energy budget, we can examine the behavior of  
145 atmosphere-to-ocean work and ocean thermal responses in CDA. This examination offers an  
146 overarching perspective on the physical processes in energy cycling of CDA, as they play a key  
147 role in maintaining equilibrium of GMOC (*R X Huang et al., 2006*). Then benefit from the  
148 interhemispheric GMOC theory, which enables a more profound depiction of dynamics of distinct  
149 regions, we can provide a deeper analysis of variability in each region. Consequently, our study  
150 provides a more comprehensive assessment of the estimated GMOC in CDA products.

151 This paper is organized as follows. After introduction, we describe methodology in section  
152 2, including two CGCMs and two ensemble multiscale CDA algorithms as well as experimental  
153 design used throughout this study. Section 3 briefly validates a new multiscale ensemble filtering  
154 CDA algorithm in terms of traditional error statistics. Sections 4 and 5 examines the contributions  
155 of various atmospheric and oceanic data constraints in the coupled model framework to the  
156 exchange fluxes at the air-sea interface and kinetic energy dissipation rate as well as their impacts  
157 on GMOC estimation. Section 6 examines the estimated GMOC in a 30-year CDA reanalysis with  
158 real atmosphere and ocean observations. The conclusions and discussions are given in Section 7.

## 159 2 Methodology

### 160 2.1 Two coupled Earth system models: CESM1.3 and CM2.1

161 In this study, we use two CGCMs, CESM1.3 and CM2.1, to detect how CDA recover the  
162 structure and variability of ocean meridional circulation by incorporating observations into  
163 assimilation models in a balance and coherent manner. Both the CESM1.3 and CM2.1 models are  
164 fully coupled global climate models that can simulate Earth's climate system, developed by the  
165 National Center for Atmospheric Research (NCAR) and Geophysical Fluid Dynamics Laboratory  
166 of National Oceanic and Atmospheric Administration (GFDL/NOAA). As important members in  
167 phases 5 and 6 of Couple Model Inter-comparison Project (CMIP5, e.g., *Taylor et al. (2012)*;  
168 CMIP6, e.g., *Eyring et al. (2016)*), the CESM1.3 and CM2.1 models are capable of providing  
169 state-of-the-art computer simulations of the past, present and future climate states of the Earth. The  
170 basic model configurations are the same as in the previous CDA studies (*Lu et al., 2023*; *Lu et al.,*  
171 *2020*; *Sun et al., 2022*), here we only comment on some relevant aspects to this study. Both models  
172 that simultaneously simulate the atmosphere, ocean, land, and sea ice of the Earth, as well as the  
173 flux exchanges at the interfaces between the components. We configure a CESM1.3 historical  
174 simulation named BHISTC5 with the resolution ne30g16 (ne30: the atmosphere and land with  
175 roughly 1° grid-spacing in 30-element spectral-element dynamical core; g16: the ocean and ice are  
176 on nominal 1° displaced pole grid of version 6) for this study. The CESM1.3 atmosphere and  
177 ocean components include the Community Atmosphere Model version 5 (CAM5) for the  
178 atmosphere, the Community Land Model version 4.0 (CLM40) for land, and the Parallel Ocean  
179 Program version 2 (POP2) for the ocean and Community Ice Code version 4 (CICE4) for sea ice.  
180 The POP2 has 60 vertical levels, while CAM5 has 30 vertical levels. The time steps of ocean and  
181 atmosphere are 1 hour and 30 minutes respectively, with a 1-hour coupling frequency between  
182 them. We chose the component set of BHISTC5 for the experiments, in which the historical  
183 radiation conditions is used as external forcing. This historical simulation is used to produce  
184 “observations” for twin experiments that will be described in section 2.3.

185 We use CM2.1 as the assimilation model. The CM2.1 combines atmosphere model 2.1 and  
186 land model 2.1 (AM2.1-LM2.1) with the Modular Ocean Model version 5 (MOM5) and the Sea  
187 Ice Simulator (SIS) (*Delworth et al., 2006*; *Gnanadesikan et al., 2006*). The atmosphere model  
188 AM2.1 is based on a finite-volume dynamical core (*Lin, 2004*) and has a horizontal resolution of  
189 2° latitude × 2.5° longitude (same as LM2.1) with 24 vertical levels. MOM5 is configured with 50  
190 vertical levels (22 levels of 10 m thickness each in the top 220 m) and 1°×1° horizontal B-grid  
191 resolution telescoping to 1/3° meridional spacing near the equator. SIS in the coupled model is a  
192 dynamical ice model with three vertical layers (one for snow and two for ice) and five  
193 ice-thickness categories. The time steps of ocean and atmosphere models are 2 hours and 30  
194 minutes respectively, with a 2-hour coupling frequency between them.

195 For convenience of description, hereafter we briefly name CESM1.3 and CM2.1 as CESM  
196 and CM2.

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### 198 2.2 A multiscale ensemble filtering CDA algorithm

199 Based on previous studies (*Anderson, 2003*; *Lu et al., 2023*; *Lu et al., 2020*; *Yu et al., 2019*;  
200 *S. Zhang et al., 2007*), a new multiscale ensemble filtering CDA algorithm is designed and tested  
201 in this study. The new CDA algorithm consists of following three parts.

## 202 a) The constraint of deep ocean model bias

203 Due to imperfect discretization and incomplete understanding for physical processes, a  
 204 coupled Earth system model is always biased with the real world (*Delworth et al.*, 2006; *S. Zhang*  
 205 *et al.*, 2009). In data assimilation, model bias is a significant obstacle to correctly extract physical  
 206 modes as observations are incorporated into the model (*Dee*, 2005; *Dee and Da Silva*, 1998),  
 207 especially in ocean data assimilation (ODA) (*Balmaseda and Anderson*, 2009). Particularly, given  
 208 most of the oceanic observations only available in upper 2000 m, deep ocean model bias could  
 209 lead to large uncertainties in ODA (*H L Johnson et al.*, 2019; *Karspeck et al.*, 2017) since the  
 210 analysis of meridional circulation requires coherent ocean stratification (*Lu et al.*, 2020). Thus, the  
 211 constraint of deep ocean model bias is critically important for the ocean meridional circulation  
 212 study by CDA approaches that combine a coupled Earth system model with the atmospheric and  
 213 oceanic observations. Here, we use the same ocean bias constraint scheme proposed by *Lu et al.*  
 214 (2020), in which the climatological temperature and salinity data (*Locarnini et al.*, 2013; *Zweng et*  
 215 *al.*, 2013) are restored into the model space by a depth-enhanced restoring strength that is identical  
 216 in all MSHea\_EnOI members. In the framework of multiscale data assimilation, the restoration of  
 217 climatological data is an important treatment for the mean state and fixed-period seasonal cycle  
 218 with observational constraint.

## 219 b) Ensemble MSHea\_EnOI

220 Based on the ensemble adjustment Kalman filter (EAKF) framework (*Anderson*, 2003; *S.*  
 221 *Zhang et al.*, 2007) and CM2 model, the previous study has developed an EnOI-like Multiscale  
 222 High-Efficiency Approximate filtering CDA system called MSHea-EnOI-CDA (*Lu et al.*, 2023).  
 223 Due to pre-structured ensemble to represent multiscale background statistics using single model  
 224 integrations, the MSHea-EnOI is a high-efficiency algorithm that is suitable for high-resolution  
 225 model application in case an ensemble model integration is unaffordable. However, in weather and  
 226 climate predictability studies and prediction applications, the probabilistic nature needs to be  
 227 addressed (*Sévellec and Drijfhout*, 2018; *D Yang et al.*, 2023). In this study, we first use the  
 228 ensemble framework of EAKF to organize multi-members of MSHea-EnOI to establish an online  
 229 MSHea-EnOI ensemble system, in which each member performs MSHea-EnOI independently.  
 230 The corresponding DA experiment is named by putting  $M_{EN}$  as prefix (i.e.,  $M_{EN}$ -CDA etc., see  
 231 **Table 1**). Here, M stands for multiscale, EN stands for ensemble. While the detailed description of  
 232 MSHea-EnOI can be found in *Lu et al.* (2023), here each member of MSHea-EnOI conducts a  
 233 two-step local least squares filtering adjustment as expressed in Eqs. (1) and (2) of *Lu et al.* (2023)  
 234 in a relatively independent manner. Each member updates its multiscale background statistics  
 235 based on its own MSHea-EnOI assimilation results.

## 236 c) MSHea\_EnOI-EAKF

237 As discussed in *Yu et al.* (2019), while the model resolution is not too high and an  
 238 affordable ensemble model integrations are available, further filtering with EAKF can improve  
 239 data assimilation quality by improving statistical parameters in high-frequency filtering. In this  
 240 study, when the computation of all members of ensemble MSHea\_EnOI are completed, we readily  
 241 conduct the EAKF filtering by collecting MSHea\_EnOI ensemble results to form the ensemble

242 analysis vector for further EAKF adjustment (*S. Zhang et al.*, 2007). We may call such a new DA  
 243 algorithm that combines MSHea\_EnOI (*Lu et al.*, 2023) and EAKF (*Anderson*, 2003) as  
 244 MSHea\_EnOI-EAKF. The corresponding DA experiment is named by putting  $M_{EF}$  as prefix (i.e.,  
 245  $M_{EF}$ -CDA etc., see **Table 1**). Here, while M again stands for multiscale, EF stands for further  
 246 ensemble filtering. The rationality of this approach lies in using MSHea\_EnOI on each ensemble  
 247 member of EAKF as a proposal density (*Evensen et al.*, 2022). Subsequently, all prior ensemble  
 248 members of EAKF can be closer to the observations than pure prior samples from model  
 249 integrations. Given the multi-scale characteristics of geophysical fluid, such proposed samples  
 250 also maintained physical sense. We will discuss more on this point in Section 2.4.

251 The ensemble update equation of multiscale ensemble CDA algorithms used in this study  
 252 can be divided into two steps. In the first step, we perform the  $M_{EN}$ -algorithm which establishes  
 253 each dynamic ensemble (DE) member by gathering the static ensembles (SE). It can be formulized  
 254 as:

$$\underbrace{\Delta x_{i,DE} = \Delta x_i^{(c)} + \sum_{\tau=1}^{\Gamma} \frac{cov(\Delta x_{i,SE}^{(\tau)}, \Delta y_{i,SE}^{(o,\tau)})}{(\sigma_{i,SE}^{(\tau)})^2} \times \Delta y_{i,SE}^{(o,\tau)}}_{M_{EN}\text{-algorithm}} \quad (1)$$

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256 Then, based on the  $M_{EN}$ -algorithm gained dynamical ensemble, we conduct EAKF  
 257 filtering:

$$\underbrace{\Delta x_i = \frac{cov(\Delta x_{DE}, \Delta y_{DE}^{(o)})}{\sigma_{DE}^2} \times \Delta y_{i,DE}^{(o)}}_{M_{EF}\text{-algorithm}} \quad (2)$$

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259 Here,  $\Delta x$  and  $\Delta y$  represent the adjusted increment of model state variable and observational  
 260 increment computed by the corresponding ensemble information (see the observational increment  
 261 formulae in *Yu et al.* (2019) and *S. Zhang et al.* (2007)), respectively. The subscript  $i$  represents the  
 262 ensemble member index, SE and DE stand for static ensemble pre-prepared but keeping updated  
 263 with individual ensemble members and dynamical ensemble instantaneously evaluated by model  
 264 integrations. The superscript (o) indicates observational information, (c) and ( $\tau$ ) represent the  
 265 increments from climatology and a particular scale  $\tau$ . Considering the fast-varying nature of  
 266 atmosphere, in this study, we only apply  $\Delta x^{(c)}$  to ODA.

## 267 2.3 Experimental design

### 268 a) Biased twin experiment design

#### 269 1) Biases between CM2 and CESM

270 Usually, the influence of model bias on data assimilation is very difficult to detect due to  
271 the scattering nature of observations and uncertainties of model. The CM2 and CESM models are  
272 independently developed at different institutions along with their own biases toward the real world  
273 (*Delworth et al.*, 2006; *Meehl et al.*, 2019). We can use them to design biased twin experiments  
274 and simulate the scenario that a biased coupled Earth system model recovers the evolution of  
275 atmosphere and ocean states by assimilating the atmospheric and oceanic observations into the  
276 model (*Lu et al.*, 2023; *Lu et al.*, 2020; *S. Zhang et al.*, 2009). Therefore, having the knowledge of  
277 CM2 bias relative to CESM is important for this study.

278 In such biased twin experiments, the model bias can be well defined as the difference of  
279 long time mean between the two models. Although the ocean model version is slightly different,  
280 the fundamental features of the bias between CM2 and CESM are the same as *Lu et al.* (2023).  
281 Here we only comment on some aspects relevant to this study. Relative to CESM, the CM2 has  
282 large warm biases in sea surface temperature (SST) over the northeast Pacific, the subtropical  
283 north Atlantic, the east Indian Ocean and along the Antarctic continent, and cold biases over the  
284 subpolar Atlantic, the northwest Pacific, and the Southern Ocean. In sea surface salinity (SSS),  
285 large salty biases are observed over the south Tropical Pacific and Atlantic and the Indian Ocean,  
286 while fresh biases appear in the Arctic, northeast and southeast Pacific along the continent and the  
287 subpolar Atlantic. For the subsurface, above 100 m, the upper ocean shows a cold bias of roughly  
288  $-0.25$  °C and a warm bias of roughly  $0.2$  °C appears between 100–500 m, while the deep ocean  
289 below 500 m has  $-0.1$  °C for cold bias. Above 1000 m, the salinity shows a salty bias of roughly 0.1  
290 psu and a fresh bias of about  $-0.02$  psu is observed below 1000 m. Relative to the CESM  
291 atmosphere, the CM2 atmosphere shows a large warm bias above 300 hPa and a small cold bias  
292 below 300 hPa. Obviously, such biases between the two coupled models are associated with their  
293 different dynamical core and physical parameterizations, etc. (*Delworth et al.*, 2006; *Meehl et al.*,  
294 2019). Due to the nature of high-frequency variability of the atmosphere, for the issue of GMOC  
295 estimation, we pay particular attention to ocean model biases and their influences on results of  
296 various CDA schemes.

#### 297 2) Biased twin experiments

298 To study how CDA estimates the ocean meridional circulation, we first use CM2 and  
299 CESM to design biased twin experiments. The atmosphere component of CESM model has a  
300 slightly higher resolution than CM2. Thus, we use its BHISTC5 simulation which is forced by  
301 historical greenhouse gas and natural aerosol (GHGNA) to define the “true” solution that produces  
302 synthetic “observations” based on 2007 Argo network. Please see Lu et al. 2020 for more detail.  
303 Then the CM2 free historical integration defines a biased simulation of the “truth” (TRUTH) as a  
304 control experiment (CTL).



305 Starting from the biased simulation of the “truth” GMOC, we conduct various CM2  $M_{EN}$   
 306 and  $M_{EF}$  DA experiments with different schemes to assess how CDA recovers the “truth” GMOC.  
 307 The synthetic “observations” of all DA experiments include “Argo” temperature and salinity  
 308 profiles, gridded SSTs for ODA and surface pressure (Ps) for atmosphere data assimilation  
 309 (ADA). The assimilation frequencies of ADA and ODA are 6 hours and 1 day respectively. All  
 310 simulation and DA experiments are listed in **Table 1**. For example, again, the CTL and TRUTH  
 311 are free model historical simulations from CM2 and CESM. While the  $M_{EN}$ -ADA (-ODA) has 12  
 312 ensemble members each of which assimilates the Ps (“Argo” profiles and SSTs) data produced by  
 313 the CESM through MSHea\_EnOI, the  $M_{EF}$ -ADA (-ODA) uses this 12-member ensemble to  
 314 further conduct the EAKF for these atmospheric (oceanic) “observations.” Correspondingly, the  
 315  $M_{EN}$ -CDA has 12 ensemble members each of which assimilates these atmospheric and oceanic  
 316 “observations” through MSHea\_EnOI along with its integration, and the  $M_{EF}$ -CDA uses this  
 317 12-member ensemble to further conduct the EAKF for these atmospheric and oceanic  
 318 “observations.” Note that in these twin experiments, the ocean data constraint includes the  
 319 restoring of climatological data derived from the CESM TRUTH integration.

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**TABLE 1. List of experiments.**

<b>Expt</b>	<b>Model</b>	<b>Period</b>	<b>Ensemble size</b>	<b>Data constraint</b>	<b>Description</b>
TRUTH	CESM1.3	1850-2000	1	Free historical run, no obs data	Prepare “true” states
CTL	CM2.1	1978-1983	1	Free historical run, no obs data	Reference for estimation
$M_{EN}$ -ADA	CM2.1	1978-1982	12	CESM1.3-produced gridded Ps	Each member conducting MSHea_EnOI ADA
$M_{EN}$ -ODA	CM2.1	1978-1982	12	CESM1.3-produced “Argo” T/S profiles and gridded SSTs, and ocean climatology	Each member conducting MSHea_EnOI ODA
$M_{EN}$ -CDA	CM2.1	1978-1982	12	The data used in $M_{EN}$ -ADA and $M_{EN}$ -ODA	Each member conducting MSHea_EnOI ADA and ODA
$M_{EF}$ -ADA	CM2.1	1978-1982	12	Same as in $M_{EN}$ -ADA	12-member $M_{EN}$ -ADA ensemble

					conducting EAKF 12-member $M_{EN}$ -ODA
$M_{EF}$ -ODA	CM2.1	1978-1982	12	Same as in $M_{EN}$ -ODA	ensemble conducting EAKF 12-member $M_{EN}$ -CDA
$M_{EF}$ -CDA	CM2.1	1978-1982	12	Same as in $M_{EN}$ -CDA	ensemble conducting EAKF
$M_{EF}$ -CDA-Robs	CM2.1	1978-2022	12	ERA5 gridded Ps and real XBT/CTD/OSD/MRB and Argo T/S profiles as well as OISST, and WOA climatology	12-member $M_{EN}$ ADA-Robs & ODA-Robs ensemble conducting EAKF

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## 325 **b) Assimilation Experiment using real observations**

326 Finally, a CDA experiment using “real” observations called  $M_{EF}$ -CDA-Robs is conducted.  
 327 For the purpose of studying reconstruction of GMOC, the  $M_{EF}$ -CDA-Robs applies the ERA5  
 328 (*Hersbach et al., 2020*) surface pressure as “observations” of the atmosphere to ADA and all ocean  
 329 real observations to ODA as shown in **Table 1**.

### 330 2.4 The assimilation quality of $M_{EF}$ -CDA vs. $M_{EN}$ -CDA

331 In the biased twin experiments, all the synthetic observations are sampled from the TRUTH  
 332 based on the network of reanalysis and the modern Earth climate observing system. Atmosphere  
 333 “observations” take the CESM Ps as gridded reanalysis format at model grids with a 2 hPa  
 334 observational error and 6-hour time interval. Ocean “observations” are produced by sampling the  
 335 CESM ocean temperature and salinity onto the 2010 Argo network repeatedly, and taking the  
 336 gridded SSTs. The ocean observational error is 0.5 °C for temperature and 0.1 PSU for salinity at  
 337 the surface and gradually decays by an e-folding depth of 2000 m. We use the 12-member  
 338 ensemble mean to compute the assimilation error for estimated states and 12 individual members  
 339 to evaluate the deviation of the assimilation errors. We summarize each the RMSE of ensemble

340 mean and the RMSE's standard deviation of 12 ensemble members of each experiment, with  
 341 statistics in last 3 years. Please see Table S1.

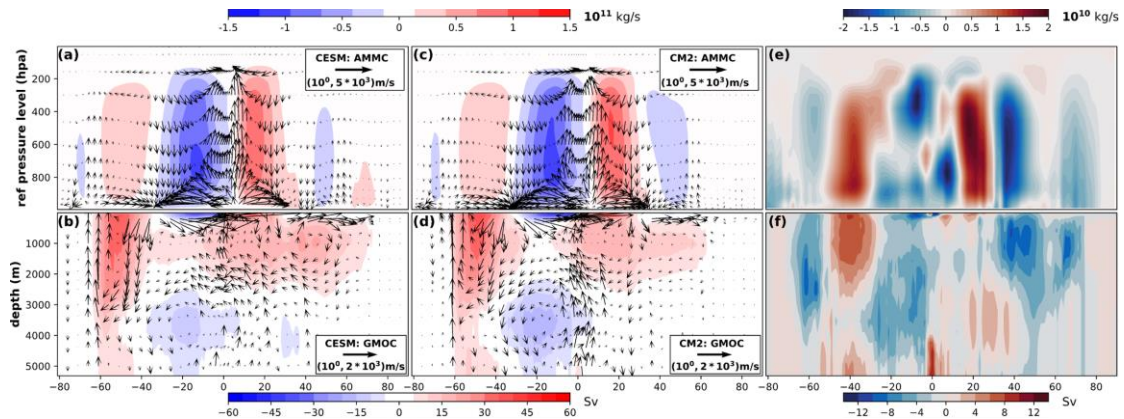
342 A thorough evaluation of errors statistics of atmosphere and ocean in various DA schemes  
 343 can be found in Supplementary materials. Here we only comment on the basic part of the  
 344 assimilation quality. Generally, both  $M_{EN-}$  and  $M_{EF-}$  have been successful in reducing RMSEs in  
 345 comparison to CTL run. Regarding the atmosphere, the difference of Ps errors between  $M_{EN-}$  and  
 346  $M_{EF-}$  is small, and error reductions over lands are relatively small compared to ones over oceans.  
 347 Among the seven twin-experiment conducted, the  $M_{EF-}$ -CDA provides the most accurate  
 348 estimation (RMSEs: 892 pascal, all others in 893-950 pascal, especially 1032 pascal in CTL)  
 349 (**Figure. S1**). However, in the ocean,  $M_{EF-}$  exhibits a more significant reduction in RMSEs.  
 350 Specifically, in upper ocean (above 2000m) where observations are more abundant, both  
 351  $M_{EF-}$ -ODA and  $M_{EF-}$ -CDA show substantial error reductions of 30% to 60% in temperature and  
 352 salinity compared to  $M_{EN-}$ -ODA and  $M_{EN-}$ -CDA (RMSEs: 0.4 °C and 0.5 psu, **Figure. S3** and  
 353 **Figure. S4 e, g**). In the abyss where the same climatology resorting scheme is employed, the  
 354 temperature and salinity errors between  $M_{EN-}$  and  $M_{EF-}$  is nearly identical (**Figure. S4 f, h**). Our  
 355 results indicating that the atmospheric mean meridional circulation (AMMC)-GMOC system in  
 356 our experiment reach a quasi-equilibrium state by the end of 1979 (**Figure. S2**). Therefore, the  
 357 analysis in this study mainly focuses on the statistics from the last three years.

### 358 **3 The problem definition and CDA solution of GMOC estimation in a “twin” experiment** 359 **framework of coupled Earth system models**

#### 360 **3.1 The definition of problem**

361 Excluding various dissipation mechanisms, the coupled atmosphere and ocean on the Earth  
 362 can be viewed as a semi enclosed system (*Stommel, 1961*) in which the atmosphere “stirring” the  
 363 ocean (*Munk, 1950*) while the ocean responds back to the atmosphere with new boundary  
 364 conditions that have redistributed thermal properties (*Manabe, 1969*). If reducing the coupled  
 365 atmosphere-ocean system to a two-dimensional vertical and meridional space, we can still view  
 366 the atmosphere and ocean as a pair of zonally-averaged self-constrained counterparts as the  
 367 AMMC and GMOC (*Wright and Stocker, 1991; Wright et al., 1998*). In this case, due to the  
 368 different dynamical-core and physical parameterizations in the CESM and CM2 models, they  
 369 simulate a pair of balance and coherent AMMC and GMOC with different features in their own  
 370 model spaces (**Figure. 1**). We see that, in both the Northern Hemisphere (NH) and Southern  
 371 Hemisphere (SH), CM2 has stronger Hadley and Ferrel cells but weaker polar cell in NH than  
 372 CESM (panels **a, c & e**). In terms of GMOC, the CM2 has a stronger Antarctic Circumpolar  
 373 Current (ACC) system than the CESM (panels **b, d & f**). While the CM2's Northern sinking at  
 374 40°N - 60°N is much weaker than the CESM's, leading to CM2's weaker NADW (North Atlantic  
 375 Deep Water). For the NADW region (40°N - 60°N), while the CESM shows a transport core  
 376 centered at (1000 m, 45°N) which is separate from the low latitude circulation cell, the CM2 only  
 377 has a weak extension from the low latitude cell. In tropical oceans, the CM2's streamfunction has  
 378 stronger meridional gradient at the equator area than the CESM's, thus CM2 appearing stronger  
 379 vertical motion around the equator. Unlike the CESM's AABW (Antarctic Bottom Water) which  
 380 extends much north beyond the equator, the CM2's anti-circulation in deep oceans is very weak in  
 381 NH.

382 In our twin experiment framework described in Section 2.3, we can use **Figure. 1** to well  
 383 define the GMOC estimation problem: Given the distinguishable differences of AMMC-GMOC  
 384 structures in the two models (panels **e & f**), how the CM2-CDA system reconstructs the  
 385 CESM-produced AMMC-GMOC (panels **a & b**) starting from the CM2-produced counterpart  
 386 (panels **c & d**) by assimilating CESM-produced atmospheric and oceanic “observations” in a  
 387 balance and coherent manner?  
 388



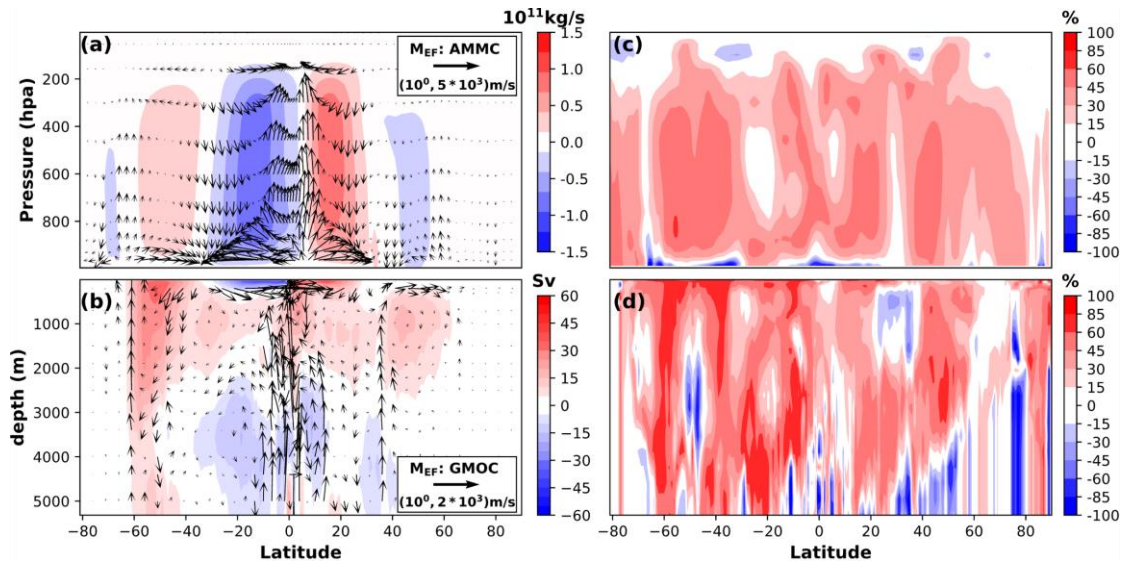
389 **Figure. 1** AMMCs (upper) and GMOCs (lower) in the CESM and CM2 models. *a-d*)  
 390 The patterns of the mean atmosphere (panels *a & c*) and ocean (panels *b & d*) meridional  
 391 overturning circulation derived from zonal mean *v*-velocities in the *y-z* space as AMMCs  
 392 and GMOCs, averaged over 1980-1999 in the historical simulations of CESM and CM2  
 393 starting from 1850. *e-f*) The difference between CM2 and CESM (defined as CM2 minus  
 394 CESM) AMMCs (panel *e*) and GMOCs (panel *f*) shown in panels *a-d*.  
 395

### 396 3.2 The solution of CDA

397 The estimation of AMMC-GMOC structure by  $M_{EF}$ -CDA and the RMSE reduction rate of  
 398 estimation relative to free model simulation (i.e., CTL) are shown in **Figure. 2**. We can see,  
 399 through coupled atmospheric and oceanic data constraints, the stronger Hadley and Ferrel cells in  
 400 CM2 has been alleviated and weaker NH polar cell has been strengthened (panels **a**). The stronger  
 401 GMOC’s ACC system and weaker NADW of CM2 are significantly improved (panels **b**). The  
 402 error reduction rate of the AMMC is greater than 15% in most of the regions (panels **c**). A transport  
 403 core in the NADW region centered at (1000 m, 45°N) has been recovered, still weak though. In  
 404 tropical oceans, stronger meridional gradient at the equator area has been mitigated. An  
 405 anti-circulation centered at (4500 m, 40°N) has been formed in deep oceans, which leads to, like  
 406 the CESM, the CM2 having its AABW extended to north beyond the equator. The error reduction  
 407 rate of the GMOC supports the above conclusions, surpassing 45% in ACC regions, 30% in  
 408 NADW regions and 85% in AABW regions (panels **d**). However, the CDA GMOC at NH’s  
 409 high-latitudes and deep oceans and AMMC below 900 hPa or above 200 hPa appear error  
 410 increases. Additionally. Substantial improvements are yet to be seen in addressing the strong  
 411 vertical motions in tropics between 1-4 km.

412 While the  $M_{EF}$ -CDA offers a relatively accurate estimation of AMMC-GMOC system, it  
 413 prompts new inquiries. The rationale underpinning the estimation needs to be clarified,  
 414 particularly concerning the attainment of physical consistency by coupled data assimilation.

415 Additionally, an assessment of the uncertainties of the estimation is important. A comprehensive  
 416 analysis of the estimation is therefore necessary.  
 417



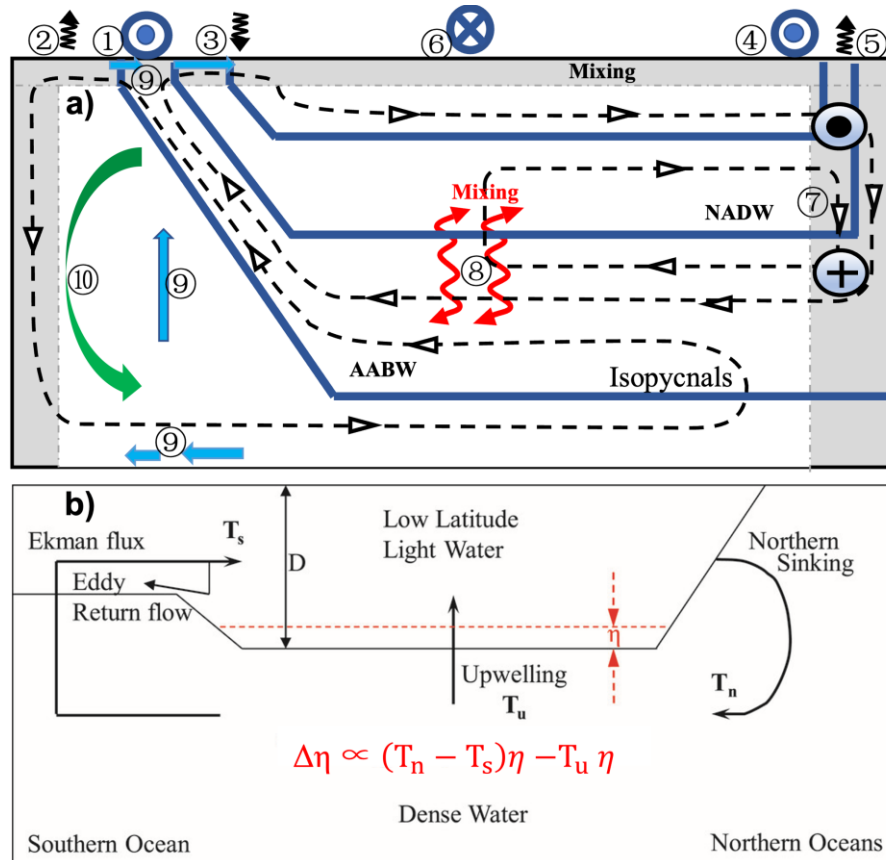
418  
 419 **Figure. 2** The recovered AMMC and GMOC through incorporating the  
 420 CESM-produced “observations” into the CM2 model by  $M_{EF}$ -CDA. a-b) Same as Figure.  
 421 1a, b but produced by  $M_{EF}$ -CDA. c-d) The reduction rate of RMSEs of AMMC (panel g)  
 422 and GMOC (panel h) made by  $M_{EF}$ -CDA from the CTL ( $RMSE_{CTL}$   
 423  $-RMSE_{MEF}/RMSE_{CTL} \times 100\%$  (unit: %)).

424 Next, starting to detect the roles of atmospheric and oceanic data constraints in GMOC  
 425 estimation, we will try to understand the physical processes in CDA reconstruction for GMOC.

#### 426 **4 The detection of the roles of atmospheric and oceanic data constraints in GMOC** 427 **estimation**

##### 428 4.1 The dynamical background of data constraints for GMOC estimation

429 In the regime of weak CDA, the transfer of observation information across different  
 430 components primarily through fluxes. In the context of air-sea interaction, the instantaneous  
 431 exchange of momentum and heat fluxes are vital to maintain global mean meridional circulation.  
 432 Then given the energy, the schematic representation of the atmosphere-ocean coupling and  
 433 oceanic internal responses can be depicted in **Figure. 3a**. Due to the difference of dynamical-core  
 434 and physical parameterizations based their own discretization systems and physical  
 435 parameterization packages, numerical models simulate a pair of balance and coherent AMMC and  
 436 GMOC in their own model spaces. As atmospheric and oceanic data are incorporated into a  
 437 coupled model by a CDA approach for reconstructing the AMMC-GMOC structure in the real  
 438 world, the adjustment mechanism for the GMOC can be summarized and understood as the  
 439 adjustment of pycnocline anomaly ( $\Delta\eta$ ) as illustrated in **Figure. 3b**. The AMMC forces the  
 440 GMOC as the consequence of the balance of three terms (*Gnanadesikan, 1999*), i.e., the difference  
 441 between the Northern Hemisphere sinking and Southern Ocean upwelling is balanced by the low  
 442 latitude dissipation by diffusive mixing.  
 443



444  
 445 **Figure. 3** The schematic illustration of processes influencing GMOC. a) Replotted  
 446 from *Nikurashin and Vallis (2012)*, the configuration of processes at the air-sea interface  
 447 include: ① Westerly jet at the ACC region, ② Ekman effects induced buoyancy gain by  
 448 ①, ③ Ekman effects induced buoyancy loss by ①, ④ Northern subpolar jet, ⑤ ④  
 449 -induced buoyancy loss, ⑥ Air-sea interactions associated with Easterlies at tropics, and  
 450 the configuration of ocean interior processes include: ⑦ ⑤-induced NH sinking to form  
 451 North Atlantic Deep Water (NADW), ⑧ Diffusive mixing at tropical oceans, ⑨ SH  
 452 wind-driven Ekman transport, ⑩ Eddy-induced circulation. ⑨ and ⑩ are important  
 453 processes associated with Antarctic Bottom Water (AABW). b) Replotted from *S. Zhang*  
 454 (2011), the summarized adjustment mechanism of pycnocline ( $\Delta\eta$ ) from panel a as  
 455 atmospheric and oceanic data are incorporated into a coupled model by a CDA approach,  
 456 based on the three-term balance model of *Gnanadesikan (1999)*: i.e. the residual between  
 457 the difference of Northern sinking and Southern upwelling and the tropical upwelling  
 458 driving the change of pycnocline depth anomaly.

459 The ocean primarily receives mechanical forcing from the atmosphere and reciprocally  
 460 provides thermal forcing to the atmosphere, compensating for the dissipation and loss of  
 461 mechanical energy caused by friction (*R X Huang et al., 2006*). From that principle, we examine  
 462 work done by atmospheric stress forces applied to the ocean (panels a & d of **Figure. 4**) and heat  
 463 fluxes of ocean to the atmosphere (panels b & e) to represent the main atmosphere-ocean  
 464 exchange processes (hereafter briefly referred to as  $W_{A2O}$  and  $HF_{O2A}$ ).

465 The  $W_{A2O}$  is defined as (*R X Huang et al., 2006*):



$$W_{A2O} = \tau_x u^o + \tau_y v^o, \#(3)$$

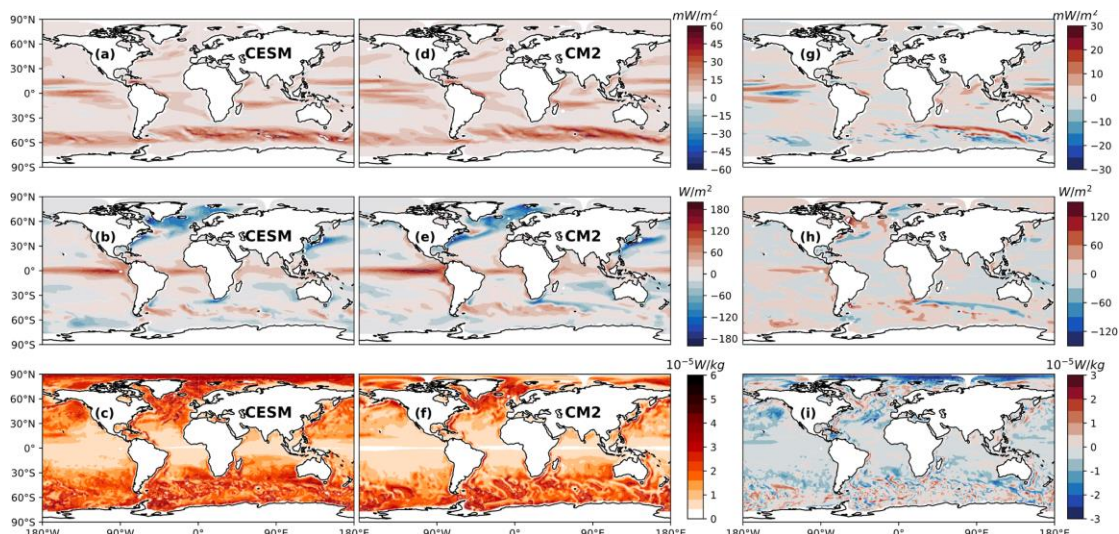
466 where  $\tau_x$  ( $u^o$ ) and  $\tau_y$  ( $v^o$ ) represent respectively the zonal and meridional components of  
 467 wind stress (ocean current). The formulae to compute  $HF_{O2A}$  can be expressed as (Cronin et al.,  
 468 2019):

$$HF_{O2A} = Q_{sen} + Q_{lat} + Q_{lw} + Q_{sw}, \#(4)$$

469 where  $Q_{sen}$  is sensible heat flux,  $Q_{lat}$  is latent heat flux,  $Q_{lw}$  is longwave heat flux  
 470 and  $Q_{sw}$  is shortwave heat flux.

471 Then, the AMMC-GMOC structures of CESM and CM2 models shown in **Figure. 2a-d**  
 472 have their own atmosphere-ocean exchange processes at the air-sea interface. Two models share  
 473 some common features in the distributions of  $W_{A2O}$  (panels **a** & **d**) and  $HF_{O2A}$  (panels **b** & **e**). On  
 474 the one hand, the maximum  $W_{A2O}$  values distribute over the Southern Ocean ACC (Antarctic  
 475 Circumpolar Current) belt areas and next large values mainly appear in the tropics. The former  
 476 represents the major Ekman pumping effects of the atmosphere to ocean while the latter reflects  
 477 the active air-sea interactions associated with warm tropical oceans. On the other hand, the  
 478 maximum positive and negative values of  $HF_{O2A}$  are respectively located in tropics and high  
 479 latitudes of the Northern Hemisphere, corresponding to the major heating of ocean to atmosphere  
 480 at tropics (Bernie et al., 2007; Sverdrup et al., 1942) and cooling at jet areas of high latitudes  
 481 associated with North Atlantic Oscillation (NAO) (Delworth and Zeng, 2016).

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**Figure. 4** Work done by atmospheric stress forces applied to the ocean ( $W_{A2O}$ )  
 (upper), heat fluxes of ocean to the atmosphere ( $HF_{O2A}$ ) (middle) and vertical mean energy  
 dissipation rate ( $\epsilon_m$ ) (lower) in the CESM and CM models. **a-f**) Same as Figure. 1a-d but  
 for the horizontal distributions of  $W_{A2O}$  (panels **a** & **d**) and  $HF_{O2A}$  (panels **b** & **e**) at the  
 air-sea interface, as well as vertical mean energy dissipation rate ( $\epsilon_m$ ) (panels **c** & **f**). **g-i**)  
 Same as Figure. 1e-f but for  $W_{A2O}$  (panel **g**) and  $HF_{O2A}$  (panel **h**) and  $\epsilon_m$  (panel **i**).

Apparently, the two models have significant differences on their  $W_{A2O}$  and  $HF_{O2A}$   
 distributions (panels **g** & **h**). We also see that the distributions of differences of  $W_{A2O}$  and  $HF_{O2A}$   
 between these two models have similar patterns with opposite sign (compare panel **g** to panel **h**),  
 especially at high latitudes. This indicates that due to the different numerical schemes used in

494 their atmosphere and ocean components, these two models have individually-different coupled  
 495 atmosphere-ocean self-balanced regimes. In the Southern Ocean, while the CM2 has smaller  
 496 atmosphere-to-ocean work than the CESM does (panel **g**), its ocean-to-atmosphere heat fluxes  
 497 appear larger (panel **h**), and vice versa. The same phenomenon can be seen in the Northern  
 498 Hemisphere high latitudes, particularly clear in the North Atlantic areas from the Labrador Sea to  
 499 the Greenland coastal seas. In the tropics, except for the east equatorial Pacific area where  
 500 CM2's smaller atmosphere-to-ocean work corresponds to larger ocean-to-atmosphere heat fluxes  
 501 compared to the CESM counterparts, no clear linkage exists in the relative biases of  $W_{A2O}$  and  
 502  $HF_{O2A}$  between the two models. In the high latitudes, quasi-stationary mechanisms exist for  
 503 maintenance of the Northern sinking (*Wright and Stocker, 1991*) and Southern upwelling such as  
 504 wind-driven Ekman transport (*Price et al., 1987*) at the upper oceans and eddy transports at the  
 505 flanks of submarine ridges (*Macdonald and Wunsch, 1996*). To sustain the balance of three terms  
 506 in GMOC (*Gnanadesikan, 1999*), each model has its own mixing processes at tropics.

507 Apart from flux exchanges at the air-sea interface, it's essential to check the mixing rate  
 508 as they play a vital role in maintaining the global circulation (*Munk and Wunsch, 1998*). As the  
 509 turbulence is not resolved in our experiment, we only compute the diagnosed turbulence kinetic  
 510 energy dissipation rate. On the basis of diapycnal advection-diffusion balance:

$$\frac{D\rho}{Dt} = \frac{\partial}{\partial z} \left( \kappa_{\rho} \frac{\partial \rho}{\partial z} \right) = \frac{\partial}{\partial z} \left( \Gamma \varepsilon N^{-2} \frac{\partial \rho}{\partial z} \right), \#(5)$$

511 where  $N^2 = -g\rho_0^{-1} \frac{\partial \rho}{\partial z}$ ,  $w$  is vertical velocity,  $\rho$  is potential density,  $\rho_0$  is the  
 512 reference density,  $\varepsilon$  is diagnosed kinetic energy dissipation rate in this study. The buoyancy flux  
 513 has been related to the turbulence kinetic energy dissipation rate  $\varepsilon$  through the constant  
 514 efficiency factor  $\Gamma$  (*Osborn, 1980*). The  $\varepsilon$  on each layer therefore can be expressed as:

$$\varepsilon(z, x, y) = \int_z^0 -\frac{g}{\Gamma \rho_0} \frac{D\rho}{Dt} dz + C(x, y) \#(6)$$

515 In this study, we set  $\Gamma = 0.2$ ,  $\rho_0 = 1026 \text{ kg/m}^3$ . The constant  $C$  is determined by  
 516 letting the minimum of the integration equals to 0. The vertical mean of  $\varepsilon$  is defined as mean  
 517 energy dissipation rate  $\varepsilon_m$ .  $\varepsilon_m$  in CESM and CM2 and their difference are shown in **Figure**  
 518 **4c, f, i**. Although distinguishable differences exist in  $\varepsilon_m$  between CESM and CM2 (panel **i**),  
 519 both models show large kinetic energy dissipation rate in the Southern Hemisphere ACC region,  
 520 North Atlantic as well as Western boundary current (panels **c** & **f**). The significant dissipation in  
 521 the Southern Ocean coincides with the location of maximum  $W_{A2O}$ , the substantial input of wind  
 522 energy corresponding to considerable kinetic energy dissipation. The dissipation in the North  
 523 Atlantic corresponds the large negative  $HF_{O2A}$  region, reflecting the cooling effect of the  
 524 atmospheric jets associated with NAO, where water loses buoyancy (*Delworth and Zeng, 2016*).

525 Next, following the mainstream of how various DA schemes improve  
 526 atmosphere-to-ocean work, ocean-to-atmosphere heat fluxes, and kinetic energy dissipation, we  
 527 elaborate the contributions of ADA and ODA for recovering the target AMMC-GMOC structure  
 528 to understand how a sound CDA approach reconstructs the GMOC decently.

#### 529 4.2 $W_{A2O}$ in various data constraints

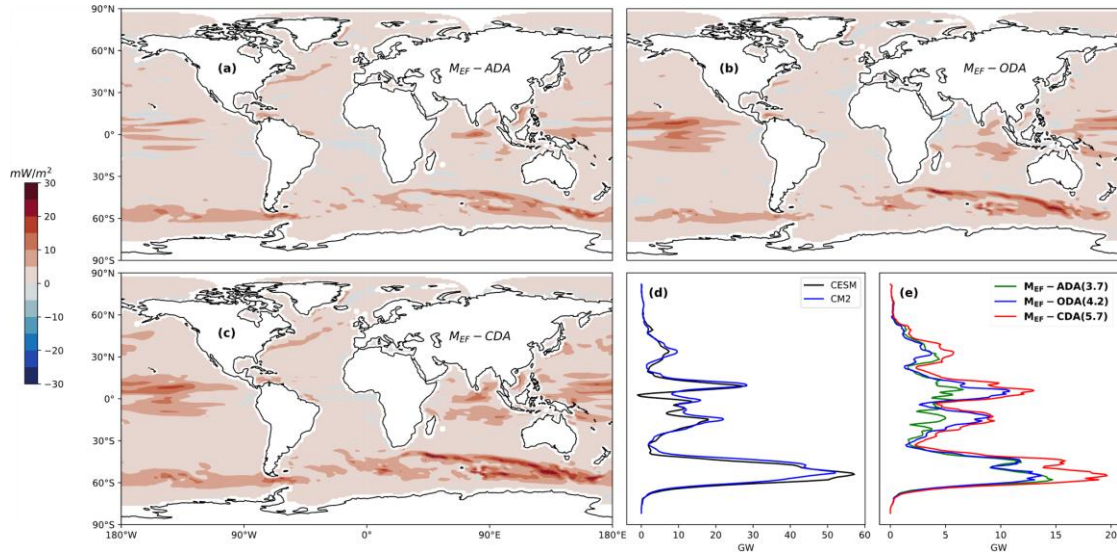
530 We present the improvement of  $W_{A2O}$  made by  $M_{EF}$ -ADA (panel **a**) and  $M_{EF}$ -ODA (panel  
 531 **b**) as well as  $M_{EF}$ -CDA (panel **c**) compared to the free model simulation of CM2 in **Figure 5**.



532 Consistent with the distribution of model simulation itself, the ADA's improvement of  $W_{A20}$   
 533 also focuses on ACC and tropical regions (panel a). In ODA, the improvement of  $W_{A20}$  reflects  
 534 the improvements of ocean surface current and responses of the atmosphere to improved SSTs.  
 535 Such improvements depend on different geographical sensitivities to SSTs. For example, in the  
 536 Southeast Atlantic, the ODA's improvement is larger than the ADA's, but in the Northwest  
 537 Indian, while the ADA improves  $W_{A20}$ , the ODA degrades it. Combining both advantages of  
 538 ADA and ODA, the CDA enhances the improvement of  $W_{A20}$  compared to individual  
 539 component DA cases (panel c).

540 We show the difference of zonal integral of  $W_{A20}$  simulated by CESM and CM2 as well  
 541 as the RMSE's reduction from the CTL made by various DA schemes in **Figure. 5d-e**. If  
 542 comparing panel e to d, we see that in a zonal mean sense, the large improvement of  $W_{A20}$  by  
 543 CDA from ADA and ODA (panel e) is at the latitudes where  $W_{A20}$  itself is large (panel d). One  
 544 can see that CDA provide the most accurate estimation of  $W_{A20}$ . In terms of the improvement  
 545 from  $M_{EN}$  to  $M_{EF}$  assimilation scheme, the  $M_{EF}$  has a nearly identical behavior to the  $M_{EN}$ . (See  
 546 **Figure. S5**).

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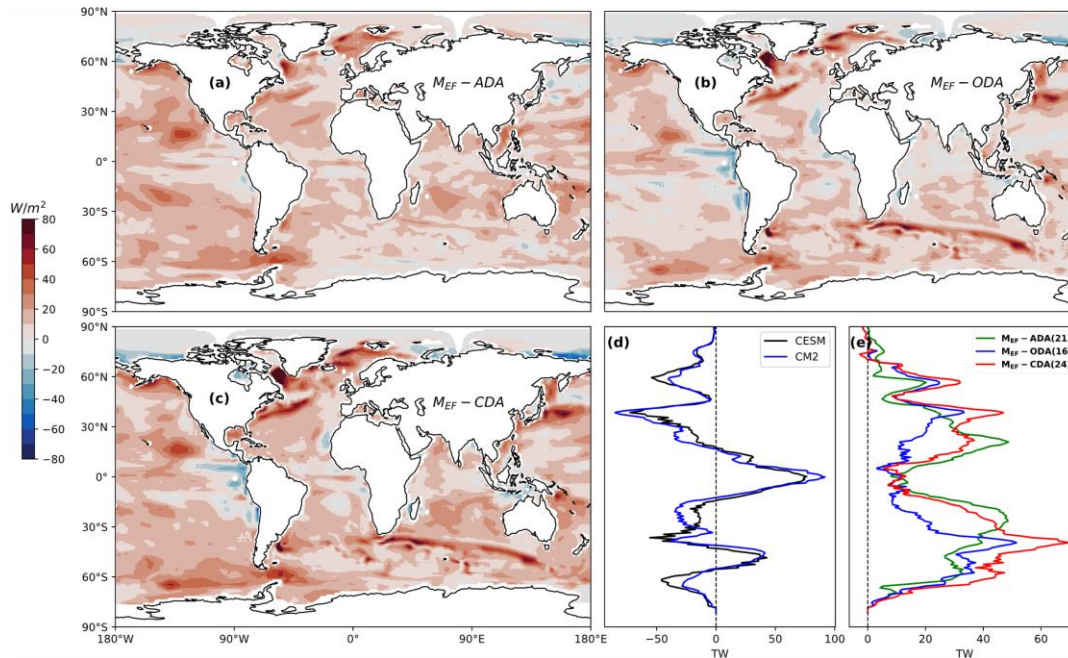
**Figure. 5** The improvement of work done by atmospheric stress forces applied to the  
 550 ocean made by ADA, ODA and CDA. a-c) The RMSE reduction of  $W_{A20}$  relative to CTL  
 551 made by  $M_{EF}$ -ADA (panel a),  $M_{EF}$ -ODA (panel b) and  $M_{EF}$ -CDA (panel c) with statistics in  
 552 last 3 years. d) The latitudinal variations of the zonal integral of  $W_{A20}$  in TRUTH and  
 553 CTL. e) The latitudinal variations of zonal integral of  $W_{A20}$  error reductions from CTL  
 554 (i.e.,  $RMSE_{CTL} - RMSE_{DA}$ ) made by  $M_{EF}$ -ADA (solid-green),  $M_{EF}$ -ODA (solid-blue) and  
 555  $M_{EF}$ -CDA (solid-red). The numbers in the parenthesis represent the latitudinal mean of  
 556 error reduction of the corresponding DA experiment from the CTL (unit: GW).

### 557 4.3 $HF_{O2A}$ in various data constraints

558 The story of the DA-made error reduction for  $HF_{O2A}$  (**Figure. 6**) is a little different from  
 559 that for  $W_{A20}$  shown in **Figure. 5**. As shown before, due the forcing effect of atmosphere to  
 560 ocean, the distribution of error reductions of  $W_{A20}$  in all DA schemes is overall consistent with  
 561 the distribution of  $W_{A20}$  itself, i.e., with major distributive belts over the Southern Ocean ACC  
 562 and Tropical Ocean regions. The distributions of error reductions of  $HF_{O2A}$  in all DA schemes

563 have a relatively uniform distribution in a global scope, even in the  $M_{EF}$ -ADA case (panel **a**) that  
 564 represents the consequence of the response of the CM2 ocean to the ADA's constraint from  
 565 CESM Ps data. Since the CM2 ocean is biased with the CESM ocean, such a response can have a  
 566 global behavior. While the error reduction of  $HF_{O2A}$  made by  $M_{EF}$ -ODA (panel **b**) mainly reflects  
 567 the decrease of ocean model bias shown in **Figure. 1e**, the biased nature of ocean model makes  
 568 difficulties in some regions for correction with direct data constraint. Such regions include the  
 569 east equatorial Pacific and Atlantic Oceans as well as the north Indian Ocean, and most of the  
 570 Arctic Ocean. With the aid of ADA effects, the large errors of the east equatorial Pacific,  
 571 Atlantic and north Indian Oceans appeared in ODA are greatly mitigated by CDA (panel **c**). In  
 572 the tropics where the model simulated  $HF_{O2A}$  have maximum values (panel **d**), the error  
 573 reductions of  $HF_{O2A}$  take the minimum values in all DA schemes. This phenomenon may be  
 574 associated with the difference of two models on dealing with very active and complex air-sea  
 575 interacting processes over tropical regions (*Delworth and Zeng, 2016; Meehl et al., 2019*). In  
 576 addition, we notice that the ODA errors in the Arctic Ocean is somewhat enlarged in CDA as the  
 577 result of combining ADA and ODA together (panel **e**). This could be associated with the sea-ice  
 578 behavior over the Arctic Ocean but it requires further research work to clarify.

579 From **Figure. 5e**, we also see that CDA produces the most accurate estimation of  $HF_{O2A}$   
 580 in ACC region and Northern Hemisphere, where the water losses buoyancy and sinks. The  
 581 minimum improvement in tropics may be attributed to the strong vertical motions shown in  
 582 **Figure 2**. The difference between these  $M_{EN}$  and  $M_{EF}$  algorithms is very subtle (See **Figure. S6**).  
 583



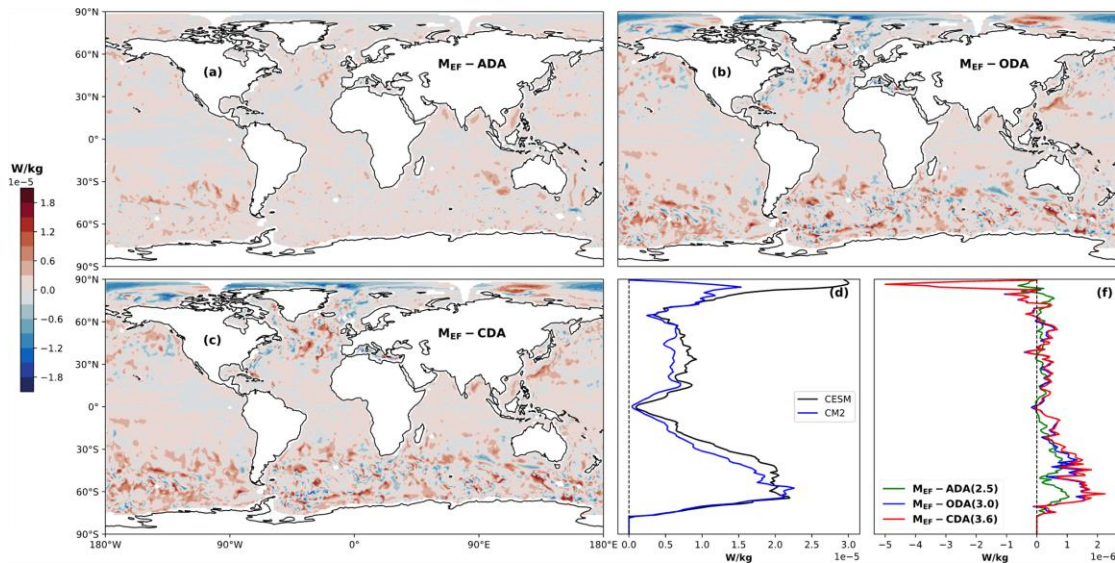
584 **Figure. 6** The improvement of  $HFO_{2A}$  made by ADA, ODA and CDA. a-e) Same as  
 585 **Figs. 5a-e** but for  $HFO_{2A}$ . The vertical dotted-black lines in panels d & e mark the zero  
 586 **flux** (panel d) or **error reduction** (panel e).  
 587

#### 588 4.4 $\epsilon_m$ in various data constraints

589 To understand the energy balance mechanisms of global ocean circulation (*Wunsch and*  
 590 *Ferrari, 2004*) in CDA, we show the global distribution of the error reductions of vertical mean

591 diagnosed turbulence kinetic energy dissipation rate ( $\epsilon_m$ ) made by various DA schemes in  
 592 **Figure. 7**. As we expected, as the result of ocean free responses to atmospheric forcing, the  
 593 ADA-induced  $\epsilon_m$  appears being improved in a large scope of global domain but in a moderate  
 594 magnitude without drastically-improved regions (see panel **a** and green lines in panel **e**). The  
 595 direct oceanic data constraints in ODA significantly improve estimation of the  $\epsilon_m$  over  
 596 Southern Ocean where air-sea interactions are very active (panel **b**). Such improvement can be  
 597 attributed to the improved estimation of stratification. However, in areas characterized by limited  
 598 observation data such as the Arctic, and regions with intricate current structure like the West  
 599 Boundary Currents in the West Pacific and Atlantic, ODA has difficulties to improve  $\epsilon_m$   
 600 estimation. Combining ADA and ODA together, CDA provides a better estimation of  $\epsilon_m$  (panel  
 601 **c**). Comparing **Figure. 7 d & e** with **Figure. 6 d & e** and **Figure. 5 d & e**, we can see that in  
 602 data assimilation, improving  $\epsilon_m$  estimation is more difficult than improving  $W_{A2O}$  and  $HF_{O2A}$   
 603 since kinetic energy dissipation tightly connects with topography, convection and eddy activities  
 604 etc. which easily produce modeling errors. Comparing  $M_{EN}$  to  $M_{EF}$  assimilation schemes,  
 605  $M_{EF}$ -ODA has more  $\epsilon_m$  error reduction while  $M_{EF}$ -ADA and  $M_{EF}$ -CDA have nearly-identical  
 606 behavior as the  $M_{EF}$  counterparts (See Figure. S7).

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610 **Figure. 7** The improvement of mean mixing rate ( $\epsilon_m$ ) in the global ocean made by  
 611 ADA, ODA and CDA. **a-e)** Same as **Figure. 5a-e** but for  $\epsilon_m$  described in the beginning of  
 612 **Section 4**. The vertical dotted-black lines in panels **d&e** mark the zero flux (panel **d**) or  
 613 error reduction (panel **e**). The numbers in the parenthesis are in unit:  $10^{-7}$  W/kg.

## 613 5 The importance of coupled data constraints in GMOC estimation

### 614 5.1 Coupled data constraints in key processes of GMOC estimation

615 In this section, we focus on the results of  $M_{EF}$ -CDA to analyze the GMOC estimation.  
 616 From **Figure. 3b**, we can see that the GMOC consist of three latitudinal regions: 1)  
 617 high-latitudes of the Southern Hemisphere on the south of  $35^\circ S$ , 2) high-latitudes of the Northern  
 618 Hemisphere between  $40^\circ N$  and  $60^\circ N$ , 3) tropical oceans in  $20^\circ S - 20^\circ N$ . The region 1)  
 619 corresponds to the ACC system linked with the processes of SH wind-driven Ekman transport  
 620 and Eddy-induced circulation denoted by ⑨ and ⑩ in **Figure. 3a**, associated with AABW.



621 The region 2) is tightly associated with the formation mechanism of NADW linked with  
 622 atmospheric jet-induced NH sinking, denoted by ⑦ in **Figure. 3a**. The region 3) corresponds to  
 623 the area of diffusive mixing at tropical oceans which have active high-frequency air-sea  
 624 interactions, denoted by ⑧ in **Figure. 3a**.

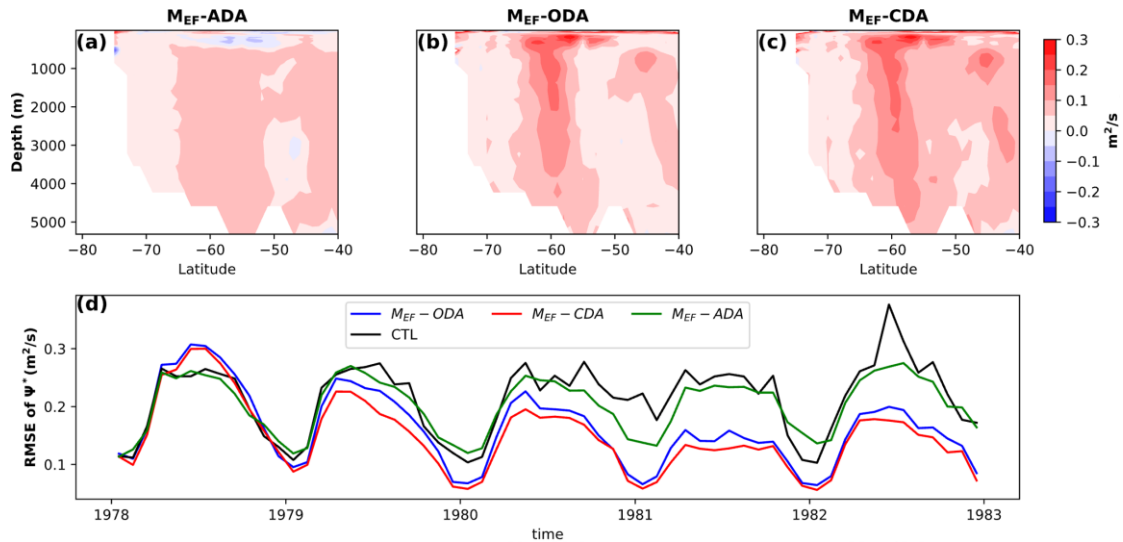
625 **a) Residual circulation of ACC system**

626 To examine the process of CDA in recovering ACC system and understand its mechanism  
 627 which is important to understand CDA's GMOC (*Rintoul, 2018*), we first compute the residual  
 628 circulation at high latitudes of SH. The residual circulation represents the net transport of Ekman  
 629 effects but compensated by the eddy-induced circulation (*Badin and Williams, 2010; McIntosh  
 630 and McDougall, 1996*). Following *Karsten and Marshall (2002)*, the streamfunction of residual  
 631 circulation ( $\psi^*$ ) can be expressed as:

$$\psi^* = -\frac{\tau}{f} + K_e S, \#(7)$$

632 where  $\tau$  and  $f$  represent wind stress and Coriolis parameter, and  $K_e$  and  $S$  are eddy  
 633 diffusivity coefficient and the slope of isopycnals respectively. Then, given the zonal-mean wind  
 634 stress and potential density, with  $K_e = 1000 \text{ m}^2/\text{s}$  (*Visbeck et al., 1997*), we calculate  $\psi^*$  in  
 635 various DA schemes and show them in **Figure. 8**.

636



637 **Figure. 8** The reduction of RMSEs of the residual circulation of ACC system  
 638 through incorporating the CESM-produced “observations” into the CM2 model in various  
 639 multiscale ensemble filtering DA approaches from the CM2 free model simulation. a-c) The  
 640 RMSE reduction of  $\psi^*$  made by  $M_{EF-ADA}$  (panel a),  $M_{EF-ODA}$  (panel b),  $M_{EF-CDA}$  (panel  
 641 c). d) The timeseries of RMSEs of  $\psi^*$  produced by  $M_{EF-ADA}$  (green),  $M_{EF-ODA}$  (blue) and  
 642  $M_{EF-CDA}$  (red). The CM2 free model control simulation (CTL) is plotted as black line as  
 643 the reference.  
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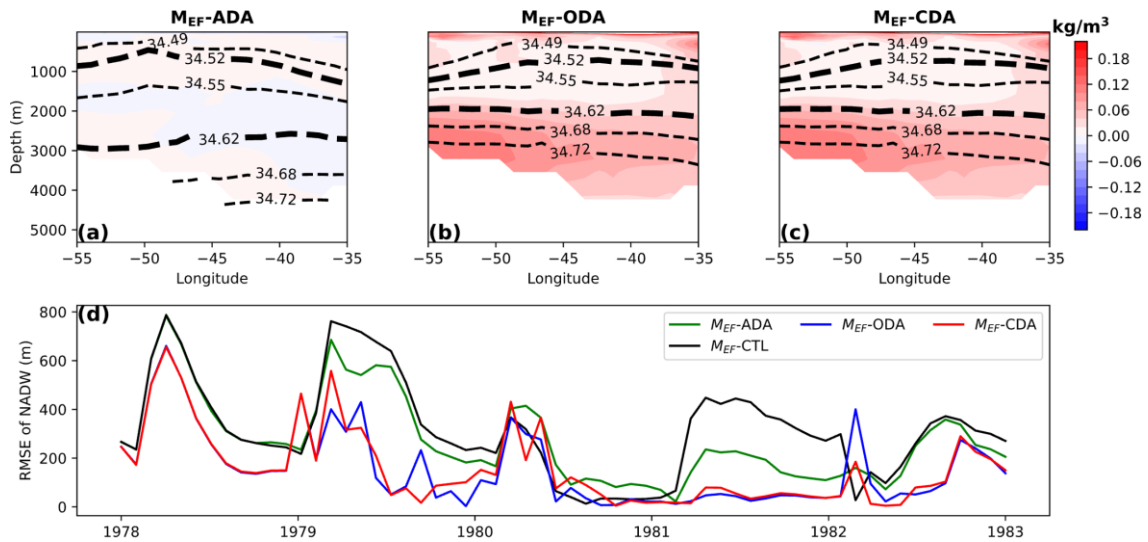
646 Relying on the response of ocean to the improved  $W_{A2O}$ , the ADA improves the residual  
647 circulation in a moderate magnitude (panel **a**). The slight degradation in the upper ocean above  
648 500 m may reflect the difference of numerical schemes expressing air-sea interactions in CESM  
649 and CM2 models. The direct oceanic data constraint in ODA improves the residual circulation in  
650 much larger magnitudes than ADA with similar large-scale patterns, and particularly it corrects  
651 the upper-ocean degradation greatly (panel **b**). Taking the advantages of ODA's ability to  
652 provide a more coherent stratification and ADA's capacity to offer more accurate wind stress,  
653 the improvement of CDA for the residual circulation appears an enhanced version of the ODA  
654 (panel **c**). While exhibiting interesting spin-up features, the timeseries of RMSEs of the residual  
655 circulation in various data constraint schemes strongly support the analysis above (panel **d**).  
656 From **Figure. 8d**, we see that ODA may introduce shocks into model at the beginning period, but  
657 by the incorporation of data and model, it can quickly constrain the model state (*S. Zhang et al.*,  
658 2009) such as the residual circulation.

659

### 660 **b) North Atlantic Deep Water**

661 The NADW is a good representation of low-frequency signals of North Atlantic  
662 convection (*Hopkins, 1991; Pickart and Spall, 2007; S. Zhang et al., 2014*). Following *Pickart*  
663 *and Spall (2007)*, we define a NADW index as the averaged thickness between two isopycnal  
664 surfaces of  $\sigma_{1.5}$  over the domain of  $55^{\circ}$ – $35^{\circ}$ W and  $45^{\circ}$ – $65^{\circ}$ N where  $\sigma_{1.5}$  is potential density  
665 referenced to 1500 m. In this case, we choose  $\sigma_{1.5} = 34.52$  and  $\sigma_{1.5} = 34.62$  as two isopycnal  
666 surfaces to identify North Atlantic deep mode water. We show the recovering degree of NADW  
667 by various data constraint schemes in **Figure. 9**. Unlike the role of ADA in recovering residual  
668 circulation of ACC system for which ADA greatly helps, the role of ADA in recovering NADW  
669 is very little (see panel **a** and green line in panel **d**), while the direct oceanic data constraint in  
670 ODA dominantly the mean state and variability of NADW (panel **b** and blue line in panel **d**).  
671 The CDA's result is nearly identical to the ODA's (panel **c** and red line in panel **d**). We may  
672 comprehend this phenomenon from two perspective. On the one hand, for slow-varying nature of  
673 NADW is primarily influenced by oceanic internal variability rather than the chaotic behavior of  
674 the atmosphere. On the other hand, this may be attributed to the large differences of two models  
675 at high-latitudes of the Northern Hemisphere in dealing with complex topography and sea-ice  
676 modeling. Therefore, it is difficult for CDA to get helps from ADA to improve the ODA's  
677 recovery in a time scale of a few years.

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**Figure. 9** The reduction of RMSEs of NADW through incorporating the CESM-produced “observations” into the CM2 model in various multiscale ensemble filtering DA approaches from the CM2 free model simulation. a-c) Same as Figure. 8 a-c but for  $\sigma_{1.5}$  (potential density referenced to 1.5 km) with statistics between  $45^{\circ}$ - $65^{\circ}$ N, while the dashed lines are contours of  $\sigma_{1.5}$  averaged between  $45^{\circ}$ - $65^{\circ}$ N. defined as d) Same as Figure. 8d but for NADW [the averaged thickness between two isopycnal surfaces (34.52 and 34.62 in this case) of  $\sigma_{1.5}$  over the domain of  $55^{\circ}$ - $35^{\circ}$ W and  $45^{\circ}$ - $65^{\circ}$ N].

### c) Diffusive mixing at tropical oceans

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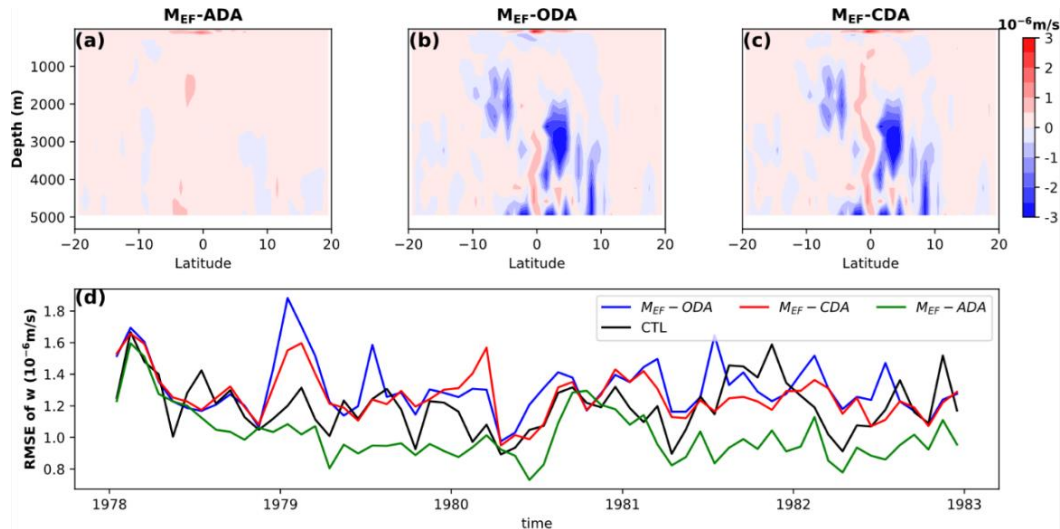
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The tropical oceans have very active air-sea interactions that can be in multiscale from hourly to seasonal-interannual (Fairall et al., 1996; McPhaden et al., 1998; Philander, 1990). Therefore, the tropics are an important adjuster for direct data constraints of ODA in ocean interior and they can serve as an outlet for unphysical influences of data when they are incorporated into the assimilation model as spurious signals input to the atmosphere that produces false variability. As shown in Figure. 10, ADA produces largest error reduction for the vertical motion of tropical oceans, and ODA is the worst, but with aids of ADA, CDA gains some mitigation from ODA. On the one hand, the free CM2 simulation has stronger vertical motions in that region (Figure. 1d), which suggests that CM2’s dynamics favor producing strong vertical motions at tropics as the balance mechanism illustrated in Figure. 3b. Then, due to the great changes of NADW and ACC system in ODA’s data constraints, the balance mechanism can produce such strong vertical motions in tropical 1000 – 4000 m. On the other hand, since many “malfunctions” of CM2’s dynamics and physics relative to the CESM’s exist, the strong vertical motion adjustment at tropical oceans could be associated with the compensation effects of such “malfunctions.” For example, the sea-ice model used in CM2, SIS (sea-ice simulator) (Winton, 2000) is quite different from the one used in CESM, CICE5 (Community Ice Code version 5) (Hunke et al., 2010). Then, the different simulations of two models at polar regions could influence on the AMMC-GMOC structure. When we incorporate the CESM-produced observations into CM2 model, such discrepancy could produce extra vertical motions at tropics as adjustment. We will discuss more on this in the Section 5.3.



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 712 **Figure. 10** The reduction of RMSEs of tropical ocean vertical motion ( $w$ ) through  
 713 incorporating the CESM-produced “observations” into the CM2 model in various  
 714 multiscale ensemble filtering DA approaches from the CM2 free model simulation. *a-d*  
 715 Same as Figure. 9*a-d* but for the vertical motion of tropical oceans ( $20^{\circ}$ S- $20^{\circ}$ N).

## 716 5.2 The reconstructed AMMC-GMOC structure by coupled data constraints

717 In this section, we examine how the major processes described Section 5.1 reflects the  
 718 efficacy of CDA in estimating the structure of AMMC-GMOC. The error reductions of  
 719 AMMC-GMOC structures estimated by  $M_{EF-ADA}$ ,  $M_{EF-ODA}$  and  $M_{EF-CDA}$  from the CTL are  
 720 shown in **Figure. 11a-f**. Different from the model state variables such as atmosphere wind,  
 721 temperature and pressure as well as ocean temperature and salinity etc. which can be directly  
 722 adjusted by observational information, the AMMC and GMOC only can be derived from these  
 723 state variables. They are not only determined by the estimated values of state variables  
 724 themselves, but also rely on the balanced and coherent properties among these variables (*Lu et*  
 725 *al.*, 2020; *S. Zhang et al.*, 2014).

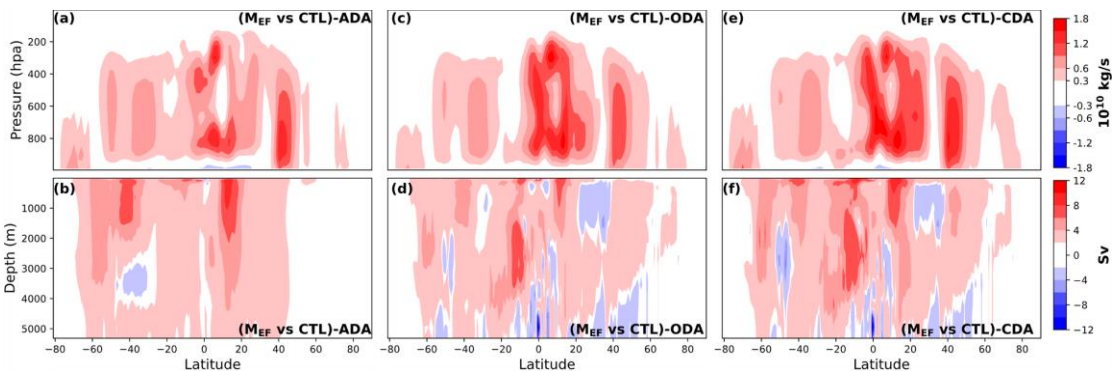
726 Generally, the incorporation of CESM-produced  $P_s$  data in  $M_{EN-ADA}$  systematically  
 727 reduces the AMMC’s difference between the CM2 and CESM (panel **a**). In this case, the wind in  
 728 ADA is adjusted through the thermal wind geostrophic balance working on the projected vertical  
 729 structure of pressure from “observational” increments of  $P_s$  data (*S. Zhang et al.*, 2014). As the  
 730 consequence of CM2-ocean’s responses to ADA effects through  $W_{A2O}$ , the  $M_{EN-ADA}$  estimated  
 731 GMOC shows significant error reductions from the CTL in a large scope (panel **b**). But again,  
 732 due to the existence of the bias of CM2-ocean vs. CESM-ocean, such responses still show light  
 733 error increases in  $20-40^{\circ}$ S and 1000-4000 m depths for the GMOC estimation of  $M_{EF-ADA}$ . In  
 734 this case, although our deep ocean bias constraining scheme largely relaxes biases there (*Lu et*  
 735 *al.*, 2020), the bias of CM2-ocean vs. CESM-ocean still exists. As the consequence of  
 736 CM2-atmosphere responding to the ODA-improved SSTs,  $M_{EF-ODA}$  shows a globally improved  
 737 AMMC (panel **c**). Nevertheless, if we compare the scope and magnitude of error reductions of  
 738 AMMC and GMOC produced by  $M_{EF-ADA}$  and  $M_{EF-ODA}$ , we found that the direct data  
 739 constraint in the atmosphere (ocean) makes a little smaller correction for AMMC (GMOC) than  
 740 the response of atmosphere (ocean) to ODA-improved SSTs (ADA-improved sea-surface

741 forcing). This addresses the importance of assimilating observations within the coupled model  
 742 framework for estimating the AMMC-GMOC structure.

743 Specifically, in the ACC region (**Figure. 11**), combining  $M_{EF}$ -ADA and  $M_{EF}$ -ODA, the  
 744 local maximum improvement in  $60^{\circ}\text{S}$  and  $40^{\circ}\text{S}$  can be attributed to the better representation of  
 745 eddy-induced circulation and Ekman transport. The same degraded estimation in  $50^{\circ}\text{S}$  2–4 km  
 746 can be attributed to the bias induced by climatology restoring scheme. In the north of  $40^{\circ}\text{N}$ , most  
 747 of the error reductions are contributed by ODA, the same as the results shown in **Figure. 9**. In  
 748 tropics between  $10^{\circ}\text{S}$  and  $10^{\circ}\text{N}$ , although the large bias of vertical velocity at  $10^{\circ}\text{N}$  still reflect on  
 749 the discrepancy in GMOC,  $M_{EN}$ -ODA still produces much larger error reduction of GMOC in  
 750 tropical ocean above 3.5 km. The AMMC-GMOC standard deviations, evaluating using 12  
 751 ensemble members in the  $M_{EF}$  algorithms, are presented in **Figure. 12**. These results  
 752 demonstrates that the combining both atmospheric and oceanic observational data has the potential  
 753 to diminish the uncertainties of data constraints. Moreover, the uncertainties of  $M_{EN}$  estimation  
 754 are shown in **Figure. S8**.

755 To get some sense on the role of CDA in retrieving the variation of GMOC, we show the  
 756 timeseries of Atlantic northward transport at  $26.5^{\circ}\text{N}$  produced by various data constraints in  
 757 **Figure. S9**. We see that the variation of GMOC is recovered well by CDA which coherently  
 758 combines effects of atmospheric and oceanic data constraints together. Recovering variability of  
 759 ocean meridional transport by CDA is critically important for both reanalysis of historical  
 760 evolution of coupled Earth system and initialization of climate prediction, and thorough  
 761 examination and evaluation shall be performed in the future studies.

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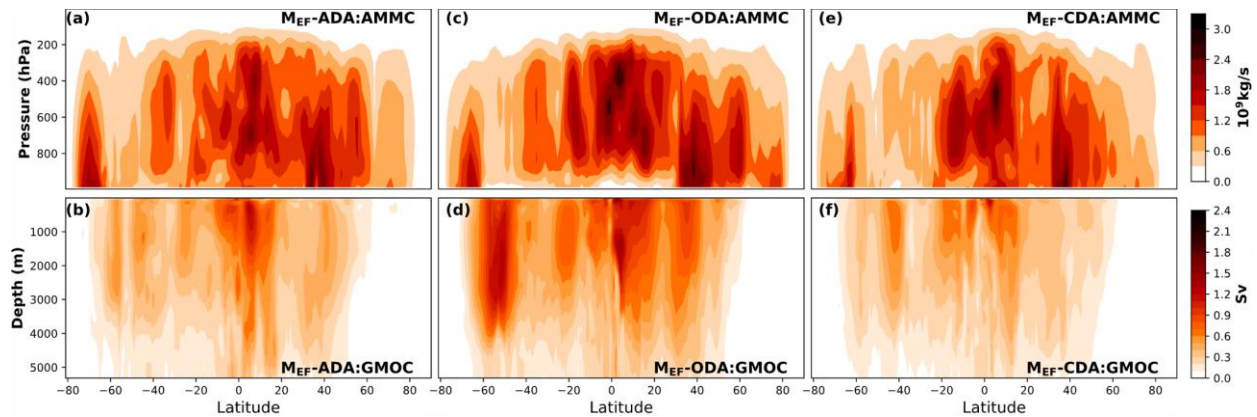
763

764 **Figure. 11** The error reductions of AMMCs and GMOCs made by various ADA, ODA and  
 765 CDA schemes. a-f) The RMSE reduction of AMMC (panels a, c & e) and GMOC (panels b,  
 766 d & f) made by  $M_{EF}$ -ADA (panels a & b),  $M_{EF}$ -ODA (panels c & d) and  $M_{EF}$ -CDA (panels e  
 767 & f) relative to the CTL's ( $RMSE_{CTL} - RMSE_{DA}$ ) with statistics in last 3 years.

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**Figure. 12** The uncertainties of AMMC-GMOC estimation by various multiscale ensemble filtering DA approaches. a-f) Same as Figure. 11a-f but for ensemble standard deviation of corresponding streamfunction.

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### 5.3 Importance of balanced and coherent coupled data constraints in GMOC estimation

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The error reduction of AMMC-GMOC structures from  $M_{EN}$  to  $M_{EF}$  shows some interesting phenomenon (**Figure. 13a-f**). Generally, it is relatively easy to improve the AMMC-GMOC structure through improving atmospheric data constraint by ADA compared to improving oceanic data constraint by ODA due to less representation of ocean model and observations for complex ocean stratification. In this case, although the analyses in section 3 show the nearly-identical assimilation quality of  $M_{EN-ADA}$  and  $M_{EF-ADA}$ , the errors of both the AMMC and GMOC estimated by  $M_{EF-ADA}$  are smaller than the ones by  $M_{EN-ADA}$ , especially in tropics (panels **a** & **b**). This means that more balance and coherence exist in ADA-estimated winds and associated ocean currents. Nevertheless, while  $M_{EF-ODA}$  shows distinguishable improvement on ocean temperature and salinity relative to  $M_{EN-ODA}$  as shown in **Figure. S2**, the  $M_{EF-ODA}$ 's improvement on GMOC is very limited (panel **d**). In fact, from  $M_{EN-ODA}$  to  $M_{EF-ODA}$ , the GMOC gets improved only in some tropics and middle and high latitudes of the Southern Hemisphere but degraded in almost the whole Northern Hemisphere. This suggests that improving GMOC requires more restricted spatial coherence of ocean temperature and salinity distributions. Although further ensemble filtering may extract more observational information that is mainly in the upper 2000 m, it is not necessarily true that the vertical structure of ocean is better. For AMMC, from  $M_{EN-ODA}$  to  $M_{EF-ODA}$ , the difference reflects the consequence of the atmosphere freely responding to the improved SSTs by  $M_{EF-ODA}$ , the improvement being the major message (panel **g**), particularly in the high latitudes of the Northern Hemisphere. The reconstruction of GMOC through combining observed data with a coupled model requires sufficient incorporation of atmospheric and oceanic observations into model atmospheric and oceanic states in a balanced and coherent manner.

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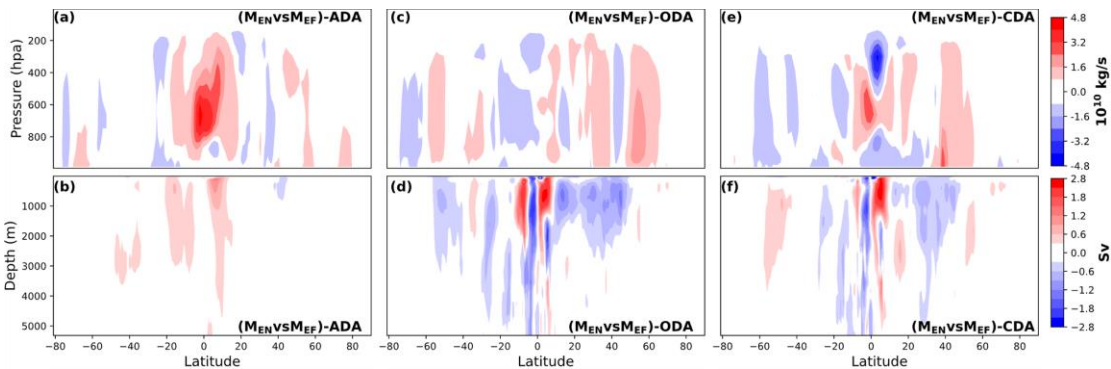
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Combining ADA and ODA, due to the addition of direct atmospheric data constraint, the ocean free responses to ADA-produced  $W_{A2O}$  significantly mitigate the degradation of  $M_{EF-CDA}$  estimated GMOC in the middle-high latitudes of the Southern Hemisphere and tropics-subtropics of the Northern Hemisphere. The maintenance of balanced physical relations between the atmosphere and ocean is very important on GMOC estimation. The atmosphere free response to ODA-produced  $HF_{O2A}$  joining with direct oceanic data constraint makes the AMMC improved in middle latitudes of the Northern Hemisphere but degraded in tropics especially low and high

804 troposphere as well as high latitudes of the Southern Hemisphere. This phenomenon implies that  
 805 the AMMC has high sensitivities to the coherent distribution of HF<sub>O2A</sub>, and great light shall be  
 806 darted on more coherent analysis of ocean states in the future.

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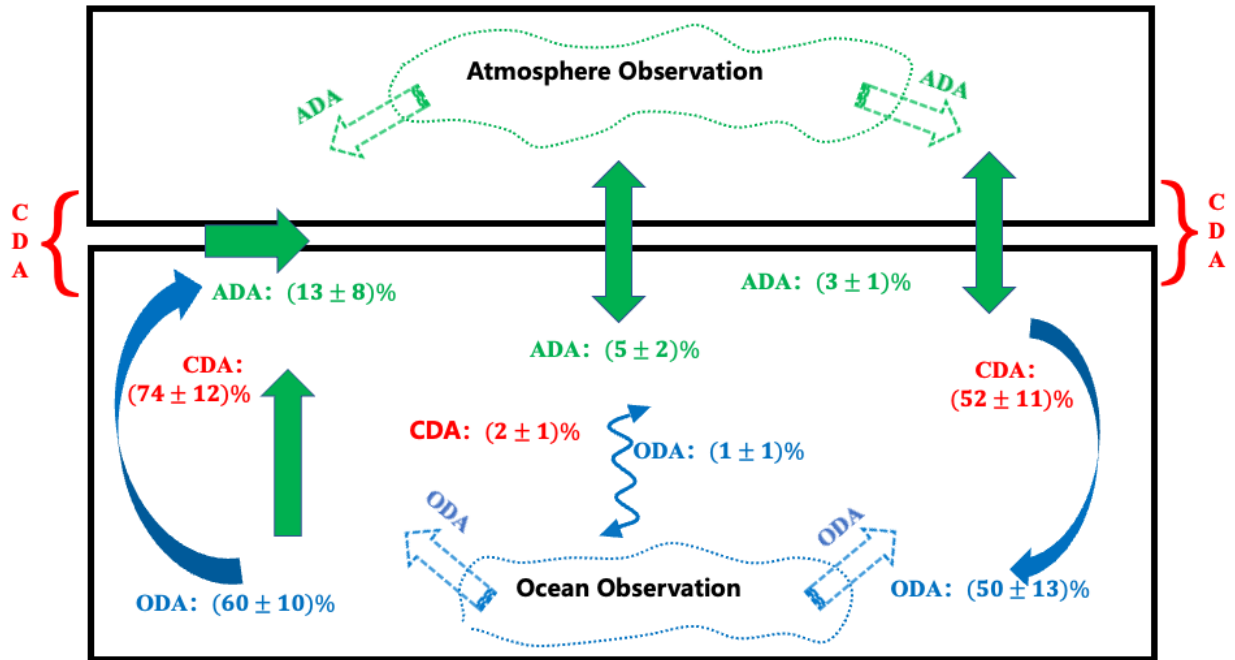
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809 **Figure. 13** The error reductions of AMMCs and GMOCs made by various ADA, ODA and  
 810 CDA schemes. a-f) Same as Figure.11 a-f but made by  $M_{EN}$ -ADA (panels a & b),  $M_{EN}$ -ODA  
 811 (panels c & d) and  $M_{EN}$ -CDA (panels e & f) relative to  $M_{EF}$ -ADA,  $M_{EF}$ -ODA and  
 812  $M_{EF}$ -CDA (i.e.,  $RMSE_{EN} - RMSE_{EF}$ ).

813 We synthesize the analyses above about the roles of various data constraints in GMOC  
 814 reconstruction of CDA as well as the uncertainties evaluated from the 12-member ensemble in  
 815 **Figure. 14**. The improvement from southern to northern is assessed by evaluating the RMSEs  
 816 improved by residual circulation in the Southern Ocean, the improved vertical velocity in  
 817 tropical areas and the improvement in NADW within their geographic domains.

818 Within this specific “twin” experiment framework, it is shown that the CDA approach is  
 819 very powerful to recover the ACC system and associated residual circulation at high latitudes of  
 820 the Southern Hemisphere by incorporating the atmospheric and oceanic observations into the  
 821 coupled model. In the CDA procedure, ADA (13%) helps ODA improve the recovery skill, in  
 822 which while the direct oceanic data constraint in ODA recovers the residual circulation by 60%,  
 823 the ADA-improved air-sea fluxes help enhance it up to 74%. The CDA skill is higher than the  
 824 sum of the ADA’s and ODA’s, suggesting that positive feedback exists in the ACC system. The  
 825 spread among ensemble members shows small uncertainties in the CDA procedure relative to  
 826 ADA and ODA. For convection and associated NADW at high latitudes of the Northern  
 827 Hemisphere, while ODA recovers 50%, ADA has a little help on them (3%) and eventually CDA  
 828 recovers 52%. On the one hand, the behavior of North Atlantic convection and associated  
 829 NADW has a slow-varying nature, and thus a few years of atmospheric data constraints may not  
 830 be sufficient to show their effects. On the other hand, as mentioned before, large differences in  
 831 topography and sea-ice modeling make difficulties for ADA to help ODA. Thus, the uncertainty  
 832 of this region is larger than the Southern ACC region. Finally, CDA recovers the tropical ocean  
 833 streamfunction by 2%, exhibiting a recovery capability considerably lower than ADA’s (5%).  
 834 However, it effectively alleviates the degradation caused by ODA (1%) in the tropical regions.  
 835 The tropical diffusive mixing activities directly link with the atmosphere through frequent air-sea  
 836 interactions. In the CDA framework, the residual of Southern upwelling and Northern sinking  
 837 not only contains unbalanced signals of these two terms, but also includes spurious variations  
 838 induced from inconsistency of data and model. The adjustment in tropical oceans can get great  
 839 impacts from ADA, but as an outlet linked to the atmosphere for accumulated unbalanced  
 840 information from extratropical oceans, it also contains much noises.

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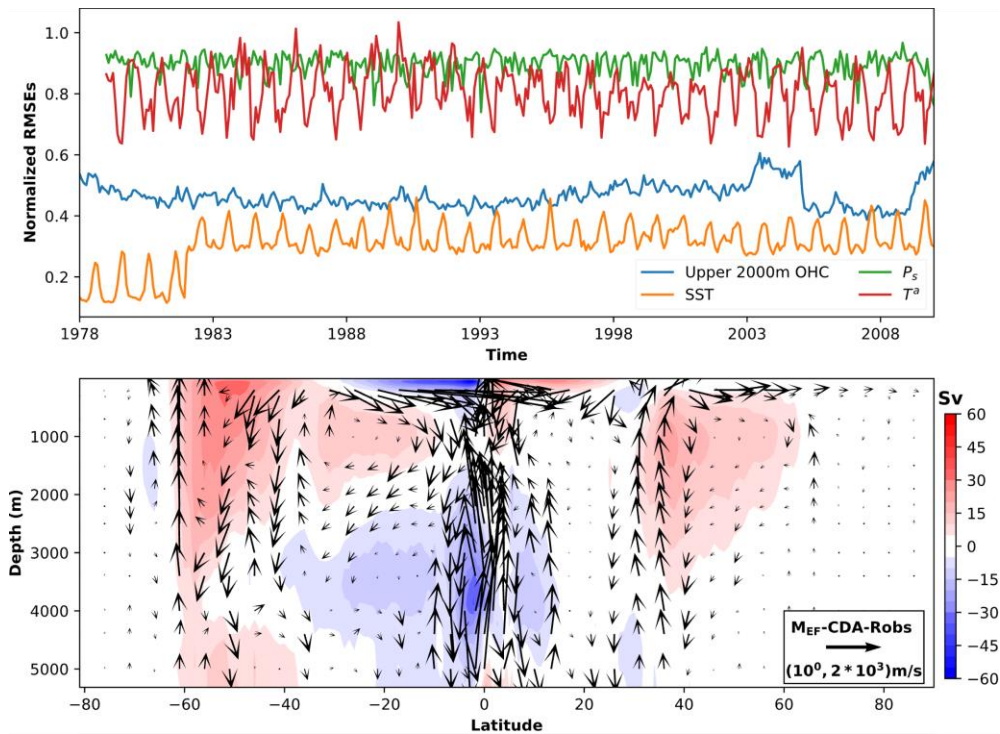
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 843 **Figure. 14** The summarized illustration of relative contributions of various data constraints  
 844 to GMOC estimation in CDA and their uncertainties. The illustration of oceanic (lower)  
 845 [atmospheric (upper)] data constraint for the ocean (atmosphere) model by ODA and  
 846 ODA's contributions (ADA and ADA's contributions) in estimation of major components  
 847 of GMOC as well as their uncertainties estimated in ensemble filtering twin experiment.  
 848 Curly braces indicate that a weakly-CDA approach is used in this study, which combines  
 849 ADA and ODA together within the coupled model through exchanged fluxes at the air-sea  
 850 interface without direct observational adjustment cross the air-sea interface.  
 851

## 852 6 The GMOC historical reanalysis by multiscale ensemble filtering CDA

853 To further confirm the understanding gained from the analyses of “twin” experiments on  
 854 the role of multiscale ensemble filtering CDA, we conduct the “real” observation CDA  
 855 experiment  $M_{EF-CDA-Robs}$  as described in Section 2.3b. The  $M_{EF-CDA-Robs}$  uses the identical  
 856 ensemble initial conditions and model configuration as  $M_{EF-CDA}$  experiments in previous  
 857 sections but substituting the ERA5 surface pressure (*Hersbach et al., 2020*) and all ocean real  
 858 observations described in **Table 1** as the observations of atmosphere and ocean. The results are  
 859 summarized in **Figure. 15 & 16**. In general, the atmosphere and ocean state estimation converge  
 860 very well (**Figure. 15a**). We notice the following phenomena. We use the HadISST product to  
 861 conduct SST verification, and the RMSEs of SSTs have a little jump around 1982 because of the  
 862 existence of discontinuous processing schemes in the HadISST product (*Rayner et al., 2003*).  
 863 While CDA of the  $M_{EF-CDA-Robs}$  cuts the RMSE of upper 2000 m ocean heat content by half,  
 864 the timeseries show oscillations with availability of observations as well as model temporal  
 865 behavior.

866 The  $M_{EF-CDA-Robs}$  estimated GMOC (**Figure. 15b**) appears having a large adjustment  
 867 from the model control as shown in **Figure. 1d**. Usually, the GMOC in free model simulations

868 exhibits a continuous single circulation cell above 2500 m and a weak anti-circulation cell at  
 869 tropical deep ocean. Compared to the CM2 free model control simulation, the GMOC estimated  
 870 by  $M_{EF}$ -CDA-Robs appears having much strengthened Northern NADW. A core of NADW is  
 871 established and the weak anti-circulation at tropical deep ocean in free model simulation  
 872 becomes much strong and extends to the upper ocean so that the continuous single circulation  
 873 cell of GMOC becomes a double-core structure (**Figure. 15b**). The Southern ACC system also  
 874 encounters some adjustment in which the Ekman transport centered at 50°S becomes weaker and  
 875 anti-circulation branch in the residual circulation apparently becomes stronger. The northward  
 876 transport in the Southern middle latitudes becomes stronger and a core centered at 35°S and 1000  
 877 m is formed. We may comprehend the changes of ACC system and NADW as consistent data  
 878 constrained signals.



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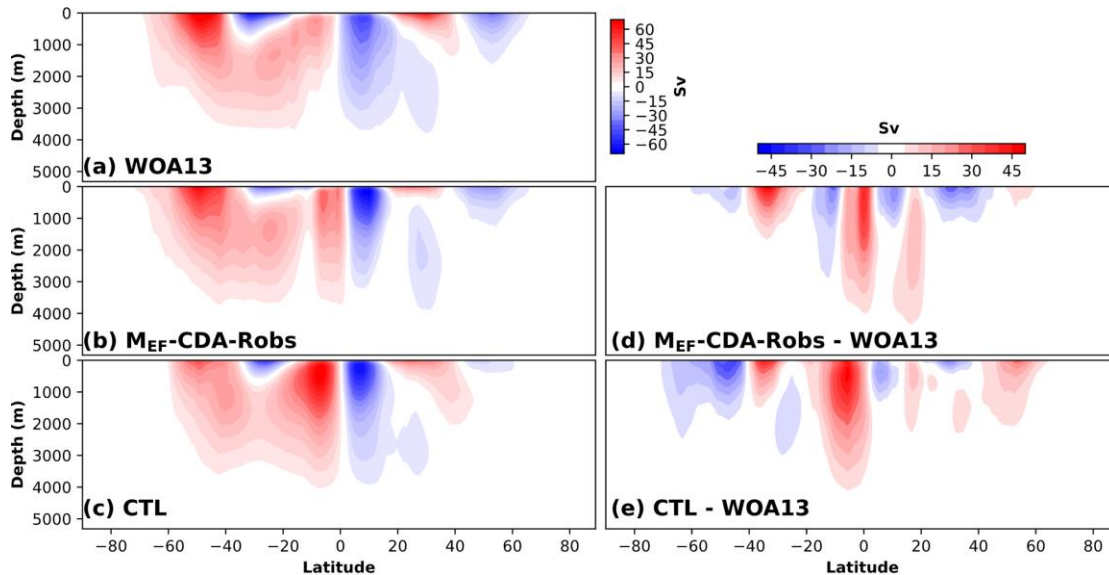
880 **Figure. 15** The convergent atmospheric and oceanic state estimation (upper) and estimated  
 881 **30-year time mean GMOC (lower) by multiscale ensemble filtering CDA approach through**  
 882 **incorporating atmospheric and oceanic observations into CM2. a) The timeseries of**  
 883 **normalized global RMSEs of surface pressure ( $P_s$ ) (solid-green), atmosphere temperature**  
 884 **( $T_a$ ) (solid-red), sea surface temperature (SST) (solid-yellow) and upper 2000 m ocean heat**  
 885 **content (solid-blue) produced by  $M_{EF}$ -CDA-Robs (see Table 1), by corresponding RMSE**  
 886 **values at the initial state. We use the HadISST and EN4 products as verification target for**  
 887 **SST and ocean heat content. Note that to sustain ensemble filtering ODA, we activate ADA**  
 888 **after 1-year of ODA, and due to the existence of discontinuous processing schemes in the**  
 889 **HadISST product, there is a little jump around 1982. b) The distribution of 1981-2010 time**  
 890 **mean meridional streamfunctions produced by  $M_{EF}$ -CDA-Robs, configured with**  
 891 **corresponding  $[v, w]$  vectors.**



892 To get some insights on the signal-to-noise ratio of estimation analyses above, especially  
 893 for the large tropical adjustments, we compute the time mean geostrophic GMOCs using ocean  
 894 temperature and salinity profiles (*Chu, 2000; Chu and Fan, 2015*) produced by the CM2 free  
 895 model simulation and  $M_{EF}$ -CDA-Robs and compared to the WOA13 climatological data (*Zweng*  
 896 *et al., 2013; Locarnini et al., 2013*) (**Figure. 16**). The geostrophic flow between  $7^{\circ}$  S- $7^{\circ}$  N is  
 897 done by using the following equations:

$$v = v * \left( |lat| \times \frac{|lat| - 14}{49} \right)^2, \# (8)$$

898 where lat is the latitude of the meridional velocity  $v$ . From **Figure. 16**, we do see the large scope  
 899 improvement of geostrophic GMOC by  $M_{EF}$ -CDA-Robs indeed from the model control, except  
 900 for slightly worse in small regions at  $35^{\circ}$ S and above 1000 m as well as at  $15^{\circ}$ N between  
 901 1000-4000 m. The largest improvements are found in the Southern ACC system and Northern  
 902 NADW regions, which strongly support our comprehension in the analysis for the appearance of  
 903 total streamfunction. Even for the tropics, the CDA procedure reduces the errors of geostrophic  
 904 GMOC by a distinguishable degree (compare panel **e** to panel **d**).



905

906 **Figure. 16** The climatologically-convergent geostrophic GMOC produced by multiscale  
 907 ensemble filtering CDA. a-c) The distributions of geostrophic meridional streamfunction  
 908 derived from WOA13 (panel a),  $M_{EF}$ -CDA-Robs-produced (panel b) and free CM2 model  
 909 control (panel c) climatological temperature and salinity data. d-e) The differences between  
 910 panels b and a (panel e) as well as between panels c and a (panel f). Note that given coarse  
 911 vertical discretization in deep ocean, to maintain deep ocean weak geostrophic information,  
 912 the integral for deriving geostrophic streamfunction is from the bottom to surface.

913 The goal of this study is to conceptually prove that it is feasible to reconstruct GMOC  
 914 through combining CGCMs with the Earth observing system, rather than a thorough examination  
 915 on GMOC reanalysis, requiring exhausted analyses for a long time CDA products which is one  
 916 of our undergoing projects. Through the analyses above, we may conclude that within a CDA  
 917 framework, simultaneously working with atmospheric data constraints, a sound multiscale

918 oceanic data constrain that makes oceanic variables having a correct vertical structure is able to  
919 produce a reliable GMOC estimation in terms of time mean structure. Once convergent  
920 variability in coupled reanalysis with multiple CGCMs using the multiscale CDA algorithm is  
921 detected, based on such multi-model multiscale ensemble filtering CDA systems, the  
922 probabilistic seamless prediction from seasonal-interannual to multidecadal scales becomes  
923 practical.

## 924 **7 Summary and Discussion**

925 With aids of two CGCMs which are biased with respect to each other, we designed a  
926 biased “twin” experiment framework to study the issue of GMOC estimation by incorporating  
927 observations into a CGCM. One of two CGCMs is used to create a “true” solution of GMOC  
928 estimation and sample the “observations” based on the realistic observing network. As the  
929 “observations” are assimilated into the other model to recover the “truth,” the degree by which  
930 the “true” GMOC is recovered is an assessment of successfulness of an assimilation scheme.  
931 With two schemes for data-model incorporation (i.e., ensemble of multiscale filtering and  
932 ensemble multiscale filtering), we configure ADA (only conducting atmospheric data constraint),  
933 ODA (only conducting oceanic data constraint), and CDA which conducts both atmospheric and  
934 oceanic data constraints together within the coupled model framework. Then we examine the  
935 role and mechanism of atmospheric and oceanic data constraints as well as the impact of  
936 coherence of data-model incorporation in GMOC estimation.

937 We find that for reconstruction of GMOC by incorporating observational information  
938 into a coupled model, the following two aspects are very important. Firstly, a sound DA  
939 algorithm that can achieve a balanced and coherent data-model incorporation (e.g., taking  
940 multiscale ensemble filtering) makes model variables having balanced physical relations and  
941 coherent spatial distributions. For oceanic data constraint, recovering a correct vertical structure  
942 is critical for retrieving variability and thus such multiscale filtering must include the correction  
943 of climatological mean state and seasonal cycle. Secondly, simultaneous data constraints in  
944 atmosphere and ocean components during the coupled model integration, which transfer  
945 observational information between the atmosphere and ocean through corrected exchange fluxes  
946 at air-sea interface, can significantly enhance the balance and coherence of the data-constrained  
947 atmosphere and ocean states. Therefore, the multiscale CDA including recovery of ocean  
948 climatology which produces balanced air-sea exchange fluxes and coherent ocean vertical water  
949 transport is able to reconstruct the GMOC in a large extent.

950 An accompanying study is conducting an exhausted analysis on climate variability of a  
951 few decades in coupled reanalyses with converged behaviors including GMOC produced by  
952 CESM and CM2 CDA systems using the multiscale CDA algorithm. That could serve as a solid  
953 sustenance for seamless seasonal-interannual to multidecadal predictability studies. Follow-up  
954 studies also include the extension of multi-model coupled reanalysis to century scales for  
955 facilitating deeper detection of GMOC variability and mechanism. Based on such multi-model  
956 multiscale ensemble filtering CDA systems, establishment of probabilistic seamless predictions  
957 from seasonal-interannual to multidecadal scales is also in the priority.

958 However, given the high sensitivities of GMOC estimation on spatial coherence of ocean  
959 states, the high-accuracy coupled reanalysis with better GMOC estimation still has a big space  
960 for improvement, for which the multi-model seamless ensemble prediction system can serve as a  
961 test platform. In the future, great lights shall be darted on improving coupled modeling and ocean

962 estimation with incorporation of model and more observational information that represents richer  
963 scales of ocean motions. By that way, more physical balance among ocean temperature, salinity  
964 and currents as well as their spatial coherence, especially for the vertical structure of temperature  
965 and salinity, can be gained and maintained. This requires four aspects of efforts for advancing  
966 coupled reanalysis.

967 First, in general, the ocean observing system in the history has far imperfect  
968 representation for the real ocean system (*Abraham et al.*, 2013), even for the modern Argo  
969 system which still has a big space for improvement (*Roemmich et al.*, 2009). Second, significant  
970 modeling errors exist in ocean and coupled system models (*S Zhang et al.*, 2023). One of  
971 outstanding issues is insufficient tropical high frequency air-sea interaction (*Bernie et al.*, 2005;  
972 *Marullo et al.*, 2016; *H Zhang et al.*, 2018) which can have significant impacts on GMOC  
973 simulation (Gnanadesikan, 1999). Third, the behaviors of oceans at polar regions have big  
974 impacts on GMOC (*Li et al.*, 2021; *Oka et al.*, 2021), for which sea ice plays an important role.  
975 Currently sea ice data assimilation is not included in the CDA system yet, whose impacts on  
976 ocean state estimation has been proved in the previous studies (*Liu et al.*, 2021). Therefore,  
977 follow-up studies shall consider improvement of sea-ice estimation which incorporates multitype  
978 of sea-ice observations with more physical balance and coherence with the atmospheric and  
979 oceanic data constraints (*Wu et al.*, 2016; *S. Zhang et al.*, 2013). Finally, refinement of deep  
980 ocean bias constraint with high-resolution coupled modeling (*S Zhang et al.*, 2023) and data  
981 assimilation (*Li et al.*, 2021) is necessary for creating a creditable coupled reanalysis dataset  
982 which has a credible GMOC. Then, the seamless weather-climate prediction of daily to  
983 multidecadal scales becomes feasible.

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## 991 **Open Research**

992 The code of CESM1.3 (*Small et al.*, 2014) and CM2.1 (*Delworth et al.*, 2006) is available at  
993 <https://www.cesm.ucar.edu/> and <https://www.gfdl.noaa.gov/cm2-5-and-flor-quickstart/>,  
994 respectively. The ERA5 reanalysis data are available from the Copernicus Climate Change  
995 Service (C3S) Climate Data Store (CDA) (*Hersbach et al.*, 2020), the OISST (*B Huang et al.*,

996 2021), World Ocean Dataset (WOD) (Boyer *et al.*, 2009) and World Ocean Atlas (WOA)  
 997 (Locarnini *et al.*, 2013; Zweng *et al.*, 2013) data is obtained from National Oceanic and  
 998 Atmospheric Administration (NOAA) website (<https://www.ncei.noaa.gov/products>). The Argo  
 999 data (Wong *et al.*, 2020) is available at <ftp://ftp.ifremer.fr/ifremer/argo/geo>. The HadISST  
 1000 (Rayner *et al.*, 2003) can be accessed in <https://www.metoffice.gov.uk/hadobs/hadisst>. Since the  
 1001 data used to produce the figures and analyses in this work are very large, they can be obtained by  
 1002 sending request to the corresponding author.

1003

1004 **References**

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