

# Assimilation of oceanic observations in a global coupled Earth system model with the SEIK filter

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## Abstract

We present results from the assimilation of observed oceanic 3-D temperature and salinity fields into the global coupled Max Planck Institute Earth system model with the SEIK filter from January 1996 to December 2010. Our study is part of an effort to perform and evaluate assimilation and prediction within the same coupled climate model without the use of re-analysis data. We use two assimilation setups, one where oceanic observations over the entire water column are assimilated, and one where only oceanic observations below 50 m depth are assimilated. We compare the results from both assimilations with an unconstrained control experiment. While we do not find significant improvements due to assimilation in terms of the root-mean-square error of simulated temperature, 0-700 m heat content, sea surface height (SSH), and the Atlantic meridional overturning circulation (AMOC) against observations, we find the variability in terms of correlation with observations significantly improved due to assimilation, most prominently in the tropical oceans. Improvements over the control experiment are stronger

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in the sub-50 m assimilation experiment and in integrated quantities (SSH, AMOC).

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## 1 **1. Introduction**

2     The natural variability of Earth’s climate is influenced by many factors.  
3     Their importance varies with the temporal scales associated with the climate  
4     under investigation. The ocean influences or may even dominate the climate  
5     variability on time scales larger than a few months due to its large heat ca-  
6     pacity. Climate predictions on these time scales therefore depend crucially  
7     on the representation of the oceanic variability by the chosen global coupled  
8     Earth system model (ESM). At seasonal to decadal time scales, the quality  
9     of the respective climate prediction is also inherently dependent on the initial  
10    conditions (Cox and Stephenson, 2007; Branstator and Teng, 2012), and in  
11    particular on a good initialization of the oceanic state prior to prediction.  
12    Any initialization should incorporate the available observations of the past  
13    state of the ocean. Oceanic observations are, however, still irregularly and  
14    sparsely distributed in both time and space, despite the development of such  
15    sophisticated profiling programs as Argo (Roemmich et al., 2009). While  
16    the accuracy of instruments is sufficiently high, the observation uncertainty  
17    depends on the representativeness of the observations. How representative  
18    any observation is to the ESM’s grid cell it is falling in remains the subject of  
19    ongoing research, and only to a certain degree this error can be approximated  
20    from large observation data sets (Forget and Wunsch, 2007; Oke and Sakov,

21 2008).

22 Given the limited number of observations and their large uncertainties to rep-  
23 resent the variability of the ocean in space and time, it has been argued that  
24 even the entire oceanic data base might currently be too small to successfully  
25 constrain an ocean model (Pohlmann et al., 2009). Hence, any oceanic re-  
26 analysis will represent both the variability seen in the observations, but also  
27 the variability native to the model that is constrained by the observations.

28 When aiming to initialize climate predictions, Pohlmann et al. (2009) ar-  
29 gued that best results may be gained when both re-analysis (assimilation)  
30 and forecast are produced with the same model. Such a model inherent ini-  
31 tialization might keep initialization shocks and model drift in forecast mode  
32 comparatively small, assuming an assimilation method is employed that does  
33 not force the model too far away from it's climatological mean state.

34 Popular assimilation methods used with temporally and spatially sparse ob-  
35 servations are based on the Ensemble Kalman filter (EnKF, Evensen, 1994).

36 All EnKFs have in common that they represent the model's state estimate  
37 and its uncertainty by an ensemble of model states. The ensemble makes  
38 the assimilation with large-scale numerical models feasible, because the full  
39 error covariance matrix is approximated by the ensemble covariance matrix  
40 computed from an ensemble of model states. They analyze the ensemble in-  
41 formation together with the observation state and uncertainty to produce an  
42 updated ensemble representing the optimized model state and uncertainty.

43 EnKFs are also known for their straightforward applicability in sequential  
44 data assimilation and potential efficiency when used on parallel computers  
45 (Keppenne and Rienecker, 2002). The EnKFs can handle model non-linearity

46 to some extent because the covariance matrix is implicitly propagated in time  
47 by integrating each ensemble state by the full model. Building on this origi-  
48 nal Ensemble Kalman filter, alternative types of EnKFs have been proposed  
49 for oceanic data assimilation, such as the error subspace transform KF (ES-  
50 TKF, Nerger et al. (2012)) or the singular evolutive interpolated KF (SEIK,  
51 Pham et al. (1998)).

52 In our study we use the SEIK filter to assimilate subsurface and surface  
53 oceanic temperature and salinity observations into the ocean component of  
54 the fully coupled global Max Planck Institute Earth System Model (MPI-  
55 ESM). Our approach is partly similar to recent studies by Karspeck et al.  
56 (2013), who also assimilated subsurface oceanic data, but only in a loosely  
57 coupled version of the Community Climate System Model (CCSM4), and by  
58 Counillon et al. (2014), who assimilated sea surface data but no subsurface  
59 observations in the fully coupled Norwegian Climate Prediction Model (Nor-  
60 CPM). Our study extends these studies, on the one hand to a fully coupled  
61 ESM including a freely running atmosphere, and on the other hand by the use  
62 of real subsurface temperature and salinity profiles from the EN3 database  
63 (Ingleby and Huddleston, 2007) for the assimilation.

64 We test two implementation strategies, one where oceanic observations over  
65 the entire water column are assimilated, and one where only oceanic ob-  
66 servations below 50 m depth are assimilated, in both cases the atmosphere  
67 is unconstrained. The latter strategy may reduce the discrepancies at the  
68 ocean-atmosphere boundary, for instance in temperature, which are implic-  
69 itly introduced when oceanic surface data are assimilated while atmospheric  
70 surface data remain unconstrained. We apply the SEIK filter on a monthly

71 basis for a time period of 15 years (1996-2010). We use 8 ensemble members,  
72 which is considerably smaller than the 30 members used by Counillon et al.  
73 (2014). The ensemble size is chosen to both comply with our computational  
74 resources and assess the feasibility, technically and scientifically, of the SEIK  
75 assimilation within MPI-ESM. However, we are aware that smaller ensemble  
76 sizes are prone to larger sampling errors and therefore an increased ensemble  
77 size may be necessary in future implementations.

78 The long-term aim of our effort is a model-inherent initialization of decadal  
79 climate predictions as proposed by Pohlmann et al. (2009), and a contribu-  
80 tion to the decadal prediction system developed within the German MiKlip  
81 project (Pohlmann et al., 2013).

82 The remainder of this paper is structured as follows: we describe the model,  
83 observations and filter characteristics used in our experimental setup in Sec. 2.  
84 Results of our experiments for the temperature field, the heat content, the  
85 sea surface height and the Atlantic meridional overturning circulation are  
86 shown in Sec. 3. We discuss our results and their implications to our future  
87 approach in Sec. 4 and conclude this paper with the main findings in Sec. 5.

## 88 **2. Experimental setup**

### 89 *2.1. Model and ensemble Kalman filter*

90 We use the Max Planck Institute Earth system model (MPI-ESM, Gior-  
91 getta et al. (2013)), version 1.0.02, which consists of ECHAM6 (Stevens et al.  
92 (2013), ECHAM is an acronym for **EC**MWF, European Centre for Medium-  
93 Range Weather Forecasts, and **H**amburg) for the atmospheric component  
94 ( $\approx 2.5^\circ$  horizontal resolution, 47 levels up to 1 hPa), and MPIOM (Max

95 Planck Institute Ocean Model, Jungclaus et al. (2013)) for the oceanic part  
96 ( $\approx 1.5^\circ$  horizontal resolution, 40 depth levels), both coupled once a day by  
97 OASIS3 (Ocean Atmosphere Sea Ice Soil, Valcke (2013)). In this study we  
98 do not apply any atmospheric assimilation nor nudging.

99 We implement the parallel data assimilation framework PDAF (Nerger and  
100 Hiller, 2013, <http://pdaf.awi.de>) in its offline mode together with the oceanic  
101 component MPIOM of MPI-ESM. PDAF has implemented several ensemble  
102 Kalman filter sub-types, we use the global SEIK filter in our experiments.

103 As with other ensemble Kalman filters, the process of assimilating observa-  
104 tions into MPI-ESM with SEIK can be sub-divided into three steps. Firstly,  
105 the forecast, where all ensemble members are independently evolved in time  
106 until an observation data set is going to be assimilated, we call this the “as-  
107 simulation interval”. Secondly, the Kalman update of the ensemble members  
108 with the observations, which we call the “analysis step”. Thirdly, the “re-  
109 initialization” of the ensemble based on the updated state and uncertainty  
110 from the analysis step. Then the re-initialized ensemble enters the forecast  
111 of the next assimilation interval.

112 In the following we give an abridged description of the global SEIK filter  
113 based on Nerger et al. (2006). A detailed description of the SEIK filter and  
114 a comparison with other sub-types of the ensemble-based Kalman filters can  
115 be found in Nerger et al. (2005).

116 We assume an already initialized ensemble of states with  $N$  members ( $\alpha =$   
117  $1, \dots, N$ ) at time  $t_i$ , with the size of the model state  $n$ :

$$\mathbf{X}_i = \{\mathbf{x}_i^\alpha\} \in \mathbb{R}^{n \times N}. \quad (1)$$

118 The non-linear model independently integrates the ensemble members for-  
 119 ward to time  $t_f$ .

$$\mathbf{X}_f = \{M_{f,i}(\mathbf{x}_i^\alpha)\} \in \mathbb{R}^{n \times N}, \quad (2)$$

120 with  $M_{f,i}$  representing the model operator. In the analysis step at time  $t_f$ , the  
 121 updated ensemble mean state  $\bar{\mathbf{x}}_a$  of size  $n$ , where the operator  $\bar{\dots}$  represents  
 122 the ensemble mean, is calculated from the forecast ensemble with

$$\bar{\mathbf{x}}_a = \bar{\mathbf{x}}_f + \mathbf{L}_f \mathbf{a}_f, \quad (3)$$

123 where the error subspace associated with the forecast ensemble is represented  
 124 by the columns of  $\mathbf{L}_f$ , which is the transformed forecast ensemble according  
 125 to:

$$\mathbf{L}_f := \mathbf{X}_f \mathbf{T} \in \mathbb{R}^{n \times (N-1)}, \quad (4)$$

$$\mathbf{T} := \begin{pmatrix} \mathbf{I}_{(N-1) \times (N-1)} \\ \mathbf{0}_{1 \times (N-1)} \end{pmatrix} - N^{-1} (\mathbf{1}_{N \times (N-1)}) \in \mathbb{R}^{N \times (N-1)}, \quad (5)$$

126 with the unit matrix  $\mathbf{I}$ , the null matrix  $\mathbf{0}$ , and  $\mathbf{1}$  is a matrix of ones. The  
 127 vector of weights  $\mathbf{a}_f$  has the size  $(N-1)$  and is calculated as

$$\mathbf{a}_f = \mathbf{U}_f (\mathbf{H}_f \mathbf{L}_f)^T \mathbf{R}_f^{-1} (\mathbf{y}_f^o - \mathbf{H}_f \bar{\mathbf{x}}_f) \quad (6)$$

128 with the observation vector  $\mathbf{y}_f^o$  of size  $o$  and it's associated measurement  
 129 operator  $\mathbf{H}_f$  and observation error covariance matrix  $\mathbf{R}_f \in \mathbb{R}^{o \times o}$ . The matrix  
 130  $\mathbf{U}_f$  is not calculated explicitly. Instead we use the LU-solver DGESV from  
 131 LAPACK (<http://www.netlib.org/lapack/>) together with  $\mathbf{U}_f^{-1}$ :

$$\mathbf{U}_f^{-1} = \rho N^{-1} (\mathbf{T}^T \mathbf{T})^{-1} + (\mathbf{H}_f \mathbf{L}_f)^T \mathbf{R}_f^{-1} \mathbf{H}_f \mathbf{L}_f \in \mathbb{R}^{(N-1) \times (N-1)}. \quad (7)$$

132 Here  $\rho$  represents the forgetting factor, which is proportional to the inverse  
 133 of the inflation factor described in Anderson and Anderson (1999). Hence,  
 134 a forgetting factor  $\rho$  smaller than 1 results in an artificial inflation of the  
 135 ensemble spread by a factor larger than 1.

136 For the re-initialization the updated ensemble of states is re-sampled accord-  
 137 ing to:

$$\mathbf{X}_a = \bar{\mathbf{X}}_a + \sqrt{N}\mathbf{L}_f\mathbf{C}_f^T\boldsymbol{\Omega}_f^T, \quad (8)$$

138 where  $\mathbf{C}_f \in \mathbb{R}^{(N-1) \times (N-1)}$  is obtained from a Cholesky decomposition applied  
 139 on  $\mathbf{U}_f^{-1}$ :

$$\mathbf{C}_f\mathbf{C}_f^T = \mathbf{U}_f^{-1}, \quad (9)$$

140 and  $\boldsymbol{\Omega}_f$  is a  $N \times (N - 1)$  random matrix with orthonormal columns.

141 Please note that neither the forecast nor the updated error covariance matrix  
 142 needs to be calculated explicitly, they are replaced according to

$$\mathbf{P} = \mathbf{L}\mathbf{C}^T\boldsymbol{\Omega}^T\boldsymbol{\Omega}\mathbf{C}\mathbf{L}^T, \quad (10)$$

143 and thus the SEIK analysis and re-initialization (Eqs. 3 and 8) only requires  
 144 the knowledge of

- the forecast ensemble  $\mathbf{x}_f^\alpha$ ,
- the observation vector  $\mathbf{y}_f^o$ ,
- the observation error covariance matrix  $\mathbf{R}_f$ ,
- and the forgetting factor  $\rho$ .

145 In our experiments, we did not use artificial inflation, leaving  $\rho = 1$ . Also,  
 146 we only use the global variant of the SEIK filter to allow for long-range and  
 147 cross-parameter covariances, no localization has been applied.

148 *2.2. Observations*

149 We assimilate observations of subsurface temperature and salinity from  
150 EN3 (Ingleby and Huddleston, 2007). In one experiment, we supplement the  
151 EN3 data with sea surface temperature from HadISST (Rayner et al., 2003),  
152 the combined data set is henceforth called EN3/HadISST. The EN3 data  
153 are used in the assimilation as unweighted averages per month and grid cell.  
154 For any grid cell and any month, all EN3 measurements, which fall within  
155 the specific grid cell in the specific month, are averaged to obtain one value  
156 per month and grid cell, both for temperature and salinity. The number of  
157 measurements within EN3 increased rapidly between 2001 and 2007 with the  
158 deployment of autonomous profiling floats from the Argo project (Roemmich  
159 et al., 2009). The HadISST data have been regridded to the MPI-ESM grid  
160 and supersede any EN3 data at the surface.

161 With the exception of the ocean surface, observations on a monthly time  
162 scale are limited, even in the upper ocean and even in the full Argo era after  
163 2007. Over the entire assimilation period (1996-2010) and on the MPI-ESM  
164 grid, EN3/HadISST provides for only 6% of the grid cells temperature data  
165 and for only 3% of the grid cells salinity data. These numbers slightly im-  
166 prove to 8% for temperature, and 7% for salinity, when only the Argo period  
167 (2004-2010) is considered (Fig. 1). In addition to the limited spatial cover-  
168 age, also the temporal coverage is limited: only a few grid cells are covered  
169 by observations on at least a yearly basis over the total assimilation time.  
170 The temporal coverage improves for the Argo era at depths above 2000 m.  
171 We heuristically chose observation uncertainties of 1 K for all temperatures  
172 and 1 psu for all salinities, so that the SEIK analysis update remains well

173 within the physically acceptable bounds of the model ( $-2^{\circ}\text{C}$  to  $40^{\circ}\text{C}$  for tem-  
174 perature and 0 psu to 52 psu for salinity). We also tested smaller uncertain-  
175 ties of 0.1 psu for salinity together with 1 K for temperature (not shown),  
176 as well as depth dependent uncertainties in the range of 0.1 K to 1 K for  
177 temperature and 0.01 psu to 0.1 psu for salinity (not shown), which showed  
178 similar gains during the analysis but more often caused updated tempera-  
179 tures and salinities outside the physically acceptable bounds of the model.  
180 In the SEIK filter no limitations are applied to the analysed field. Therefore  
181 it may generate unwanted temperatures and salinities while trying to honor  
182 sparse observations with small uncertainties, especially in it's global variant  
183 and with only 8 ensemble members.

### 184 *2.3. Assimilation experiments*

185 Three experiments are carried out, using the same model setup and the  
186 same initial conditions: (*i*) an unconstrained simulation without assimilation  
187 (NoAssim), (*ii*) an assimilation experiment using all subsurface temperature  
188 and salinity observations from EN3 supplemented by HadISST sea surface  
189 temperature (AllAssim), and (*iii*) an assimilation experiment using only sub-  
190 surface temperature and salinity observations from EN3 below 50 m depth  
191 (SubAssim).

192 The experimental configuration is summarized in Tab. 1. All three ex-  
193 periments are initialized at January 1st, 1996 from the long-term MiKlip  
194 baseline-1 assimilation (Pohlmann et al., 2013). Here, anomaly restoring  
195 to the European Centre for Medium-Range Weather Forecasts oceanic re-  
196 analysis ORAS4 and atmospheric re-analysis ERA and ERA Interim is ap-  
197 plied to keep the assimilation close to the climatological state of the model.

198 The three experiments consist of eight ensemble members each. The initial-  
199 ization ensembles for all experiments are calculated from a daily data set of  
200 baseline-1 in January 1996. For the assimilation experiments we use mini-  
201 mum second order exact sampling (Pham, 2001; Nerger et al., 2005), such  
202 that the ensemble mean and covariance matrix of the January 1996 baseline-1  
203 assimilation is exactly represented by the initialization ensemble. This differs  
204 slightly from NoAssim, where each of the eight ensemble members has been  
205 assigned with the state of the baseline-1 experiment at the end of days 1 to  
206 8 in January 1996. The analysis is conducted at the end of each month, and  
207 only observations from this month are considered in the SEIK update. All  
208 experiments are carried out for 15 years (from January 1, 1996 to December  
209 31, 2010).

#### 210 *2.4. Model-observation comparison*

211 In our study our prime interest is in the assimilation of the observed  
212 oceanic variability in terms of deviations from the seasonal cycle. For the  
213 comparison with observations, we therefore calculate the monthly averaged  
214 ensemble mean, which includes the state prior to the analysis step at the end  
215 of the month, and remove the mean seasonal cycle and any linear trend for  
216 each experiment, except for the Atlantic meridional overturning circulation,  
217 see below. Then we compute the root mean square error, RMSE, and corre-  
218 lation coefficient against observations for each grid cell.

219 We calculate RMSE and correlation coefficients for the global average as well  
220 as for regional averages in the following regions: Northern Atlantic Ocean,  
221 Indian Ocean, and Niño 3.4. The regions are outlined in Fig. 1.

222 For each experiment we compute the significance of the calculated RMSE and

223 correlation coefficient against observations as following: For each grid cell we  
224 apply a bootstrapping scheme with 500 bootstraps of the 15-year monthly  
225 averaged ensemble mean. We then calculate the corresponding probability  
226 distribution and determine the significance at the 95% level with a two-tailed  
227 test of this distribution.

228 For sea surface temperature (SST) and potential temperature at 100 m depth  
229 (T100), we compare the simulated temperature field against the observations  
230 from EN3/HadISST. Times and grid cells without EN3/HadISST data are  
231 omitted. At the surface, in most grid cells the time series consists of 180  
232 points, since there is an observation from HadISST in each month. At 100 m  
233 depth, the time series often consists of less than 10 points, given the lack of  
234 sub-surface oceanic observations (Fig. 1a). Here, and also at larger depths,  
235 the calculation of a meaningful RMSE or correlation coefficient becomes dif-  
236 ficult.

237 For the ocean heat content (HC700), we compare the simulated heat con-  
238 tent from the surface down to 700 m depth with the heat content data set  
239 from the National Oceanic and Atmospheric Administration Ocean Climate  
240 Laboratory (NOAA OCL) (Levitus et al., 2012). The NOAA OCL data set  
241 comprises seasonal (3 monthly) heat contents, we apply a 3 month averaging  
242 to our data accordingly.

243 For the simulated sea surface height (SSH), we compare our experiments  
244 with satellite based measurements of the absolute dynamic topography. The  
245 altimeter products were produced by Ssalto/Duacs and distributed by Aviso,  
246 with support from CNES (<http://www.aviso.altimetry.fr/duacs/>), hereafter  
247 AVISO.

248 We compare the simulated Atlantic meridional overturning circulation (AMOC)  
249 time series at 26°N from 2004 to 2010 at 1020 m with the observations from  
250 the Rapid Climate Change-Meridional Overturning Circulation and Heatflux  
251 Array (RAPID-MOCHA, Cunningham et al. (2007); Smeed et al. (2014)).  
252 In the model, the AMOC is derived from the simulated meridional velocity  
253 field. There is an overlap of only 6 years between simulations and observa-  
254 tions. We therefore do not remove the linear trend nor the seasonal cycle  
255 from the simulated AMOC, rather we apply a three months running mean  
256 to the time series. We use the ensemble mean time series and its standard  
257 deviation to estimate significant changes between the experiments.

258

### 259 **3. Results**

260 In this section we assess the simulated temperature, ocean heat content,  
261 sea surface height and Atlantic meridional overturning circulation in terms  
262 of RMSE and correlation coefficient against observations and with reference  
263 to the unconstrained experiment NoAssim.

#### 264 *3.1. Surface temperature*

265 The observed SST from EN3/HadISST has been directly assimilated in  
266 AllAssim, but not in SubAssim. The RMSE of the simulated SST against  
267 observations shows similar patterns for all three experiments: large RMSE  
268 ( $>0.7$  K) in the Northern Atlantic, equatorial East Pacific, Northwest Pacific,  
269 and Southern Ocean, and small RMSE ( $<0.7$  K) in other regions. The mag-  
270 nitude of the RMSE for the global averaged SST does not differ very much  
271 between the two assimilation experiments (AllAssim: 0.55 K, SubAssim:

272 0.59 K). However, it is larger in both assimilations than in the unconstrained  
273 experiment NoAssim (0.45 K, Fig. 2 a,c,e), although the latter is not sig-  
274 nificant at the 95% level. Areas with significant RMSE values are the trop-  
275 ical Pacific Ocean, and some parts of the Indian Ocean as well. In the  
276 Indian Ocean both assimilation experiments degrade the RMSE (0.47 K for  
277 AllAssim, 0.52 K for SubAssim) compared to NoAssim (0.37 K, Tab 2). In  
278 the Niño 3.4 region the RMSE is smaller in the assimilation experiments than  
279 in NoAssim: 0.89 K in AllAssim and 0.82 K in SubAssim, 0.95 K in NoAssim.  
280 In the Northern Atlantic Ocean the RMSE of the assimilation experiments  
281 (0.90 K for AllAssim, 1.0 K for SubAssim) is larger than in NoAssim (0.67 K).  
282 However, these values are not significant at the 95% level.

283 It is not surprising that the RMSE is not improved at every individual grid  
284 cell, however, the degradation of the RMSE on the regional and global scale  
285 is an issue with regard to the SEIK implementation and will be discussed in  
286 Sec. 4.

287 Compared to the RMSE the patterns for the correlation coefficient of the  
288 simulated SST against observations show larger differences between the three  
289 experiments (compare Fig. 2 a,c,e and b,d,f). The correlation of the global av-  
290 eraged SST is higher for the two assimilation experiments (0.09 for AllAssim,  
291 0.13 for SubAssim) than for NoAssim (0.06) with a significance level  $\pm 0.02$   
292 (Tab. 2). The improvements in both AllAssim and SubAssim are most  
293 prominent in the Tropics, and are generally stronger in SubAssim than in  
294 AllAssim. The averaged correlation coefficient in the Niño 3.4 region is 0.14  
295 for NoAssim, 0.38 for AllAssim, and 0.56 for SubAssim with a significance  
296 level of  $\pm 0.13$ . In the Northern Atlantic the averaged correlation coefficient

297 is degraded due to the assimilation (0.04 in AllAssim, 0.02 in SubAssim,  
298 from 0.05 in NoAssim, although all coefficients are too small to be significant  
299 ( $\pm 0.05$ )). In the Indian Ocean only SubAssim (0.14) shows improvement  
300 over NoAssim (0.09), the significance level is at  $\pm 0.04$ .  
301 Hence, for SST, the SEIK assimilation does not improve the RMSE against  
302 observations, except for the Niño 3.4 region. In contrast, the SEIK assim-  
303 ilations does improve the correlation coefficient against observations on the  
304 global average, largest improvements are in the tropical oceans, especially the  
305 tropical Pacific. The largest region with degradation is in the Northwestern  
306 Pacific in SubAssim (Fig. 2f).

307

### 308 *3.2. Sub-surface temperature*

309 The observed T100 from EN3 has been directly assimilated in both as-  
310 simulation experiments. The RMSE of the globally averaged simulated T100  
311 against observations (Fig. 3a,c,e and Tab. 2) is smaller in NoAssim(0.48 K)  
312 than in either of the assimilations (0.68 K in AllAssim and 0.74 K in SubAssim).  
313 Even in the Niño 3.4 region the RMSE is smaller in NoAssim (0.90 K) com-  
314 pared to AllAssim (0.95 K) and SubAssim (1.1 K). However, over most areas  
315 the RMSE is not significant in either experiment, which may be caused by  
316 the large undersampling in time of the T100 grid cells due to the sparsity  
317 of T100 observations. For the same reason the correlation coefficient against  
318 observations for T100 is spatially very noisy and not significant for almost  
319 any grid cell (Fig. 3b,d,f).

320 For the three selected regions, the depth profiles down to 500 m of the area  
321 averaged RMSE of simulated temperature against observations show degra-

322 dation due to assimilation (Fig. 4a,c,e). In the Northern Atlantic Ocean and  
323 in the Indian Ocean the RMSE is for all depths smallest in NoAssim, the  
324 difference between AllAssim and SubAssim is negligible. In the Niño 3.4 re-  
325 gion the RMSE is improved due to the assimilation only at the surface. For  
326 depths below the surface down to 150 m the RMSE is degraded in AllAssim  
327 and even more in SubAssim when compared to NoAssim. Below 150 m, the  
328 RMSE is the same in all three experiments. The depth profiles of the area av-  
329 eraged correlation coefficient of simulated temperature against observations  
330 (Fig. 4b,d,f) show little difference between the three experiments, except for  
331 the upper 100 m in the Niño 3.4 region, where both assimilation experiments  
332 show higher correlation coefficients than NoAssim, and for depths between  
333 200 m and 300 m in the Niño 3.4 region, where AllAssim shows higher cor-  
334 relation than both NoAssim and SubAssim.

335

### 336 *3.3. Heat content*

337 The observed 0-700 m heat content (HC700) from NOAA OCL has not  
338 been directly assimilated in our experiments. The global patterns in HC700  
339 RMSE against observations (not shown) are similar to those from SST in  
340 Fig. 2. The SEIK assimilation does not improve the RMSE of the global  
341 averaged or the regional averaged HC700, except for a small improvement  
342 in SubAssim in the Niño 3.4 region (Tab. 2). The correlation coefficients  
343 against observations are shown in Fig. 5. The correlation of the global aver-  
344 aged HC700 is improved due to SEIK assimilation (0.08 for both AllAssim  
345 and SubAssim compared to 0.05 for NoAssim), significance level  $\pm 0.02$ . On  
346 the regional scale, improvements due to the assimilation are confined to the

347 equatorial Pacific, e.g. in the Niño 3.4 region the correlation of the averaged  
348 HC700 is 0.30 for AllAssim, 0.45 for SubAssim, against 0.08 for NoAssim,  
349 significance level ( $\pm 0.22$ ). We find degradations in some parts of the North-  
350 eastern Pacific and Northeastern Atlantic. The correlation of the averaged  
351 HC700 over the Northern Atlantic is 0.09 for AllAssim, 0.08 for SubAssim,  
352 from 0.10 for NoAssim, significance level ( $\pm 0.05$ ).

### 353 *3.4. Sea surface height*

354 The observed SSH from AVISO has not been directly assimilated in our  
355 experiments. The RMSE of SSH with respect to observations shows similar  
356 patterns and significant areas as the RMSE of SST, they are not shown here.  
357 The averaged RMSE for the three selected regions are given in Tab. 2, there  
358 is hardly any difference between the three experiments. The global patterns  
359 in the correlation coefficient against observations resemble those from SST  
360 in an attenuated form (Fig. 6 versus Fig. 2b,d,f). The SEIK assimilation  
361 improves the correlation in the global average from 0.05 in NoAssim to 0.09  
362 in both AllAssim and SubAssim, significance level  $\pm 0.01$ . We find most im-  
363 provements in the tropical oceans, e.g. the correlation of the averaged SSH  
364 over the Indian Ocean is increased from 0.00 in NoAssim to 0.12 in AllAssim  
365 and 0.13 in SubAssim, significance level  $\pm 0.04$ , and the correlation of the  
366 averaged SSH over the Niño 3.4 region is increased from 0.15 in NoAssim to  
367 0.36 in AllAssim and 0.51 in SubAssim, with a significance level of  $\pm 0.16$ .  
368 The SEIK assimilation degrades the correlation in some parts of the Northern  
369 Pacific, while in the Northern Atlantic there is hardly any difference between  
370 the three experiments.

371

372 *3.5. AMOC*

373 The observed AMOC has not been directly assimilated in our experi-  
374 ments. Compared to temperature, HC700, and SSH, the AMOC represents  
375 a highly integrated quantity.

376 The three experiments have a similar 15-year mean AMOC cell (Fig. 7),  
377 with the maximum AMOC at 35°N and at 1020 m depth. However, there  
378 are noticeable small-scale differences between the three experiments. Firstly,  
379 the maximum strength of the AMOC, which is 22 Sv in NoAssim, 20 Sv in  
380 AllAssim, and 22 Sv in SubAssim. Secondly, between 20°N and 50°N, the  
381 maximum AMOC in SubAssim is generally larger than 20 Sv, whereas it is  
382 only 18 Sv in NoAssim and AllAssim. Thirdly, between 20°N and 50°N, the  
383 minimum AMOC of -2 Sv is maintained as far as 40°N in NoAssim, as far as  
384 50°N in AllAssim, but only as far as 25°N in SubAssim. As a consequence,  
385 between 20°N and 50°N the boundary between positive and negative simu-  
386 lated AMOC is shifted 100 m up in AllAssim, but 100 m down in SubAssim,  
387 when compared to NoAssim. There is a noticeable difference in the depth of  
388 this boundary between the two assimilations of about 200 m.

389 As there are no observations available to compare the full AMOC cell with,  
390 we now turn to the observed 26°N time series from RAPID-MOCHA (Fig. 8a,  
391 Tab. 3). The RMSE against observations does not show significant differ-  
392 ences between the three experiments ( $3.2 \pm 0.4$  Sv for both AllAssim and  
393 SubAssim,  $3.1 \pm 0.6$  Sv for NoAssim). The correlation with the observed  
394 AMOC is decreased in AllAssim ( $0.32 \pm 0.16$ ) and increased in SubAssim  
395 ( $0.59 \pm 0.17$ ) when compared to NoAssim ( $0.42 \pm 0.29$ ), but only the im-  
396 provement of SubAssim over AllAssim is significant.

397 In our experiments, we do not expect that an unconstrained atmosphere cap-  
398 tures the correct zonal-mean wind variability. It is therefore not surprising  
399 that none of our experiments matches the anomalous weak observed AMOC  
400 in 2009/2010, which was related to anomalous surface winds in 2009/2010  
401 and the resulting anomalous wind-driven transport.

402 We remove the direct atmospheric influence on the AMOC at 26°N by sub-  
403 tracting the zonal-mean wind driven transport, which is calculated from  
404 the simulated zonal wind stress at the ocean’s surface (Mielke et al., 2013).  
405 Within the three experiments the RMSE of AMOC minus Ekman (Fig. 8b)  
406 differs more than the RMSE of the full AMOC. It is smallest in SubAssim  
407 with  $2.4 \pm 0.1$  Sv, compared to  $2.6 \pm 0.5$  Sv in NoAssim and  $3.1 \pm 0.1$  Sv  
408 in AllAssim. The correlation with observations is smaller in AMOC mi-  
409 nus Ekman than in the full AMOC. Nevertheless, within the three experi-  
410 ments the correlation of AMOC minus Ekman with observations is improved  
411 from  $0.23 \pm 0.38$  in NoAssim to  $0.28 \pm 0.04$  in AllAssim and  $0.41 \pm 0.04$   
412 in SubAssim. Based on the standard deviation, the improvement of both  
413 RMSE and correlation against observations in AMOC-Ekman from AllAssim  
414 to SubAssim are significant, while the other changes are not significant.

415 We notice that the standard deviation for RMSE and correlation, along  
416 with the ensemble spread, is always larger in NoAssim than in AllAssim  
417 and SubAssim, while the difference between the latter two is negligible. For  
418 AMOC the standard deviations of NoAssim are larger by a factor of 1.5 to  
419 2, for AMOC minus Ekman by a factor of 5 to 10 (Tab. 3). The SEIK as-  
420 similation reduces the RMSE and correlation variability within the ensemble  
421 for the AMOC, and even more for AMOC minus Ekman, where the direct

422 atmospheric influence is largely reduced.  
423 Summarizing the results, for all analyzed variables there is little improve-  
424 ment over NoAssim due to the SEIK assimilation in the RMSE against ob-  
425 servations, but some improvement in the correlation against observations.  
426 However, improvements over NoAssim are more often stronger in SubAssim  
427 than in AllAssim.

#### 428 **4. Discussion**

429 The main questions arising from our results are: Why is the impact of  
430 the SEIK assimilations AllAssim and SubAssim, when compared to the un-  
431 restricted experiment NoAssim, small on the global scale? Why are improve-  
432 ments from assimilation restricted to the correlation of simulated against  
433 observed temperatures and SSH in the tropical oceans, and to correlation im-  
434 provements in the AMOC and AMOC minus Ekman at 26°N in SubAssim?  
435 Firstly, the atmosphere in our assimilation is as unconstrained as in NoAssim.  
436 Therefore any change of the oceanic fields due to assimilation is quickly offset  
437 by the influence of the unconstrained atmosphere, the number of oceanic ob-  
438 servations is too small to maintain the gains expected from their assimilation  
439 over the whole assimilation interval, this supports the result of (Pohlmann  
440 et al., 2009) that there are too few oceanic observations to have an im-  
441 pact. On a monthly scale, the offset is strong in the mid-latitudes, leading  
442 to a poorer performance of the assimilation system, and weak in the Trop-  
443 ics, where assimilation gains are retained over the assimilation interval. A  
444 shorter assimilation interval than one month would be desirable for the mid-  
445 latitudes, however, in this case the number of available observations would

446 drop even more. Also, the lower atmosphere’s high frequency variability may  
447 be in conflict with the upper ocean variability, which leads to the significantly  
448 poorer performance of AllAssim against SubAssim in terms of SST correla-  
449 tion. A simultaneously constrained atmosphere may help here, but only if  
450 it does not destroy the oceanic assimilation effort. The variabilities on both  
451 side of the atmosphere-ocean boundary have to be addressed in a reconciled  
452 way, which is beyond the scope of our study.

453 Secondly, we are aware of the fact that we only use a basic setup of the SEIK  
454 filter: the ensemble size of 8 is small, together with the global variant of the  
455 SEIK filter the covariance matrices are strongly rank-deficient. As a result  
456 the filter performance is limited, accounting for analyzed temperatures and  
457 salinities being outside the physical bounds of the model, and also accounting  
458 for degradation of temperature RMSE on a large scale. A larger ensemble  
459 size together with the localized variant of the SEIK filter would be more  
460 appropriate.

461 Thirdly, the uncertainty assigned to the oceanic observations, i.e. their rep-  
462 resentativeness, needs to be properly utilized for the benefit of a better per-  
463 formance of the SEIK assimilation. For the reason of model stability and  
464 setup simplicity we chose uncertainties of 1 K for temperature and 1 psu for  
465 salinity, both independent in time and space. The model uncertainty, which  
466 is ultimately calculated from the variability within the simulated ensemble, is  
467 smaller than 1 K or 1 psu at almost any grid cell. Thus, a large weight is put  
468 on the model and a small one on the observations. We see two possibilities to  
469 put more weight on observations and improve the SEIK performance without  
470 compromising the model stability: Firstly, the use of sub-surface observation

471 uncertainties based on either the true or modeled representativeness of ob-  
472 servations, and secondly, the inflation of the ensemble.

473 It is also almost certain that the model's preferential oceanic circulation pat-  
474 tern deviates from the one established in the real ocean. An assimilation,  
475 which puts too strong an emphasis on the observed state may actually coun-  
476 teract any potential improvement in the circulation pattern. Müller et al.  
477 (2015) showed that strong restoring of ocean temperature and salinity to  
478 re-analysis data eventually draws the model's state closer to the observed  
479 ocean but results in a wrongly simulated AMOC. In this sense, model errors  
480 in terms of biases in the circulation cannot and perhaps should not always  
481 be corrected too strongly by data assimilation.

482 Further studies are needed with the ensemble Kalman filter to address the  
483 direct assimilation of oceanic observations in a global coupled climate model:  
484 the filter setup needs to be improved (including localization), as well as the  
485 weighting of the observations and the calibration of the ensemble. However,  
486 for a successful oceanic assimilation in a coupled climate model the influence  
487 of the atmosphere needs to be properly handled. In the context of coupled  
488 data assimilation Zhang et al. (2013) showed that a consistent and balanced  
489 atmosphere-ocean constraint is mandatory to initialize predictions, especially  
490 on the decadal scale, the corresponding atmosphere-only and ocean-only as-  
491 similation, respectively, perform worse than the coupled approach.

492

493 **5. Conclusion**

494 We assimilate temperature and salinity observations with a global en-  
495 semble Kalman filter into the global coupled model MPI-ESM at a monthly  
496 time interval over the period 1996 to 2010. Comparing the results of two  
497 assimilation experiments and an unconstrained experiment, we conclude:

- 498 • For the analyzed quantities, the ensemble Kalman filter assimilation  
499 improves the model’s sea surface temperature, heat content and sea  
500 surface height variability with respect to observations in the tropical  
501 oceans. Improvements due to assimilation are largest for the sea surface  
502 temperature in the Niño 3.4 region.
  
- 503 • The assimilation experiment that only incorporates oceanic observa-  
504 tions below 50 m depth results in larger improvements of the simulated  
505 variability with respect to observations than the assimilation experi-  
506 ment that incorporates oceanic observations over the entire water col-  
507 umn. These results suggest that surface variability in a coupled model  
508 assimilation with an unconstrained atmosphere can potentially be im-  
509 proved when the boundary between ocean and atmosphere is not too  
510 strongly restricted by assimilation, and the variability at the boundary  
511 is thus determined by the model dynamics.
  
- 512 • In addition to changes in the directly assimilated temperature field, the  
513 assimilation experiment with observations only below 50 m depth im-  
514 proves the variability of the simulated Atlantic Meridional Overturning  
515 Circulation at 26°N over the unconstrained experiment.

516 Given the basic implementation of the ensemble Kalman filter we used, our  
517 study is only the first, and successful, step towards a weakly coupled data  
518 assimilation system with the global coupled model MPI-ESM.

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Table 1: Overview of the three experiments carried out. AllAssim: assimilation of EN3/HadISST oceanic temperatures and salinities at all model levels, SubAssim: assimilation of EN3 temperatures and salinities below 50 m only, NoAssim: no assimilation in the ocean. All three experiments use an identical setup for the remaining components of MPI-ESM. They are all initialized from the January 1996 MiKlip baseline-1 assimilation (Pohlmann et al., 2013).

	AllAssim	SubAssim	NoAssim
assim. data	EN3 and HadISST	EN3 only below 50m	- -
assim. interval	1 month		-
init. method	minimum 2nd order exact sampling		1 day lagged
init. data	January 1996 MiKlip baseline-1		
resolution	GR15L40 ocean, T63L47 atmosphere		
start date	1996-01-01		
end date	2010-12-31		
ens. size	8		

Table 2: RMSE and correlation of area averaged monthly sea surface temperature (SST, against HadISST), monthly 100 m potential temperature (T100, against EN3), three-monthly 0-700 m heat content (HC700, against NOAA OCL heat content), and monthly sea surface height (SSH, against AVISO) for the three experiments NoAssim, AllAssim, SubAssim. The quantities have been averaged over the globe and over three selected regions: Northern Atlantic Ocean, Indian Ocean, and Niño 3.4 region. The units for RMSE are K (SST, T100), EJ (HC700), cm (SSH). Values, which are not significant at the 95% level, are written in italics. For each parameter and basin the lowest RMSE and highest correlation coefficient is underlined.

	RMSE			correlation		
	NoAssim	AllAssim	SubAssim	NoAssim	AllAssim	SubAssim
global						
SST	<u>0.45</u>	0.55	0.59	0.06	0.09	<u>0.13</u>
T100	<u>0.48</u>	0.68	0.74	0.03	0.03	<u>0.05</u>
HC700	<u>10</u>	14	15	0.05	0.08	<u>0.08</u>
SSH	<u>6.0</u>	6.5	6.7	0.05	0.09	<u>0.09</u>
North Atl.						
SST	<u>0.67</u>	0.90	1.0	<u>0.05</u>	0.04	0.02
T100	<u>0.55</u>	0.93	0.94	-0.01	-0.01	0.03
HC700	<u>7.4</u>	9.4	9.5	<u>0.10</u>	0.09	0.08
SSH	<u>7.5</u>	8.3	8.6	0.01	<u>0.05</u>	0.04
Indian O.						
SST	<u>0.37</u>	0.47	0.52	0.09	0.09	<u>0.14</u>
T100	<u>0.64</u>	0.88	0.95	0.03	0.06	<u>0.10</u>
HC700	<u>11</u>	15	16	0.00	0.10	<u>0.15</u>
SSH	<u>7.4</u>	7.5	7.8	0.00	0.12	<u>0.13</u>
Niño 3.4						
SST	0.95	0.89	<sup>31</sup> <u>0.82</u>	0.14	0.38	<u>0.56</u>
T100	<u>0.90</u>	0.95	1.1	0.11	0.17	<u>0.18</u>
HC700	15	14	<u>13</u>	0.08	0.30	<u>0.43</u>
SSH	7.5	7.1	<u>6.7</u>	0.15	0.36	<u>0.51</u>

Table 3: RMSE (in Sv) and correlation of AMOC and AMOC minus Ekman at 26°N with respect to RAPID-MOCHA, monthly averaged data 2004-2010 with three month running mean. The experiment with the lowest RMSE and higher correlation coefficient is indicated in bold.

	RMSE			correlation		
	NoAssim	AllAssim	SubAssim	NoAssim	AllAssim	SubAssim
AMOC	<b>3.1</b>	3.2	3.2	0.42	0.32	<b>0.59</b>
spread	2.8-4.4	2.8-4.0	2.8-4.0	-0.20-0.60	0.04-0.52	0.25-0.69
std.-dev.	0.6	0.4	0.4	0.29	0.16	0.17
AMOC-Ekman	2.6	3.1	<b>2.4</b>	0.23	0.28	<b>0.41</b>
spread	2.2-3.6	3.0-3.2	2.3-2.6	-0.30-0.60	0.23-0.37	0.32-0.46
std.-dev.	0.5	0.1	0.1	0.38	0.04	0.04

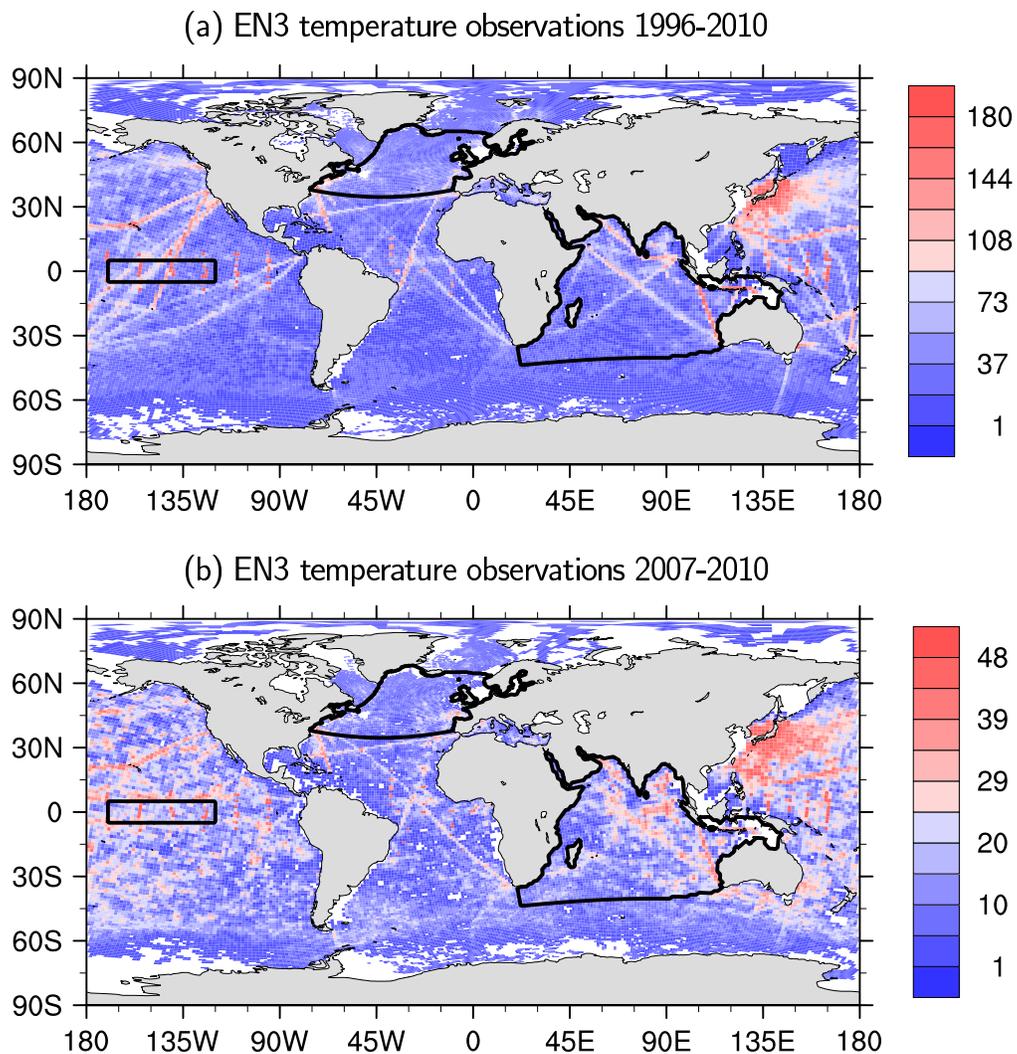


Figure 1: Number of available temperature observations from EN3 at the model's 100 m level as prepared for the monthly assimilation interval for (a) total assimilation time from January 1996 to December 2010 (180 monthly observations possible), and (b) full Argo era overlapping with our experiments from January 2007 to December 2010 (48 monthly observations possible). White grid cells do not contain any EN3 data.

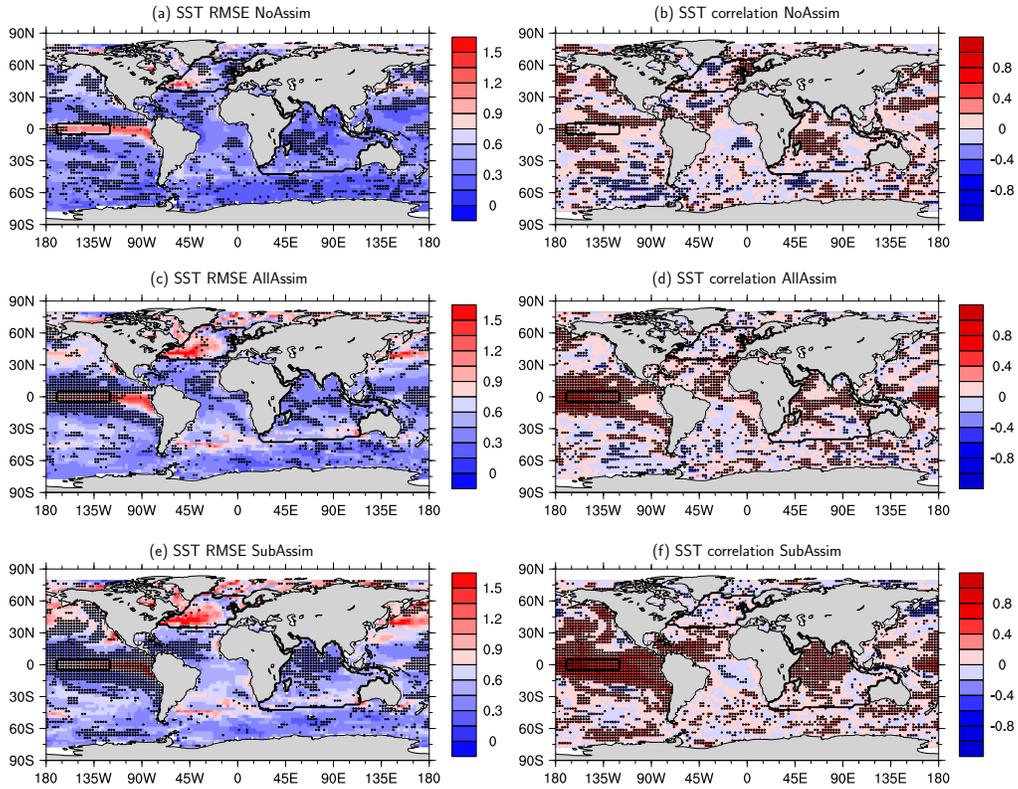


Figure 2: RMSE (a,c,e) and correlation (b,d,f) over 15 years of potential temperature with respect to EN3/HadISST in K at the surface for NoAssim (a,b), AllAssim (c,d), and SubAssim (e,f). Stippling indicates values, which are significant at the 95% level. White grid cells do not contain any EN3/HadISST data. The black outlines represent the three regions, which have been closer examined: the Northern Atlantic Ocean, the Niño 3.4 region in the equatorial Pacific Ocean, and the Indian Ocean.

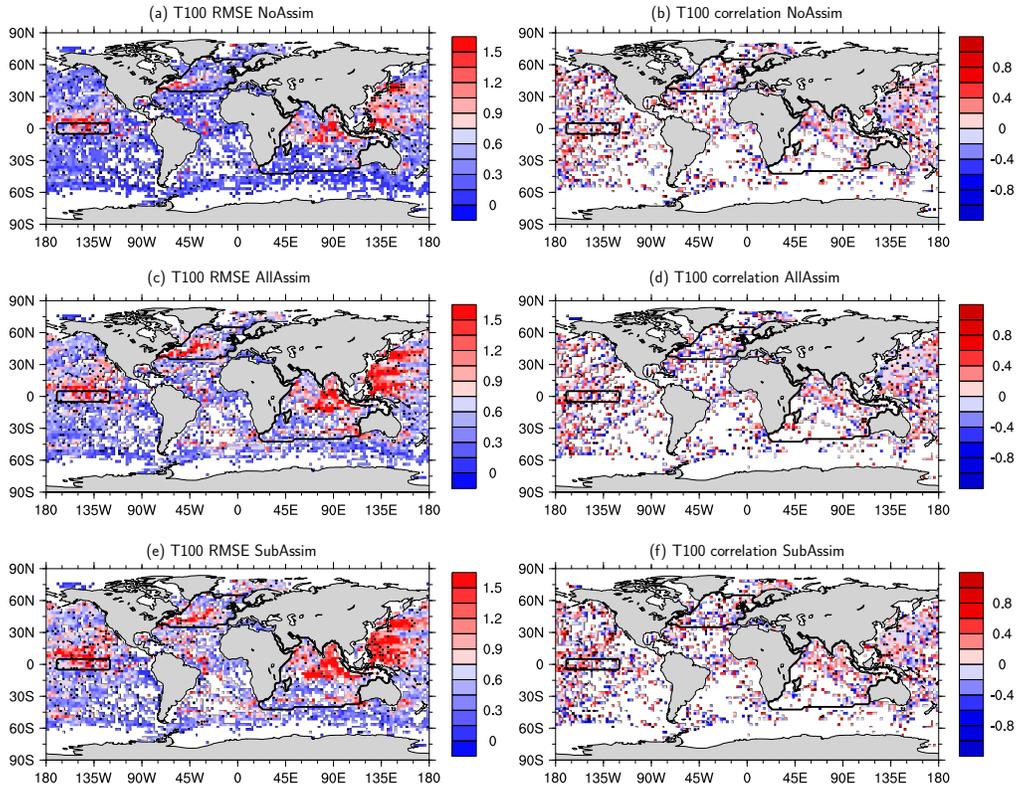


Figure 3: RMSE (a,c,e) and correlation (b,d,f) over 15 years of potential temperature with EN3/HadISST at 100 m depth for NoAssim (a,b), AllAssim (c,d), and SubAssim (e,f). Stippling indicates values, which are significant at the 95% level. White grid cells do not contain any EN3/HadISST data. The black outlines represent the Northern Atlantic Ocean, the Niño 3.4 region in the equatorial Pacific Ocean, and the Indian Ocean.

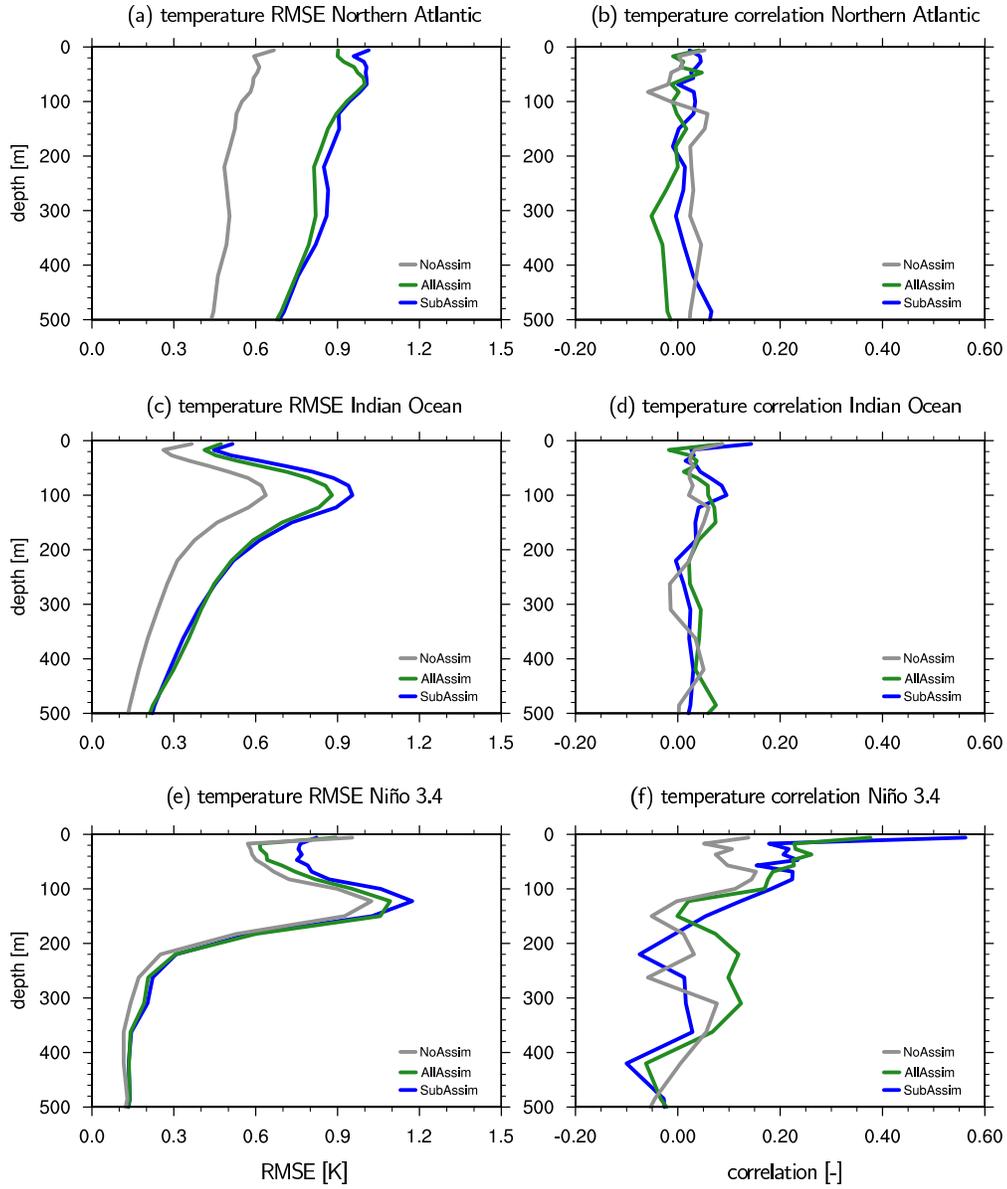


Figure 4: Area average of 15-year RMSE (a,c,e, in K) and correlation (b,d,f) of potential temperature with respect to EN3/HadISST for depths down to 500 m for NoAssim (gray), AllAssim (green), and SubAssim (blue) for the Northern Atlantic Ocean (a,b), the Indian Ocean (c,d), and the Niño 3.4 region (e,f).

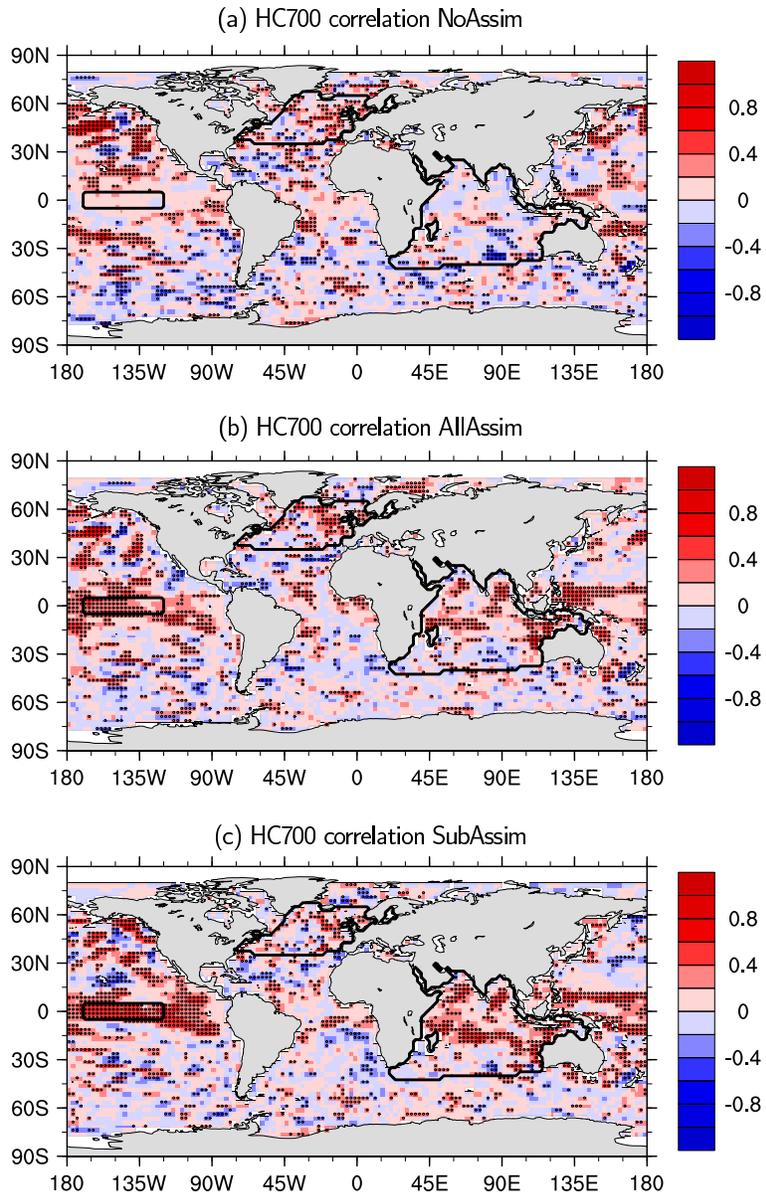


Figure 5: Correlation over 15 years of 3-month average 0-700 m heat content with NOAA OCL, (a) NoAssim, (b) AllAssim, (c) SubAssim. Stippling indicates values, which are significant at the 95% level. White grid cells do not contain any NOAA OCL data. The black outlines represent the Northern Atlantic Ocean, the Niño 3.4 region in the equatorial Pacific Ocean, and the Indian Ocean.

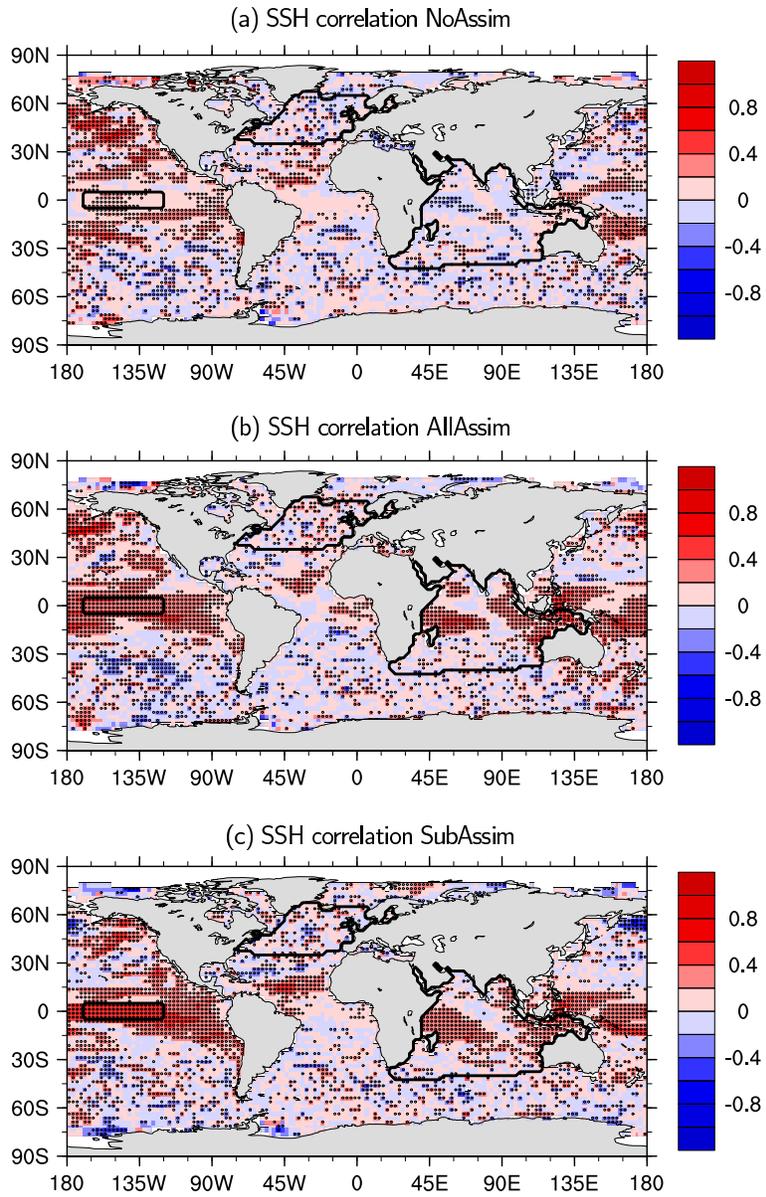


Figure 6: Correlation over 15 years of sea surface height with AVISO, (a) NoAssim, (b) AllAssim, (c) SubAssim. Stippling indicates values, which are significant at the 95% level. White grid cells do not contain any AVISO data. The black outlines represent the Northern Atlantic Ocean, the Niño 3.4 region in the equatorial Pacific Ocean, and the Indian Ocean.

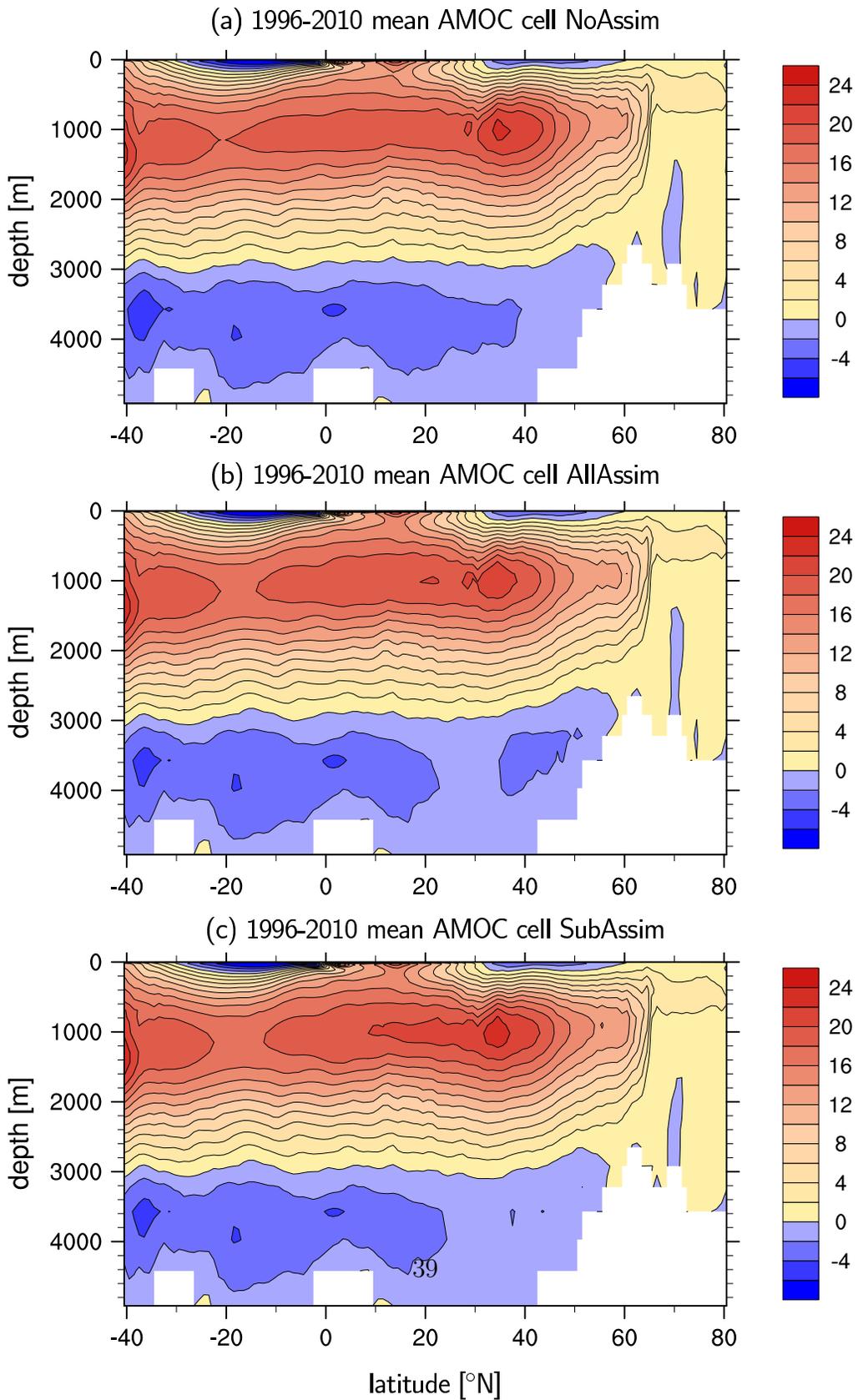


Figure 7: The 15-year mean Atlantic meridional overturning circulation in Sv as simulated

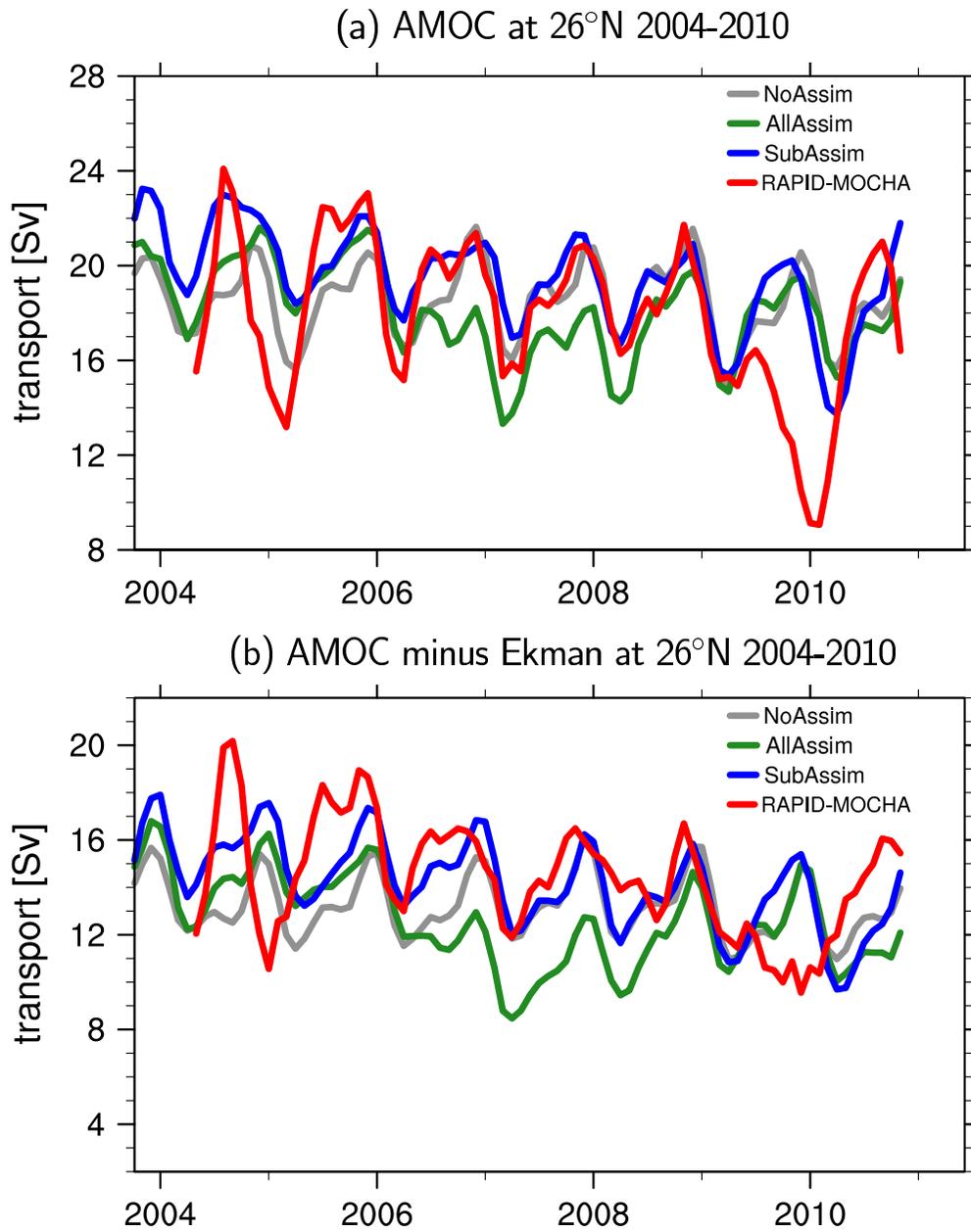


Figure 8: (a) Atlantic meridional overturning circulation (AMOC) and (b) AMOC with zonal-mean wind driven transport removed (AMOC minus Ekman) at 26°N of NoAssim (gray), AllAssim (green), SubAssim (blue), and observations from RAPID-MOCHA (red, Cunningham et al. (2007); Smeed et al. (2014)). A three month running mean filter has been applied to the monthly data.