Dear Editor of Geoscientific Model Development,

We modified the manuscript according to the comments and queries from the three reviewers. To fulfill their requests, we

1) Clarified several sections of the main text by focusing our analysis on the root-mean squared error (RMSE) and removing information on the difference between modeled and observed spatial variability ( $\Delta\sigma$ ). We included supplementary figures to several sections in order to support our hypotheses and strengthen our analysis.

2) Included one additional IPCC-class Earth system model (ESM) to our analyses. This extends the current analysis to an ensemble of 15 IPCC-class ESMs. Accordingly, we have revised all computations and updated all figures of the manuscript.

3) Added two new subsections to the revised manuscript to satisfy the request to include further discussion on the limitation of our framework. These are a new subsection dealing with the assessment of the simple drift model with IPSL-CM5A-LR as well as an extended discussion of the limitations of our framework.

Finally, we also introduce two co-authors (O. Aumont and A. Romanou) for their expertise on their model and their help to address the comments and queries from the three reviewers.

Please find a detailed response to each question/comment hereafter in blue (text fragments are *in blue italics*).

# # Editor

The column for model INMCM4 is shown in a colour (red) that does not appear in the key to the figure. Presumably this colour is a simple error as the text does not identify INMCM4 as undertaking a unique spin-up strategy.

We thank the Editor for his comment. It was indeed an error. Figure 1 was updated to improve its readability (bar plot enlarged and cross hatching modified). An additional model (CNRM-ESM1) was added to the analysis. The model is detailed in Séférian et al. (2015).

# Referee #1

Inconsistent strategies to spin up models in CMIP5: implications for ocean biogeochemical model performance assessment. Séférian et al

This study examines spin-up and drift in ocean biogeochemical properties using a spinup run from a single model and archived model output from CMIP5. In particular the study demonstrates the need to take drift into account when assessing model skill. I think that this is a useful study that highlights an important issue that is probably not given enough attention. I do have some issues with the analysis undertaken however that need to be addressed or clarified before I think this manuscript is ready for publication.

We appreciate the reviewer's careful reading and suggestions for corrections. Most of his suggestions are addressed in the revised manuscript.

# 8754:

However, since these models are typically initialized from observations, initialization and equilibration of climate variables are the most model-dependent protocols that could introduce errors or drifts in modeled fields with consequences on skill score metrics.

By 'equilibration' do you mean spin-up procedure. Sentence isn't very clear

We agree that the use of "equilibration" might be confusing.

We consider the spin-up procedure to encompass: (1) the initial conditions, (2) the spinup time (duration of the spin-up simulation at the end of which a "quasi-steady-state equilibrium" is declared) and (3) the method to achieve this quasi-steady-state equilibrium (it can consist in an offline mode simulation or a coupled mode simulation called online in the manuscript).

We modified the sentence as follows:

# Revised:

"However, since these models are typically initialized from observations, the spin-up procedure of climate variables are the most model-dependent protocols that could introduce errors or drifts in modeled fields with consequences on skill score metrics."

# 8755:

# First paragraph

There is an assumption here that the model will reach an equilibrium. This is not clear. Sen Gupta et al 2013 show little evidence for equilibration in many physical variables. Work by Will Hobbs and collaborators (soon to be published) shows that a large component of drift in physical variables is associated with spurious energy leaks in the models that are independent of model state. As such the models just keep drifting. Indeed in your Fig 2b I don't really see clear evidence for equilibration.

'quasi-equilibrium state is assumed for the interior ocean tracers.'

I don't think its assumed its either corrected for or neglected.

We agree with the reviewer that "reaching an equilibrium" is a strong assumption. It is, however, mentioned in several published papers: In (Dunne et al., 2013): "The fully coupled models were then integrated over 1000 model years with 1860 solar and radiative forcing before <u>declaring</u> "quasi-steady-state equilibrium" and beginning the 1860 control and perturbation integrations. In addition to the many qualitative requirements, we define acceptable quasi-steady-state equilibrium with quantitative metrics: net top-of-the-atmosphere radiative fluxes less than 0.5 W m-2, surface temperature drifts less than 0.18C century-1, stable Atlantic meridional overturning circulation (AMOC; Delworth et al. 1993) above 10 Sv (1 Sv [ 106 m3 s-1), local sea surface tem- perature (SST) biases less than ;98C, global 708S–708N root-mean-square SST errors less than 1.98C, and global net CO2 fluxes between the atmosphere and both land and ocean lower than 20 PgC century-1 (averaged over two centuries)."

#### In (Mignot et al., 2013):

"First of all, although it is clear that the oceanic adjustment requires several hundreds of years, this figure illustrates that all simulations <u>approaches an equilibrium state after 300</u> <u>years</u>. The latter is nevertheless not reached and may require thousands of years, as it was necessary in CM5\_piCtrl."

#### In (Stouffer et al., 2004):

"The initialization of coupled atmosphere-ocean climate models (AOGCMs) has been a long-standing problem in models used to study climate change on multi-century time scales (Moore et al. 2001). To perform simulations of the twentieth century and into the future, <u>modellers must start with an initial equilibrium prior</u> to extensive industrialization (typically near year 1850)."

#### In (Vichi et al., 2011):

"Oceanic DIC and alkalinity pools have been initialized from current climate data reconstructions (Key et al. 2004) and DIC <u>has been spun up to equilibrium with the preindustrial atmospheric CO2 concentration</u> by means of an acceleration method (adapted from Alessandri 2006 and Alessandri et al. 2011) consisting of increasing the air–sea CO2 outgassing flux of a factor 20 and removing the corresponding DIC amount homogeneously from the oceanic pool."

Besides, in most of the reference papers we reviewed for this study it is indicated that a near steady-state equilibrium is declared or assumed before performing any CMIP5 control and 20<sup>th</sup> century simulation. Therefore, we prefer to keep the term "assumed" in the revised version of the manuscript.

#### 8757:

It ranges from 1500 to 4000 years depending on the ocean circulation and can reach up to 10 000 years in the deeper domains of the ocean

Doesnt really make sense to give a range of 1500 to 4000 and then say some regions are 10,000. That means the range is 1500 to 10,000.

We have amended the sentence as follows.

# Revised:

"Depending on ocean circulation, it ranges from 1500 years for subsurface water masses to 10000 years for deep water masses (Wunsch and Heimbach, 2008)."

8759: Gupta et al. (2012, 2013). Should be 'Sen Gupta et al'

Done and acknowledged.

8763 last paragraph:

The metrics (2-4) are not very well defined can you be more precise? Does 2 mean you calculate the difference between model and obs at each grid point and then average? Is 3 just the spatial correlation between model and observations. 4 I dont really understand. Is this the difference between the spatial standard deviation for model and obs?

In the revised version of the manuscript, we chose to simplify the methodology and to concentrate the analysis on:

- The error or bias (metric 2 in the submitted manuscript)

- The root-mean-squared error (RMSE, the metric 5 in the submitted manuscript)

Since most of the analyses were performed with the RMSE, we have chosen to remove mention to the metrics 4 ( $\Delta\sigma$ ) in the revised manuscript.

Consequently, we have amended the sentence as follows.

Original:

"The skill score metrics are (1) the global averaged concentrations for overall drift; (2) the average error or bias for mismatches between modeled and observed fields; (3) spatial correlation for mismatches between modeled and observed large-scale structures; (4) the difference between modeled and observed spatial variability ( $\Delta\sigma$ ) and (5) the root-mean squared error (RMSE) to assess the total cumulative errors between modeled and observed fields."

Revised:

"The skill score metrics are (1) the global averaged concentrations for overall drift; (2) the error or bias between modeled and observed fields at each grid-cell; (3) spatial correlation between model and observations to assess mismatches between modeled and observed large-scale structures; (4) the root-mean squared error (RMSE) to assess the total cumulative errors between modeled and observed fields."

Figure 1:

In Fig 1 I think that the direction of the cross hatching for initial conditions are the opposite way round for 'model' and 'mixed' in the figure and the legend.

As stated above in the response to the Editor, we updated Figure 1 in order to improve its readability: we have enlarged the barplot and made cross hatching in only one way direction.

# 8766:

except some recommendations for the decadal prediction exercise ...

I presume however that there was no simulation of BGC in the decadal prediction simulations

At least one ESM participating in the CMIP5 decadal prediction exercise included BGC, namely IPSL-CM5A-LR (Séférian et al., 2014)).

# 8767:

Figure 2b also shows that the drift in the global sea-to-air carbon flux reduces slowly after the first 50 years of the spin-up simulation. While this drift is about 0.001 PgCyr-2 from year 250 to 500, it is much weaker over the last century of the simulation  $(5_{10-4} PgCy-2)$ 

The drift looks pretty linear after about year 50. Are the differences you discuss really significant? For example, if you shifted your analysis 50 years earlier i.e using 150 to 450 do you get robust results?

We appreciate the reviewer's careful reading. To address this question, we have computed the drift in fgCO2 over several time windows (Table R1):

Time	window	251-350	301-400	401-500
(model year)	)			
Drift (PgC y	-1 y-1)	0.0030	0.0004	0.0007

Table R1: Drift in ocean carbon flux (fgCO2 in PgC y-2) over various time window of 100 years.

Drift estimates differ by one order of magnitude between each other and they decrease with time. Although our computations show drift to fluctuate in course of the spin-up simulation, only the two last time window (301-400 and 401-500) are statistically different from the long-term drift of 0.001 PgC y-2 at 90% confidence level.

the simulated sea-to-air carbon flux would reach a steady state after  $\sim 500$  supplemental years of spin-up.

I'm a bit confused. By steady state do you mean when the air-sea flux is zero? But this isn't steady state. Steady state is when dF/dt=0, which will never happen under an exponential model, which is why you have a decay timescale.

Also your time estimates seem strange. If the decay timescale was only 73 years we would expect to see a large slowdown in drift over the course of the experiment, whereas it looks pretty linear. Also, if the trend at the end of the control is 5e-4, and the carbon flux is just less than -0.5PgCy-1 it would take almost 1000years to reach 0 and a further 950 years to reach 0.45. This is without any further reduction in the rate of the drift. Am I missing something?

We apologize for the confusion. The subsection discusses two distinct criteria:

(1) The ocean carbon flux: the model set up includes a prescribed input of riverine carbon which should induce an outgassing of about 0.45-0.6 PgC y-1 at preindustrial state and under quasi-steady-state equilibrium (see (Aumont et al., 2001)).

(2) The drift in ocean carbon flux: the simple drift model is used to track the temporal evolution of drift until it approaches a value close to zero. At this stage, we consider that the variable has reached a quasi-steady-state equilibrium.



Figure R1: Comparison of linear (solid blue line) and exponential (dashed magenta and green lines) regression in ocean carbon fluxes from years 250 to 500.

To address the first point, we fitted a linear model (in solid blue line in Fig R1) and two exponential models (in green and magenta dashed lines in Fig R1) to the time series of carbon flux. The linear model was fitted over 251-500 years. The exponential models were fitted over years 251-500, respectively 351-500. While the differences between the three models are overall small, the two exponential models show a flattening of the long-term tendency towards the end of the simulation (Fig. R1).

From these fits, we estimated that fgCO2 would reach the range of 0.44-0.56 PgC y-1 after 1627-1838 years of simulation, This range corresponds to the multi-model inverse estimate of preindustrial fluxes of CO2 estimated by (Mikaloff Fletcher et al., 2007) plus a river-induced outgassing of 0.45 PgC y-1.

Since the model has already completed 500 years of spin-up, we substracted this duration and concluded that the model would fit the target flux after an additional of 1127-1338 years of simulation.

The above is consistent with the estimate computed by the referee considering that he/she did not account for the 500 years of spin-up simulation already performed by the model. After correction, his/her estimate of 1450 years is close to ours.

To improve the readability, we modified the following subsection.

#### Original:

"The temporal evolution of sea-to-air  $CO_2$  fluxes was used in phase 2 of the Ocean Carbon Model Intercomparison Project (OCMIP-2, (Orr, 2002)) as an equilibration metric for the marine biogeochemistry and was still widely used during CMIP5. Figure

2b presents its evolution in the 500-year long spin-up simulation. The global ocean seato-air  $CO_2$  flux is ~-0.7 Pg C y<sup>-1</sup> over the last decades of the spin-up simulation (negative values indicate ocean  $CO_2$  uptake). The global sea-to-air carbon flux does not fit the range of values estimated from preindustrial natural ocean carbon flux inversions (e.g. (Gerber and Joos, 2010) or (Mikaloff Fletcher et al., 2007), referred to as MF2007 on Figure 2), which amounts to  $0.03 \pm 0.08$  Pg C y<sup>-1</sup> (to which an open-ocean river-induced carbon outgassing of 0.45 Pg C y<sup>-1</sup> has to be added on Figure 2 accordingly to (IPCC, 2013; Le Quéré et al., 2015). This indicates that the ocean carbon cycle has not reached a steady state in the model system following the 500 years of integration.

Figure 2b also shows that the drift in the global sea-to-air carbon flux reduces slowly after the first 50 years of the spin-up simulation. While this drift is about 0.001 Pg C  $y^2$ from year 250 to 500, it is much weaker over the last century of the simulation  $(5xI0^4 Pg)$  $C y^2$ ). Using an approximate relaxation time of 73 years estimated from the simple drift model (Equation 1) over years 250-500 and the drift of 0.001 Pg C y<sup>-2</sup>, we find that the simulated sea-to-air carbon flux would reach a steady state after ~500 supplemental years of spin-up. After the additional 500 supplemental years of spin-up, sea-air carbon flux would fall into the range of inverse estimates of MF2007 with accounting for outgassing of river carbon of  $0.45 \text{ Pg C y}^{-1}$ . This estimate does not account for the nonlinearity of the ocean carbon cycle and the associated process uncertainties (Schwinger et al., 2014). This estimation potentially underestimates the time required to equilibrate the ocean carbon cycle and sea-to-air carbon fluxes in the range of inversion estimates. The duration of the spin-up simulation would have to be increased by an additional 500 years to account for the estimated river-induced natural  $CO_2$  outgassing of about 0.45 Pg C y<sup>-1</sup> (IPCC, 2013). The drift of 0.001 Pg C y<sup>-2</sup> is, however, much smaller than the oceanic sink for anthropogenic carbon. Even if not fully equilibrated in terms of carbon balance, it is likely that this run would have given consistent estimates of anthropogenic carbon uptake in transient historical hindcasts." Revised:

"The temporal evolution of sea-to-air  $CO_2$  fluxes was used in phase 2 of the Ocean Carbon Model Intercomparison Project (OCMIP-2, Orr (2002)) as an equilibration metric for the marine biogeochemistry and was still widely used during CMIP5. Figure 2b presents its evolution in the 500-year long spin-up simulation. The global ocean sea-to-air  $CO_2$  flux is ~-0.7 Pg C y<sup>-1</sup> over the last decades of the spin-up simulation (negative values indicate ocean  $CO_2$  uptake).

To assess the global sea-to-air carbon flux, we use the range of values estimated from preindustrial natural ocean carbon flux inversions (e.g. Gerber and Joos (2010) or Mikaloff Fletcher et al. (2007)). Since, these estimates do not account for the preindustrial carbon outgassing induced by the river input, while our model does, we have added a constant outgassing of 0.45 Pg C y<sup>-1</sup> to the range of 0.03  $\pm$  0.08 Pg C y<sup>-1</sup> (Mikaloff Fletcher et al. 2007). This value of 0.45 Pg C y<sup>-1</sup> corresponds to the global open-ocean river-induced carbon outgassing accordingly to IPCC (2013) or Le Quéré et al. (2015). Consequently, in our modeling framework, the target value of the global seato-air carbon flux ranges between 0.4 and 0.56 Pg C y<sup>-1</sup>.

Figure 2b shows that the global sea-to-air carbon flux does not fit our range of values estimated from preindustrial natural ocean carbon flux inversions. Besides, Figure 2b shows that the drift in the global sea-to-air carbon flux reduces more slowly after a strong decline during the first 50 years of the spin-up simulation. While this drift is about 0.001 Pg C  $y^2$  from year 250 to 500, it is weaker over the last century of the simulation  $(7x10^4 Pg C y^2)$ . Using a linear fit over the last century of the simulation with a drift of  $7x10^4 Pg C y^2$ , we estimate that the simulated sea-to-air carbon flux would reach the range of 0.4-0.56 Pg C  $y^1$  after 1100 to 1300 supplemental years of spin-up simulation. Our simple drift model (Equation 1) gives a relaxation time of around 160 years, which

indicates that drift in ocean carbon flux should range between  $2x10^{-7}$  and  $7x10^{-7}$  Pg C y<sup>-2</sup> after this 1100 to 1300 supplemental years of spin-up simulation."

8770:

# ... over the last century of spin-up ...

Is 100 years really sufficient to get a good estimate? While you need to remove the period of initial coupling shock, this seems to only affect the first 100yrs or so in Fig 2.

These decay timescales seem very short. The tracers dont look like they would reach equilibrium on O[50yr] timescales. Indeed given that there is still substantial drift at the end of the 500yr control, when you exclude the initial coupling shock the timescale for reaching steady conditions look to be much longer.

I would like to see more detail on how you are fitting your drift model as it seems something is going wrong.

The reviewer is right. We apologize for errors in reporting results of our computation. Fig R2 presents the fit of the drift model at three depth levels. For this Figure, we computed drift in oxygen RMSE over a time window of 100 years starting from model year 200 to model year 400 every 5 years. The simple drift model was fitted to the resulting drift estimates presented with black circles in Fig R2.



Figure R2: Evaluation of a simple drift model to fit drift in O2 RMSE for time windows of 100 years starting every 5 years from year 200 to 400 as simulated by IPSL-CM5A-LR 500-year-long spin-up simulation. Top: surface, middle 150m, bottom 2000m.

The corrected relaxation times of drift in the oxygen field are 90, 564 and 1149 years at surface, 150 m, respectively 2000 m depth.

We agree with the referee's comment on the noise in the fit (below). Figure R2 clearly shows that there are substantial fluctuations in the drift across the spin-up simulation. To assess uncertainty in relaxation time, we repeated the analysis for time windows of 100, 150, 200 and 250 years. Table R2 presents the relaxation time for oxygen RMSE for these time windows.

Depth levels	100 years	150 years	200 years	250 years	Mean±sd
surface	90	200	126	40	114±67
150 m	564	391	238	306	375±140
2000 m	1149	590	895	1829	1116±527

Table R2: Relaxation time estimated from the 500-year-long spin-up simulation performed with IPSL-CM5A-LR using a simple drift model and different time windows.

We modified the subsection as follows.

Original:

"From these two metrics, the simple drift model (Equation 1) enables us to determine the relaxation time  $\tau$  required to reach equilibration over the last century of spin-up simulation. The relaxation times for oxygen RMSE are about 4, 13 and 140 y at the surface 150 m and 2000 m, respectively. Different values are derived for oxygen  $\Delta\sigma$  with

8, 7 and 46 y at surface, 150 and 2000 m, respectively. Values for other biogeochemical fields are quite similar to those for  $O_2$  except for  $NO_3$  at 150 m. This contrasting result between the two skill score metrics expresses the fact that RMSE accounts for the total distance between modeled and observed oxygen distributions, while  $\Delta\sigma$  considers solely the difference in spatial structure between model fields and observations. This shows that the time scale for equilibration of spatial structure is not necessarily the same as the drift."

Revised:

#### "3-5 Drifts in IPSL-CM5A-LR spin-up simulation

With the evolution of the RMSE established, we can use the simple drift model (Equation 1) to determine the relaxation time,  $\tau$ , required to reach equilibration after a longer of spin-up simulation. To use this simple drift model, we compute the drift in RMSE determined from time segments of 100 years distributed evenly every 5 years from year 250 to 500 for  $O_2$ ,  $NO_3$  and Alk-DIC tracers. The drift model (magenta lines in Figure 8) is fitted level to the 80 drift values for each field and each depth (colored crosses in Figure 8).

The simple drift model fits well the evolution of the drift in RMSE for the biogeochemical variables along the spin-up simulation of IPSL-CM5A-LR (Figure 8). Correlation coefficients are mostly significant at 90% confidence level ( $r^*=0.14$  determined with a student distribution with significance level of 90% and 80 degrees of freedom), except for  $NO_3$  at surface and Alk-DIC at 150 m. Another exception is found for  $NO_3$  at 150 m where the drift does not correspond to an exponential decay of the drift as function of time. The large confidence interval of the fit indicates that the fit would have been considered as non-significant given a longer spin-up simulation or a higher confidence threshold.

When significant, estimates of  $\tau$  for  $O_2$  RMSE are  $\approx 90$ , 564 and 1149 y at the surface 150 m and 2000 m, respectively. These values match reasonably well  $\tau$  estimated for  $NO_3$  RMSE at 2000 m (1130 y) and those for Alk-DIC RMSE at surface and 2000 m (137 and 1163 y). However, these estimates are sensitive to the time windows used to compute the drift. For a subset of time windows between 100 and 250 years by step of 50 years,  $\tau$  estimates for  $O_2$  RMSE are  $\approx 114\pm67$ ,  $375\pm140$  and  $1116\pm527$  y at the surface 150 m and 2000 m depth. These large uncertainties associated with  $\tau$  estimates are essentially due to the length of the spin-up simulation. A longer spin-up simulation would improve the quality of the fit (see Figure S1)."

We added Figure S1 to the supplementary materials to show how the fit is sensitive to the time-window. Estimates of the relaxation time are quite similar when using a time-window greater than 80 years. Below this threshold, the quality of the fit is significantly reduced (R<0.3)

#### ... across depth over the first century of simulation for each ESM ...

Given that the minimum control is 250yrs I don't see why you would only consider 100ys to obtain your drift estimate. The shorter the time period the more likely it is that you are aliasing low frequency natural variability. Indeed you are assuming that the drift follows an exponential model so why wouldn't you use the full control run to estimate the decay timescale?

At the very least I would like to see error bars on the drift estimates based on the rest of the control runs (the full period should be subject to the same drift timescale, if your model is appropriate)

We thank the referee for his/her thoughtful comment. Accordingly, we re-run the analysis for the different CMIP5 models using the full available control simulation and a time window of 100 years. We modified Figure 8 which now presents this new computation and includes error bars for each model drift.

We removed the fit performed with the IPSL spin-up simulation from the Figure 9 (previous Fig. 8), acknowledging that extrapolation IPSL drift up to 11900 years is subject to large uncertainties. We have nonetheless included results of the drift computation performed with this simulation in the Figure to strengthen our conclusions. They are represented in magenta cross over the available period (1 to 500 model year).

8771:

... between the drift in RMSE and the spin-up duration. The relationship is with the log of the spin up time

Please see response below

fall outside the 90% ... Do you mean 'below' not outside

Please refer to text changes presented below.

This low significance level must be put into perspective given the large diversity of spin-up protocols and initial conditions (Fig. 1 and Table 1) that can deteriorate the drift-spin up duration relationship in this ensemble of models. In addition you are unlikely to find the same drift rates in different models anyway

Please see the modification of the text below.

#### extrapolated over the 250–11900 spin-up duration range

This is a massive extrapolation. I would like to see the raw data this is based on displayed on the graph as I suspect the drift estimates from the 100yr chunks are very noisy

You might also consider doing this analysis for all depths (and plotting R vs depth) to see how robust the relationship is, although I appreciate that this might be a big task given all the data required

As mentioned above, we have removed the extrapolation from the original version of Figure 8. Besides, we have introduced a new subsection in the revised manuscript with new Figures. Previous section 3.4 and 3.5 are now splitted in 3.4 3.5 and 3.6. Major changes are presented below.

Please note that a new Figure has been introduced as Figure 8 (see modification below). Therefore, the Figure 8 of the submitted manuscript now becomes Figure 9 in the revised manuscript.

# "3-5 Drifts in IPSL-CM5A-LR spin-up simulation

With the evolution of the RMSE established, we can use the simple drift model (Equation 1) to determine the relaxation time,  $\tau$ , required to reach equilibration after a longer of spin-up simulation. To use this simple drift model, we compute the drift in RMSE determined from time segments of 100 years distributed evenly every 5 years from year 250 to 500 for  $O_2$ ,  $NO_3$  and Alk-DIC tracers. The drift model (magenta lines in Figure 8) is fitted level to the 80 drift values for each field and each depth (colored crosses in Figure 8).

The simple drift model fits well the evolution of the drift in RMSE for the biogeochemical variables along the spin-up simulation of IPSL-CM5A-LR (Figure 8). Correlation coefficients are mostly significant at 90% confidence level ( $r^*=0.14$  determined with a student distribution with significance level of 90% and 80 degrees of freedom), except for NO<sub>3</sub> at surface and Alk-DIC at 150 m. Another exception is found for NO<sub>3</sub> at 150 m where the drift does not correspond to an exponential decay of the drift as function of time. The large confidence interval of the fit indicates that the fit would have been considered as non-significant given a longer spin-up simulation or a higher confidence threshold.

When significant, estimates of  $\tau$  for  $O_2$  RMSE are  $\approx 90$ , 564 and 1149 y at the surface 150 m and 2000 m, respectively. These values match reasonably well  $\tau$  estimated for  $NO_3$  RMSE at 2000 m (1130 y) and those for Alk-DIC RMSE at surface and 2000 m (137 and 1163 y). However, these estimates are sensitive to the time windows used to compute the drift. For a subset of time windows between 100 and 250 years by step of 50 years,  $\tau$  estimates for  $O_2$  RMSE are  $\approx 114\pm67$ , 375 $\pm140$  and 1116 $\pm527$  y at the surface 150 m and 2000 m depth. These large uncertainties associated with  $\tau$  estimates are essentially due to the length of the spin-up simulation. A longer spin-up simulation would improve the quality of the fit (see Figure S1).

#### 3-6 Drifts in CMIP5 ESMs preindustrial simulations

In this subsection, the analysis is extended to the CMIP5 archive. We focus on oxygen fields in the long preindustrial simulation, piControl, for the 15 available CMIP5 ESMs. From these simulations that span from 250 to 1000 years, we compute the drift in  $O_2$  RMSE across depth from several time segments of 100 years distributed evenly every 5 years from the beginning until the end of the piControl simulation. These drifts are used as a surrogate for drift computed from the spin-up of each model since such simulations are not available through the data portal.

Figure 9 represents the drift in  $O_2$  RMSE versus the spin-up duration for each CMIP5 ESM. The analysis shows that the drift in  $O_2$  RMSE differs substantially between models. For a given model, drifts in other biogeochemical tracers (NO<sub>3</sub> and Alk-DIC) display similar features (not shown). The between-model differences in drift are not surprising since there are no reasons for different models to exhibit similar drift for a given field. Yet, Figure 9 shows that a global relationship emerges from this ensemble when using the simple drift model to fit the drift in  $O_2$  RMSE as function of the spin-up duration (solid green lines in Figure 9). With a 90% confidence level, this relationship suggests a general decrease of the drift as a function of spin-up duration for all depth levels. At the surface and at 2000 m depth, the quality of fits is low with correlation coefficients of about ~0.4. These are however significant at 90% confidence level ( $r^*=0.34$  determined with a student distribution with significance level of 90% and 15 models as degree of freedom). The weakest correlation coefficient is found for the fit at 150 m depth and hence indicating that there is no link between the drift in  $O_2$ RMSE and the duration of the spin-up simulation. This low significance level must be put into perspective given the large diversity of spin-up protocols and initial conditions (Figure 1 and Table 1) that can deteriorate the drift-spin up duration relationship in this ensemble of models.

The drift versus spin up duration relationship established from the 15 CMIP5 ESMs is nonetheless consistent with the results obtained with IPSL-CM5A-LR (The results in Figure 8 have been reported in Figure 9 with magenta crosses). Consistency is indicated by the sign of the drift versus spin up duration relationship of the IPSL-CM5A-LR model at the various depth levels, although their magnitudes differ. This difference in magnitude is not surprising if one considers that drift is highly model and protocol dependent and that the length of the IPSL-CM5A-LR spin-up simulation is potentially too short to determine accurate estimates of the long-term drift in  $O_2$  RMSE. Despite these differences, our analyses show that a relationship between the drift in  $O_2$  RMSE versus the spin-up duration emerges from an ensemble of models and is broadly consistent with our theoretical framework of a drift model established from the results of the IPSL-CM5A-LR model (Figure 8)."

#### 8773:

#### We employ $\Delta RMSE$ to penalize the normalized distance ...

Im not really clear what has been done here. Is the following correct?

1. You have taken the RMSE for the mean 1985-2005 historical period relative to available observations

2. You then calculate the drift timescale for each model based on the first 100yrs of picontrol

3. You then calculate the additional RMSE you would expect for a further 3000 years worth of integration and add it to the original RMSE.

#### Correct.

If so, some problems I see with this:

1. It assumes that 100yrs from the picontrol is sufficient to get an accurate estimate of the drift.

2. It assumes that the drift at the start of the control is representative of the 1985-2000 period. This depends on when the historical simulation was branched off the control.

#### The referee is right.

In the revised version of the manuscript, we updated the different computations taking into account the referee's comments. In particular, we accounted for uncertainties associated with the long-term drift estimate and those due to the different starting dates of the historical hindcast. In the revised version, we now use

(1) The average of several drift estimates computed over a time window of 100 years from year 1 to the end of the preindustrial simulation every 5 years.

(2) The ensemble-mean of all historical hindcast members (over 1986-2005).

We preferred this approach rather than computing a single drift estimate from the full control simulation (since this latter is not equal between models).

We updated Figure 9 (now Figure 10 in the revised manuscript) accordingly of the manuscript and we have amended the text as follows. Original:

"To assess the impact of model drift inherited from the diversity of spin-up strategies (Figure 1 and Table 1) on model performance metrics, the incremental deviation due to drift in biogeochemical fields is estimated from the simple drift model (Equation 1). The incremental deviation,  $\Delta RMSE$ , is computed using the relaxation time  $\tau$  determined from the piControl simulations of each CMIP5 model (Figure 8) and a common duration of T=3000 years for all models:

$$\Delta RMSE = \int_{0}^{t} drift(t=0) \times \exp(-\frac{1}{\tau}t)dt$$
(2)

where  $\Delta RMSE$  has the same unit as RMSE. The common duration T is used to bring model drift close to zero and hence to make models comparable to each other.

We employ  $\Delta RMSE$  to penalize the normalized distance from the observations assuming that this drift-induced deviation in tracer fields can be added to RMSE. This means that the effect of the penalty is to increase the normalized distance giving a consistent measure of the equilibration error."

#### Revised:

"To assess the impact of model drift inherited from the diversity of spin-up strategies (Figure 1 and Table 1) on the performance metrics, we use a simple additive assumption to incorporate an incremental error due to the drift,  $\Delta RMSE$ , to the above-mentioned RMSE. This incremental error due to the drift is computed using the relaxation time  $\tau$  determined from the piControl simulations of each CMIP5 model at each depth level (Equation 1 and Figure 9) and a common duration of T=3000 years for all models (m):

$$\Delta RMSE_m(z) = \int_0^{\infty} drift_m(z,t=0) \times \exp(-\frac{1}{\tau(z)}t)dt \qquad (2)$$

where  $\Delta RMSE$  has the same unit as RMSE.

The common duration T is used to bring model drift close to zero and hence to make models comparable to each other.

We employ  $\Delta RMSE$  to penalize the distance from the observations assuming that this drift-induced deviation in tracer fields can be added to RMSE. This means that the effect of the penalty is to increase the distance giving a consistent measure of the equilibration error."

In addition to this modification, we extended the discussion of our approach in a new subsection :

# *"4-4 Limitations of the framework*

In this work, the analyses focus on the globally averaged  $O_2$  RMSE across a diverse ensemble of CMIP5 models, which differ in terms of represented processes, spatial

resolution and performance in addition to differences in spin-up protocols. Major limitations of the framework are presented below.

Due to their specificities in terms of processes and resolution (e.g., Cabré et al., (2015), Laufkötter et al. (2015)), regional drift in CMIP5 models may differ from the drift computed from globally averaged skill-score metrics (see Figure S2 and S3). These differences may lead to different estimates of the relaxation time  $\tau$  at regional scale. Moreover, the combination of regional ocean physics and biogeochemical processes in each individual model may drive an evolution of regional drift in RMSE that does not fit the hypothesis of an exponential decay of the drift during the course of the spin-up simulation.

The above-mentioned remark can explain the relatively low confidence level of the fit to drift across the multi-model CMIP5 ensemble (Figure 9). The relatively low significance level of the fit directly reflects not only the large diversity of spin-up protocols and initial conditions (Figure 1 and Table 1) but also the large diversity of processes and resolution of the CMIP5 models. An improved derivation of the penalization would require access to output from spin-up simulations for each individual model or, at least, a better quantification of model-model differences in terms of initial conditions.

Finally, it is unlikely that model fields drift at the same rate along the spin-up simulation, even under the same spin-up protocols. Indeed, as shown in Kriest and Oschlies (2015), various parameterizations of the particles sinking speeds in a common physical framework may lead to a similar evolution of the globally averaged RMSE in the first century of the spin-up simulation but display very different behaviour within a time-scale of  $O(10^3)$  years. As such, drift and  $\tau$  estimates need to be used with caution when computed from short spin-up simulation because they can be subject to large uncertainties."

# (i.e., CMCC-CESM, IPSL-CM5B-LR, NorESM1-ME, CNRM-CM5) what about the GFDL ESM2M?

Our focus is on the identification of main patterns, rather than on the description of individual models. We nevertheless added a sentence specific to GFDL ESM2: *"The ranking of GFDL-ESM2G and GFDL-ESM2M slightly evolves with penalization but both models stay close to the ensemble median and ensemble mean."* 

#### 8774:

... errors in ocean biogeochemical fields amplify and propagate... not sure what you mean by propogate in this context

#### We removed the word 'propagate' from the revised manuscript.

Mignot et al. (2013) with the same model simulation showed that the large-scale ocean circulation reaches quasi-equilibrium after 250 years of spin-up, but our analyzes indicate that biogeochemical tracers do not ...

But all the characteristic timescales you have calculated are <150yrs. This does not match with your assertions of long equilibrium times

As mentioned above, we have corrected the relaxation time in the revised manuscript. Except at surface, subsurface and deep ocean relaxation times are greater than 150 years.

#### 8777: that have drifted further away from their initial states ...

This doesn't seem to be true always. Examination of Fig 3 shows that in many cases the initial coupling shock is in the opposite direction to the long term drift. Eg in 3e, NO3 is almost back to its initial state after the spin up period

In the ideal case of a model perfectly reproducing all the processes occurring in the real world (which is not the case), the model field will fit the observed field some time after the initial coupling shock (years to thousand of years).

Figure 9 abc confirms that none of the CMIP5 model represents an ideal case since none of them displays an RMSE close to zero for oxygen fields.

However, we acknowledge that a 500-year-long spin-up simulation might be too short to accurately determine the long-term drift of the model. The use of output from the spin-up simulations performed for CMIP5 would have provided a solution to the problem, but these have not been archived. We included further discussion on the limitation of our framework in the revised manuscript.

#### Swart and Fyfe (2011)

I'm not sure about the relevance of this study here - please explain

#### We removed this sentence from the text and the reference list.

#### 8778:

One issue is that the penalization relates to what the model state will look like around the time of full equilibration. However the transient (historical/RCP) runs are potentially done when the model state is closer to the initial observed state than the final equilibrium state. As such the transient response to greenhouse forcing may be more correct (even if the model is going to keep drifting). In the end the scores are there to help identify the models that produce the most realistic projections

This is not always true. Indeed Figure 1 indicates that several CMIP5 modelling groups have used previous simulations to initialize their model, some others have used mixed sources of initialization (both models and observations).

Nonetheless, we agree with the referee that drift in model field are one or two order of magnitude smaller than the climate change trends. This is why we emphasize the fact that our penalization approach does not totally turn upside down model standard ranking (i.e., done with standard RMSE over the historical period).

Besides, we have already mentioned this point in the submitted manuscript:

"The drift of 0.001 Pg C  $y^2$  is, however, much smaller than the oceanic sink for anthropogenic carbon. Even if not fully equilibrated in terms of carbon balance, it is

likely that this run would have given consistent estimates of anthropogenic carbon uptake in transient historical hindcasts."

The low confidence level of the fit to drift ... Where in your analysis do you demonstrate this low confidence?

Please see the response below.

The impact of this penalization approach on model ranking calls for the consideration of spin-up and initialization strategies in the determination of skill assessment metrics...

I don't follow this. Your penalisation process doesn't involve the spin up. It just requires an estimate of the drift which is estimated by looking at the control simulation. However I agree that it would be very useful to have more spin up information (including the spin up run output) as part of the available archive.

In this section, we have discussed our results.

First, we have highlighted the fact that the fit of our model is quite low. Even if, correlation coefficients are larger than zero with a 90% confidence interval at surface and 2000m, there are substantial uncertainties on the drift estimates (shown in the revised Figure 8 with error bars). These uncertainties influence the confidence we can have on the fit of the exponential model.

Next, we have attributed the large diversity in drift to both the protocols employed for spin-up and the initial condition (observations, models, mixing of both or constant values). These have to be considered to explain part of the model drift. As mentioned above, we introduce a new subsection "4-4 Limitations of this framework" where we further discuss the limitations and caveats of our approach.

8779:

CMIP7 ...

What happened to CMIP6?

We have corrected this error.

Yet, we acknowledge that CMIP6 has been omitted purposely since we (all of the coauthors) that it is/was too late to agree on a common set of spin-up protocol for CMIP6.

agree on a set of recommendations for initialization, spin-up protocols and duration

I'm not sure that it makes sense to have a common duration as different models drift at different rates

We understand the referee's point of view. Therefore, we have simplified the message with "the community should agree on a set of simple recommendations for spin-up protocols". Yet, we could agree that drift is a direct metrics of model performance. Consequently, a common set of recommendations including the duration of the spin-up simulation should contribute to valuable information for model assessment protocols. This suggestion needs further discussion and, of course, to be tested in a forthcoming study

# Referee #2 (F. Joos)

This is a nice and timely paper that addresses an important issue – model drift. It reflects the authors' broad knowledge in the field of coupled modelling. The authors show that short spin-up simulations initialized with observations lead to a too optimistic error statistic and biases model ranking. The authors also make proposal how model drift may be accounted for in future model assessments. This is an important and original contribution to the field.

I recommend publication after the following comments have been addressed

We appreciate the thoughtful suggestions from F. Joos. We incorporated most of the suggestions in the revised manuscript.

1) I am concerned about the way the drift model is presented and introduced and that the drift model may be used inappropriately in future work. The authors apply an exponential model with a single relaxation time scale to approximate the evolution of drift. However, the application of a single time scale is most likely not appropriate to determine the drift in whole ocean RMSE or other global error statistics. For example, this is implicitly demonstrated by the results in section 3.5 where the authors apply the drift models for different depth levels individually and show that time scales are different between depth levels.

In my opinion, the following point should be made very clear in this manuscript and in the method, results and discussion/conclusion section: different relaxation time scales apply for different regions (and variables). This requires that the drift in RMSE and other metrics is to be determined for different regions or even for different grid boxes individually before the drift in RMSE for the whole ocean is to be determined. In this way, multiple time scales would be applied to estimate the evolution of whole ocean RMSE and to correct error statistics for drift.

#### Please see our response below.

2) I am not convinced that selecting depth levels as regions is a good approach. For example, drift at 2000 m in the well-ventilated North Atlantic Deep Water may be quite different from drift in the slowly ventilated North Pacific. It would be illustrative to compute the relaxation time scale, tau, individually for each grid cell and plot tau along sections in the Atlantic, Pacific and Indian (or similar). A grid-cell based approach is generally also applied when removing model drift from projections by using a control simulation. Computing tau for individual grid cells would be comparable with such an approach.

We agree with F. Joos and his comments are addressed in the revised manuscript by adding in a new subsection "4.4 Limitations of the framework" and including corresponding results to the supplementary material. At the scale of individual grid cells, drift displays a large temporal and spatial variability. The larger variability reflects the mismatch between model output and observations, i.e. model fields vary on inter-annual

to decadal timescales, while observations are climatological means based on sparse observations. A similar problem arises when analyzing temporal trends and requires to be solved using either longer time series or smoothing procedures. Extending the analysis of drift to basin-scale improves the signal-to-noise ratio and facilitates the determination of drift without smoothing procedure.

The preceding is addressed in a new subsection:

# *"4-4 Limitations of the framework*

In this work, the analyses focus on the globally averaged  $O_2$  RMSE across a diverse ensemble of CMIP5 models, which differ in terms of represented processes, spatial resolution and performance in addition to differences in spin-up protocols. Major limitations of the framework are presented below.

Due to their specificities in terms of processes and resolution (e.g., Cabré et al., (2015), Laufkötter et al. (2015)), regional drift in CMIP5 models may differ from the drift computed from globally averaged skill-score metrics (see Figure S2 and S3). These differences may lead to different estimates of the relaxation time  $\tau$  at regional scale. Moreover, the combination of regional ocean physics and biogeochemical processes in each individual model may drive an evolution of regional drift in RMSE that does not fit the hypothesis of an exponential decay of the drift during the course of the spin-up simulation.

The above-mentioned remark can explain the relatively low confidence level of the fit to drift across the multi-model CMIP5 ensemble (Figure 9). The relatively low significance level of the fit directly reflects not only the large diversity of spin-up protocols and initial conditions (Figure 1 and Table 1) but also the large diversity of processes and resolution of the CMIP5 models. An improved derivation of the penalization would require access to output from spin-up simulations for each individual model or, at least, a better quantification of model-model differences in terms of initial conditions.

Finally, it is unlikely that model fields drift at the same rate along the spin-up simulation, even under the same spin-up protocols. Indeed, as shown in Kriest and Oschlies (2015), various parameterizations of the particles sinking speeds in a common physical framework may lead to a similar evolution of the globally averaged RMSE in the first century of the spin-up simulation but display very different behaviour within a time-scale of  $O(10^3)$  years. As such, drift and  $\tau$  estimates need to be used with caution when computed from short spin-up simulation because they can be subject to large uncertainties."

The discussion of limitations is supported by two new supplementary Figures:

- Figure S2 presents the sensitivity of the drift profile computed either from globalaveraged RMSE or form 3D RMSE. The figure suggests that while the approach selected for computing global drift might impact its magnitude, the general form of vertical profiles appears robust.

- Figure S3 presents basin-scale drift in  $O_2$  RMSE and its structure for the ensemble of CMIP5 models. The results are broadly consistent with the outcome of the penalization approach (Figure 10) with models displaying the largest drift having the greatest penalization.

Further comments:

1) A sufficiently long spin up over several hundred years is a prerequisite to estimate drift in error statistics and other variables. (High-resolution) models that are initialized with observed fields and not spun-up over several centuries very likely suffer from serious drift problems. It may be very difficult to estimate the future evolution of the drift from a short spin-up. This should be mentioned explicitly in the manuscript. (May be this could even be quantitatively illustrated by estimating relaxation time scales from an initial period, e.g., first 50 or 100 yr as compared to time scales from the last 100 year of the simulation as already presented for three different depth levels.)

As mentioned above, we have introduced a new subsection in the revised version of the manuscript in which we further discussed the limitation of our approach. One of the limitations is of course the duration of the spin-up simulation employed to determine the drift.

It is worth mentioning that the scope of the study emphasizes the impact of drift on skillscore assessment and not the assessment time required, for each CMIP5 models, to reach a quasi-steady-state equilibrium.

2) The authors may also note that rate of drifts (e.g. in the surface) may increase when the mode of model operation is changed, e.g. from prescribed atmospheric CO2 to freely simulated atmospheric CO2.

We agree with F. Joos. But this point was already mentioned in the submitted version of the manuscript:

"These developments will go along with an increase in the diversity and complexity of spin-up protocols applied to Earth system models, especially those including an interactive atmospheric  $CO_2$  or interactive nitrogen cycle (Dunne et al., 2013; Lindsay et al., 2014). The additional challenge of spinning-up emission-driven simulations with interactive carbon cycle will also require us to extend the assessment of the impact of spin-up protocols to the terrestrial carbon cycle. Processes such as soil carbon accumulation, peat formation as well as shift in biomes such as tropical and boreal ecosystems for dynamic vegetation models require several long time-scales to equilibrate (Brovkin et al., 2010; Koven et al., 2015)."

3) The authors do hardly evaluate the validity of their exponential model. It would be nice if this model could be validated, e.g. in the context of a millennium long control simulation or similar?

An important part of the analysis was dedicated to the evaluation of the simple drift model. However, we did not present any material to support its reliability in the submitted version of the manuscript. Consequently, in agreement with F. Joos suggestion, we included the assessment of our simple drift model with a long millennial-scale control simulation of IPSL-CM5A-LR. The result of this assessment is presented in Figure S1.

In response to a suggestion by reviewer 1, Figure S1 shows sensitivity tests on the length of the time-window to compute the drift in  $O_2$  RMSE. It supports the fact that long time series are required to accurately estimate the time of relaxation (R<0.3 with a time-window < 80 years).

Sec 3.6: It is not entirely clear whether the same time scale is applied here across all models considered. Please make this clear. It is also not clear whether different time scales are used for different depth levels. Please clarify.

We apologize for the lack of clarity. Pending on your comments and those of reviewer 1, we have amended the following section.

# Original:

"To assess the impact of model drift inherited from the diversity of spin-up strategies (Figure 1 and Table 1) on model performance metrics, the incremental deviation due to drift in biogeochemical fields is estimated from the simple drift model (Equation 1). The incremental deviation,  $\Delta RMSE$ , is computed using the relaxation time  $\tau$  determined from the piControl simulations of each CMIP5 model (Figure 8) and a common duration of T=3000 years for all models:

$$\Delta RMSE = \int_{0}^{1} drift(t=0) \times \exp(-\frac{1}{\tau}t)dt$$
 (2)

where  $\Delta RMSE$  has the same unit as RMSE. The common duration T is used to bring model drift close to zero and hence to make models comparable to each other.

We employ  $\Delta RMSE$  to penalize the normalized distance from the observations assuming that this drift-induced deviation in tracer fields can be added to RMSE. This means that the effect of the penalty is to increase the normalized distance giving a consistent measure of the equilibration error."

Revised:

"To assess the impact of model drift inherited from the diversity of spin-up strategies (Figure 1 and Table 1) on the performance metrics, we use a simple additive assumption to incorporate an incremental error due to the drift,  $\Delta RMSE$ , to the above-mentioned RMSE. This incremental error due to the drift is computed using the relaxation time  $\tau$  determined from the piControl simulations of each CMIP5 model at each depth level (Equation 1 and Figure 9) and a common duration of T=3000 years for all models (m):

$$\Delta RMSE_m(z) = \int_0^t drift_m(z,t=0) \times \exp(-\frac{1}{\tau(z)}t)dt \qquad (2)$$

where  $\Delta RMSE$  has the same unit as RMSE.

The common duration T is used to bring model drift close to zero and hence to make models comparable to each other.

We employ  $\Delta RMSE$  to penalize the distance from the observations assuming that this drift-induced deviation in tracer fields can be added to RMSE. This means that the effect of the penalty is to increase the distance giving a consistent measure of the equilibration error."

Sec 3.2: I am somewhat confused here about the role of river outgassing. The clarity of the text should be increased. It is not readily clear whether the model should actually achieve a flux of 0 GtC/yr or an outgassing of  $\sim$ 0.4 to 0.6 GtC/yr at equilibrium.

# Reviewer #1 also critized the lack of clarity of this section. To improve its readability and to clarify our computation, we modified this subsection as follows. Original:

"The temporal evolution of sea-to-air  $CO_2$  fluxes was used in phase 2 of the Ocean Carbon Model Intercomparison Project (OCMIP-2, (Orr, 2002)) as an equilibration metric for the marine biogeochemistry and was still widely used during CMIP5. Figure 2b presents its evolution in the 500-year long spin-up simulation. The global ocean seato-air  $CO_2$  flux is ~-0.7 Pg C y<sup>-1</sup> over the last decades of the spin-up simulation (negative values indicate ocean  $CO_2$  uptake). The global sea-to-air carbon flux does not fit the range of values estimated from preindustrial natural ocean carbon flux inversions (e.g. (Gerber and Joos, 2010) or (Mikaloff Fletcher et al., 2007), referred to as MF2007 on Figure 2), which amounts to  $0.03 \pm 0.08$  Pg C y<sup>-1</sup> (to which an open-ocean river-induced carbon outgassing of 0.45 Pg C y<sup>-1</sup> has to be added on Figure 2 accordingly to (IPCC, 2013; Le Quéré et al., 2015). This indicates that the ocean carbon cycle has not reached a steady state in the model system following the 500 years of integration.

Figure 2b also shows that the drift in the global sea-to-air carbon flux reduces slowly after the first 50 years of the spin-up simulation. While this drift is about 0.001 Pg C  $y^{-2}$ from year 250 to 500, it is much weaker over the last century of the simulation  $(5x10^4)$  Pg  $C y^2$ ). Using an approximate relaxation time of 73 years estimated from the simple drift model (Equation 1) over years 250-500 and the drift of 0.001 Pg C  $y^2$ , we find that the simulated sea-to-air carbon flux would reach a steady state after ~500 supplemental years of spin-up. After the additional 500 supplemental years of spin-up, sea-air carbon flux would fall into the range of inverse estimates of MF2007 with accounting for outgassing of river carbon of  $0.45 Pg C y^{-1}$ . This estimate does not account for the nonlinearity of the ocean carbon cycle and the associated process uncertainties (Schwinger et al., 2014). This estimation potentially underestimates the time required to equilibrate the ocean carbon cycle and sea-to-air carbon fluxes in the range of inversion estimates. The duration of the spin-up simulation would have to be increased by an additional 500 years to account for the estimated river-induced natural  $CO_2$  outgassing of about 0.45 Pg C y<sup>-1</sup> (IPCC, 2013). The drift of 0.001 Pg C y<sup>-2</sup> is, however, much smaller than the oceanic sink for anthropogenic carbon. Even if not fully equilibrated in terms of carbon balance, it is likely that this run would have given consistent estimates of anthropogenic carbon uptake in transient historical hindcasts."

Revised:

"The temporal evolution of sea-to-air  $CO_2$  fluxes was used in phase 2 of the Ocean Carbon Model Intercomparison Project (OCMIP-2, Orr (2002)) as an equilibration metric for the marine biogeochemistry and was still widely used during CMIP5. Figure 2b presents its evolution in the 500-year long spin-up simulation. The global ocean sea-to-air  $CO_2$  flux is ~-0.7 Pg C y<sup>-1</sup> over the last decades of the spin-up simulation (negative values indicate ocean  $CO_2$  uptake).

To assess the global sea-to-air carbon flux, we use the range of values estimated from preindustrial natural ocean carbon flux inversions (e.g. Gerber and Joos (2010) or Mikaloff Fletcher et al. (2007)). Since, these estimates do not account for the preindustrial carbon outgassing induced by the river input, while our model does, we have added a constant outgassing of 0.45 Pg C y<sup>-1</sup> to the range of 0.03  $\pm$  0.08 Pg C y<sup>-1</sup> (Mikaloff Fletcher et al. 2007). This value of 0.45 Pg C y<sup>-1</sup> corresponds to the global open-ocean river-induced carbon outgassing accordingly to IPCC (2013) or Le Quéré et

al. (2015). Consequently, in our modeling framework, the target value of the global seato-air carbon flux ranges between 0.4 and 0.56 Pg C  $y^{-1}$ .

Figure 2b shows that the global sea-to-air carbon flux does not fit our range of values estimated from preindustrial natural ocean carbon flux inversions. Besides, Figure 2b shows that the drift in the global sea-to-air carbon flux reduces more slowly after a strong decline during the first 50 years of the spin-up simulation. While this drift is about 0.001 Pg C  $y^2$  from year 250 to 500, it is weaker over the last century of the simulation  $(7x10^4 Pg C y^2)$ . Using a linear fit over the last century of the simulation with a drift of  $7x10^4 Pg C y^2$ , we estimate that the simulated sea-to-air carbon flux would reach the range of 0.4-0.56 Pg C  $y^1$  after 1100 to 1300 supplemental years of spin-up simulation. Our simple drift model (Equation 1) gives a relaxation time of around 160 years, which indicates that drift in ocean carbon flux should range between  $2x10^7$  and  $7x10^7 Pg C y^2$  after this 1100 to 1300 supplemental years.

8767, line 17: additional compared to what? Please refer to the modification of the text above.

8778 line 24: conclusion: Is it sufficient to report the drift in global RMSE? Perhaps this clause should be deleted or refined

This section has been amended as follows.

Original:

"Skill-score metrics are expected to be widely used in the framework of the future CMIP6 (Meehl et al., 2014) with the development of international community benchmarking tools like the ESMValTool (<u>http://www.pa.op.dlr.de/ESMValTool</u> (Eyring et al., 2015)). The assessment of model skill to reproduce observations will focus on the modern period. In order to increase the reliability of these traditional metrics, additional metrics that allow us to determine the equilibrium state of the model like the 3-dimensional growth rate or drift of relevant skill score metrics (e.g., RMSE) over the last decades or centuries of the spin-up, should be included in the set of standard assessment tools for CMIP6." Revised:

"Skill-score metrics are expected to be widely used in the framework of the future CMIP6 (Meehl et al., 2014) with the development of international community benchmarking tools like the ESMValTool (<u>http://www.pa.op.dlr.de/ESMValTool</u> (Eyring et al., 2015)). The assessment of model skill to reproduce observations will focus on the modern period. Complementary to this approach, our results call for the consideration of spin-up and initialization strategies in the determination of skill assessment metrics (Friedrichs et al., 2009; Stow et al., 2009) and, by extension, to model weighting (Steinacher et al., 2010) and model ranking (Anav et al., 2013). Indeed, the use of equilibrium-state metrics of the model like the 3-dimensional growth rate or drift of relevant skill score metrics (e.g. RMSE) could be employed to increase the reliability of these traditional metrics and, as such, should be included in the set of standard assessment tools for CMIP6."

#### Referee #3 (I. Kriest)

This paper examines the impact of different initialization procedures and spinup times in CMIP5 models, the resulting drift, and its impact on model skill assessement. I am

delighted to see that finally the issue of spinup times and drift is addressed comprehensively for the CMIP5 model suite. However, I have two concerns or comments, that I think should be kept in mind, and a few minor issues.

We appreciate I. Kriest careful reading. We included most of her suggestions and corrections in the revised version of the manuscript.

(1) As far as I understand, the core model experiment, IPSL-CM5A-LR, was spun up from rest for 500 years. I am aware that it is sometimes quite expensive - in terms of computational cost - to simulate global or earth system models over a long time. However, I am not quite sure that a spinup time of 500 years, as used for this experiment, is always sufficient to draw conclusions about the long-term model drift. As has been shown recently (Kriest and Oschlies, 2015; www.geosci-model-dev.net/8/2929/2015/), simulated global average oxygen, nitrate, or total fixed nitrogen can exhibit a non-linear trajectory over time, sometimes with inflection points within the first few centuries of spinup; i.e., the model drift may not only decrease or increase, but change its sign. In practice, it means that, due to the many timescales involved, a model that shows a bad fit and negative trend within the first few hundred years e.g., with respect to global average oxygen, may cease to do so after some more centuries, and finally show a quite good fit to observed oxygen after some millenia.

We agree with the referee. In the revised version of the manuscript, we clearly stated that our 500-year-long spin-up simulation, as used for this study, is maybe too short to draw robust conclusions on the long-term drift. An ideal solution would have been to use output of the spin-up simulation performed in the context of CMIP5 but these latter have not been archived. This will be tested in a forthcoming study in the context of CMIP6 for which we hope some modeling groups will store output from the spin-up simulation.

(2) The above doesn't have to hold for all model types. It can depend on the biogeochemical time scales involved, i.e. on particle sinking speed or remineralization (Kriest and Oschlies, 2015), circulation, and probably other parameters as well. Given that the CMIP5 biogeochemical models involve a huge variety of these parameterizations (e.g., Cabre et al., 2015; www.biogeosciences.net/12/5429/2015/; Fig. 6), together with very different circulations, resolutions, etc., the time scales associated with model equilibration, as well as their transient may be very different, and not always follow linear relationships for the decay term.

Therefore, I would suggest to include some discussion on this in the paper. Overall, nevertheless I think this paper gives a helpful and timely overview about potential limitations of model-model and model-data comparison of this suite of models.

As mentioned above to the first referee and to F. Joos, we have amended the manuscript with the inclusion of this new subsection:

# "4-4 Limitations of the framework

In this work, the analyses focus on the globally averaged  $O_2$  RMSE across a diverse ensemble of CMIP5 models, which differ in terms of represented processes, spatial

resolution and performance in addition to differences in spin-up protocols. Major limitations of the framework are presented below.

Due to their specificities in terms of processes and resolution (e.g., Cabré et al., (2015), Laufkötter et al. (2015)), regional drift in CMIP5 models may differ from the drift computed from globally averaged skill-score metrics (see Figure S2 and S3). These differences may lead to different estimates of the relaxation time  $\tau$  at regional scale. Moreover, the combination of regional ocean physics and biogeochemical processes in each individual model may drive an evolution of regional drift in RMSE that does not fit the hypothesis of an exponential decay of the drift during the course of the spin-up simulation.

The above-mentioned remark can explain the relatively low confidence level of the fit to drift across the multi-model CMIP5 ensemble (Figure 9). The relatively low significance level of the fit directly reflects not only the large diversity of spin-up protocols and initial conditions (Figure 1 and Table 1) but also the large diversity of processes and resolution of the CMIP5 models. An improved derivation of the penalization would require access to output from spin-up simulations for each individual model or, at least, a better quantification of model-model differences in terms of initial conditions.

Finally, it is unlikely that model fields drift at the same rate along the spin-up simulation, even under the same spin-up protocols. Indeed, as shown in Kriest and Oschlies (2015), various parameterizations of the particles sinking speeds in a common physical framework may lead to a similar evolution of the globally averaged RMSE in the first century of the spin-up simulation but display very different behaviour within a time-scale of  $O(10^3)$  years. As such, drift and  $\tau$  estimates need to be used with caution when computed from short spin-up simulation because they can be subject to large uncertainties."

Other comments:

p. 8760, line 27ff: "Oxygen is prognostically simulated using two different oxygen-tocarbon ratios, one for the oxic remineralization of matter and one for the sub-oxic pathway (Sarmiento and Gruber, 2006)." - It is not clear to me what is meant with "oxygento-carbon ratios": the ratio of organic matter, or of the process itself? If the latter, how can oxygen be used in sub-oxic pathways? If the former: doesn't this imply that either oxygen or carbon is not conserved when switching between these processes? E.g. consider that - implicitly - organic matter built during photosynthesis has a composition according to Anderson (1995, Deep-Sea Res. I, 42(9), 1675-1680), with C:H:O:N:P = 106:175:42:16:1. Of course, one usually does not describe OM in models exactly this way; but the assumption particularly about C:H:O (in some way: the amount of carbohydrates) is reflected in the stoichiometry for O2 release and CO2 consumption. If then the C:O-ratio of OM is different between remineralization and denitritification/anammox (whatever is considered), wouldn't this affect mass conservation of either C or O?

We apologize for this misleading information. We have amended the description of

#### PISCES accordingly. <u>Original:</u>

"Oxygen is prognostically simulated using two different oxygen-to-carbon ratios, one for the oxic remineralization of organic matter and one for the sub-oxic pathway (Sarmiento and Gruber, 2006)."

# Revised:

"Oxygen is prognostically simulated. The model distinguishes between oxic and suboxic remineralization pathways, the former relying on oxygen as electron acceptor, the latter on nitrate."

Therefore the total amount of C and O is conserved in PISCES.

p. 8763, subsection 2.3: I would suggest to more clearly define drift, to make this term more easily accessible for users outside the modeling or CMIP5 community.

We refined the subsection describing the way we determine the drift. In addition, in the revised subsection, we briefly discuss the sensitivity to the time-window used to compute the drift.

Original:

"The drift is determined for either concentrations in simulated biogeochemical fields or for skill score metrics (e.g., RMSE or  $\Delta\sigma$ ) using a linear regression fit over a time window of 100 years. This time window of 100 years was chosen as a trade off between longer time window (>200 years) that smoothes the drift signal and shorter time window (<80 years) that introduces fluctuations due to internal variability." Revised:

"The drift is determined for either concentrations in simulated biogeochemical fields or for skill score metrics (e.g., RMSE) using a linear regression fit over a time window of 100 years. This time window of 100 years was chosen as a trade off between a longer time window (>200 years) that smoothes the drift signal and a shorter time window (<100 years) that introduces fluctuations due to internal variability and hence impacting the quality of the fit (see the assessment performed with the millennial-long CMIP5 piControl simulation of IPSL-CM5A-LR in Figure S1)."

p. 8773, lines 10-11: "We employ  $\Delta$ RMSE to penalize the normalized distance from the observations assuming that this drift-induced deviation in tracer fields can be added to RMSE." - Why choose an additive model?

We acknowledge that there is no justification to employ a simple additive model rather than a multiplicative model in our case. That said, we aimed at keeping our framework as simple as possible for this study.

The additive approach is coherent with current 'drift-correction' approaches which are based on an additive hypothesis. As indicated in the submitted version of the manuscript: "So far, the most frequent approach relies on the use of long preindustrial control simulations to 'remove' the drift embedded in the simulated fields over the historical period or future projections (Bopp et al., 2013; Cocco et al., 2013; Friedlingstein et al., 2006; 2013; Frölicher et al., 2014; Gehlen et al., 2014; Keller et al., 2014; Steinacher et

al., 2010; Tjiputra et al., 2014). Although this approach allows to determine relative changes, it does not allow to investigate the underlying reasons of the spread between models in terms of processes, variability and response to climate change. The "drift-correction" approach, much as the one used for this study, assumes that drift-induced errors in the simulated fields can be isolated from the signal of interest."

Testing the validity of both hypothesis (additive or multiplicative amplification of the errors) is not easy. We think that it would have required for example a large ensemble of historical simulations starting at various date of the spin-up, with an important computation cost. To our knowledge, this question remains an uncharted territory that would require further analyses to be answered.

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- 1 Inconsistent strategies to spin up models in CMIP5: implications for
- 2 ocean biogeochemical model performance assessment
- 3
- 4 | Roland Séférian<sup>1\*</sup>, Marion Gehlen<sup>2</sup>, Laurent Bopp<sup>2</sup>, Laure Resplandy<sup>3,2</sup>, James C.
- 5 Orr<sup>2</sup>, Olivier Marti<sup>2</sup>, John P. Dunne<sup>4</sup>, James R. Christian<sup>5</sup>, Scott C. Doney<sup>6</sup>,
- 6 Tatiana Ilyina<sup>7</sup>, Keith Lindsay<sup>8</sup>, Paul Halloran<sup>9</sup>, Christoph Heinze<sup>10,11</sup>, Joachim
- 7 Segschneider<sup>12</sup>, Jerry Tjiputra<sup>11</sup>, Olivier Aumont<sup>13</sup>, Anastasia Romanou<sup>14,15</sup>

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- 8 <sup>1</sup> CNRM-GAME, Centre National de Recherches Météorologiques-Groupe d'Etude
- 9 de l'Atmosphère Météorologique, Météo-France/CNRS, 42 Avenue Gaspard Coriolis,
- 10 31057 Toulouse, France
- 11 <sup>2</sup> LSCE/IPSL, Laboratoire des Sciences du Climat et de l'Environnement, Orme des
- 12 Merisiers, CEA/Saclay 91198 Gif-sur-Yvette Cedex, France
- <sup>3</sup> Scripps Institution of Oceanography, UCSD, La Jolla, CA, USA
- 14 4 Geophysical Fluid Dynamics Laboratory, NOAA, Princeton, New Jersey, USA
- 15 <sup>5</sup> Fisheries and Oceans Canada and Canadian Centre for Climate Modelling and
- 16 Analysis, Victoria, B.C., Canada
- 17 <sup>6</sup>Marine Chemistry and Geochemistry Department, Woods Hole Oceanographic
- 18 Institution, Woods Hole MA, USA
- <sup>7</sup> Max Planck Institute for Meteorology, Bundesstraße 53, 20146 Hamburg, Germany
- 20 <sup>8</sup> Climate and Global Dynamics Division, National Center for Atmospheric Research,
- 21 Boulder, Colorado
- 22 <sup>9</sup> College of Life and Environmental Sciences, University of Exeter, EX4
- 23 4RJ, UK

24	<sup>10</sup> Geophysical Institute, University of Bergen and Bjerknes Centre for Climate	
25	Research, Bergen, Norway	
26	<sup>11</sup> Uni Research Climate, Allegt. 55, 5007 Bergen and Bjerknes Centre for Climate	
27	Research, Bergen, Norway	
28	<sup>12</sup> University of Kiel, Kiel, Germany	
29	<sup>13</sup> Sorbonne Universités (UPMC, Univ Paris 06)-CNRS-IRD-MNHN, LOCEAN-	
30	IPSL Laboratory, 4 Place Jussieu, F-75005 Paris, France	
31	<sup>14</sup> Dept. of Applied Math. and Phys., Columbia University, 2880 Broadway, New	roland seferian 28/1/16 19:35
32	York, NY 10025, USA	roland seferian 28/1/16 19:35
33	<sup>15</sup> NASA-GISS, NY, USA	pt roland seferian 28/1/16 19:35
34		Formatted: Font:Times New Roman, 12 pt, Superscript
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36	*Corresponding author address: Roland Séférian, CNRM-GAME, 42 av. Gaspard	pt roland seferian 28/1/16 19:35
37	Coriolis 31100 Toulouse. E-mail: roland.seferian@meteo.fr	Formatted
38		
39	Abstract	
40	During the fifth phase of the Coupled Model Intercomparison Project (CMIP5)	
41	substantial efforts were made on the systematic assessment of the skill of Earth	roland seferian 28/1/16 09:08
42	system models. One goal was to check how realistically representative marine	Deleted: carried out
43	biogeochemical tracer distributions could be reproduced by models. Mean-state	
44	assessments routinely compared model hindcasts to available modern biogeochemical	
45	observations. However, these assessments considered neither the extent of equilibrium	
46	in modeled biogeochemical reservoirs nor the sensitivity of model performance to	
47	initial conditions or to the spin-up protocols. Here, we explore how the large diversity	
48	in spin-up protocols used for marine biogeochemistry in CMIP5 Earth system models	

49	(ESM) contribute to model-to-model differences in the simulated fields. We take
50	advantage of a 500-year spin-up simulation of IPSL-CM5A-LR to quantify the
51	influence of the spin-up protocol on model ability to reproduce relevant data fields.
52	Amplification of biases in selected biogeochemical fields (O <sub>2</sub> , NO <sub>3</sub> , Alk-DIC) is
53	assessed as a function of spin-up duration. We demonstrate that a relationship
54	between spin-up duration and assessment metrics emerges from our model results and
55	is consistent when confronted against a larger ensemble of CMIP5 models. This
56	shows that drift has implications on performance assessment in addition to possibly
57	aliasing estimates of climate change impact. Our study suggests that differences in
58	spin-up protocols could explain a substantial part of model disparities, constituting a
59	source of model-to-model uncertainty. This requires more attention in future model
60	intercomparison exercises in order to provide realistic ESM results on marine
61	biogeochemistry and carbon cycle feedbacks.
62	
63	1- Introduction
64	1-1 Context
65	Earth system models (ESM) are recognized as the current state-of-the-art global
66	coupled models used for climate research (e.g., Hajima et al., 2014; IPCC, 2013).
67	They expand the numerical representation of the climate system used during the $4^{th}$
68	IPCC assessment report (AR4) that was limited to coupled physical general
69	circulation models, to the inclusion of biogeochemical and biophysical interactions
70	between the physical climate system and the biosphere. ESMs that contributed to
71	CMIP5 substantially differ in terms of their simulations of physical and
72	biogeochemical components. These differences in design translate into a significant
73	variability of the models' ability to reproduce the observed biogeochemistry and

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74	carbon cycle, which in turn may impact projected climate change responses (IPCC,

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74	<u>carbon</u>
75	2013).

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77	In the typical objective evaluation and intercomparison of these models, a suite of
78	standardized statistical metrics (e.g., correlation, root-mean-squared errors) is applied
79	to quantify differences between modeled and observed variables (e.g., Doney et al.,
80	2009; Rose et al., 2009; Stow et al., 2009; Romanou et al., 2014; 2015). With the goal
81	of constraining future projections, statistical metrics are often used for model ranking
82	(e.g., Anav et al., 2013), weighting of model projections (e.g., Steinacher et al., 2010)
83	or selection of the most skillful models across a wider ensemble (e.g., Cox et al.,
84	2013; Massonnet et al., 2012; Wenzel et al., 2014). Most of these approaches can be
85	considered as "blind" given that they are routinely applied without considering
86	models' specific characteristics and treat models a priori as equivalently independent
87	of observations. However, since these models are typically initialized from
88	observations, the spin-up procedure of climate variables are the most model-
89	dependent protocols that could introduce errors or drifts in modeled fields with
90	consequences on skill score metrics.
91	
92	1-2 Initialization of biogeochemical fields and spin-up protocols in CMIP5
93	Ocean initialization protocols aim at obtaining stable and equilibrated distributions of
94	model state variables, such as temperature or concentrations of dissolved tracers. Most
95	commonly used initialization protocols consist of initializing both physical and
96	biogeochemical variables with either climatologies of the observed fields or constant
97	values before running the model to equilibrium. In theory, equilibrium corresponds to

98 steady-state and, hence, temporal derivatives of tracer fields close to zero. The time

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99	needed to equilibrate tracer distributions or, in other words, the integration time
100	needed by the model to converge towards its own attractor (which is different from
101	the true state of the climate system) varies greatly between components of the climate
102	system. It spans from several weeks for the atmosphere (e.g., Phillips et al., 2004) to
103	several centuries for ocean and sea ice components (e.g., Stouffer et al., 2004). The
104	equilibration of ocean biogeochemical tracers across the entire water column amounts
105	to several thousands of years (e.g., Heinze et al., 1999; Wunsch and Heimbach, 2008)
106	and depends on the state of background ocean circulation as well as the turbulent
107	mixing and eddy stirring parameterizations (e.g., Aumont et al., 1998; Bryan, 1984; Deleted: diapycnal diffusivity
108	Gnanadesikan, 2004; Marinov et al., 2008). In practice, these simulations, called
109	"spin-up", span in general only several hundreds of years at the end of which a quasi-
110	equilibrium state is assumed for the interior ocean tracers.
111	
112	The present degree of complexity and increasing spatial as well as temporal resolution
113	of marine biogeochemical ESM components, however, often precludes a spin-up to
114	reach adequate equilibration of biogeochemical tracers. This is a consequence of the
115	increasing number of state variables present in most of the current generation of
116	biogeochemical models (e.g., for each tracer a separate advection equation has to be
117	solved via a numerical CPU time demanding algorithm), more complex process
118	descriptions (e.g., including more plankton functional types than before), and
119	increasing spatial as well as temporal resolution. This number has continuously
120	increased from simple biogeochemical models (e.g., HAMOCC3, Maier-Reimer and
121	Hasselmann (1987)) to marine biodiversity models (e.g., Follows et al., 2007).
122	Current generation biogeochemical models embedded in CMIP5 ESMs contain
123	roughly two to four times more state variables than the physical models (e.g.,
124	atmosphere, ocean, sea-ice), which makes their equilibration computationally costly
-----	------------------------------------------------------------------------------------------
125	and difficult. The initialization of biogeochemical state variables is further
126	complicated by the scarcity of biogeochemical observations as compared to
127	observations of physical variables (e.g., temperature, salinity). While three-
128	dimensional observation-based climatologies exist for macro-nutrients, oxygen,
129	dissolved carbon and alkalinity, for other tracers such as dissolved iron, dissolved
130	organic carbon and biomass of the various plankton functional types data are still
131	sparse and represent measurements done over different time periods and climate
132	conditions (in-spite of considerable efforts such as the GEOTRACES program for
133	trace elements, or MAREDAT for biomasses of plankton functional types). The latter
134	are initialized either with constant values (e.g. global average estimates) or with
135	output from a previous model run. An additional difficulty stems from the use of
136	modern climatologies to initialize the ocean state, implicitly assuming a long-term
137	steady state, which does not necessarily represent the preindustrial state of the ocean.
138	These climatologies incorporate the ongoing anthropogenic perturbation of marine
139	biogeochemical fields, be it the uptake of anthropogenic $\text{CO}_2$ or the excess of
140	nutrients inputs and pollutants (e.g., Doney, 2010). Although methods exist to remove
141	the anthropogenic perturbation from observed ocean carbon tracer fields, their use is
142	still debated since they lead to non-unique results (e.g., Tanhua et al., 2007; Yool et
143	al., 2010).
144	
145	The equilibration of marine biogeochemical tracer distributions is driven not only by
146	the ocean circulation but also by numerous internal biogeochemical processes acting

- 147 at various time scales. For example, while the transport and degradation of sinking
- 148 organic matter spans days to perhaps several months, the associated impact on deep

149	water chemistry accumulates over several decades to centuries as zones of differential
150	remineralization are mixed across water masses and follows the ocean circulation
151	(Wunsch and Heimbach, 2008). For models including interactive sediment modules,
152	the sediment equilibration takes even longer ( $O(10^4)$ years; e.g., Archer et al. (2009)
153	and Heinze et al. (1999)). As a consequence of the interplay between ocean
154	circulation and biogeochemical processes, biogeochemical models require long spin-
155	up times to equilibrate (e.g., Khatiwala et al., 2005; Wunsch and Heimbach, 2008).
156	Modeling studies of paleo-oceanographic passive tracers such as $\delta^{18}O$ or $\Delta^{14}C$
157	(Duplessy et al., 1991), or global ocean passive tracers (Wunsch and Heimbach,
158	2008), as well as more recently available modern global scale data compilations (e.g.,
159	Key et al., 2004; Sarmiento and Gruber, 2006) and GEOTRACES Intermediate Data
160	product 2014 (Version 2) http://www.bodc.ac.uk/geotraces/data/idp2014/) provide an
161	estimate of the time required for the ocean biogeochemical reservoir to equilibrate
162	with the climate systems (excluding continental weathering and reaction with marine
163	sediments). Depending on ocean circulation, it ranges from 1500 years for subsurface
164	water masses to 10000 years for the deep water masses (Wunsch and Heimbach,
165	2008).
166	
167	In a context of model-to-model intercomparison, this time range contributes to the
168	model uncertainty. Lessons from the previous OCMIP-2 exercise have demonstrated
169	that some models required ~10,000 years to equilibrate to a global sea-air carbon flux
170	of 0.01 Pg C $y^{-1}$ .

172 While it is recognized that long time-scale processes influence the length of spin-up to

173 equilibrium, the spin-up duration is usually defined *ad hoc* based on external

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174	constraints or internal biogeochemical criteria. The computational cost is commonly				
175	invoked as external constraint to shorten and limit the spin-up duration. It is directly				
176	related to model complexity (e.g., Tjiputra et al., 2013; Vichi et al., 2011; Yool et al.,				
177	2013) and spatial resolution (Ito et al., 2010). The internal biogeochemical criteria				
178	applied to derive the duration of the spin-up simulations are generally defined by (i)				
179	reaching a steady-state, quasi equilibrium of the long-term global-mean $\text{CO}_2$ fluxes				
180	between the ocean and the atmosphere (e.g., Dunne et al., 2013; Ilyina et al., 2013;				
181	Lindsay et al., 2014; <u>Romanou et al., 2013;</u> Séférian et al., 2013), (ii) determining the				
182	amount of carbon stored into the ocean at preindustrial state (e.g., Dunne et al., 2013;				
183	Vichi et al., 2011) or (iii) representing relevant biogeochemical tracer patterns (e.g.,				
184	oxygen minimum zone in Ito and Deutsch (2013)).				
185					
186	Despite its importance, only limited information on spin-up procedures is available				
187	through the CMIP5 metadata portal (http://metaforclimate.eu/trac). Information on				
188	spin-up protocols and model initialization is usually not taken into account in model				
189	intercomparison studies (e.g., Andrews et al., 2013; Bopp et al., 2013; Cocco et al.,				
190	2013; Frölicher et al., 2014; Gehlen et al., 2014; Keller et al., 2014; Resplandy et al.,				
191	2013; 2015; Rodgers et al., 2014; Séférian et al., 2014). This information, if available,				
192	can only be found separately in the reference papers of individual models (e.g.,				
193	Adachi et al., 2013; Arora et al., 2011; Collins et al., 2011; Dunne et al., 2013; Ilyina				
194	et al., 2013; Lindsay et al., 2014; Romanou et al., 2013; Séférian et al., 2013 <u>; Séférian</u>				
195	et al., 2015; Tjiputra et al., 2013; Vichi et al., 2011; Volodin et al., 2010; Watanabe et				
196	al., 2011; Wu et al., 2013). The duration of spin-up simulations of CMIP5 ocean				
197	biogeochemical components spans from one hundred years (e.g., CMCC-CESM) to				
198	several thousand years (e.g., MPI-ESM-LR, MPI-ESM-MR) (Figure 1 and Table 1).				

199 Model initialization and spin-up procedures are equally variable across the model

200 ensemble (Figure 1 and Table 1). Four different sources of initialization and four

201 different procedures of model equilibration emerge from the 24 ESMs reviewed for
 202 this study.

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204 Biogeochemical state variables were mostly initialized from observations, although 205 from various releases of the same World Ocean Atlas global climatology (WOA1994, 206 WOA2001, WOA2006, WOA2010). A small subset of ESMs relied either on a mix 207 between previous model output and observations or solely on model output from a 208 previous simulation for initialization. Similarly, spin-up procedures fall into two 209 categories. The first one may be called "sequential": it consists in decomposing the 210 spin-up integration into one long offline simulation (~200-10000 years) and one 211 shorter online simulation (~100-1000 years). During the offline simulation, the 212 biogeochemical model is forced by dynamical fields from the climate model or from 213 reanalysis (CanESM2, MRI-ESM, Figure 1 and Table 1). Some modeling groups have 214 adopted a "direct" strategy, which consists in running solely one online or coupled 215 spin-up simulation (e.g., <u>CNRM-ESM1</u>, GFDL-ESM2M, GFDL-ESM2G, <u>GISS-E2-</u> 216 H-CC, GISS-E2-R-CC, NorESM1-ME). Finally, a spin-up "acceleration" procedure is 217 used by CMCC-CESM. This technique consists of enhancing the ocean carbon 218 outgassing to remove anthropogenic carbon from the ocean, a legacy from 219 initialization with modern data (Global Data Analysis Project or GLODAP following 220 Key et al., 2004). None of these spin-up procedures, durations and sources of 221 initialization can be considered as "standard"; each of them is unique and subjectively 222 employed by one modeling group.

223

224	Objective arguments and hypotheses justifying the choice of one method of spin-up
225	rather than the others have been the focus of previous studies (e.g., Dunne et al., 2013;
226	Heinze and Ilyina, 2015; Tjiputra et al., 2013). Similarly, modeling groups discussed
227	impacts of their particular spin-up procedure on model performance (e.g., Dunne et
228	al., 2013; Lindsay et al., 2014; Séférian et al., 2013; Vichi et al., 2011). However, no
229	study has addressed the potential for the large diversity of spin-up procedures found
230	across the CMIP5 ensemble to translate into model-to-model differences in terms of
231	comparative model performance assessments or model evaluations in terms of future
232	projections.

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#### 234 1-3 Objectives of this study

235 This study assesses the role of the spin-up protocol in the representation of 236 biogeochemical fields and subsequent model skill assessment, providing a 237 complementary analysis from the studies of <u>Sen</u> Gupta et al. (2012; 2013). It relies on 238 a 500-year long spin-up simulation from a state-of-the-art Earth system model, IPSL-239 CM5A-LR to investigate the impacts of spin-up strategy on selected biogeochemical 240 tracers and residual model drift across the various ESMs of the CMIP5 ensemble. We 241 demonstrate that the duration of the spin-up has implications for the determination of 242 robust and meaningful skill-score metrics that should improve future intercomparison 243 studies such as CMIP6 (Meehl et al., 2014). 244

245 Section 2 describes the model, the observations, the model experiments, as well as the 246 methods used for assessing the impacts of spin-up protocols on the representation of 247 biogeochemical fields in IPSL-CM5A-LR, as well as across the ensemble of CMIP5 248 ESMs. Section 3 presents the analysis developed for the assessment of the impact of

249 spin-up duration on the representation of biogeochemical structures. Implications and

250 recommendations are discussed in Sections 4 and 5, respectively.

#### 251

#### 252 **2- Methods**

#### 253 **2-1- Model simulations**

This study exploits in particular results from one simulation performed with IPSL-254 255 CM5A-LR (Dufresne et al., 2013) as representative for other CMIP5 Earth system 256 models. As a typical representative of the current generation of ESMs, IPSL-CM5A-257 LR combines the major components of the climate system (Chap 9, Table 9.1, (IPCC, 258 2013). The atmosphere is represented by the atmospheric general circulation model 259 LMDZ (Hourdin et al., 2006) with a horizontal resolution of 3.75°x1.87° and 39 260 levels. The land surface is simulated with ORCHIDEE (Krinner et al., 2005). The 261 oceanic component is NEMOv3.2 in its ORCA2 global configuration (Madec, 2008). 262 It has a horizontal resolution of about 2° with enhanced resolution at the equator 263 (0.5°) and 31 vertical levels. NEMOv3.2 includes the sea-ice model LIM2 (Fichefet 264 and Maqueda, 1997), and the marine biogeochemistry model PISCES (Aumont and 265 Bopp, 2006). PISCES simulates the biogeochemical cycles of oxygen, carbon and the 266 main nutrients with 24 state variables. The model simulates dissolved inorganic 267 carbon and total alkalinity (carbonate alkalinity + borate + water) and the distributions 268 of macronutrients (nitrate and ammonium, phosphate, and silicate) and micronutrient 269 iron. PISCES represents two sizes of phytoplankton (i.e., nanophytoplankton and 270 diatoms) and two zooplankton size-classes: microzooplankton and mesozooplankton. 271 PISCES simulates semi-labile dissolved organic matter, and small and large sinking particles with different sinking speeds (3 m d<sup>-1</sup> and 50 to 200 m d<sup>-1</sup>, respectively). 272 273 While fixed elemental stoichiometric C:N:P-O2 ratios after Takahashi et al. (1985) are

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274	imposed for these three compartments the internal concentrations of iron, silica and
275	calcite are simulated prognostically . The carbon system is represented by dissolved
276	inorganic carbon, alkalinity and calcite. Calcite is prognostically simulated following
277	Maier-Reimer (1993) and Moore et al. (2002). Alkalinity in the model system
278	includes the contribution of carbonate, bicarbonate, borate, protons, and hydroxide
279	ions. <u>Oxygen is prognostically simulated</u> . The model distinguishes between oxic and
280	suboxic remineralization pathways, the former relying on oxygen as electron acceptor,
281	the latter on nitrate, For carbon and oxygen pools, air-sea exchange follows the
282	Wanninkhof (1992) formulation.
I	
283	The boundary conditions account for nutrient supplies from three different sources:
284	atmospheric dust deposition for iron, phosphorus and silica (Jickells and Spokes,
285	2001; Moore et al., 2004; Tegen and Fung, 1995), rivers for nutrients, alkalinity and
286	carbon (Ludwig et al., 1996) and sediment mobilization for sedimentary iron (de Baar
287	and de Jong, 2001; Johnson et al., 1999). To ensure conservation of nitrogen in the
288	ocean, annual total nitrogen fixation is adjusted to balance losses from denitrification.
289	For the other macronutrients, alkalinity and organic carbon, the conservation is
290	ensured by tuning the sedimental loss to the total external input from rivers and dust.
291	In PISCES, an adequate treatment of external boundary conditions has been
292	demonstrated to be essential for the accurate simulation of nutrient distributions
293	(Aumont and Bopp, 2006; Aumont et al., 2003). Riverine carbon inputs induce a
294	natural outgassing of carbon of 0.6 Pg C $y^{-1}$ which has been shown essential to model
295	the inter-hemispheric gradient of atmospheric CO <sub>2</sub> under preindustrial state (Aumont
296	et al., 2001).

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298 The core simulation of this study is a 500-year long coupled preindustrial run. It uses 299 the same atmospheric, land surface and ocean configurations as IPSL-CM5A-LR 300 (Dufresne et al., 2013) for which the marine biogeochemistry has been extensively 301 evaluated (see e.g., Séférian et al. (2013) for modern-state evaluation). The only 302 difference between the "standard" preindustrial simulation contributed to CMIP5 and 303 the present one is the initial conditions. While the CMIP5 preindustrial simulation 304 starts from an ocean circulation after several thousand years of online physical 305 adjustment, the present simulation starts from an ocean at rest using the January 306 temperature and salinity fields from the World Ocean Atlas (Levitus and Boyer, 307 1994). Biogeochemical state variables were initialized from data compilations or 308 climatologies as explained in the following section. Atmospheric CO<sub>2</sub> and other 309 greenhouse gases, as well as natural aerosols, were set to their 1850 preindustrial 310 values. The simulation is extensively described in terms of ocean physics by Mignot 311 et al. (2013). Mignot and coworkers show that the strength of the Atlantic meridional 312 overturning circulation and the Antarctic circumpolar current as well as the upper 300 313 m ocean heat content stabilize after 250 years of simulation. 314

315 Although the spin-up protocol used to conduct this 500-year long simulation is not 316 readily comparable to the one used to produce the initial conditions for the CMIP5 317 preindustrial simulation, its duration is greater than the median length of on-line 318 adjustment computed from the multiple spin-up protocols applied during CMIP5 319 (~395 years, Figure 1 and Table 1). Besides, the methodology of initializing 320 biogeochemical state variables from data fields is not broadly employed by the 321 various modeling groups that have contributed to CMIP5. Despite the above-322 mentioned methodological shortcuts, we take this 500-year long preindustrial

323 simulation as a representative example of a spin-up protocol for the diversity of

324 approaches used by CMIP5 models.

325

32	6	2-2- Ob	servations	for	initia	lization	and	eval	luaf	tion
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- 327 Two streams of data sets were used in this study. The first stream combines data from
- the World Ocean Atlas 1994 (WOA94, Levitus and Boyer (1994) and Levitus et al.,
- 329 (1993)) for the initialization of 3-dimensional fields of temperature and salinity,
- dissolved nitrate, silicate, phosphate and oxygen, and data from GLODAP (Key et al.,

331 2004) for preindustrial dissolved inorganic carbon and total alkalinity. This stream of

- data was chosen purposely in our experimental setup to be slightly different than the
- 333 second stream of data, World Ocean Atlas 2013 (WOA2013, Levitus et al. (2013)),
- the evaluation data set.
- 335

- 337 includes up-to-date observed climatologies of nitrate and oxygen from the WOA2013.
- 338 This database is based on samples collected since 1965, and incorporates also data
- 339 from WOA94 onwards. For the concentrations of preindustrial dissolved inorganic
- 340 carbon and total alkalinity, we still use GLODAP. The second stream of data was
- 341 selected to be as close as possible to the "standard" evaluation procedure of skill-
- 342 assessment protocols found in CMIP5 model reference papers (Adachi et al., 2013;
- 343 Arora et al., 2011; Collins et al., 2011; Dunne et al., 2013; Ilyina et al., 2013; Lindsay
- 344 et al., 2014; Romanou et al., 2013; Séférian et al., 2013<u>; Séférian et al., 2015</u>; Tjiputra
- 345 et al., 2013; Vichi et al., 2011; Volodin et al., 2010; Watanabe et al., 2011; Wu et al.,
- 346 2013). Differences between these two streams of data are minor and are further
- detailed below.

349	2-3- Approach and statistical analysis
350	To quantify the impacts of a large diversity of spin-up procedures on the
351	representation of biogeochemical fields in CMIP5, we employ a three-fold approach.
352	(1) The 500-year long spin-up simulation described in Section 2.1 is used to
353	determine the influence of the spin-up procedure on the representation of
354	biogeochemical fields in IPSL-CM5A-LR.
355	(2) In the next step, relationships between biases in modeled fields, model-data
356	mismatches and the duration of the spin-up simulation are identified across the
357	CMIP5 ensemble. For this step, drifts in biogeochemical fields are determined from
358	the first century of the preindustrial simulation (referred to as <i>piControl</i> ) of each
359	CMIP5 ESM.
360	(3) Finally, the <u>various ensemble of</u> modern hindcast (referred to as <i>historical</i> ) from
361	each available CMIP5 ESM are used to estimate the impact of these drifts in
362	biogeochemical fields on the ability of models to replicate modern observations. For a
363	given model, we use the <u>ensemble average</u> of the <u>available</u> 'historical' <u>members</u> if
364	several realizations are available.
365	For this purpose, several statistical skill score metrics are computed following Rose et
366	al. (2009) and Stow et al. (2009) from model fields interpolated on a regular 1° grid
367	and to fixed depth levels. The skill score metrics are (1) the global averaged
368	concentrations for overall drift; (2) the error or bias between modeled and observed
369	fields at each grid-cell; (3) spatial correlation between model and observations to
370	assess mismatches between modeled and observed large-scale structures; (4) the root-
371	mean squared error (RMSE) to assess the total cumulative errors between modeled
372	and observed fields. These statistical metrics are computed across the water column,

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373	but for clarity we focus on surface, 150 m (thermocline) and 2000 m (deep) levels.	
374	These statistical metrics were chosen among those described in the literature, because	
375	they proved to yield the most indicative scores for tracking model errors or	
376	improvement along the various intercomparison exercises (IPCC, 2013).	roland seferian 5/1/16 16:02 Formatted: French
377		
378	The drift is determined for either concentrations in simulated biogeochemical fields or	
379	for skill score metrics (e.g., RMSE) using a linear regression fit over a time window	roland seferian 11/1/16 19:20 Deleted: or $\Delta\sigma$
380	of 100 years. This time window of 100 years was chosen as a trade off between $\underline{a}$	
381	longer time window (>200 years) that smoothes the drift signal and <u>a</u> shorter time	
382	window (< <u>100</u> years) that introduces fluctuations due to internal variability and hence	roland seferian 14/1/16 10:38 Deleted: 8
383	impacting the quality of the fit (see the assessment performed with the millennial-long	
384	CMIP5 piControl simulation of IPSL-CM5A-LR in Figure S1),	roland seferian 14/1/16 10:40 Formatted: Font:Italic
385	The drift is assumed to decrease exponentially during the spin-up simulation and is	roland seferian 14/1/16 10:38 Deleted:
386	described by a simple drift model:	
387	$driff(t) = drift(t=0) \times \exp(-\frac{1}{\tau}t) $ (1)	
388	where $\tau$ is the relaxation time of the respective field at a given depth level. It	
389	corresponds to the time required to nullify the drift.	
390		
391	Our analyses focus on the global distribution of nitrate (NO <sub>3</sub> ), dissolved oxygen (O <sub>2</sub> )	
392	and the difference between total alkalinity and dissolved inorganic carbon (Alk-DIC).	
393	The latter serves as an approximation of carbonate ion concentration following Zeebe	
394	and Wolf-Gladrow (2001). We use this approximation of the carbonate ion	
395	concentration rather than its concentration, $[CO_3^{2-}]$ , since the latter was poorly	
396	assessed in CMIP5 reference papers and was not provided by a majority of ESMs.	
397	These three biogeochemical tracers were chosen because (1) most current	
	16	

398	biogeochemical models simulate Alk, DIC, $NO_3$ and $O_2$ prognostically and (2) they
399	are frequently used in state-of-the-art model performance assessment (e.g., Anav et
400	al., 2013; Bopp et al., 2013; Doney et al., 2009; Friedrichs et al., 2009; 2007; Stow et
401	al., 2009), and (3) DIC and Alk are both used as "master tracers" for the carbonate
402	system in the ocean biogeochemistry models (while $[CO_3^{2-}]$ , e.g., is not explicitly
403	advected as a tracer but diagnosed from temperature, salinity, DIC, Alk, $[H^+]$ , and
404	$p\mathrm{CO}_2$ when needed) . Modeled distributions of $\mathrm{NO}_3,\mathrm{O}_2$ and Alk-DIC reflect the
405	representation of biogeochemical processes related to the biological pump ( $CO_2$ , $NO_3$ ,
406	$O_2$ ), the air-sea gas exchange and ocean ventilation (CO <sub>2</sub> and $O_2$ ), as well as carbonate
407	chemistry (Alk-DIC). These biogeochemical processes are of particular relevance for
408	investigating the impact of climate change on marine productivity (e.g., Henson et al.,
409	2010), ocean deoxygenation (e.g., Gruber, 2011; Keeling et al., 2009) and the ocean
410	carbon sink, processes for which future projections with the current generation of
411	ESMs yield large inter-model spreads (e.g., Friedlingstein et al., 2013; Resplandy et
412	al., 2015; Séférian et al., 2014; Tjiputra et al., 2014).
413	
414	3 Results
415	3-1 Comparison of observational datasets

416 Our review of spin-up protocols for CMIP5 ESM shows that several modeling groups

417 have employed different streams of datasets to initialize their biogeochemical models

418 (e.g., WOA1994, WOA2001), while model evaluation relies on the most up-to-date

419 stream of data. Differences between the two data streams used for initializing and

420 assessing, respectively,  $NO_3$  and  $O_2$  concentrations are analyzed. Table 2 summarizes

421 RMSE and correlation between WOA1994 and WOA2013 for these two

422 biogeochemical fields.

- 424 Table 2 indicates that differences between the two streams of data are fairly small. 425 The total difference (RMSE) represents a departure between 5 to 10% from the global 426 average concentrations of WOA2013 across depth levels. It is generally lower in 427 regions where the sampling density has not increased markedly between the two 428 releases. These values can be used as a baseline for model-to-model comparison 429 assuming that errors attributed to the various sources of initialization cannot be larger 430 than 10%. Considering that some models have used outputs from previous model 431 simulations or globally averaged concentrations as initial conditions, we acknowledge 432 that this baseline is not a perfect criterion for benchmarking model performance. 433 There is, however, no ideal solution to address this issue since there is no standardized 434 set of initial conditions in CMIP5 except some recommendations for the decadal 435 prediction exercise in which specific attention was paid to initialization (e.g., 436 Keenlyside et al., 2008; Kim et al., 2012; Matei et al., 2012; Meehl et al., 2013; 2009; 437 Servonnat et al., 2014; Smith et al., 2007; Swingedouw et al., 2013). 438 439 **3-2 Equilibration state metrics in IPSL-CM5A-LR** 440 The global mean sea surface temperature (SST) is a common metric to quantify the 441 energetic equilibrium of the model. This metric has been widely used in various
- 442 papers referenced in this study to determine the equilibration of ESM physical
- 443 components. Figure 2a shows the evolution of this metric during the 500-year long
- 444 spin-up simulation. The global average SST sharply decreases during the first 250
- 445 years of the simulation. In the last 250 years of the simulation, the global averaged
- 446 SST displays a small residual drift of  $\sim -10^{-4}$  °C y<sup>-1</sup> which falls into the range of the
- 447 drifts reported for CMIP5 ESMs. The evolution over the last 250 years is comparable

- 448 to those of other physical equilibration metrics, such as the ocean heat content or the
- 449 meridional overturning circulation (Mignot et al., 2013).
- 450

451	The temporal evolution of sea-to-air $\text{CO}_2$ fluxes was used in phase 2 of the Ocean		
452	Carbon Model Intercomparison Project (OCMIP-2, Orr (2002)) as an equilibration		
453	metric for the marine biogeochemistry and was still widely used during CMIP5.		
454	Figure 2b presents its evolution in the 500-year long spin-up simulation. The global		
455	ocean sea-to-air $CO_2$ flux is ~-0.7 Pg C y <sup>-1</sup> over the last decades of the spin-up		
456	simulation (negative values indicate ocean CO <sub>2</sub> uptake).		
457	To assess the global sea-to-air carbon flux, we use the range of values estimated from		
458	preindustrial natural ocean carbon flux inversions (e.g. Gerber and Joos (2010) or		
459	Mikaloff Fletcher et al. (2007)). Since, these estimates do not account for the		
460	preindustrial carbon outgassing induced by the river input, while our model does, we		
461	have added a constant outgassing of 0.45 Pg C y <sup>-1</sup> to the range of $0.03 \pm 0.08$ Pg C y <sup>-1</sup>		
462	(Mikaloff Fletcher et al. 2007). This value of 0.45 Pg C y <sup>-1</sup> corresponds to the global		
463	open-ocean river-induced carbon outgassing accordingly to IPCC (2013) or Le Quéré		
464	et al. (2015). Consequently, in our modeling framework, the target value of the global		
465	sea-to-air carbon flux ranges between 0.4 and 0.56 Pg C y <sup>-1</sup> .		
466			
467	Figure 2b shows that the global sea-to-air carbon flux does not fit our range of values		
468	estimated from preindustrial natural ocean carbon flux inversions, <u>Besides</u> , Figure 2b		
469	shows that the drift in the global sea-to-air carbon flux reduces more slowly after <u>a</u>		
470	strong decline during the first 50 years of the spin-up simulation. While this drift is		
471	about 0.001 Pg C y <sup>-2</sup> from year 250 to 500, it is weaker over the last century of the		
472	simulation (7x10 <sup>-4</sup> Pg C y <sup>-2</sup> ). Using a linear fit over the last century of the simulation		

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<b>Deleted:</b> (e.g. Gerber and Joos (2010) or Mikaloff Fletcher et al. (2007), referred to as MF2007 on Figure 2), which amounts to 0.03 $\pm$ 0.08 Pg C y <sup>-1</sup> (to which an open-ocean river- induced carbon outgassing of 0.45 Pg C y <sup>-1</sup> has to be added on Figure 2 accordingly to IPCC (2013) or Le Quéré et al. (2015). This indicates that the ocean carbon cycle has not reached a steady state in the model system following the 500 years of integration
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<b>Deleted:</b> an approximate relaxation time of 73 years estimated from the simple drift model (Equation 1) over years 250-500

473	with a drift of $\frac{7 \times 10^{-4} \text{ Pg C y}^2}{2}$ , we estimate that the simulated sea-to-air carbon flux
474	would reach the range of 0.4-0.56 Pg C y <sup>-1</sup> after 1100 to 1300 supplemental years of
475	spin-up simulation. Our simple drift model (Equation 1) gives a relaxation time of
476	around 160 years, which indicates that drift in ocean carbon flux should range
477	between $2x10^{-7}$ and $7x10^{-7}$ Pg C y <sup>-2</sup> after this 1100 to 1300 supplemental years of spin-
478	up simulation.
479	

480 These estimates do not account for the non-linearity of the ocean carbon cycle and the 481 associated process uncertainties (Schwinger et al., 2014), and hence potentially 482 underestimate the time required to equilibrate the ocean carbon cycle and sea-to-air carbon fluxes in the range of inversion estimates. The drift of 0.001 Pg C y<sup>-2</sup> is\_ 483 484 however, much smaller than the oceanic sink for anthropogenic carbon. Even if not 485 fully equilibrated in terms of carbon balance, it is likely that this run would have 486 given consistent estimates of anthropogenic carbon uptake in transient historical 487 hindcasts.

488

#### 489 3-3 Temporal evolution of model errors in IPSL-CM5A-LR

Figure 3 shows the temporal evolution of globally averaged concentrations for  $O_2$ , NO<sub>3</sub> and Alk-DIC at the surface (panels a, b and c), 150 m (panels d, e and f) and 2000 m (panels g, h, and i). Globally averaged concentrations of  $O_2$ , NO<sub>3</sub> and Alk-DIC (solid lines) reach steady state after 100 to 250 years of spin-up at the surface. While modeled nominal values for  $O_2$  concentration converge toward the observed concentration (i.e., 172.3  $\mu$ mol L<sup>-1</sup>), that of NO<sub>3</sub> and to a lesser extent Alk-DIC present persistent deviations from WOA2013 and GLODAP. At the surface, the

497 convergence of the simulated oxygen to observed value is expected since the

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498	dominant governing process of thermodynamic saturation (through the air-sea gas
499	exchange) is well understood and modeled. The deviation in surface NO <sub>3</sub> highlights
500	uncertainty related to near surface biological processes and upper ocean physics.
501	Below the surface, concentrations of biogeochemical tracers drift away from the
502	globally averaged concentrations computed from WOA2013 or GLODAP (Figure 3,
503	panels d-i). At 150 and 2000 meters, the drift in global averaged concentrations for
504	these fields, computed over the last 250 years, is still significant with $p<10^4$ (Table 3).
505	Dashed lines in Figure 3 indicate the temporal evolution of RMSE, which quantifies
506	the total mismatch between simulated and observed fields. Except for the surface
507	fields, Figure 3 shows that RMSE globally increases with time for all biogeochemical
508	fields. The linear drift in RMSE over the last 250 years of the spin-up simulation falls
509	within the 2-3 $\%$ ky $^{\text{-1}}$ range at the surface. It is much larger at 2000 m (144-280 $\%$ ky $^{\text{-1}}$
510	; Table 3). This is also the case regionally, because the latitudinal maximum in RMSE
511	$(RMSE_{max})$ is similar to the global RMSE. Table 3 also shows that the magnitude of
512	drift in RMSE for O <sub>2</sub> , NO <sub>3</sub> and Alk-DIC differs at a given depth as different processes
513	affect the interior distribution of these biogeochemical fields.
514	
515	3-4 Evolution of geographical mismatches in IPSL-CM5A-LR
516	To further explore the evolution of mismatch in biogeochemical distributions, we

517 analyze differences ( $\epsilon$ ) between simulated and observed fields of  $O_2$ ,  $NO_3$  from

518 WOA2013 and Alk-DIC from GLODAP after the initialization and at the end of the

519 spin-up, i.e., the first year and the last year of the core spin-up simulation performed

520 with the IPSL-CM5A-LR model (Figures 4, 5 and 6).

521

522 Figure 4 (panels a, c, and e) shows that surface concentrations of biogeochemical

523	fields are associated with small biases at initialization. This error represents less than	
524	5% of the observed surface concentrations for $O_2$ , NO <sub>3</sub> and Alk-DIC and reflects the	
525	weak difference between the data stream employed for initialization and validation.	
526	After 500 years of spin-up, deviations between the modeled and observed fields at the	
527	surface have increased locally by up to $\sim 40\%$ (Figure 4, panels b, d, and f). The	
528	largest deviations are found in high-latitude oceans for $O_2$ and $NO_3$ and also to some	
529	extent in the tropics for NO <sub>3</sub> and Alk-DIC.	
530		
531	Below the surface, distributions of modeled biogeochemical fields compare well to	
532	the observations at 150 m at initialization with averaged errors close to zero (Figure 5,	
533	panels a, c, and e). This result was expected since WOA2013 and WOA1994 differ	roland seferian 6/1/16 14:23
534	weakly at these depth levels. Subsurface distributions at initialization strongly contrast	Deleted. ac
535	with the concentrations that resulted from 500 years of spin-up (Figure 5, panels b, d,	roland seferian 6/1/16 14:23
536	and f). After 500 years of spin-up, strong mismatches characterize the distribution of	Deleted. bu
537	$O_2$ , $NO_3$ and Alk-DIC fields in the high-latitude oceans and in the tropics. Figure 5	
538	illustrates that pattern of errors are well correlated. It directly translates the	
539	assumptions employed in the biogeochemical model (here the elemental C:N:-O2	roland seferian 26/1/16 14:09
540	stochiometry of PISCES). Figure 6 shows that model-data deviations at 2000 m have	
541	substantially increased regionally after 500 years of simulation, showing large errors	
542	in the southern hemisphere oceans. This appears clearly in Figure 6, panels d and f for	
543	NO <sub>3</sub> and Alk-DIC fields, respectively.	
544		
545	The temporal evolution of the total mismatch between modeled and observed fields of	
546	$O_2$ , NO <sub>3</sub> and Alk-DIC over the whole water column is presented in Figure 7 in terms	
547	of RMSE (Figure 7, panels a-c), As expected, Figure 7 illustrates that there is a good	roland seferian 6/1/16 14:24 <b>Deleted:</b> and the difference in

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22

- 548 match during the first years of simulation for all biogeochemical fields at all depth
- 549 levels with low RMSE, After a few centuries, patterns of error evolve differently

550 across depth for  $O_2$ ,  $NO_3$  and Alk-DIC.

551	The temporal evolution of <u>RMSE</u> shows that patterns of error have reached a steady
552	state after few decades within the upper hundred meters of the ocean but continue to
553	evolve at greater depths, even after 500 years. Patterns of errors within the
554	thermocline and deep water masses evolve at time scales of few decades and few
555	centuries, respectively in relation with the structure of the large-scale ocean
556	circulation. Mid-depth (~1500-2500m) RMSE evolves much slower because this
557	depth corresponds to the depth of the very old radiocarbon age (e.g., Wunsch and
558	Heimbach, 2007; 2008) whose characteristics time scale spans over thousand of years.
559	At the end of the spin-up simulation, two maxima of comparable amplitude are found
560	for RMSE at 150 and 3750 m for $O_2$ and at 50 m and 3800 m for Alk-DIC.
561	
562	3-5 Drifts in IPSL-CM5A-LR spin-up simulation
563	With the evolution of the RMSE established, we can use the simple drift model
563 564	With the evolution of the RMSE established, we can use the simple drift model (Equation 1), to determine the relaxation time, $\tau$ , required to reach equilibration after a
563 564 565	With the evolution of the RMSE established, we can use the simple drift model (Equation 1), to determine the relaxation time, $\tau$ , required to reach equilibration after a longer of spin-up simulation. To use this simple drift model, we compute the drift in
563 564 565 566	With the evolution of the RMSE established, we can use the simple drift model (Equation 1), to determine the relaxation time, $\tau_2$ , required to reach equilibration after a longer of spin-up simulation. To use this simple drift model, we compute the drift in RMSE determined from time segments of 100 years distributed evenly every 5 years
563 564 565 566 567	With the evolution of the RMSE established, we can use the simple drift model (Equation 1), to determine the relaxation time $_{\tau}$ , required to reach equilibration after a longer of spin-up simulation. To use this simple drift model, we compute the drift in RMSE determined from time segments of 100 years distributed evenly every 5 years from year 250 to 500 for O <sub>2</sub> , NO <sub>3</sub> and Alk-DIC tracers. The drift model (magenta
563 564 565 566 567 568	With the evolution of the RMSE established, we can use the simple drift model (Equation 1), to determine the relaxation time, $\tau_2$ , required to reach equilibration after a longer of spin-up simulation. To use this simple drift model, we compute the drift in RMSE determined from time segments of 100 years distributed evenly every 5 years from year 250 to 500 for O <sub>2</sub> , NO <sub>3</sub> and Alk-DIC tracers. The drift model (magenta lines in Figure 8) is fitted level to the 80 drift values for each field and each depth
563 564 565 566 567 568 569	With the evolution of the RMSE established, we can use the simple drift model (Equation 1), to determine the relaxation time, $\tau_2$ , required to reach equilibration after a longer of spin-up simulation. To use this simple drift model, we compute the drift in RMSE determined from time segments of 100 years distributed evenly every 5 years from year 250 to 500 for O <sub>2</sub> , NO <sub>3</sub> and Alk-DIC tracers. The drift model (magenta lines in Figure 8) is fitted level to the 80 drift values for each field and each depth (colored crosses in Figure 8).
563 564 565 566 567 568 569 570	With the evolution of the RMSE established, we can use the simple drift model (Equation 1) to determine the relaxation time, $\tau_2$ required to reach equilibration after a longer of spin-up simulation. To use this simple drift model, we compute the drift in RMSE determined from time segments of 100 years distributed evenly every 5 years from year 250 to 500 for O <sub>2</sub> , NO <sub>3</sub> and Alk-DIC tracers. The drift model (magenta lines in Figure 8) is fitted level to the 80 drift values for each field and each depth (colored crosses in Figure 8).
563 564 565 566 567 568 569 570 571	With the evolution of the RMSE established, we can use the simple drift model (Equation 1), to determine the relaxation time, $\tau_2$ , required to reach equilibration after a longer of spin-up simulation. To use this simple drift model, we compute the drift in RMSE determined from time segments of 100 years distributed evenly every 5 years from year 250 to 500 for O <sub>2</sub> , NO <sub>3</sub> and Alk-DIC tracers. The drift model (magenta lines in Figure 8) is fitted level to the 80 drift values for each field and each depth (colored crosses in Figure 8).
563 564 565 566 567 568 569 570 571 572	With the evolution of the RMSE established, we can use the simple drift model (Equation 1) to determine the relaxation time, $\tau$ , required to reach equilibration after a longer of spin-up simulation. To use this simple drift model, we compute the drift in RMSE determined from time segments of 100 years distributed evenly every 5 years from year 250 to 500 for O <sub>2</sub> , NO <sub>3</sub> and Alk-DIC tracers. The drift model (magenta lines in Figure 8) is fitted level to the 80 drift values for each field and each depth (colored crosses in Figure 8). The simple drift model fits well the evolution of the drift in RMSE for the biogeochemical variables along the spin-up simulation of IPSL-CM5A-LR (Figure 8).

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**Deleted:** Patterns of Δσ present different features than those of RMSE and demonstrate that the simulated fields substantially underestimate the spatial variation of observed biogeochemical fields on subsurface depth surfaces except for Alk-DIC. roland seferian 6/1/16 14:25 **Deleted:** both metrics

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From these two metrics, the simple drift model
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573	Correlation coefficients are mostly significant at 90% confidence level ( $r^*=0.14$	
574	determined with a student distribution with significance level of 90% and 80 degrees	
575	of freedom), except for NOg at surface and Alk-DIC at 150 m. Another exception is	roland seferian 13/1/16 15:52
576	found for NO <sub>2</sub> at 150 m where the drift does not correspond to an exponential decay	([1])
577	of the drift as function of time. The large confidence interval of the fit indicates that	
578	the fit would have been considered as non-significant given a longer spin-up	
579	simulation or a higher confidence threshold.	
580		
581	<u>When significant, estimates of <math>\tau</math> for O<sub>2</sub> <u>RMSE</u> are <math>\approx</math> 90, 564 and 1149 y at the surface</u>	roland seferian 6/1/16 14:27
582	150 m and 2000 m, respectively. These values match reasonably well $\tau$ estimated for	RMSE about41340[2]
583	NO <sub>3</sub> RMSE at 2000 m (1130 y) and those for Alk-DIC RMSE at surface and 2000 m	roland seferian 13/1/16 16:18
584	(137 and 1163 y). However, these estimates are sensitive to the time windows used to	
585	compute the drift. For a subset of time windows between 100 and 250 years by step of	
586	50 years, $\tau$ estimates for O <sub>2</sub> RMSE are $\approx$ 114±67, 375±140 and 1116±527 y at the	roland seferian 6/1/16 14:28
587	surface 150 m and 2000 m depth. These large uncertainties associated with $\tau_{z}$	oxygen $\Delta\sigma$ with 8, 7 and 46 y at surface, 150 and 2000 m, respectivelyValues for
588	estimates are essentially due to the length of the spin-up simulation. A longer spin-up	other biogeochemical fields are quite similar to those for $O_2$ except for $NO_3$ at 150 m[3]
589	simulation would improve the quality of the fit (see Figure S1),	roland seferian 13/1/16 16:19
590	Υ	Roman
591	3-6 Drifts in CMIP5 ESMs preindustrial simulations	<b>Deleted:</b> This contrasting result between the two skill score metrics expresses the fact that
592	In this subsection, the analysis is extended to the CMIP5 archive. We focus on oxygen	RMSE accounts for the total distance between modeled and observed oxygen distributions, while $\Delta\sigma$ considers solely the difference in
593	fields in the long preindustrial simulation, <i>piControl</i> , for the 15 available CMIP5	spatial structure between model fields and observations. This shows that the time scale
594	ESMs. From these simulations that span from 250 to 1000 years, we compute the drift	necessarily the same as the drift
595	in O2 RMSE across depth from several time segments of 100 years distributed evenly	Deleted: 5
596	every 5 years from the beginning until the end of the piControl simulation, These	<b>Deleted:</b> we extend our4While the duration of CMIP5 <i>piControl</i> simulations
597	drift <u>s are used as a surrogate for drift computed from the spin-up of each model since</u>	ranges from 250 to 1000 years, we choose torelativeand $\Delta \sigma$ over the first century of simulation for each ESM (Figure 8). isis[4]

such simulations are not available through the data portal. 598

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## 599

600	Figure $\underline{9}$ represents the drift in $\underline{0}_2$ RMSE versus the spin-up duration for each CMIP5	roland seferian 13/1/16 16:29
601	ESM. The analysis shows that the drift in $O_2 RMSE$ differs substantially between	b, and c) and $\Delta\sigma$ (Figure 8, panels d, e, and f) for O <sub>2</sub> concentrations (log scale)
602	models. For a given model, drifts in other biogeochemical tracers (NO <sub>3</sub> and Alk-DIC)	with aconcentrationgreater than 10% over the first century of the CMIP5
603	display similar features (not shown). The between-model differences in drift are not	preindustrial simulationDshowThe magnitude of the drifts in RMSE and $\Delta\sigma$ tends to increase with depth. It spans within 0-35%
604	surprising since there are no reasons for different models to exhibit similar drift for a	range at the surface up to a 0-400% range at 2000 m8alsothe best-fit linear regression relationship (or exponential in
605	given field. Yet, Figure 9, shows that a global relationship emerges from this ensemble	linear scale) between t (or $\Delta \sigma$ )andThis relationship suggests a general decrease of the
606	when using the simple drift model to fit the drift in $\underline{O}_2$ RMSE as function of the spin-	drift as a function of spin-up duration for all depth levels. This decrease in drift displays low significance thegenerallyranging
607	up duration (solid green lines in Figure 9). With a 90% confidence level, this	between 0.3 and 0.7The lower correlation coefficients fall outside the 90% significance thre shold 6 4 C of RMSE at 150 m is
608	relationship suggests a general decrease of the drift as a function of spin-up duration	even lower than the 66% significance threshold (0.1),decrease in drift as a
609	for all depth levels. At the surface and at 2000 m depth, the quality of fits is low with	tunction of spin-up duration [5]
610	correlation <u>coefficients of about ~0.4</u> . These are however significant at 90%	
611	<u>confidence level</u> ( $r^*=0.34$ , determined with a student distribution with significance	
612	level of 90% and 15 models as degree of freedom). The weakest correlation	
613	coefficient is found for the fit at 150 m depth and hence indicating that there is no link	
614	between the drift in $O_2$ RMSE and the duration of the spin-up simulation. This low	
615	significance level must be put into perspective given the large diversity of spin-up	
616	protocols and initial conditions (Figure 1 and Table 1) that can deteriorate the drift-	
617	spin up duration relationship in this ensemble of models.	
618		
619	The drift versus spin up duration relationship established from the 15 CMIP5 ESMs is	roland seferian 23/1/16 13:12
620	nonetheless consistent with the results obtained with IPSL-CM5A-LR, (The results in	modelshown as solid red lines in8, for which the relationship was (1) determined
621	Figure 8 have been reported in Figure 9 with magenta crosses), Consistency is	year 250 to 500 and (2) extrapolated over the 250-1190 spin-up duration range [6]

indicated by the sign of the drift versus spin up duration relationship of the IPSL-622

25

[ ... [6]

623	CM5A-LR model at the various depth levels, although their magnitudes differ. This	
624	difference in magnitude is not surprising if one considers that drift is highly model	
625	and protocol dependent and that the length of the IPSL-CM5A-LR spin-up simulation	
626	is potentially too short to determine accurate estimates of the long-term drift in $O_2$	
627	<u>RMSE</u> . Despite these differences, our analyses show that a relationship between the	roland seferian 6/1/16 18:56
628	drift in $O_2 RMSE$ versus the spin-up duration emerges from an ensemble of models	emphasized by the fact that the regression fit (red line on Figure 8 determined from the spin- up simulation) and data point (blue point on
629	and is broadly consistent with our theoretical framework of a drift model established	Figure 8 determined from the first century of the CMIP5 piControl simulation) derived from IPSL-CM5A-LR results differ at some denth
630	from the results of the IPSL-CM5A-LR model (Figure 8).	levels.
631		reland asferies 40/4/40 45-04
632	<b>3-7</b> Impact of the drift on model skill score assessment metrics across CMIP5	Deleted: 6
633	ESMs	roland seferian 13/1/16 16:37
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634	In the following, we investigate the influence of model drift on skill score assessment	roland seferian 13/1/16 16:36
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635	metrics that are routinely used to benchmark model performance. For this purpose, we	roland seferian 13/1/16 16:37
$\omega$		roland soferian 12/1/16 16:27
636	use the ensemble-mean $O_2$ RMSE as a metrics to assess the distance petween the	Deleted:
637	biogeochemical observations and model results. For this purpose, we compute 0.	roland seferian 13/1/16 16:40
057	biogeoenemical observations and <u>model results. For any purpose</u> , we compute op	Formatted: Subscript
638	RMSE from each ensemble member of the CMIP5 models averaged from 1986 to	roland seferian 13/1/16 16:41
639	2005 with respect to WOA2013 observations. The model-data distance is then	of individual CMIP5 ESMs is computed following the approach widely employed to
640	determined for each CMIP5 model using the mean across the available ensemble	evaluate CMIP5 models (Adachi et al., 2013; Arora et al., 2011; Collins et al., 2011; Dunne et al., 2013; Ilyina et al., 2013; Lindsay et al.,
641	members.	2014; Romanou et al., 2013; Séférian et al., 2013; Tjiputra et al., 2013; Vichi et al., 2011; Volodin et al., 2010; Watanabe et al., 2011;
642	▼	Wu et al., 2013). The normalized distance consists of the scaled RMSE of model output averaged from 1985 to 2005.
643	The left hand side panels of Figure <u>10</u> present the performance of available CMIP5	roland seferian 13/1/16 16:35
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644	models in terms of distance to oxygen observations at the surface, 150 m and 2000 m,	roland seferian 11/1/16 12:09
645	respectively. In these panels, the various CMIP5 models are ordered as function of	Deleted: normalized distance to oxygen observations
646	their distance to the oxygen observations, Following Knutti et al. (2013), either the	Deleted: The normalized distance is used for model ranking
647	ensemble mean or the ensemble median is used to identify groups of models with	roland seferian 13/1/16 18:19 Deleted: 9
648	similar skill within the CMIP5 ensemble. <u>The left hand side panels of Figure 10 show</u>	roland seferian 13/1/16 18:22 Deleted: s

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649	that the ability of models to reproduce oxygen observations varies across depth levels.	
650	The RMSE in the simulated O <sub>2</sub> fields in <u>CESM1-BGC</u> , HadGEM2- <u>ES</u> , HadGEM2-	roland seferian 11/1/16 13:48
651	CC, GFDL-ESM2M, MPI-ESM-LR and MPI-ESM-MR is generally smaller than the	Deleted: CC roland seferian 11/1/16 13:48
652	ensemble mean or ensemble median RMSE across the various depth levels (Figure 10	roland seferian 11/1/16 13:51 Deleted: and CESM1-BGC
653	panels a, b and c). On the other side of the ranking, <u>CMCC-CESM</u> , CNRM-CM5.	roland seferian 13/1/16 21:25
654	CNRM-CM5-2, IPSL-CM5B-LR, and NorESM1-ME exhibit RMSE generally higher	<b>Deleted:</b> For the HadGEM2 models, this result might arise from the fact that these models (1) are closer to the initial state since they have been spun up for a relatively short
655	than the ensemble mean and median RMSE across the various depth levels. The other	integration time or (2) display a better representation of the observed ocean. In either
656	models, i.e., CNRM-ESM1, GFDL-ESM2G, IPSL-CM5A-LR and IPSL-CM5A-MR	case, this would lead to a departure from the initial state that is smaller than for models that have a longer spin-up duration.
657	display O <sub>2</sub> RMSE that is generally close to the ensemble mean or the ensemble	roland seferian 13/1/16 21:22
650	modian	roland seferian 13/1/16 21:22
038	median.	Deleted: CMCC-CESM
659		roland seferian 13/1/16 21:24
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660	To assess the impact of model's drift inherited from the diversity of spin-up strategies	
661	(Figure 1 and Table 1) on the performance metrics, we use a simple additive	roland seferian 13/1/16 21:25
		Deleted: model
662	assumption to incorporate an incremental error due to the drift, ARMSE, to the above-	
663	mentioned RMSE. This incremental error due to the drift is computed using the	roland seferian 7/1/16 12:28
664	relaxation time $\tau$ determined from the <i>piControl</i> simulations of each CMIP5 model <u>at</u>	<b>Deleted:</b> the incremental deviation due to drift in biogeochemical fields is estimated from the simple drift model (Equation 1). The incremental deviation, ΔRMSE,
665	each depth level (Equation 1 and Figure 9) and a common duration of T=3000 years	roland seferian 13/1/16 18:20
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666	for all models ( <u>m</u> ):	roland seferian 7/1/16 12:41
	T	roland seferian 7/1/16 12:28
667	$\Delta RMSE_{m}(z) = \int dr i f t_{m}(z, t=0) \times \exp(-\frac{1}{(z)}t) dt \qquad (2)$	Formatted: Font:(Default) Times
	$\int_{0}^{\infty} \tau(z) $	roland seferian 7/1/16 12:37
668	where $\Delta RMSE$ has the same unit as RMSE.	Formatted: Font:Times, Font color: Auto, English (US), Lowered by 13 pt
669	The common duration T is used to bring model drift close to zero and hence to make	
670	models comparable to each other.	
671	We employ $\Delta RMSE$ to penalize the distance from the observations assuming that this	roland seferian 7/1/16 12:44
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672	drift-induced deviation in tracer fields can be added to RMSE. This means that the	Deleted: normalized

673 effect of the penalty is to increase the distance giving a consistent measure of the

674 equilibration error.

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675

676	Right hand side panels of Figure <u>10</u> show the influence of this penalization approach	roland seferian 13/1/16 18:20
677	on the model ranking at the various depth levels. They show that several models have	Deleted: 9
678	been upgraded in the ranking while others have not. For example, both MPI-ESM-LR,	
679	MPI-ESM-MR have been upgraded at the surface and 2000 m. On the other hand, the	roland seferian 11/1/16 16:43
680	rank of HadGEM2-ES and HadGEM2-CC has been downgraded to the $5^{\text{th}}$ and $3^{\text{th}}$	models that roland seferian 11/1/16 16:44
681	position due to the large drift in surface oxygen concentrations in comparison to that	Deleted: models roland seferian 11/1/16 16:44
682	of the other models. The surface drift might be attributed to drivers in oxygen fluxes	Deleted: 6 roland seferian 11/1/16 16:44
683	(e.g., SST, SSS). The ranking of GFDL-ESM2G and GFDL-ESM2M slightly changes	Deleted: 7
684	with penalization but both models stay close to the ensemble mean or the ensemble	
685	median. At the bottom of the ranking, models with large deviation from the oxygen	
686	observations (i.e., CMCC-CESM, IPSL-CM5B-LR, NorESM1-ME, CNRM-CM5) are	
687	found. For these models, the computed $\Delta RMSE$ and RMSE result in similar ranking,	
688	because even a small drift and hence relatively low $\Delta RMSE$ cannot compensate for	
689	their large RMSE.	roland seferian 13/1/16 21:28 Deleted:
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691	4- <u>Discussion</u>	roland seferian 11/1/16 18:59 Deleted: Implications
692	4-1 Implications for biogeochemical processes	
693	Our results show that errors in ocean biogeochemical fields amplify during the spin-	roland seferian 7/1/16 13:44 Deleted: and propagate
694	up simulation but not at the same rate at all depths. These differences in error	
695	evolution are consistent with an increasing contribution of biogeochemical processes	
696	in setting the distribution of tracers at depth. Indeed, Mignot et al. (2013) with the	
697	same model simulation showed that the large-scale ocean circulation reaches quasi-	

698	equilibrium after 250 years of spin-up, but our analyses indicate that biogeochemical	roland seferian 28/1/16 09:17
699	tracers do not (Figure <u>3</u> ).	roland seferian 26/1/16 14:11
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701	Besides, our analysis demonstrates that error propagation and biogeochemical drift are	
702	highly model dependent. For example, despite having the same initialization strategy	
703	and comparable spin up duration, the GFDL-ESM2G, GFDL-ESM2M, and	
704	NorESM1-ME models display considerable difference in drift (Figures <u>9</u> and <u>10</u> ) that	roland seferian 26/1/16 14:11 Deleted: 8
705	mirror large differences in model performance and properties (e.g., resolution,	roland seferian 26/1/16 14:11 Deleted: 9
706	simulated processes).	
707		
708	The identification of the dynamical or biogeochemical processes responsible for these	
709	errors is not within the scope of this study and would required additional long	
710	simulations with additional tracers targeted for attribution of the various	
711	biogeochemical processes and the underlying ocean physics (e.g., Doney <u>et al.</u> , 2004)	
712	involved (e.g. using abiotic, passive tracers as suggested in Walin et al. (2014)). Some	
713	mechanisms can be nonetheless invoked to explain differences or similarities in	
714	behavior between biogeochemical fields. For example, the evolution of surface	
715	concentrations for $O_2$ and Alk-DIC is controlled by the solubility of $O_2$ and $CO_2$ in	
716	seawater and the concentration of these gases in the atmosphere (set to the observed	
717	values and kept constant in all experiments performed with IPSL-CM5A-LR	
718	discussed here) and the biological soft-tissue and calcium carbonate counter pumps	
719	(in relation with the vertical transport of nutrients and alkalinity). Therefore, the	
720	equilibration of the $O_2$ and Alk-DIC surface fields once the physical equilibrium is	
721	reached (~250 years of spin-up) is expected (Figure 3, panels a and c and Figure 7).	roland seferian 26/1/16 14:11
722	Nevertheless, spatial errors could increase depending on the physical state of the	Deleteu

723	model (Figure 4, panels b and f). By contrast, the evolution of $NO_3$ concentration is
724	predominantly determined by ocean circulation, biological processes, and to a lesser
725	extent by external supplies from rivers and atmosphere. Below the surface,
726	concentrations of $O_2$ , $NO_3$ , and Alk-DIC evolve in response to the combined effect of
727	ocean circulation and biogeochemical processes. The combination of dynamical and
728	biogeochemical processes on the one hand, and the spin-up strategy on the other hand
729	both shape the modeled distributions of large-scale biogeochemical tracers.
730	
731	Consequences of the difficulty in achieving the correct equilibration procedure are
732	even larger for biogeochemical features that are defined by regional characteristics in
733	tracer concentrations, such as high nutrient/low chlorophyll regions, oxygen minimum
734	zones and nutrient-to-light colimitation patterns. This point is illustrated by recent
735	studies focusing on future changes in phytoplankton productivity (e.g. Vancoppenolle
736	et al. (2013) and Laufkötter et al. (2015). Vancoppenolle and co-workers report a
737	wide spread of surface mean $NO_3$ concentrations (1980-1999) in the Arctic with a
738	range from 1.7 to 8.9 $\mu$ mol L <sup>-1</sup> across a subset of 11 CMIP5 models. The spread in
739	present day NO <sub>3</sub> concentrations translates into a large model-to-model uncertainty in
740	future net primary production. Laufkötter and colleagues determined limitation terms
741	of phytoplankton production for a subset of CMIP5 and MAREMIP (Marine
742	Ecosystem Model Intercomparison Project) models. The authors demonstrate that
743	nutrient-to-light colimitation patterns differ in strength, location and type between
744	models and arise from large differences in the simulated nutrient concentrations.
745	Although large differences between models were reported by Vancoppenolle et al.
746	(2013) and Laufkötter et al. (2015) such as the spatial resolution and the complexity
747	of biogeochemical models, differences in nutrient concentrations were identified as

748	the largest source of model-to-model spread in addition to simply model error. The
749	authors of both studies qualitatively invoked differences in spin-up duration to explain
750	this spread. Besides, a recent assessment of interannual to decadal variability of ocean
751	$\mathrm{CO}_2$ and $\mathrm{O}_2$ fluxes in CMIP5 models, suggests that decadal variability can range
752	regionally from 10 to 50% of the total natural variability among a subset of 6 ESMs
753	(Resplandy et al., 2015). In that study, the authors demonstrate that, despite the
754	robustness of driving mechanisms (mostly related to vertical transport of water
755	masses) across the model ensemble, model-to-model spread can be related to
756	differences in modeled carbon and oxygen concentrations. In light of present results,
757	it appears likely that differences in spin-up strategy and sources of initialization could
758	<u>also</u> contribute to the amplitude of the natural variability of the ocean $\text{CO}_2$ and $\text{O}_2$
759	fluxes.
760	
761	4-2 Implications for future projections

762 The inconsistent strategy to spin-up models in CMIP5 is a significant source of model 763 uncertainty. It needs to be better constrained in order to draw robust conclusions on 764 the impact of climate change on the carbon cycle as well as its climate feedback (e.g., 765 Arora et al., 2013; Friedlingstein et al., 2013; Roy et al., 2011; Schwinger et al., 2014; 766 Séférian et al., 2012) and on marine ecosystems (e.g., Bopp et al., 2013; Boyd et al., 767 2015; Cheung et al., 2012; Doney et al., 2012; Gattuso et al., 2015; Lehodey et al., 768 2006). So far, the most frequent approach relies on the use of long preindustrial 769 control simulations to 'remove' the drift embedded in the simulated fields over the 770 historical period or future projections (e.g., Bopp et al., 2013; Cocco et al., 2013; 771 Friedlingstein et al., 2013; 2006; Frölicher et al., 2014; Gehlen et al., 2014; Keller et 772 al., 2014; Steinacher et al., 2010; Tjiputra et al., 2014). Although this approach allows

773	to determine relative changes, it does not allow to investigate the underlying reasons
774	of the spread between models in terms of processes, variability and response to
775	climate change. The "drift-correction" approach, much as the one used for this study,
776	assumes that drift-induced errors in the simulated fields can be isolated from the
777	signal of interest. Verification of this fundamental hypothesis would require a specific
778	experimental set-up consisting of the perturbation of model fields (e.g., nutrients or
779	carbon-related fields) to assess by how much the model projections would be
780	modified. So far, several modeling groups have generated ensemble simulation in
781	CMIP5 using a similar approach. However, the perturbations were applied either to
782	physical fields only or to both the physical and marine biogeochemical fields. To
783	assess impacts of different spin-up strategies and/or initial conditions on future
784	projections of marine biogeochemical tracer distributions, ensemble simulations in
785	which only biogeochemical fields are perturbed would be needed.
786	
787	4-3 Implications for multi-model skill-score assessments.
788	While the importance of spin-up protocols is well accepted in the modeling
789	community, the link between spin-up strategy and the ability of a model to reproduce
790	modern observations remains to be addressed.
791	
792	Most of the recent CMIP5 skill assessment approaches were based on historical
793	hindcasts that were started from preindustrial runs of varying duration and from
794	various spin-up strategies. Therefore, in typical intercomparison exercises, Earth
795	system models with a short spin-up, and hence modeled distributions still close to
796	initial fields, are confronted with Earth system models with a longer spin-up duration
797	and modeled distributions that have drifted further away from their initial states. Our

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798	study highlights that such inconsistencies in spin-up protocols and initial conditions	
799	across CMIP5 Earth system models (Figure 1 and Table 1) could significantly	
800	contribute to model-to-model spread in performance metrics. The analysis of the first	roland seferian 11/1/16 17:09
801	century of CMIP5 <i>piControl</i> simulations demonstrated a significant spread of drift	<b>Deleted:</b> These inconsistencies result in systematic model biases, somewhat in line with Swart and Fyfe (2011), and affect model reliability
802	between CMIP5 models (Figure 2). An approximate exponential relationship between	roland seferian 26/1/16 14:12
803	the amplitude of drift and the spin up duration emerges from the ensemble of CMIP5	Deleted: 8
804	models, which is consistent with results from IPSL-CM5A-LR. For example, while	
805	the global average root-mean square error increased up to 70% during a 500-year	
806	spin-up simulation with IPSL-CM5A-LR, its rate of increase (or drift) decreased with	
807	time to a very small rate (0.001 Pg C y <sup>-1</sup> ), Combining a simple drift model and this	roland seferian 11/1/16 18:38
808	relationship, we propose a penalization approach in an effort to assess more	<b>Deleted:</b> , suggesting that results should be reliable in the context of transient historical hindcast or future projections
809	objectively the influence of documented model differences on model-data biases.	
810	Figure <u>10</u> compares the state-of-the-art approach to assess model performance (left	roland seferian 26/1/16 14:12
811	hand side panels) to the drift-penalized approach (right hand side panels). This novel	
812	approach penalizes models with larger drift without affecting the models with smaller	
813	drift, Taking into account drift in modeled fields results in subtle adjustments in	roland seferian 11/1/16 18:40
814	ranking, which reflect differences in spin-up and initialization strategies.	<b>Deleted:</b> , while not inducing major changes in model ranking
815		
816	4-4 Limitations of the framework	
817	In this work, the analyses focus on the globally averaged O <sub>2</sub> RMSE across a diverse	roland seferian 15/1/16 10:48 Formatted: Subscript
818	ensemble of CMIP5 models, which differ in terms of represented processes, spatial	roland seferian 15/1/16 11:17
819	resolution and performance in addition to differences in spin-up protocols. Major	Formatted: English (US) roland seferian 15/1/16 12:39
820	limitations of the framework are presented below.	<b>Formatted:</b> Justified, Don't adjust space between Latin and Asian text, Don't adjust space between Asian text and numbers, Tabs: 0,99 cm, Left + 1,98 cm, Left +
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822 Due to their specificities in terms of processes and resolution (e.g., Cabré et al.,

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823	(2015), Laufkötter et al. (2015)), regional drift in CMIP5 models may differ from the
824	drift computed from globally averaged skill-score metrics (see Figure S2 and S3).
825	These differences may lead to different estimates of the relaxation time $\tau$ at regional
826	scale. Moreover, the combination of regional ocean physics and biogeochemical
827	processes in each individual model may drive an evolution of regional drift in RMSE
828	that does not fit the hypothesis of an exponential decay of the drift during the course
829	of the spin-up simulation.
830	
831	The above-mentioned remark can explain the relatively low confidence level of the fit
832	to drift across the multi-model CMIP5 ensemble (Figure 9). The relatively low
833	significance level of the fit directly reflects not only the large diversity of spin-up
834	protocols and initial conditions (Figure 1 and Table 1) but also the large diversity of
835	processes and resolution of the CMIP5 models. An improved derivation of the
836	penalization would require access to output from spin-up simulations for each
837	individual model or, at least, a better quantification of model-model differences in
838	terms of initial conditions.
839	
840	Finally, it is unlikely that model fields drift at the same rate along the spin-up
841	simulation, even under the same spin-up protocols. Indeed, as shown in Kriest and
842	Oschlies (2015), various parameterizations of the particles sinking speeds in a
843	common physical framework may lead to a similar evolution of the globally averaged
844	RMSE in the first century of the spin-up simulation but display very different
845	behaviour within a time-scale of $O(10^3)$ years. As such, drift and $\tau$ estimates need to
846	be used with caution when computed from short spin-up simulation because they can
847	be subject to large uncertainties.

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848	
849	5- Conclusions and recommendation for future intercomparison exercises
850	Skill-score metrics are expected to be widely used in the framework of the future
851	CMIP6 (Meehl et al., 2014) with the development of international community
852	benchmarking tools like the ESMValTool (http://www.pa.op.dlr.de/ESMValTool, see
853	also Eyring et al. (2015)). The assessment of model skill to reproduce observations
854	will focus on the modern period. Complementary to this approach, our results call for
855	the consideration of spin-up and initialization strategies in the determination of skill
856	assessment metrics (e.g., Friedrichs et al., 2009; Stow et al., 2009) and, by extension,
857	to model weighting (e.g., Steinacher et al., 2010) and model ranking (e.g., Anav et al.,
858	2013). Indeed, the use of equilibrium-state metrics of the model like the 3-
859	dimensional growth rate or drift of relevant skill score metrics (e.g. RMSE) could be
860	employed to increase the reliability of these traditional metrics and, as such, should be
861	included in the set of standard assessment tools for CMIP6.
862	x
863	In an effort to better represent interactions between marine biogeochemistry and
864	climate (Smith et al., 2014), future generations of Earth system models are likely to
865	include more complex ocean biogeochemical models, be it in terms of processes (e.g.,
866	Tagliabue and Völker, 2011; Tagliabue et al., 2011) or interactions with other
867	biogeochemical cycles (e.g., Gruber and Galloway, 2008) or increased spatial
868	resolution (e.g., Dufour et al., 2013; Lévy et al., 2012) in order to better represent
869	mesoscale biogeochemical dynamics. These developments will go along with an
870	increase in the diversity and complexity of spin-up protocols applied to Earth system
871	models, especially those including an interactive atmospheric CO <sub>2</sub> or interactive
872	nitrogen cycle (e.g., Dunne et al., 2013; Lindsay et al., 2014). The additional

Deleted: The low confidence level of the fit to drift across the multi-model CMIP5 ensemble is a limitation of our approach and the robustness of the fit used to penalize models might be criticized. The low significance level of the fit directly reflects the large diversity of spin-up protocols and initial conditions (Figure 1 and Table 1). The improved derivation of the penalization factor would require access to output from spin-up simulations for each individual model or, at least, a better quantification of model-model differences in terms of initial conditions. The impact of this penalization approach on model ranking calls for the consideration of spin-up and initialization strategies in the determination of skill assessment metrics (e.g., Friedrichs et al., 2009; Stow et al., 2009) and, by extension, to model weighting (e.g., Steinacher et al., 2010) and model ranking (e.g., Anav et al., 2013).

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**Deleted:** In order to increase the reliability of these traditional metrics, additional metrics that allow us to determine the equilibrium state of the model like the 3-dimensional growth rate or drift of relevant skill score metrics (e.g., RMSE) over the last decades or centuries of the spin-up,

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873	challenge of spinning-up emission-driven simulations with interactive carbon cycle	
874	will also require us to extend the assessment of the impact of spin-up protocols to the	
875	terrestrial carbon cycle. Processes such as soil carbon accumulation, peat formation as	
876	well as shift in biomes such as tropical and boreal ecosystems for dynamic vegetation	
877	models require several long time-scales to equilibrate (Brovkin et al., 2010; Koven et	
878	al., 2015). In addition, the terrestrial carbon cycle has large uncertainties in terms of	
879	carbon sink/source behavior (Anav et al., 2013; Dalmonech et al., 2014; Friedlingstein	
880	et al., 2013) which might affect ocean CO <sub>2</sub> uptake (Brovkin et al., 2010). <u>A novel</u>	
881	numerical algorithm to accelerate the spin-up integration time for computationally	
882	expensive ocean biogeochemical models has emerged (Khatiwala, 2008), which could	
883	further complicate the determination of inter-model spreads.	
884		
885	To evaluate the contribution of variable spin-up and initialization strategies to model	
886	performance, these should be documented extensively and the corresponding model	
887	output should be archived. Ideally, for future <u>coupled model</u> intercomparision	
888	exercises (i.e., CMIP6, CMIP7, Meehl et al., (2014)), the community should agree on	roland seferian 15/1/16 11:52
889	a set of simple recommendations for spin-up protocols, following past projects such	roland seferian 15/1/16 11:53
890	as OCMIP-2. In parallel, any trade-off between model equilibration and	roland seferian 15/1/16 11:53
891	computationally efficient spin-up procedures has to be linked with efforts to reduce	Deleted: and duration
892	model errors due to the physical and biogeochemical parameterizations.	
893		
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- 895 Acknowledgement:
- 896 We sincerely thank I. Kriest, F. Joos, the anonymous reviewer and A Yool for
   897 their useful comments on this paper. This work was supported by the H2020 project

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- 898 CRESCENDO "Coordinated Research in Earth Systems and Climate : Experiments,
- 899 kNowledge, Dissemination and Outreach" which received funding from the European
- 900 Union's Horizon 2020 research and innovation programme under grant agreement
- 901 No 641816 and by the EU FP7 project CARBOCHANGE "Changes in carbon uptake 902 and missions by oceans in a changing climate" which received funding from the 903
  - European community's Seventh Framework Programme under grant agreement no.
- 904 264879. Supercomputing time was provided by GENCI (Grand Equipement National 905 de Calcul Intensif) at CCRT (Centre de Calcul Recherche et Technologie), allocation
- 906 016178. Finally, we are grateful to the ESGF project which make data available for
- 907 all the community. R.S. is grateful Aurélien Ribes for his kind advices on statistics. JT
- 908 acknowledges ORGANIC project (239965/F20) funded by the Research Council of
- 909 Norway. CH and TJ are grateful for support through project EVA - Earth system
- 910 modelling of climate variations in the Anthropocene (229771/E10) funded by the
- 911 Research Council of Norway, as well as CPU-time and mass storage provided
- 912 through NOTUR project NN2345K as well as NorStore project NS2345K. K.L. and
- 913 S.C.D. acknowledge support from the National Science Foundation. 914

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	spin-up	initial	offline	online	spin-up	
	procedure	conditions	time	time	duration	
		WOA2001,				(Wu et al.,
BCC-CSM1-1	sequential	GLODAP	200	100	300	2013)
		WOA2001,				(Wu et al.,
BCC-CSM1-1-m	sequential	GLODAP	200	100	300	2013)
	sequential	OCMIP				
	(forced w/	profiles,				(Arora et al.,
CanESM2	obs.)	CanESM1	6000	600	6600	2011)
						(Lindsay et
CESM1-BGC	direct	CCSM4	0	1000	1000	al., 2014)
	sequential	WOA2001,				(Vichi et al.,
CMCC-CESM	(w/ acc.)	GLODAP	100	100	200	2011)
		WOA1994,				
		GLODAP,				(Séférian et
CNRM-CM5	sequential	IPSL	3000	100	3100	al., 2013)
		WOA1994,				
		GLODAP,				(Schwinger et
CNRM-CM5-2	sequential	CNRM	3000	100	3100	al., 2014)
		<u>CNRM-</u>				(Séférian et
CNRM-ESM1	sequential	<u>CM5</u>	<u>0</u>	<u>1300</u>	<u>1300</u>	<u>al., 2015)</u>
GFDL-ESM2G	direct	WOA2005,	0	1000	1000	(Dunne et al.,

		GLODAP				2013)
		WOA2005,				(Dunne et al.,
GFDL-ESM2M	direct	GLODAP	0	1000	1000	2013)
		WOA2005,				
		GLODAP				(Romanou et
GISS-E2-H-CC	direct	DIC*	0	3300	3300	al., 2013)
		WOA2005.				, ,
		GLODAP				(Romanou et
GISS-E2-R-CC	direct	DIC*	0	3300	3300	al., 2013)
		210		0000		(Collins et
						al 2011.
		HadCM3LC				Wassmann et
HadGEM2-CC	sequential	WOA2011	400	100	500	2010
HaddEM2-CC	sequentiai	HadCM3LC	-100	100	500	(Collins et
HadGEM2 ES	sequential	WOA 2010	400	100	500	(0.00000000000000000000000000000000000
HaddEWIZ-ES	sequentiai	, WOA2010	400	100	500	(Volodin et
INIMCM4	a a grantial	DIC	2000	200	2200	(volouin et al. 2010)
	sequentiai	WOA 1004	3000	200	3200	al., 2010)
		CLODAD				(Sáfánian at
IDEL CM5A LD		GLODAP,	2000	600	2600	(Selerian et)
IPSL-CMJA-LK	sequential	IPSL WOA1004	3000	000	3000	al., 2013)
		WUA1994,				
		GLODAP,	2000	200	2200	(Dufresne et
IPSL-CM5A-MR	sequential	IPSL	3000	300	3300	al., 2013)
		IPSL-	0	200	200	(Dufresne et
IPSL-CM5B-LR	sequential	CM5A-LR	0	300	300	al., 2013)
		GLODAP/c				
		onstant				(Watanabe et
MIROC-ESM	sequential	values	1245	480	1725	al., 2011)
		GLODAP/c				
MIROC-ESM-		onstant				(Watanabe et
CHEM	sequential	values	1245	484	1729	al., 2011)
		HAMOCC/				
		constant				(Ilyina et al.,
MPI-ESM-LR	sequential	values	10000	1900	11900	2013)
		HAMOCC/				
		constant				(Ilyina et al.,
MPI-ESM-MR	sequential	values	10000	1500	11500	2013)
	sequential					
	(forced w/					(Adachi et
MRI-ESM1	obs.)	GLODAP	550	395	945	al., 2013)
		WOA2010.				(Tjiputra et
NorESM	direct	GLODAP	0	900	900	al., 2013)

1446 **Table 1:** Summary of spin-up strategy, sources of initial conditions, offline/online

1447 durations and references used to equilibrate ocean biogeochemistry in CMIP5 ESMs.

1448 The so-called direct and sequential strategies inform whether the spin-up of the ocean

- 1449 biogeochemical model is run directly in online/coupled mode or <u>first</u> in offline (ocean
- 1450 biogeochemistry only) and <u>then in online/coupled mode. DIC\* refers to the</u>
- 1451 observation-derived estimates of preindustrial dissolved inorganic carbon
- 1452 | concentration using the  $\Delta C^*$  method. w/ acc. and forced w/ obs. indicates the strategy
- 1453 using 'acceleration' and observed atmospheric forcings during the spin-up,
- 1454 respectively.
- 1455

	O <sub>2</sub>			NO <sub>3</sub>				
Depth	surface	150 m	2000 m	surface	150 m	2000 m		
RMSE	7.19	8.75	5.50	2.07	2.90	2.08		
R <sup>2</sup>	0.98	0.98	0.99	0.96	0.92	0.94		

1457

1458 **Table 2:** Differences between the oxygen  $(O_2, \mu \text{mol } L^{-1})$  and nitrate  $(NO_3, \mu \text{mol } L^{-1})$ 

1459 datasets used for initializing IPSL-CM5A-LR (WOA1994) and the datasets used for

1460 assessing its performances (WOA2013).

- 1461
- 1462

	$O_2$			NO <sub>3</sub>			Alk-DIC			
metrics	mean RMSE RMSE <sub>max</sub>			mean RMSE RMSE <sub>max</sub>			mean	RMSE	RMSE <sub>max</sub>	
Surf										
	-0.2	2.6	55.8	-0.1	-0.1	34.2	1.6	-0.1	-0.1	
150 m										
	3.4	39.0	31.5	-15.9	33.4	55.2	6.1	27.9	24.7	

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200	0 m											
1463	Та	-30.4	144.3	-40.1	$\frac{2}{(0)}$ nitr	51.8	-34.8	-69.6	281.8	47.5	roland se	ferian 28/1/16 09:24
1403	1 a		t III 70 Ky	ioi oxygen	$(O_2)$ , intra	$(100_3)$		unnty m	liius DIC		Deleted:	in
1464	(Alk-DIC) at surface, 150 and 2000 meters as simulated by the IPSL-CM5A-LR											
1465	model. The drift has been computed over the last 250 years of the spin-up simulation											
1466	using a linear regression fit of the globally averaged concentrations, root-mean											
1467	squ	ared error	(RMSE) a	nd latitudina	ıl maximu	m root-me	ean squared e	error (RM	(ISE <sub>max</sub> )			
1468	wit	h respect t	o the value	es at year 250	Э.							
1469												
1470												
1471												
1472	Fig	<b>ure 1</b> : Spi	n-up proto	cols of CMI	P5 Earth s	system mo	dels. Color s	hading r	epresents			
1473	stra	tegies of t	he various	modeling gr	coups. On	<i>line</i> and <i>O</i>	<i>ffline</i> steps re	efer to ru	n <u>s</u>			
1474	per	formed wi	th coupled	climate mod	del and wi	th stand-a	lone ocean b	iogeoche	emistry			
1475	mo	del, respec	ctively. Sou	urces of initia	al condition	ons for bio	geochemical	compon	ent of		roland se	ferian 28/1/16 09:25
1476	CM	IIP5 Earth	system me	odels are ind	icated <u>as l</u>	<u>natching</u> b	elow the barj	olot.			Deleted:	for
1477												
1478	Fig	ure 2: Tin	ne series o	f two climate	e indices o	over the 50	0-year spin-	up simul	ation of 🕇		roland se	ferian 28/1/16 09:26
1479	IPS	SL-CM5A-	LR. They	represent the	e global av	veraged se	a surface terr	perature	(a) and		Formatte space be	d: Hyphenate, Don't adjust tween Asian text and numbers,
1480	the	global me	an sea-air	carbon flux (	(b). For se	a-air carbo	on flux, nega	tive valu	ie		Tabs:Not cm + 3,9	at 0,99 cm + 1,98 cm + 2,96 5 cm + 4,94 cm + 5,93 cm +
1481	ind	icates upta	ke of carb	on. Steady st	tate equili	brium of p	hysical comp	ponents a	as		6,91 cm + 10,86 cm	+ 7,9 cm + 8,89 cm + 9,88 cm + 1 + 11,85 cm
1482	des	cribed in N	Mignot et a	ıl., (2013) is	reached a	t ~250 yea	rs and is indi	icated wi	ith a			
1483	ver	tical dashe	d line. Dri	fts in sea sur	face temp	erature an	d global cart	on flux	are			
1484	ind	icated with	n dashed b	lue lines. Th	ey are cor	nputed usi	ng a linear re	gression	i fit over			
1485	yea	rs 250 to 5	500. Hatch	ing on panel	(b) repres	sents the ra	inge of inver	se mode	ling			
1486	esti	mates for	preindustr	ial global car	rbon flux a	as describe	ed in Mikalof	ff Fletche	er et al.,			
1487	(20	07), i.e., 0	.03±0.08 F	g C y <sup>-1</sup> plus	0.45 Pg C	y <sup>-1</sup> corres	ponding to the	he riveri	ne-			
1488	ind	uced natur	al CO <sub>2</sub> out	tgassing outs	ide of nea	r-shore re	gions consist	ently wi	th Le		roland se	ferian 28/1/16 09:26
1489	Que	éré et al. (2	2015).								Deleted:	to
1490											roland se Deleted:	terian 28/1/16 09:26

1491		Figure 3: Time series of globally averaged concentration ([X] in solid lines) and
1492	ĺ	globally averaged root-mean squared error (RMSE in dashed lines) for dissolved
1493	I	oxygen (O <sub>2</sub> ), nitrate (NO <sub>3</sub> ) and difference between alkalinity and dissolved inorganic
1494		carbon (Alk-DIC) as simulated by IPSL-CM5A-LR. [X] and RMSE are given at
1495		surface (a,b and c), 150 m (d, e and f), and 2000 m (g, h and i) for these three
1496	1	biogeochemical fields. Their values are indicated on the left-side and right-side y-axis,
1497	I	respectively. Hatching represents the $\pm \sigma$ observational uncertainty due to optimal
1498		interpolation of in situ concentrations around the observed [X].
1499		
1500		Figure 4: Snap-shots of spatial biases, $\epsilon$ , in surface concentrations (µmol L <sup>-1</sup> ) in
1501		biogeochemical fields during the 500-year spin-up simulation of IPSL-CM5A-LR. $\boldsymbol{\epsilon}$
1502		in dissolved oxygen (O <sub>2</sub> ), nitrate (NO <sub>3</sub> ) and difference between alkalinity and
1503		dissolved inorganic carbon (Alk-DIC) is given for the first year (a, c and e,
1504		respectively) and for the last year of spin-up simulation (b, d and f, respectively).
1505		
1506		Figure 5: As Figure 4 but for concentrations at 150 m. Note that color shading does
1507		not represent the same amplitude in spatial biases as in Figures 4 and 6.
1508	•	
1509		Figure 6: As Figure 4 but for concentrations at 2000 m. Note that color shading does
1510		not represent the same amplitude in spatial biases as in Figures 4 and 5.
1511		
1512		Figure 7: Temporal-vertical evolution in root-mean squared error (RMSE) for
1513		biogeochemical tracers during the 500-year-long spin-up simulation of IPSL-CM5A-
1514		LR. RMSE is given for (a) dissolved oxygen O <sub>2</sub> , (b) nitrate NO <sub>3</sub> , and (c) difference
1515		between alkalinity and dissolved inorganic carbon Alk-DIC
1516		
1517		Figure 8: Temporal evolution of drift in root-mean squared error (RMSE) for
1518		dissolved oxygen (O <sub>2</sub> , blue crosses), nitrate (NO <sub>3</sub> , green crosses) and difference
1519		between alkalinity and dissolved inorganic carbon (Alk-DIC, orange crosses) during
1520		the 500-year-long spin-up simulation of IPSL-CM5A-LR. Drift in RMSE is given at
1521		surface (a,b and c), 150 m (d, e and f), and 2000 m (g, h and i) for these three
1522		biogeochemical fields. Drift in RMSE is computed from time segments of 100 years
1523		begenning every 5 years from the beginning until year 400 of the spin-up simulation
1524		for O <sub>2</sub> , NO <sub>3</sub> and Alk-DIC tracers. The best-fit linear regressions between drifts in

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**Deleted:** and difference in spatial standard deviation between observations and model fields  $(\Delta \sigma)$ roland seferian 14/1/16 07:40 **Deleted:** and  $\Delta \sigma$ roland seferian 28/1/16 09:27 Deleted: are roland seferian 28/1/16 09:27 Deleted: ( roland seferian 28/1/16 09:27 Deleted: ) roland seferian 28/1/16 09:27 Deleted: ( Deleted: ) Deleted: ( **Deleted:** ) in panels (a,d), (b,e) and (c,f), respectively

1525	RMSE and spin-up duration over year 250 to 500 are indicated in solid magenta lines;		
1526	their 90% confidence intervals are given by thin dashed envelopes.		
1527			
1528	Figure 2: Scatterplot of drifts in root-mean squared error (RMSE) in O <sub>2</sub> concentration		roland seferian 14/1/16 07:42
1529	versus the duration of the spin-up simulation, for the available CMIP5 Earth system	$\square$	<b>Deleted:</b> 8relativeand difference in spatial standard deviation $(\Delta \sigma)$ (in
1530	models. Drifts in $\underline{O_2}$ RMSE are respectively given for surface (a), 150 m (b) and 2000	///	logscale)Relative d and $\Delta\sigma$
1531	m (c) for oxygen concentrations. Drift in O <sub>2</sub> RMSE is computed from several time		the first century of the piControl simulation relative and $\Delta \sigma$ in R 6 similar best-
1532	segments of 100 years begenning every 5 years from the beginning until the end of the		fit linear regressions haven derived; they are indicated in solid red line They have
1533	piControl simulation for the available CMIP5 models. Coloured symbols indicate the	/ //	been obtained from drifts computed over 100- year-long overlapping time slices of O <sub>2</sub> RMSE
1534	mean drift in O <sub>2</sub> RMSE while vertical lines represent the associated 90% confidence		from years 250 to 500 at each depth levels and (2) extrapolated over the CMIP5 spin-up
1535	interval. The best-fit linear regressions between models' mean drifts in RMSE and	//	duration range (250-10190 years).
1536	spin-up duration are indicated as solid green lines; their 90% confidence intervals are		
1537	given by thin dashed envelopes. Fits are assumed robust if correlation coefficients are		
1538	significant at 90% (i.e., <u>r*&gt;0.34</u> ). For comparison, <u>drift in O<sub>2</sub> RMSE</u> from our spin-up		
1539	simulation with IPSL-CM5A-LR (Figure 8) are represented by magenta crosses,		
1540			
1541	Figure 10; Rankings of CMIP5 Earth system models based on standard and penalized		roland seferian 14/1/16 07:55
1542	version of the distance from oxygen observations. The standard distance metric is	$\square$	Deleted: 9normalizednormalized
1543	calculated as the ensemble-mean root-mean squared error (RMSE) for $O_2$	$\square$	roland seferian 14/1/16 07:46
1544	concentrations at surface (a), 150 m (b) and 2000 m (c). The penalized distance metric		Formatted: Subscript
1545	incorporates drift-induced changes in $\underline{O_2}$ RMSE ( $\Delta$ RMSE) to $\underline{O_2}$ RMSE at surface (d),		
1546	150 m (e) and 2000 m (f). Ensemble-mean RMSE are calculated using available		
1547	ensemble members of Earth system models oxygen concentrations averaged over the		
1548	198 $\underline{6}$ -2005 historical period relative to WOA2013 observations. $\Delta RMSE$ is		roland seferian 14/1/16 07:47
1549	determined using Equation 2 and fits derived from first century of the CMIP5		<b>Deleted:</b> 5Red sand dashedmean and median fordifferent ensembles
1550	piControl simulations. Solid red and magenta lines indicate the multi-model mean		
1551	standard and penalized distance from O2 observations, respectively. With the same		
1552	colour pattern, dashed lines are indicative of the multi-model median for the standard		
1553	and penalized distance from O <sub>2</sub> observations.		
1554			



Figure 1:



Figure 2:



Figure 3:



Figure 4:



Figure 5:



Figure 6:







Figure 8:



Figure 9:



Figure 10:



Figure S 1: Temporal evolution of the drift in  $O_2$  root-mean squared error (RMSE) at 2000 m over the 1000-year-long CMIP5 piControl simulation of IPSL-CM5A-LR. Drift in  $O_2$  RMSE is computed from time segments of (a) 20, (b) 50, (c) 80, and (d) 100 years distributed evenly every 5 years from the beginning until the end of the piControl simulation. The best-fit linear regressions between drifts in  $O_2$  RMSE and simulation duration are indicated in solid magenta lines; their 90% confidence intervals are given by thin dashed envelope.

## - Supplementary Figures -



Figure S 2: Vertical profiles of the globally averaged drift in O<sub>2</sub> root-mean squared error (in  $10^{-3} \mu \text{mol}$  L<sup>-1</sup> kyr<sup>-1</sup>) from the 15 CMIP5 Earth system models used in this study. Two ways to determine the globally averaged drift are presented in this Figure: vertical profiles determined from global-averaged O<sub>2</sub> RMSE are indicated in blue while those computed from the globally averaged 3-dimensionnal drift (i.e., estimated from 3-dimensionnal O<sub>2</sub> RMSE over domains where the drift in O<sub>2</sub> RMSE fits the simple drift model) are given in red. Solid lines represent the mean vertical profile of the drift in O<sub>2</sub> RMSE; the 90% confidence interval around the mean profile is represented with hatching patterns.



Figure S 3: Vertical structures of the basin-scale drift in  $O_2$  root-mean squared error (in  $10^{-3} \mu \text{mol}$   $\text{L}^{-1} \text{kyr}^{-1}$ ) from the 15 CMIP5 Earth system models used in this study. Basin-scale drift in  $O_2$  RMSE has been computed from 3-dimensionnal drift averaged over Atlantic and Pacific oceans (i.e., estimated from 3-dimensionnal  $O_2$  RMSE over domains where the drift in  $O_2$  RMSE fits the simple drift model).