Improving GCM-based decadal ocean carbon flux predictions using observationally-constrained statistical models

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Abstract

Initialized climate model simulations have proven skillful for near-term predictability of the key physical climate variables. By comparison, predictions of biogeochemical fields like ocean carbon flux, are still emerging. Initial studies indicate skillful predictions are possible for lead-times up to six years at global scale for some CMIP6 models. However, unlike core physical variables, biogeochemical variables are not directly initialized in existing decadal preciction systems, and extensive empirical parametrization of ocean-biogeochemistry in Earth System Models introduces a significant source of uncertainty. Here, we propose a new approach for improving the skill of decadal ocean carbon flux predictions using observationally-constrained statistical models, as alternatives to the ocean-biogeochemistry models. We use observations to train multi-linear and neural-network models to predict the ocean carbon flux. To account for observational uncertainties, we train using six different observational estimates of the flux. We then apply these trained statistical models using input predictors from the Canadian Earth System Model (CanESM5) decadal prediction system to produce new decadal predictions. Our hybrid GCM-statistical approach significantly improves prediction skill, relative to the raw CanESM5 hindcast predictions over 1990-2019. Our hybrid-model skill is also larger than that obtained by any available CMIP6 model. Using bias-corrected CanESM5 predictors, we make forecasts for ocean carbon flux over 2020-2029. Both statistical models predict increases in the ocean carbon flux larger than the changes predicted from CanESM5 forecasts. Our work highlights the ability to improve decadal ocean carbon flux predictions by using observationally-trained statistical models together with robust input predictors from GCM-based decadal predictions.

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Key Points:

- We use observationally trained statistical models to obtain decadal predictions of ocean carbon flux from initialized GCM-based predictors.
- The hybrid GCM-statistical ocean carbon flux predictions show improved skill over hindcast predictions from the GCM's biogeochemical models.
- The hybrid models are used to make decadal predictions for the ocean-atmosphere carbon flux over the decade ending in 2029.

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Abstract

Initialized climate model simulations have proven skillful for near-term predictability of the key physical climate variables. By comparison, predictions of biogeochemical fields like ocean carbon flux, are still emerging. Initial studies indicate skillful predictions are possible for lead-times up to six years at global scale for some CMIP6 models. However, unlike core physical variables, biogeochemical variables are not directly initialized in existing decadal preciction systems, and extensive empirical parametrization of ocean-biogeochemistry in Earth System Models introduces a significant source of uncertainty. Here we propose a new approach for improving the skill of decadal ocean carbon flux predictions using observationally-constrained statistical models, as alternatives to the ocean-biogeochemistry models. We use observations to train multi-linear and neural-network models to predict the ocean carbon flux. To account for observational uncertainties, we train using six different observational estimates of the flux. We then apply these trained statistical models using input predictors from the Canadian Earth System Model (CanESM5) decadal prediction system to produce new decadal predictions. Our hybrid GCM-statistical approach significantly improves prediction skill, relative to the raw CanESM5 hindcast predictions over 1990-2019. Our hybrid-model skill is also larger than that obtained by any available CMIP6 model. Using bias-corrected CanESM5 predictors, we make forecasts for ocean carbon flux over 2020-2029. Both statistical models predict increases in the ocean carbon flux larger than the changes predicted from CanESM5 forecasts. Our work highlights the ability to improve decadal ocean carbon flux predictions by using observationally-trained statistical models together with robust input predictors from GCM-based decadal predictions.

Plain Language Summary

Using initialized Earth system model simulations for near term predictions of ocean biogeochemichal variables is an emerging field of research. In particular, near term predictability of ocean carbon flux is central to efforts for planing and limiting climate change. Unlike physical variables whose predictability have been established, these simulations are only indirectly initialized and rely on heavily parameterized ocean biogeochemistry models. Here, we propose a new approach to acquire decadal predictions of air-sea carbon flux as alternatives to those based on ocean biogeochemistry models. Our methodology combines the explanatory power of statistical models that have widely been used for gap filling purposes for informing full coverage ocean carbon flux data products, and well established predictability skill of key physical predictors. We provide hybrid GCM-statistical ocean carbon flux hindcasts using predictors from CanESM5 and doing so, show that we can beat all CMIP6 decadal prediction system hindcast skills. We use our models to provide near future hybrid model forecast for ocean carbon flux. Our results shows the potential for improving predictability skill of ocean carbon sink by combining GCMs and observationally trained statistical models.

1 Introduction

The ocean accounts for sequestering nearly 25% percent of human CO_2 emissions annually (Hauck et al., 2020; Friedlingstein et al., 2022, 2020), playing a key role in mitigating climate change. Future changes in the ocean carbon flux are of direct relevance to climate change science (Friedlingstein et al., 2022) and policy making related to climate and emissions targets. Ocean carbon uptake has increased substantially over the past several decades in response to human induced increases in atmospheric CO_2 concentrations (Gooya et al., 2023; Rodgers et al., 2020; Lovenduski et al., 2016; McKinley et al., 2016; Wang et al., 2016). However, there is also substantial internal variability in the magnitude of the flux on seasonal to decadal time scales both regionally and globally (Landschützer et al., 2016; McKinley et al., 2017; Gruber et al., 2019; McKinley et al., 2020). Decadal scale variability of ocean carbon flux is believed to be driven largely by variability in external forcing (McKinley et al., 2020), and specifically, the deviations of atmospheric growth of CO_2 from the long term trend but also changes in circulation (DeVries et al., 2019; Keppler & Landschützer, 2019). Higher frequency interannual variability is largely attributable to modes of climate variability such as ENSO on global scale and other modes of high latitude variability on regional scales (McKinley et al., 2017). Predicting future variations in the ocean carbon sink on inter-annual to decadal time scales in the face of these mulitple drivers is therefore challenging.

Decadal predictions, such as those made under the Decadal Climate Prediction Project (DCCP) are produced by Global Climate Models (GCMs) that are that are initialized with observations and also driven by external forcing (Kirtman et al., 2013). Predictive skill of key physical climate variables from such simulations have been well established in the literature (Boer et al., 2016). However, near term predictability of the ocean carbon flux and other biogeochemical variables have only become possible with the recent advent of Earth System Models (ESMs) (Meehl et al., 2021) and are still at their infancy. Previous studies have shown potential predictability of the ocean carbon flux for up to 7 years (Li et al., 2019; Séférian et al., 2018) and actual skill versus observation based estimates for 2-6 years based on different ESMs (Li et al., 2019; Ilyina et al., 2021). However, ESM simulations are subject to biases, drifts (Kharin et al., 2012) and exhibit a wide range of prediction skill globally and regionally (Ilyina et al., 2021). Predictions of ocean carbon flux using ESMs are especially challenging given that ocean biogeochemical variables are not directly initialized in current decadal prediction systems (Sospedra-Alfonso et al., 2021), and that the ocean biogeochmical models themselves are heavily parameterized using empirical parameterizations (Christian et al., 2022).

Here we propose using observationally-trained statistical models forced by predictors from GCM/ESM-based decadal predictions, as an alternative to using the raw predictions of ocean carbon flux obtained from the ESMs ocean biogeochemistry models. It is well established that the surface ocean partial pressure of CO_2, and by extension the surface carbon flux, is closely related to physical predictors, such as sea-surface temperature and salinity, atmospheric CO_2 concentration and wind speed. These empirical relationships are widely exploited in the observational community to infill sparse direct observations of the ocean carbonate system (e.g., Surface Ocean CO_2 Atlas, SOCAT), using indirect but more widely sampled physical variables (Landschützer et al., 2016). It is also common to post-process raw GCM results to produce more skillful predictions, for example through bias correction (Kharin et al., 2012). Our proposal is a logical extension of these two established practises that combines the explanatory power that statistical models learn from the relationships between observational predictors, and the established prediction skill of the process based physical models. Our principal goal is to establish a methodology that allows us to improve near-term predictions of the ocean carbon sink over and above the skill obtained from raw ESM predictions.

We begin by introducing the methodology and our statistical models of choice in Section 2. In section 3 we evaluate observational uncertainties and the performance of our statistical models when forced by observation based predictors. In section 4, we apply the observationally trained statistical models to physical predictors from CanESM5 simulations, and evaluate the skill of this hybrid approach relative to the raw CanESM5 predictions over the hindcast period of 1990 to 2019. We go on to provide forecasts for ocean carbon flux over the decade 2019 to 2029 in section 5. We conclude by reflecting on how our approach could be improved and expanded on in future work.

2 Materials and Methods

2.1 Surface CO_2 flux data

For observations of the atmosphere-ocean CO_2 flux we use the SeaFlux Ocean carbon sink ensemble product (Gregor & Fay, 2021). SeaFlux contains an ensemble of flux estimates, based on six global observation-based mapping products for surface ocean partial pressure of CO_2 (pCO_2), and wind speeds from ERA5. The six products include three neural-network-derived products (CMEMS-FFNN, MPI-SOMFFN, NIES-FNN), a mixed layer scheme product (JENA-MLS), a multiple linear regression (JMA-MLR), and a machine learning ensemble (CSIR-ML6) (Fay et al., 2021). We also use the mean across the products, which we refer to as SF-MEAN. Given the sparseness of actual pCO_2 measurements, using the ensemble of products allows us to quantify uncertainties associated with the data infilling and mapping techniques, and avoids overfitting to a single product.

All six SeaFlux products show strong agreement in the long term (trended) changes in ocean carbon flux (not shown here). Comparing linearly detrended versions of the SeaFlux products shows cross correlation coefficients between them ranging from 0.47 to 0.95 (Fig. S1). The MPI-SOM-FFN and JENA-MLS are least correlated with others. The lower correlation skills for the two show that there are variabilities specific to these products that are not common to other datasets, and known biases linked to data sparsity (Gloege et al., 2021; Hauck et al., 2023). The averaged SF-MEAN contains signals common to all of the products, and we use this as the most reliable estimate moving forward.

2.2 Statistical models and observed predictors

For each individual SeaFlux input dataset and SF-MEAN, we train a multi-linear regression model and a neural network (NN) model to predict the surface atmosphere ocean carbon flux, using three observation-based physical predictors - sea surface temperature (SST), sea surface salinity (SSS), surface wind speed (sfcWind), one biological predictor -surface chlorophyll concentrations (CHL), as well as atmospheric CO_2 concentrations (xCO_2) (table S1). These are mainly physical predictors for which full coverage observational products are available and are believed to drive the variability in ocean carbon flux (Landschützer et al., 2016). Linear models are trained for each grid cell on a standard one degree grid, while the NN models are trained over 16 biomes (Landschützer et al., 2016), as explained further in SI (Sect. S1.1). By combining these biomes, we can produce spatially resolved maps of the surface CO_2 flux, given the set of five input predictors at any point. In total that gives us 14 sets of models (7 set of linear models, and 7 NN models, one for each SeaFlux target predictand) that are later used to make hindcasts and forecasts using modelled predictors from CanESM5. We have chosen to illustrate our approach using the linear and NN models, which have different structures and levels of complexity, as illustrative examples. However, alternative models and predictor variables could be used.

2.3 Decadal predictions using GCM base predictors

To make predictions the five predictors from Table S1 are obtained from CanESM5 simulations (Swart et al., 2019; Sospedra-Alfonso et al., 2021). We use a range of simulations, including standard free running CMIP6 historical simulations (Eyring et al., 2016), as well as assimilation and hindcast and forecast runs (Boer et al., 2016). In assimilation runs, CanESM5 is nudged towards observations for key physical variables (Sospedra-Alfonso et al., 2021). For historical, hindcast and forecast simulations, the five predictors are bias corrected to the same observational predictors used for training the models following the approach of (Kharin et al., 2012). This bias correction adjusts the mean and trend of the predictors to be consistent with observations. These CanESM5 predictors are fed to the each of the 14 statistical model sets mentioned above to produce hy-

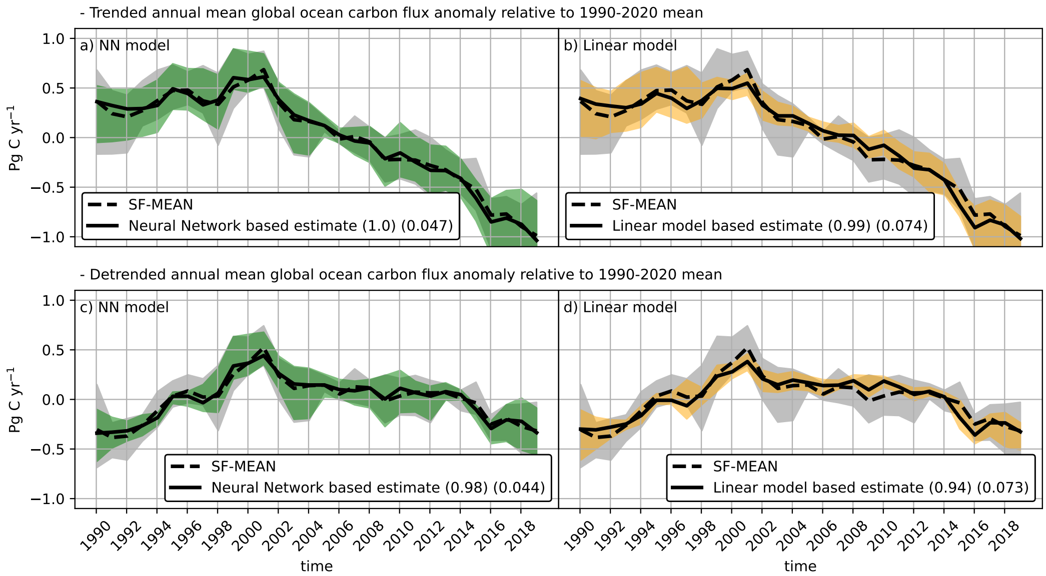

Figure 1. Time series of the global ocean CO_2 flux anomalies for the (a) NN model (left panel) and (b) linear model (right panel) reconstruction using obervational predictors. The black lines shows reconstruction using models that are trained on mean of SeaFlux products (SF-MEAN; solid) as well the mean product itself (dashed). The shadings represent the range estimates from the six different SeaFlux products (grey) and from NN and linear models reconstructions (green and orange). The numbers in the legends are correlation coefficients between the solid black lines and dashed black lines (first number) and root mean square error of the two time series (second number). (c) and (d) are same as (a) and (b) but are linearly detrended.

brid predictions of surface ocean CO_2 flux. For hindcasts and forecasts, predictions are made for lead years 1 to 10. To test significance of prediction skill differences, we use a 1000 iteration bootstrap to test of (Goddard et al., 2013).

3 Evaluation of statistical models

In this section, we consider the performance of the statistical models trained on the SeaFlux ensemble and using observed predictors, for predicting the global mean surface carbon flux as defined by SF-MEAN (Fig. 1). When trained on SF-MEAN, both the NN and linear models can accurately reconstruct the changes of the SF-MEAN ($r > 0.9$), indicating that the statistical models are able to capture the majority of the variance in the global mean surface flux. The NN model shows higher skill in reconstructing SF-MEAN relative to the linear model, reflected in higher correlations and lower root mean square error (Fig. 1). Similarly, both linear and NN models are able to successfully reproduce individual SeaFlux products on which they are trained (Fig. S2), with the NN models again achieving tighter fits than the linear models. The orange and green shading in Fig. 1 represents the spread across models trained on individual SeaFlux products. These models are still able to successfully reproduce SF-MEAN, which gives an indication of their generalizability. The smaller spread for the linear models (Fig. 1b, orange shading), suggests they may be more generalizable (i.e. successful in predicting data they were not trained on) than the NN models. We further explore the idea of generalizability when using model-derived predictors in the following section.

4 Applying statistical models to physical predictors from the ESM

4.1 Assimilation run

The CanESM5 assimilation run is relaxed towards the observed physical state of the system, which forces physical variables, including our input predictors, to be close to observations. However, the detrended CO_2 flux from the CanESM5 biogeochemical component is not in good agreement with observations (Fig. 2 bottom row). We have identified issue in the model derived CO_2 flux, including seasonality that is out of phase with observations (not shown here), and it appears that the data ingestion in the assimilation run degrades the biogeochemical models performance. Indeed, previous results have shown that atmosphere-ocean CO_2 flux predictability is low in CanESM5, and particularly poor in the early lead years immediately following the assimilation run (Ilyina et al., 2021). A major goal of our effort is to see whether by replacing the CanESM5 biogeochemical model derived flux with one computed based on the statistical models leads to improvement.

We use the linear and NN models previously trained using observed predictors, and for each of the six individual SeaFlux products and SF-MEAN as predictands (for a total of 14 model sets). We then extract the five input predictors from the (ensemble mean of 10) CanESM5 DCPP assimilation runs, apply the statistical models on these GCM-based predictors, and compare their skill against the original SeaFlux observational products (Fig 2).

The statistical models forced by CanESM5 assimilation predictors obtain similar skills in reproducing the individual SeaFlux products to the skills of the reconstructions that used predictors from observations (compare Fig. 2 and supplementary Fig. S2). This is a somewhat expected result given that assimilation runs assimilate physical predictors and are very close to the observations, but nonetheless it is first step in applying the models on data on which they were not directly trained. For both the linear and NN statistical models, the skill is in all cases is significantly higher than than skill of the raw CanESM5 CO_2 flux. These results indicate that statistical models trained on observations can usefully be applied to GCM-derived predictors. By using this approach we are able to avoid biases in the CanESM5 biogeochemical model by combining the observationally constrained statistical models with the directly initialized physical predictors from CanESM.

We compute the cross-correlation matrix for statistical models trained on one SeaFlux product in reproducing all the other five product and SF-MEAN (Fig. 2). This allows us to assess the impacts of observational uncertainty, and the potential consequences of overfitting statistical models to a single observational product. As expected, the statistical models are most skillful in reproducing the product on which they were trained (diagonal in Fig. 2). Correlation in reproducing other products can be lower than 0.5. The extent to which a model trained on one observational product can be generalized to others is measured with the mean of scores versus all other observational data products (mean of rows excluding the diagonal values as indicated in Fig. 2 EXT column). Overall, the linear models have larger extendibility scores, while the NN models produce better fits for the products on which they were trained. Our results illustrate that care should be taken in tightly fitting statistical models to a single observation based CO_2 flux product, as uncertainties exist. Moving forward, we will use statistical model trained on the SF-MEAN product as the best estimate. Based on the encouraging success so far, in the next section we will apply our approach to decadal predictions.

4.2 Prediction skill of CO_2 flux over the hindcast period

Hindcasts are ESM simulations that use the observationally constrained assimilation simulation as initial conditions, and which are then run freely under standard CMIP6

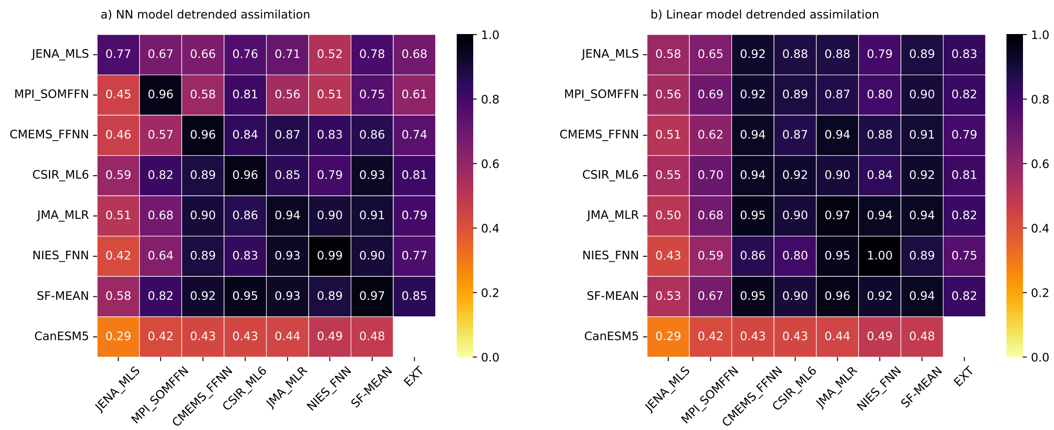

Figure 2. (a) Correlation matrix for the detrended global ocean carbon flux anomaly. The y axis indicate the product on which the NN model is trained and the x axis shows the data products against which the skill is evaluated. The EXT column measures the mean of skills excluding the diagonal element for each row. (b) Same as (a) but for the Linear model.

external forcings for ten years (Boer et al., 2016). Generally, as lead years increase (i.e. number of year since initialization) the hindcasts simulations lose memory of initializaton and drift towards the preferred state of the model (historical simulations). However, raw CanESM5 ocean carbon flux DCPP scores show a decrease in the skill after initialization in hindcast compared to the historical free runs (Ilyina et al., 2021). This is not the expected result of initialization and indicates possible discrepancies with interactions between initialization and the CanESM5 biogeochemical decadal prediction system (initialization "shocks").

As an alternative to the biogeochmical model flux, we apply our SF-MEAN trained statistical models on predictors from the CanESM5 hindcast simulations over the period 1990 to 2019. The hindcast skill from both the linear and NN model when trained and evaluated against SF-MEAN are significantly larger than raw CanESM5 skills, with NN yielding slightly better scores (Fig. 3). Both statistical models show increase in skill after initialization, as expected and seen in physical predictors, and a gradual drop with lead time. As an even more stringent test, we compare the skill of the statistical models driven by CanESM5 predictors against the skill from all other available CMIP6 models that participated in DCPP. The NN model skill is higher than that shown by any raw CMIP6 model, when evaluated against SF-MEAN (Fig. S3) over 1990-2017 that is the period common to all models. Linear model score are higher than all CMIP6 models on all lead years except lead year 3 where CESM1 (Danabasoglu, 2019) yields slightly larger score (Fig. S3). These results clearly show the potential of our approach for improving the decadal CO_2 flux prediction skills.

To this point we have considered the absolute skill in predicting global mean surface CO_2 flux. An important concept in decadal prediction is the relative contribution to the absolute skill that is provided by the initialization. To asses whether initialization has added additional value to the predictions, the hindcast simulation skill can be compared to that found in standard, non-initialized CMIP6 historical simulations (Fig. 3). For the linear statistical models, hindcast skills are close to the corresponding historical skill, and do not show statistically significant improvement. That is, the linear model scores do not show significant added skill due to initialization. For the NN model, the hindcast skills are significantly larger than the historical skills at least for the first three years, based on a bootstrapping test (Fig. 3). This is the range where tempera-

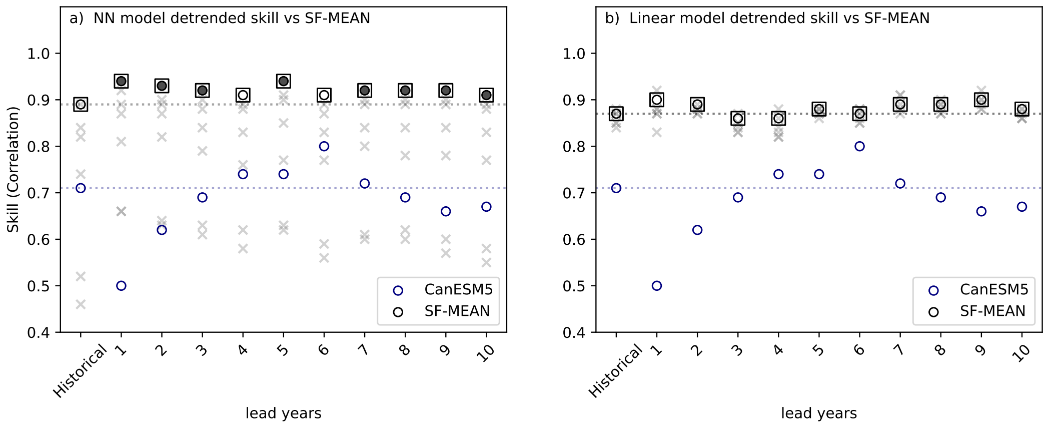

Figure 3. (a) Detrended global ocean carbon flux skills versus SF-MEAN for raw CanESM5 model (blue dots) and NN model trained on the SF-MEAN using bias corrected historical/hindcast predictors from CanESM5 (black dots). The scores that are statistically better than the raw CanESM5 score based on 1000 iteration bootstrap tests are shown with black boxes and the lead years where scores are significantly better than the corresponding historical score are filled. The grey marks in the background show scores from models trained on individual SeaFlux products versus the SF-MEAN. (b) Same as (a) but for the linear model.

ture variations largely control short term predictability of ocean carbon sink (Li et al., 2019). The NN hindcast scores are not significantly better than historical for lead years 4 to 6, but show re-emergence of significance afterward. NN models consistently show better fits to the dataset used for training them (Fig S2), but are also more subject to overfitting than the linear models (Fig. 2). While more work is needed to understand difference in model structure, our results show that initialization does add value to predictions made with the NN models (see also Fig. S4).

Both the hindcasts and historical run used observed atmospheric CO_2 concentrations (as do our statistical models, as an input predictor). We expect that skills estimated from the hindcast are higher than those achievable in true forecasts, because in true forecasts the atmospheric CO_2 concentration will not be known. It is not just the background rate of increase that is relevant, but deviations in the growth rate of atmospheric CO_2 are also known to be a key driver of decadal scale variability in the ocean CO_2 sink (McKinley et al., 2020). This is an issue common to any DCPP-style hindcast. Regardless, the improved skill that the statistical models driven by CanESM5 based predictors show over and above CanESM5 or other raw CMIP6 DCPP model hindcast skills encourages us to apply our methods to making future predictions in the following section. First however, we turn to considering the spatial pattern of skill over the hindcast period.

We compare spatially resolved temporal correlations between SF-MEAN, the CanESM5 raw biogeochemical model, and the two statistical models for the historical, assimilation and lead years 1 to 10 of the hindcast experiments. Both the NN and linear models show large correlations for the detrended flux over the majority of global ocean, when driven by predictors from the CanESM5 assimilation run (Fig. 4). Compared to the raw flux from the CanESM5 assimilation run, the statistical models significantly improve skill over more than 55% of the global ocean (56% for NN and 65% for linear). The linear model shows better average grid scale correlation compared to the NN model for assimilation and lead year one hindcast. This is most likely due to the high grid scale training resolution of the linear model as opposed to biome scale resolution of the NN model (see

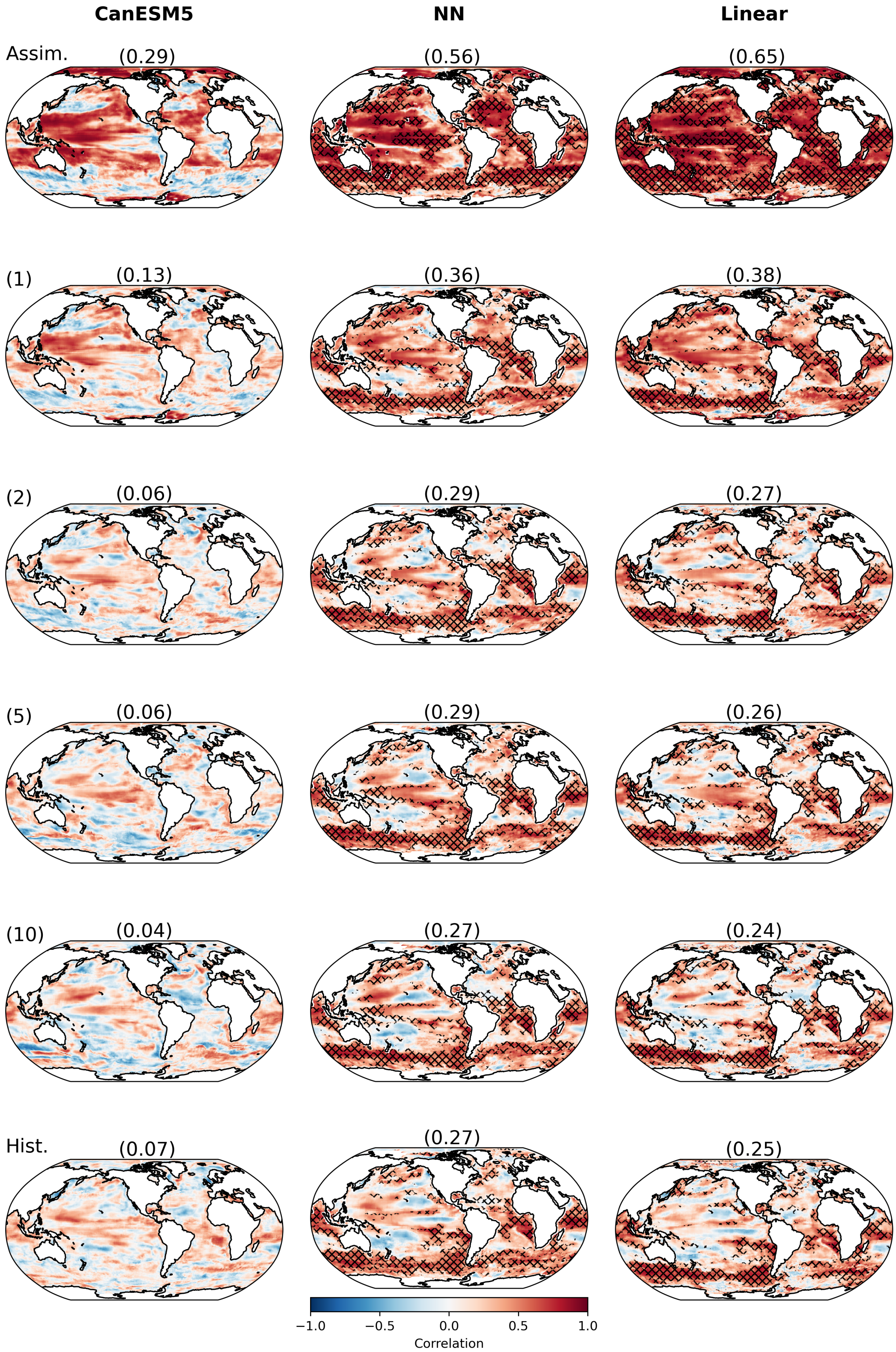

Figure 4. Grid wise correlation for the anomalous detrended ocean carbon flux versus SF-using assimilation, historical as well as lead years 1, 2, 5 10 predictors from CanESM5. The first column shows raw CanESM5 model skills, while the second and third columns show the NN and linear model based simulations. Hatches show regions where there is an statistically significant improvement in skill using a 1000 iteration bootstrap test compared to the raw CanESM5 results. The numbers on top of each panel are global mean of correlations.

supplements). Notably, the linear models has improved skill regionally, while the skill of the globally integrated sink is better from the NN model. On longer hindcasts lead yaers, the mean grid scale skill for the linear models drop faster than NN model and NN model beats the linear model with small offsets and more percentage of grid cell (not shown here) with significantly improved skills.

The regions that show significant improvements relative to raw CanESM5 model include but are not limited to the highly active regions for the sink (Gooya et al., 2023) which makes them important for both the flux magnitude and uncertainty. These are regions where the largest sink is concentrated in smallest ocean surface area and where internal and model uncertainty tend to be largest. Specifically, significant improvements over the Southern Ocean is the common feature to all simulations. The Southern Ocean is of key importance for ocean carbon sink (Gruber et al., 2019) where the models disagree most (Gooya et al., 2023; Frölicher et al., 2015). In the hindcast simulations, skills decrease with lead year, approaching the corresponding historical simulation skill on longer lead times (>7), as expected. For all lead years there is significant improvement beyond the raw CanESM5 results regionally over more than 30% of the global ocean (hatched areas in Fig. 4). Our results offer a potential pathway to better quantification of ocean carbon sink predictions both regionally and globally.

5 Hybrid forecast of the 2020-2029 ocean carbon sink

The ultimate purpose of decadal prediction systems is to provide forecasts of the short term future evolution of the climate system, including the ocean carbon flux. In this section, we use the statistical models trained on the SF-MEAN, and evaluated over the hindcast period, to make predictions for the near term evolution of ocean carbon flux. We extract ensemble means of our five predictors from CanESM5 DCPP forecasts for the period 2019-2029, and bias correct them according to lead time following (Kharin et al., 2012). We apply the statistical models on these predictors, and include the atmospheric concentration of CO_2 from SSP245 (Eyring et al., 2016), which is the same procedure applied to the hindcasts in the previous section.

Both NN model and linear model based forecasts predict that ocean carbon sink is going to grow with a faster than linear rate over the next decade under the SSP245 scenario (Fig. 5). The linear model predicts slower rate of increase until 2022 compared to the NN model, and an accelerated increase after to nearly 1.29 pgC yr^{-1} relative to 2019 by 2029. The rate of change in the linear model is consistent with the rate of change of the atmospheric CO_2 concentrations under the SSP245 scenario. The NN model predicts a more steady yet faster than linear increase of approximately 1.09 pgC yr^{-1} in global ocean carbon sink relative to 2019. Both models are in close agreement regarding decadal scale changes in the flux and predict larger changes compared to the bias corrected flux from the CanESM5 biogeochemical component. The fact that the results show are largely consistent between the two statistical models over 1990-2019 as well as the future forecast globally and regionally (Fig. S5), increases our confidence in the results. Based on the skill demonstrated in the hindcasts, we assert that our hybrid statistical-GCM predictions represent a more reliable estimate of future changes in the ocean carbon flux than the raw model predictions.

6 Discussion and conclusions

We have proposed a methodology to improve the decadal predictability of the ocean carbon flux by using statistical models as alternatives to the ocean biogeochemistry components of decadal prediction systems. Through their training, the statistical models encode the relationships between physical predictors and the surface carbon flux found in observations. Predictions are made by applying these observationally trained statistical models on (largely) physical predictors obtained from the GCM-based decadal pre-

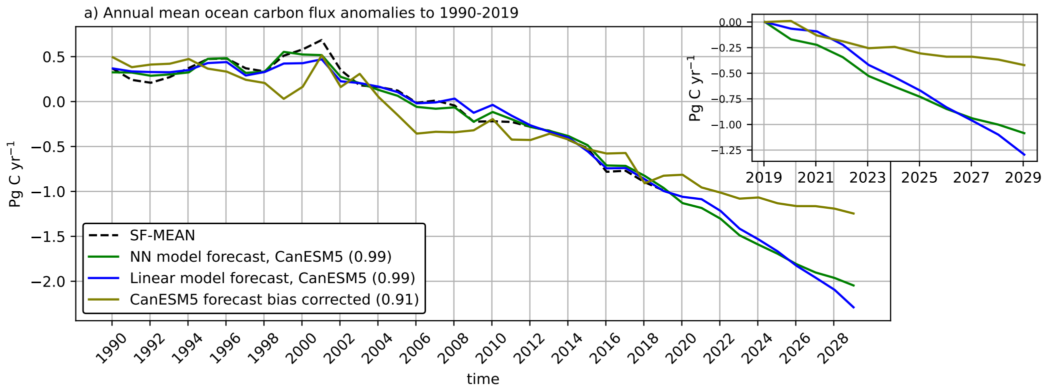

Figure 5. Global ocean carbon flux decadal forecast based on bias corrected CanESM5 (olive), NN model (green), and linear model (blue) trained on SF-MEAN. The dashed black line shows SF-MEAN over the period of 1990-2019. The Forecasts show assimilation runs over this period and forecast initialized in 2019 after. The subplot shows anomalies relative to the 2019 ocean carbon flux on each product and shows the predicted changes until 2029 from different estimates. All global timeseries are scaled based on the spatial coverage of the SF-MEAN to account for differences in coverage.

diction systems. Unlike biogeochemical variables, the physical variables are directly initialized in current prediction systems, have a more established track record of skill, and are based on less heavily parameterized processes than ocean biogeochemistry. In principal, our approach can be thought of as an extension of traditional bias correction (Kharin et al., 2012). Statistical bias correction schemes using linear/NN algorithms have previously been used for physical parameters in decadal prediction system (citation). Unlike those, our approach does not use the same variable that is being bias corrected. Instead, it relies primarily on key physical predictors whose predictability have been well evaluated.

We have demonstrated that in hindcasts, our hybrid statistical-GCM system improves prediction skill for the surface ocean carbon flux relative to the ocean biogeochemical model, both in the global mean, and regionally over broad areas of the ocean. Indeed, for the global mean flux, our hybrid skills based on CanESM5 predictors beat all available CMIP6 DCPP models. Globally, the NN model can retain the memory of initialization of the predictors at least up to lead year three after initialization.

We have demonstrated our approach using two examples of observationally constrained statistical models of different complexities; a linear and a neural network model. The two statistical models used here have different structures and use different combinations of predictors. Both statistical models are able to reconstruct observed CO_2 fluxes when forced by observed predictors, and both perform well in hindcast evaluations driven by CanESM5-based predictoris (i.e. beating the skill of the raw CanESM5 flux). In general, the NN model was able to achieve higher correlations when trained and evaluated against a given surface flux product, but the linear model showed more "generalizability" across products. In addition, while the linear model was quite robust to changes in structure (predictors), the NN model was quite sensitive to changes in the number of predictors or neurons used. This shows the need for carefully adjusting such complex models and validation against other such models to avoid possible overfitting and to make reliable estimates.

We emphasize that the two statistical models we have used are just examples of our more general approach of applying observationally trained statistical models to GCM predictors. Our method is not limited to the choice of ESM, observation based product, or to the choice of the alternative model. Future work should test the ability of different types of statistical models to improve upon our results, and could draw upon the large body of work in developing empirical relationships for the purposes of infilling sparse pCO_2 observations (Fay et al., 2021). Currently, CanESM5 is the only model with sufficient number of simulations publicly available for 10-year hindcasts and forecast for all of the required predictors. More robust estimates of the future changes of ocean carbon sink would be possible with multimodel averages of predictors, since such multi-model predictions are generally more skillful (Tebaldi & Knutti, 2007). We also note that our approach is not limited to surface ocean carbon flux, but could also be applied to other biogeochemical predictors, or even less certain physical variables that could benefit from exploiting empirical relationships based on well predicted quantities such as SST.

Based on the demonstrated skill of our hybrid approach in hindcasts, we have made forecasts of the near term evolution of ocean carbon flux using both the linear and NN models under ssp245 scenario. Both hybrid statistical models show consistent changes over the period of 2019-2029 with faster than linear increase in the sink that are larger than bias corrected CanESM5 forecasts. This information about predicted future changes in the ocean carbon sink might be useful to climate science and policy effort, for example the assessment of the global carbon budget (Friedlingstein et al., 2022). Moving forward we encourage further research into improving decadal predictions by optimally exploiting all available observational information, and data science techniques, in conjunction with traditional GCM based predictions.

Open Research

The SeaFlux observation based ensemble is available publicly at `https://zenodo.org/record/5482547`. All model data used in this study are part of the World Climate Research Programme's (WCRP) 6th Coupled Model Intercomparison Project (CMIP6) and open-access through Earth System Grid Federation (ESGF) repositories. Observational predictors used for training the statistical models are available through institutional public repositories as cited in the Supplements. All other inquiries should be directed to P. Gooya.

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Improving GCM-based decadal ocean carbon flux predictions using observationally-constrained statistical models

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Key Points:

- We use observationally trained statistical models to obtain decadal predictions of ocean carbon flux from initialized GCM-based predictors.
- The hybrid GCM-statistical ocean carbon flux predictions show improved skill over hindcast predictions from the GCM's biogeochemical models.
- The hybrid models are used to make decadal predictions for the ocean-atmosphere carbon flux over the decade ending in 2029.

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Abstract

Initialized climate model simulations have proven skillful for near-term predictability of the key physical climate variables. By comparison, predictions of biogeochemical fields like ocean carbon flux, are still emerging. Initial studies indicate skillful predictions are possible for lead-times up to six years at global scale for some CMIP6 models. However, unlike core physical variables, biogeochemical variables are not directly initialized in existing decadal preciction systems, and extensive empirical parametrization of ocean-biogeochemistry in Earth System Models introduces a significant source of uncertainty. Here we propose a new approach for improving the skill of decadal ocean carbon flux predictions using observationally-constrained statistical models, as alternatives to the ocean-biogeochemistry models. We use observations to train multi-linear and neural-network models to predict the ocean carbon flux. To account for observational uncertainties, we train using six different observational estimates of the flux. We then apply these trained statistical models using input predictors from the Canadian Earth System Model (CanESM5) decadal prediction system to produce new decadal predictions. Our hybrid GCM-statistical approach significantly improves prediction skill, relative to the raw CanESM5 hindcast predictions over 1990-2019. Our hybrid-model skill is also larger than that obtained by any available CMIP6 model. Using bias-corrected CanESM5 predictors, we make forecasts for ocean carbon flux over 2020-2029. Both statistical models predict increases in the ocean carbon flux larger than the changes predicted from CanESM5 forecasts. Our work highlights the ability to improve decadal ocean carbon flux predictions by using observationally-trained statistical models together with robust input predictors from GCM-based decadal predictions.

Plain Language Summary

Using initialized Earth system model simulations for near term predictions of ocean biogeochemichal variables is an emerging field of research. In particular, near term predictability of ocean carbon flux is central to efforts for planing and limiting climate change. Unlike physical variables whose predictability have been established, these simulations are only indirectly initialized and rely on heavily parameterized ocean biogeochemistry models. Here, we propose a new approach to acquire decadal predictions of air-sea carbon flux as alternatives to those based on ocean biogeochemistry models. Our methodology combines the explanatory power of statistical models that have widely been used for gap filling purposes for informing full coverage ocean carbon flux data products, and well established predictability skill of key physical predictors. We provide hybrid GCM-statistical ocean carbon flux hindcasts using predictors from CanESM5 and doing so, show that we can beat all CMIP6 decadal prediction system hindcast skills. We use our models to provide near future hybrid model forecast for ocean carbon flux. Our results shows the potential for improving predictability skill of ocean carbon sink by combining GCMs and observationally trained statistical models.

1 Introduction

The ocean accounts for sequestering nearly 25% percent of human CO_2 emissions annually (Hauck et al., 2020; Friedlingstein et al., 2022, 2020), playing a key role in mitigating climate change. Future changes in the ocean carbon flux are of direct relevance to climate change science (Friedlingstein et al., 2022) and policy making related to climate and emissions targets. Ocean carbon uptake has increased substantially over the past several decades in response to human induced increases in atmospheric CO_2 concentrations (Gooya et al., 2023; Rodgers et al., 2020; Lovenduski et al., 2016; McKinley et al., 2016; Wang et al., 2016). However, there is also substantial internal variability in the magnitude of the flux on seasonal to decadal time scales both regionally and globally (Landschützer et al., 2016; McKinley et al., 2017; Gruber et al., 2019; McKinley et al., 2020). Decadal scale variability of ocean carbon flux is believed to be driven largely by variability in external forcing (McKinley et al., 2020), and specifically, the deviations of atmospheric growth of CO_2 from the long term trend but also changes in circulation (DeVries et al., 2019; Keppler & Landschützer, 2019). Higher frequency interannual variability is largely attributable to modes of climate variability such as ENSO on global scale and other modes of high latitude variability on regional scales (McKinley et al., 2017). Predicting future variations in the ocean carbon sink on inter-annual to decadal time scales in the face of these mulitple drivers is therefore challenging.

Decadal predictions, such as those made under the Decadal Climate Prediction Project (DCCP) are produced by Global Climate Models (GCMs) that are that are initialized with observations and also driven by external forcing (Kirtman et al., 2013). Predictive skill of key physical climate variables from such simulations have been well established in the literature (Boer et al., 2016). However, near term predictability of the ocean carbon flux and other biogeochemical variables have only become possible with the recent advent of Earth System Models (ESMs) (Meehl et al., 2021) and are still at their infancy. Previous studies have shown potential predictability of the ocean carbon flux for up to 7 years (Li et al., 2019; Séférian et al., 2018) and actual skill versus observation based estimates for 2-6 years based on different ESMs (Li et al., 2019; Ilyina et al., 2021). However, ESM simulations are subject to biases, drifts (Kharin et al., 2012) and exhibit a wide range of prediction skill globally and regionally (Ilyina et al., 2021). Predictions of ocean carbon flux using ESMs are especially challenging given that ocean biogeochemical variables are not directly initialized in current decadal prediction systems (Sospedra-Alfonso et al., 2021), and that the ocean biogeochmical models themselves are heavily parameterized using empirical parameterizations (Christian et al., 2022).

Here we propose using observationally-trained statistical models forced by predictors from GCM/ESM-based decadal predictions, as an alternative to using the raw predictions of ocean carbon flux obtained from the ESMs ocean biogeochemistry models. It is well established that the surface ocean partial pressure of CO_2, and by extension the surface carbon flux, is closely related to physical predictors, such as sea-surface temperature and salinity, atmospheric CO_2 concentration and wind speed. These empirical relationships are widely exploited in the observational community to infill sparse direct observations of the ocean carbonate system (e.g., Surface Ocean CO_2 Atlas, SOCAT), using indirect but more widely sampled physical variables (Landschützer et al., 2016). It is also common to post-process raw GCM results to produce more skillful predictions, for example through bias correction (Kharin et al., 2012). Our proposal is a logical extension of these two established practises that combines the explanatory power that statistical models learn from the relationships between observational predictors, and the established prediction skill of the process based physical models. Our principal goal is to establish a methodology that allows us to improve near-term predictions of the ocean carbon sink over and above the skill obtained from raw ESM predictions.

We begin by introducing the methodology and our statistical models of choice in Section 2. In section 3 we evaluate observational uncertainties and the performance of our statistical models when forced by observation based predictors. In section 4, we apply the observationally trained statistical models to physical predictors from CanESM5 simulations, and evaluate the skill of this hybrid approach relative to the raw CanESM5 predictions over the hindcast period of 1990 to 2019. We go on to provide forecasts for ocean carbon flux over the decade 2019 to 2029 in section 5. We conclude by reflecting on how our approach could be improved and expanded on in future work.

2 Materials and Methods

2.1 Surface CO_2 flux data

For observations of the atmosphere-ocean CO_2 flux we use the SeaFlux Ocean carbon sink ensemble product (Gregor & Fay, 2021). SeaFlux contains an ensemble of flux estimates, based on six global observation-based mapping products for surface ocean partial pressure of CO_2 (pCO_2), and wind speeds from ERA5. The six products include three neural-network-derived products (CMEMS-FFNN, MPI-SOMFFN, NIES-FNN), a mixed layer scheme product (JENA-MLS), a multiple linear regression (JMA-MLR), and a machine learning ensemble (CSIR-ML6) (Fay et al., 2021). We also use the mean across the products, which we refer to as SF-MEAN. Given the sparseness of actual pCO_2 measurements, using the ensemble of products allows us to quantify uncertainties associated with the data infilling and mapping techniques, and avoids overfitting to a single product.

All six SeaFlux products show strong agreement in the long term (trended) changes in ocean carbon flux (not shown here). Comparing linearly detrended versions of the SeaFlux products shows cross correlation coefficients between them ranging from 0.47 to 0.95 (Fig. S1). The MPI-SOM-FFN and JENA-MLS are least correlated with others. The lower correlation skills for the two show that there are variabilities specific to these products that are not common to other datasets, and known biases linked to data sparsity (Gloege et al., 2021; Hauck et al., 2023). The averaged SF-MEAN contains signals common to all of the products, and we use this as the most reliable estimate moving forward.

2.2 Statistical models and observed predictors

For each individual SeaFlux input dataset and SF-MEAN, we train a multi-linear regression model and a neural network (NN) model to predict the surface atmosphere ocean carbon flux, using three observation-based physical predictors - sea surface temperature (SST), sea surface salinity (SSS), surface wind speed (sfcWind), one biological predictor -surface chlorophyll concentrations (CHL), as well as atmospheric CO_2 concentrations (xCO_2) (table S1). These are mainly physical predictors for which full coverage observational products are available and are believed to drive the variability in ocean carbon flux (Landschützer et al., 2016). Linear models are trained for each grid cell on a standard one degree grid, while the NN models are trained over 16 biomes (Landschützer et al., 2016), as explained further in SI (Sect. S1.1). By combining these biomes, we can produce spatially resolved maps of the surface CO_2 flux, given the set of five input predictors at any point. In total that gives us 14 sets of models (7 set of linear models, and 7 NN models, one for each SeaFlux target predictand) that are later used to make hindcasts and forecasts using modelled predictors from CanESM5. We have chosen to illustrate our approach using the linear and NN models, which have different structures and levels of complexity, as illustrative examples. However, alternative models and predictor variables could be used.

2.3 Decadal predictions using GCM base predictors

To make predictions the five predictors from Table S1 are obtained from CanESM5 simulations (Swart et al., 2019; Sospedra-Alfonso et al., 2021). We use a range of simulations, including standard free running CMIP6 historical simulations (Eyring et al., 2016), as well as assimilation and hindcast and forecast runs (Boer et al., 2016). In assimilation runs, CanESM5 is nudged towards observations for key physical variables (Sospedra-Alfonso et al., 2021). For historical, hindcast and forecast simulations, the five predictors are bias corrected to the same observational predictors used for training the models following the approach of (Kharin et al., 2012). This bias correction adjusts the mean and trend of the predictors to be consistent with observations. These CanESM5 predictors are fed to the each of the 14 statistical model sets mentioned above to produce hy-

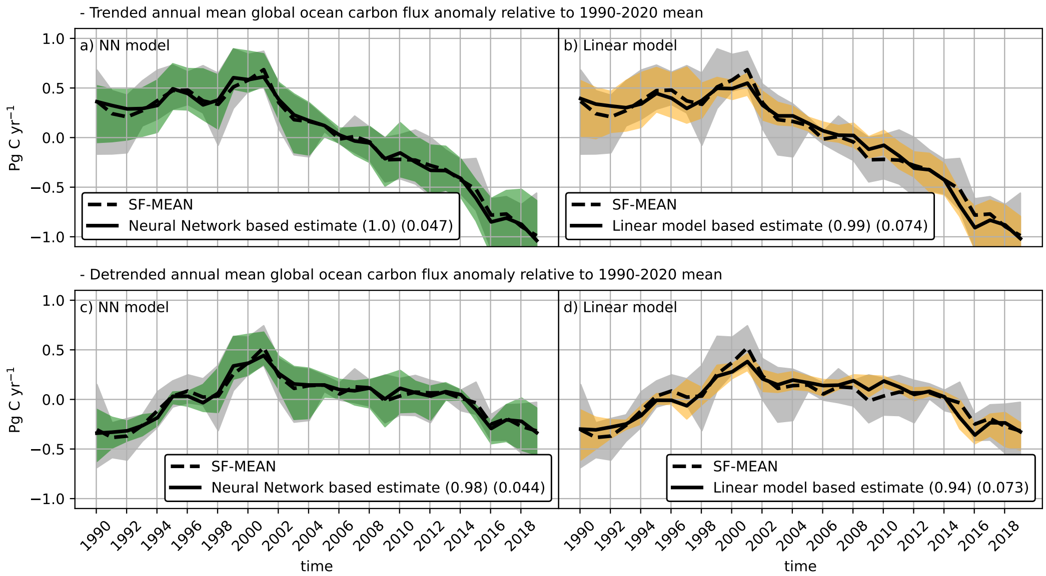

Figure 1. Time series of the global ocean CO_2 flux anomalies for the (a) NN model (left panel) and (b) linear model (right panel) reconstruction using obervational predictors. The black lines shows reconstruction using models that are trained on mean of SeaFlux products (SF-MEAN; solid) as well the mean product itself (dashed). The shadings represent the range estimates from the six different SeaFlux products (grey) and from NN and linear models reconstructions (green and orange). The numbers in the legends are correlation coefficients between the solid black lines and dashed black lines (first number) and root mean square error of the two time series (second number). (c) and (d) are same as (a) and (b) but are linearly detrended.

brid predictions of surface ocean CO_2 flux. For hindcasts and forecasts, predictions are made for lead years 1 to 10. To test significance of prediction skill differences, we use a 1000 iteration bootstrap to test of (Goddard et al., 2013).

3 Evaluation of statistical models

In this section, we consider the performance of the statistical models trained on the SeaFlux ensemble and using observed predictors, for predicting the global mean surface carbon flux as defined by SF-MEAN (Fig. 1). When trained on SF-MEAN, both the NN and linear models can accurately reconstruct the changes of the SF-MEAN ($r > 0.9$), indicating that the statistical models are able to capture the majority of the variance in the global mean surface flux. The NN model shows higher skill in reconstructing SF-MEAN relative to the linear model, reflected in higher correlations and lower root mean square error (Fig. 1). Similarly, both linear and NN models are able to successfully reproduce individual SeaFlux products on which they are trained (Fig. S2), with the NN models again achieving tighter fits than the linear models. The orange and green shading in Fig. 1 represents the spread across models trained on individual SeaFlux products. These models are still able to successfully reproduce SF-MEAN, which gives an indication of their generalizability. The smaller spread for the linear models (Fig. 1b, orange shading), suggests they may be more generalizable (i.e. successful in predicting data they were not trained on) than the NN models. We further explore the idea of generalizability when using model-derived predictors in the following section.

4 Applying statistical models to physical predictors from the ESM

4.1 Assimilation run

The CanESM5 assimilation run is relaxed towards the observed physical state of the system, which forces physical variables, including our input predictors, to be close to observations. However, the detrended CO_2 flux from the CanESM5 biogeochemical component is not in good agreement with observations (Fig. 2 bottom row). We have identified issue in the model derived CO_2 flux, including seasonality that is out of phase with observations (not shown here), and it appears that the data ingestion in the assimilation run degrades the biogeochemical models performance. Indeed, previous results have shown that atmosphere-ocean CO_2 flux predictability is low in CanESM5, and particularly poor in the early lead years immediately following the assimilation run (Ilyina et al., 2021). A major goal of our effort is to see whether by replacing the CanESM5 biogeochemical model derived flux with one computed based on the statistical models leads to improvement.

We use the linear and NN models previously trained using observed predictors, and for each of the six individual SeaFlux products and SF-MEAN as predictands (for a total of 14 model sets). We then extract the five input predictors from the (ensemble mean of 10) CanESM5 DCPP assimilation runs, apply the statistical models on these GCM-based predictors, and compare their skill against the original SeaFlux observational products (Fig 2).

The statistical models forced by CanESM5 assimilation predictors obtain similar skills in reproducing the individual SeaFlux products to the skills of the reconstructions that used predictors from observations (compare Fig. 2 and supplementary Fig. S2). This is a somewhat expected result given that assimilation runs assimilate physical predictors and are very close to the observations, but nonetheless it is first step in applying the models on data on which they were not directly trained. For both the linear and NN statistical models, the skill is in all cases is significantly higher than than skill of the raw CanESM5 CO_2 flux. These results indicate that statistical models trained on observations can usefully be applied to GCM-derived predictors. By using this approach we are able to avoid biases in the CanESM5 biogeochemical model by combining the observationally constrained statistical models with the directly initialized physical predictors from CanESM.

We compute the cross-correlation matrix for statistical models trained on one SeaFlux product in reproducing all the other five product and SF-MEAN (Fig. 2). This allows us to assess the impacts of observational uncertainty, and the potential consequences of overfitting statistical models to a single observational product. As expected, the statistical models are most skillful in reproducing the product on which they were trained (diagonal in Fig. 2). Correlation in reproducing other products can be lower than 0.5. The extent to which a model trained on one observational product can be generalized to others is measured with the mean of scores versus all other observational data products (mean of rows excluding the diagonal values as indicated in Fig. 2 EXT column). Overall, the linear models have larger extendibility scores, while the NN models produce better fits for the products on which they were trained. Our results illustrate that care should be taken in tightly fitting statistical models to a single observation based CO_2 flux product, as uncertainties exist. Moving forward, we will use statistical model trained on the SF-MEAN product as the best estimate. Based on the encouraging success so far, in the next section we will apply our approach to decadal predictions.

4.2 Prediction skill of CO_2 flux over the hindcast period

Hindcasts are ESM simulations that use the observationally constrained assimilation simulation as initial conditions, and which are then run freely under standard CMIP6

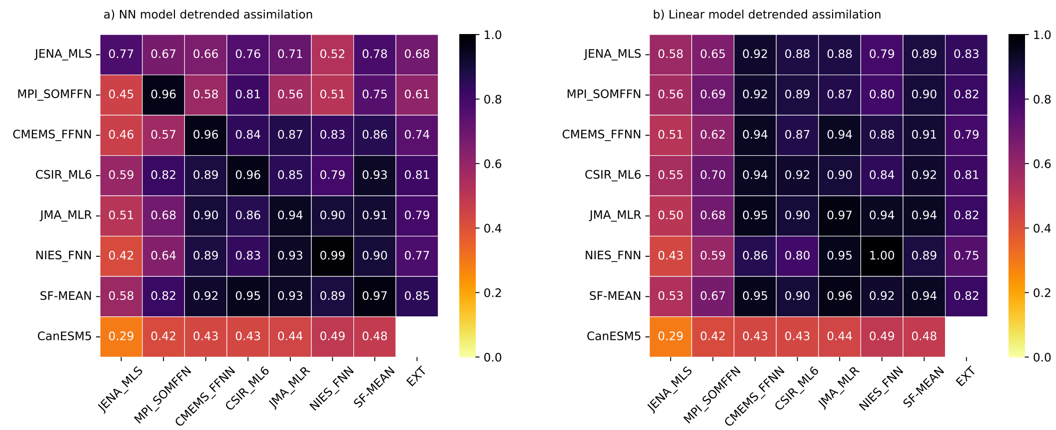

Figure 2. (a) Correlation matrix for the detrended global ocean carbon flux anomaly. The y axis indicate the product on which the NN model is trained and the x axis shows the data products against which the skill is evaluated. The EXT column measures the mean of skills excluding the diagonal element for each row. (b) Same as (a) but for the Linear model.

external forcings for ten years (Boer et al., 2016). Generally, as lead years increase (i.e. number of year since initialization) the hindcasts simulations lose memory of initializaton and drift towards the preferred state of the model (historical simulations). However, raw CanESM5 ocean carbon flux DCPP scores show a decrease in the skill after initialization in hindcast compared to the historical free runs (Ilyina et al., 2021). This is not the expected result of initialization and indicates possible discrepancies with interactions between initialization and the CanESM5 biogeochemical decadal prediction system (initialization "shocks").

As an alternative to the biogeochmical model flux, we apply our SF-MEAN trained statistical models on predictors from the CanESM5 hindcast simulations over the period 1990 to 2019. The hindcast skill from both the linear and NN model when trained and evaluated against SF-MEAN are significantly larger than raw CanESM5 skills, with NN yielding slightly better scores (Fig. 3). Both statistical models show increase in skill after initialization, as expected and seen in physical predictors, and a gradual drop with lead time. As an even more stringent test, we compare the skill of the statistical models driven by CanESM5 predictors against the skill from all other available CMIP6 models that participated in DCPP. The NN model skill is higher than that shown by any raw CMIP6 model, when evaluated against SF-MEAN (Fig. S3) over 1990-2017 that is the period common to all models. Linear model score are higher than all CMIP6 models on all lead years except lead year 3 where CESM1 (Danabasoglu, 2019) yields slightly larger score (Fig. S3). These results clearly show the potential of our approach for improving the decadal CO_2 flux prediction skills.

To this point we have considered the absolute skill in predicting global mean surface CO_2 flux. An important concept in decadal prediction is the relative contribution to the absolute skill that is provided by the initialization. To asses whether initialization has added additional value to the predictions, the hindcast simulation skill can be compared to that found in standard, non-initialized CMIP6 historical simulations (Fig. 3). For the linear statistical models, hindcast skills are close to the corresponding historical skill, and do not show statistically significant improvement. That is, the linear model scores do not show significant added skill due to initialization. For the NN model, the hindcast skills are significantly larger than the historical skills at least for the first three years, based on a bootstrapping test (Fig. 3). This is the range where tempera-

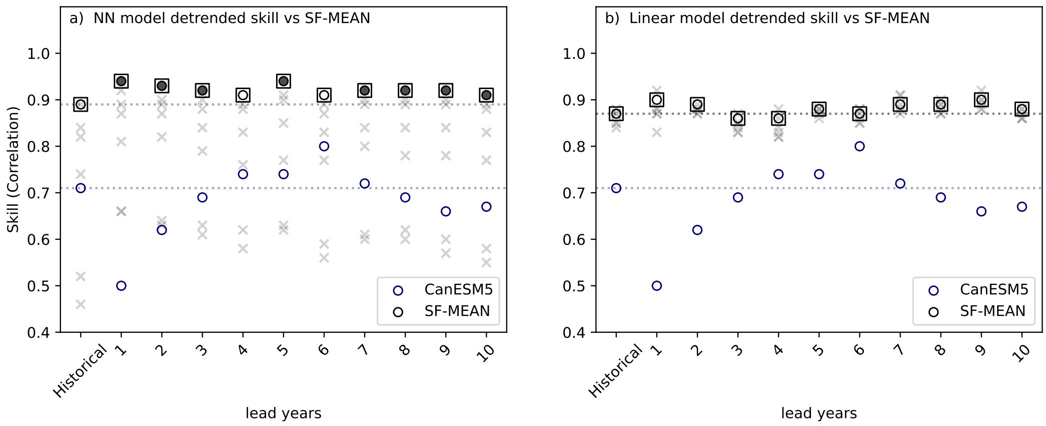

Figure 3. (a) Detrended global ocean carbon flux skills versus SF-MEAN for raw CanESM5 model (blue dots) and NN model trained on the SF-MEAN using bias corrected historical/hindcast predictors from CanESM5 (black dots). The scores that are statistically better than the raw CanESM5 score based on 1000 iteration bootstrap tests are shown with black boxes and the lead years where scores are significantly better than the corresponding historical score are filled. The grey marks in the background show scores from models trained on individual SeaFlux products versus the SF-MEAN. (b) Same as (a) but for the linear model.

ture variations largely control short term predictability of ocean carbon sink (Li et al., 2019). The NN hindcast scores are not significantly better than historical for lead years 4 to 6, but show re-emergence of significance afterward. NN models consistently show better fits to the dataset used for training them (Fig S2), but are also more subject to overfitting than the linear models (Fig. 2). While more work is needed to understand difference in model structure, our results show that initialization does add value to predictions made with the NN models (see also Fig. S4).

Both the hindcasts and historical run used observed atmospheric CO_2 concentrations (as do our statistical models, as an input predictor). We expect that skills estimated from the hindcast are higher than those achievable in true forecasts, because in true forecasts the atmospheric CO_2 concentration will not be known. It is not just the background rate of increase that is relevant, but deviations in the growth rate of atmospheric CO_2 are also known to be a key driver of decadal scale variability in the ocean CO_2 sink (McKinley et al., 2020). This is an issue common to any DCPP-style hindcast. Regardless, the improved skill that the statistical models driven by CanESM5 based predictors show over and above CanESM5 or other raw CMIP6 DCPP model hindcast skills encourages us to apply our methods to making future predictions in the following section. First however, we turn to considering the spatial pattern of skill over the hindcast period.

We compare spatially resolved temporal correlations between SF-MEAN, the CanESM5 raw biogeochemical model, and the two statistical models for the historical, assimilation and lead years 1 to 10 of the hindcast experiments. Both the NN and linear models show large correlations for the detrended flux over the majority of global ocean, when driven by predictors from the CanESM5 assimilation run (Fig. 4). Compared to the raw flux from the CanESM5 assimilation run, the statistical models significantly improve skill over more than 55% of the global ocean (56% for NN and 65% for linear). The linear model shows better average grid scale correlation compared to the NN model for assimilation and lead year one hindcast. This is most likely due to the high grid scale training resolution of the linear model as opposed to biome scale resolution of the NN model (see

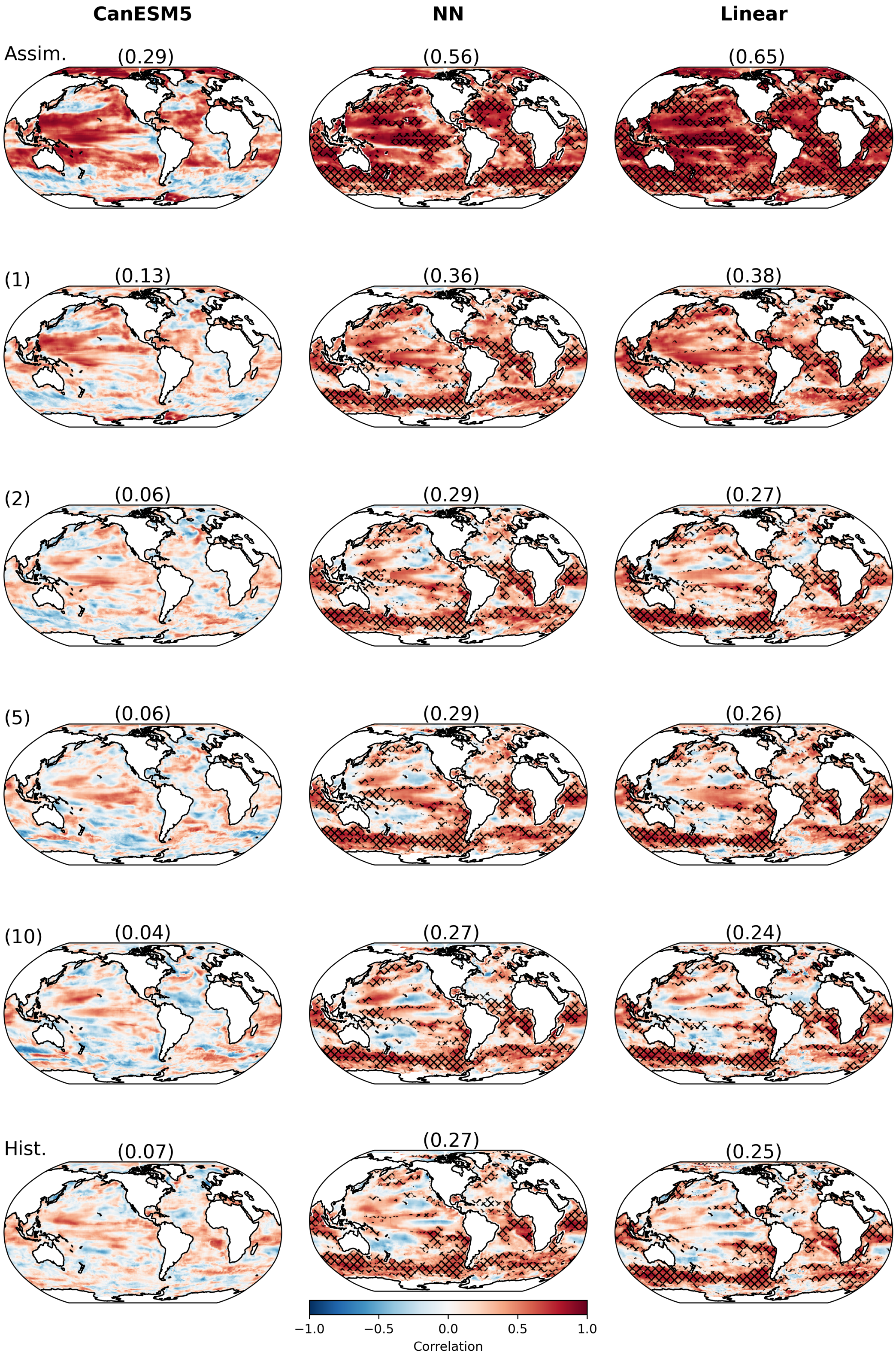

Figure 4. Grid wise correlation for the anomalous detrended ocean carbon flux versus SF-using assimilation, historical as well as lead years 1, 2, 5 10 predictors from CanESM5. The first column shows raw CanESM5 model skills, while the second and third columns show the NN and linear model based simulations. Hatches show regions where there is an statistically significant improvement in skill using a 1000 iteration bootstrap test compared to the raw CanESM5 results. The numbers on top of each panel are global mean of correlations.

supplements). Notably, the linear models has improved skill regionally, while the skill of the globally integrated sink is better from the NN model. On longer hindcasts lead yaers, the mean grid scale skill for the linear models drop faster than NN model and NN model beats the linear model with small offsets and more percentage of grid cell (not shown here) with significantly improved skills.

The regions that show significant improvements relative to raw CanESM5 model include but are not limited to the highly active regions for the sink (Gooya et al., 2023) which makes them important for both the flux magnitude and uncertainty. These are regions where the largest sink is concentrated in smallest ocean surface area and where internal and model uncertainty tend to be largest. Specifically, significant improvements over the Southern Ocean is the common feature to all simulations. The Southern Ocean is of key importance for ocean carbon sink (Gruber et al., 2019) where the models disagree most (Gooya et al., 2023; Frölicher et al., 2015). In the hindcast simulations, skills decrease with lead year, approaching the corresponding historical simulation skill on longer lead times (>7), as expected. For all lead years there is significant improvement beyond the raw CanESM5 results regionally over more than 30% of the global ocean (hatched areas in Fig. 4). Our results offer a potential pathway to better quantification of ocean carbon sink predictions both regionally and globally.

5 Hybrid forecast of the 2020-2029 ocean carbon sink

The ultimate purpose of decadal prediction systems is to provide forecasts of the short term future evolution of the climate system, including the ocean carbon flux. In this section, we use the statistical models trained on the SF-MEAN, and evaluated over the hindcast period, to make predictions for the near term evolution of ocean carbon flux. We extract ensemble means of our five predictors from CanESM5 DCPP forecasts for the period 2019-2029, and bias correct them according to lead time following (Kharin et al., 2012). We apply the statistical models on these predictors, and include the atmospheric concentration of CO_2 from SSP245 (Eyring et al., 2016), which is the same procedure applied to the hindcasts in the previous section.

Both NN model and linear model based forecasts predict that ocean carbon sink is going to grow with a faster than linear rate over the next decade under the SSP245 scenario (Fig. 5). The linear model predicts slower rate of increase until 2022 compared to the NN model, and an accelerated increase after to nearly 1.29 pgC yr^{-1} relative to 2019 by 2029. The rate of change in the linear model is consistent with the rate of change of the atmospheric CO_2 concentrations under the SSP245 scenario. The NN model predicts a more steady yet faster than linear increase of approximately 1.09 pgC yr^{-1} in global ocean carbon sink relative to 2019. Both models are in close agreement regarding decadal scale changes in the flux and predict larger changes compared to the bias corrected flux from the CanESM5 biogeochemical component. The fact that the results show are largely consistent between the two statistical models over 1990-2019 as well as the future forecast globally and regionally (Fig. S5), increases our confidence in the results. Based on the skill demonstrated in the hindcasts, we assert that our hybrid statistical-GCM predictions represent a more reliable estimate of future changes in the ocean carbon flux than the raw model predictions.

6 Discussion and conclusions

We have proposed a methodology to improve the decadal predictability of the ocean carbon flux by using statistical models as alternatives to the ocean biogeochemistry components of decadal prediction systems. Through their training, the statistical models encode the relationships between physical predictors and the surface carbon flux found in observations. Predictions are made by applying these observationally trained statistical models on (largely) physical predictors obtained from the GCM-based decadal pre-

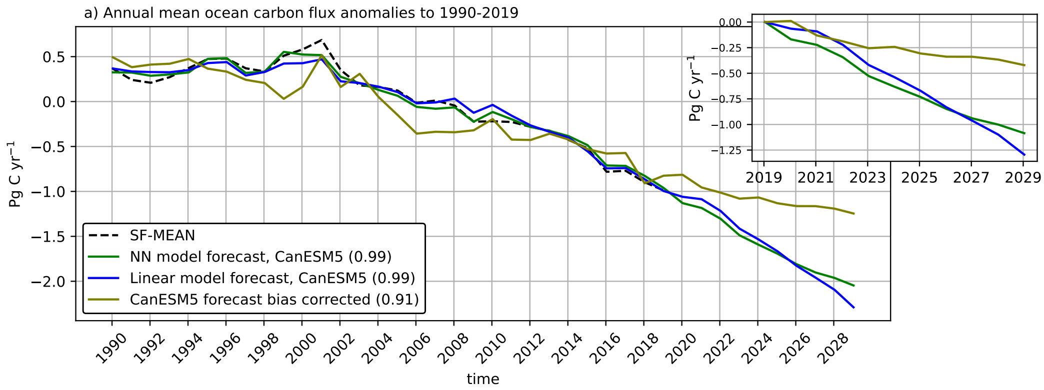

Figure 5. Global ocean carbon flux decadal forecast based on bias corrected CanESM5 (olive), NN model (green), and linear model (blue) trained on SF-MEAN. The dashed black line shows SF-MEAN over the period of 1990-2019. The Forecasts show assimilation runs over this period and forecast initialized in 2019 after. The subplot shows anomalies relative to the 2019 ocean carbon flux on each product and shows the predicted changes until 2029 from different estimates. All global timeseries are scaled based on the spatial coverage of the SF-MEAN to account for differences in coverage.

diction systems. Unlike biogeochemical variables, the physical variables are directly initialized in current prediction systems, have a more established track record of skill, and are based on less heavily parameterized processes than ocean biogeochemistry. In principal, our approach can be thought of as an extension of traditional bias correction (Kharin et al., 2012). Statistical bias correction schemes using linear/NN algorithms have previously been used for physical parameters in decadal prediction system (citation). Unlike those, our approach does not use the same variable that is being bias corrected. Instead, it relies primarily on key physical predictors whose predictability have been well evaluated.

We have demonstrated that in hindcasts, our hybrid statistical-GCM system improves prediction skill for the surface ocean carbon flux relative to the ocean biogeochemical model, both in the global mean, and regionally over broad areas of the ocean. Indeed, for the global mean flux, our hybrid skills based on CanESM5 predictors beat all available CMIP6 DCPP models. Globally, the NN model can retain the memory of initialization of the predictors at least up to lead year three after initialization.

We have demonstrated our approach using two examples of observationally constrained statistical models of different complexities; a linear and a neural network model. The two statistical models used here have different structures and use different combinations of predictors. Both statistical models are able to reconstruct observed CO_2 fluxes when forced by observed predictors, and both perform well in hindcast evaluations driven by CanESM5-based predictoris (i.e. beating the skill of the raw CanESM5 flux). In general, the NN model was able to achieve higher correlations when trained and evaluated against a given surface flux product, but the linear model showed more "generalizability" across products. In addition, while the linear model was quite robust to changes in structure (predictors), the NN model was quite sensitive to changes in the number of predictors or neurons used. This shows the need for carefully adjusting such complex models and validation against other such models to avoid possible overfitting and to make reliable estimates.

We emphasize that the two statistical models we have used are just examples of our more general approach of applying observationally trained statistical models to GCM predictors. Our method is not limited to the choice of ESM, observation based product, or to the choice of the alternative model. Future work should test the ability of different types of statistical models to improve upon our results, and could draw upon the large body of work in developing empirical relationships for the purposes of infilling sparse pCO_2 observations (Fay et al., 2021). Currently, CanESM5 is the only model with sufficient number of simulations publicly available for 10-year hindcasts and forecast for all of the required predictors. More robust estimates of the future changes of ocean carbon sink would be possible with multimodel averages of predictors, since such multi-model predictions are generally more skillful (Tebaldi & Knutti, 2007). We also note that our approach is not limited to surface ocean carbon flux, but could also be applied to other biogeochemical predictors, or even less certain physical variables that could benefit from exploiting empirical relationships based on well predicted quantities such as SST.

Based on the demonstrated skill of our hybrid approach in hindcasts, we have made forecasts of the near term evolution of ocean carbon flux using both the linear and NN models under ssp245 scenario. Both hybrid statistical models show consistent changes over the period of 2019-2029 with faster than linear increase in the sink that are larger than bias corrected CanESM5 forecasts. This information about predicted future changes in the ocean carbon sink might be useful to climate science and policy effort, for example the assessment of the global carbon budget (Friedlingstein et al., 2022). Moving forward we encourage further research into improving decadal predictions by optimally exploiting all available observational information, and data science techniques, in conjunction with traditional GCM based predictions.

Open Research

The SeaFlux observation based ensemble is available publicly at `https://zenodo.org/record/5482547`. All model data used in this study are part of the World Climate Research Programme's (WCRP) 6th Coupled Model Intercomparison Project (CMIP6) and open-access through Earth System Grid Federation (ESGF) repositories. Observational predictors used for training the statistical models are available through institutional public repositories as cited in the Supplements. All other inquiries should be directed to P. Gooya.

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Supporting Information for "Improving GCM-based decadal ocean carbon flux predictions using observationally-constrained statistical models"

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S1. Statistical models

S1.1. Linear model

The linear model used in this study is a least square multi linear regression model. For this model, training is done on monthly mean time resolution at each grid cell on a normal one-by-one grid. The predictands are deseasonalized monthly mean ocean carbon flux time series at each ocean grid cell. For the linear model, the predictors are: SST, SSS, log(CHL), sfcWind squared, linear xCO_2 trend, and detrended xCO_2. Each of the predictors are monthly mean time series that are deseasonalized using a repeating seasonal cycle over 1990-2019 period. This combination of predictors was chosen to represent variability across different time scales. For instance, the linear atmospheric trend is the dominant driver of long term changes in ocean carbon flux, deviations of atmospheric

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forcing from the trend are the main drivers of the decadal variability of the sink, and other predictors are believed to drive variabilities on inter-annual to sub decadal scales. After trial and error with different combinations of our five predictors, this combination yielded best skills of reconstruction. Moreover, a repeating seasonal cycle over the period of study is removed to acquire the deseasonalized time series to reduce the variability of the variables. This showed however, to only marginally increase the skills. Finally, the training was done once with CHL and once without CHL and the results were combined with priority given to the model with CHL. This step was taken to account for possible missing CHL data point as satellite imaging of surface chlorophyll concentrations is not possible in time and space grids where clouds block the surface ocean.

S1.2. Neural Network model

NN models establish non-linear relationships between the target variable and the predictors through the use of non-linear activation functions and interconnected networks of neurons. Here, the predictant is the annual mean ocean carbon flux anomaly relative to the 1990-2019 period coming from each of the six SeaFlux data products (Fay et al., 2021). The predictors are annual mean anomalies of SST, SSS, log(CHL), sfcWind square, xCO_2 over the same period of time. These predictors are sufficient to reproduce the variability on different time scales on each data product with very high skill (Fig. S2). The NN model used in this study is a modified and simplified version of the SOM-FFN model from (Landschützer et al., 2016). The network was designed using Python Tensorflow as a dense fully connected Keras model with one hidden layer with sigmoid activation and an output layer with linear activation function. The criteria for the number of hidden layer neurons is not only minimizing the root mean square error in a randomly generated evaluation sample from training data, but more importantly, not overfitting over the forecast period, i.e., consistency of the forecast with the expected near term future behaviour of the global flux based on the evolution of the atmospheric forcing. More concisely, we already have observational references over the historical period. What we want are models that are consistent with these observation based estimates over the historical period, yet, are not overfitting to the same period of training and are extendable to future time period for actual forecasts. This is the ultimate goal of decadal prediction systems. The number of neurons was set to 15 after trial and error with a variety of neuron numbers. Comparison with the linear model where a different combination for external forcing is utilized, serve as a validation tool for the products, and against what theory suggests.

Unlike the linear model, the training resolution of the NN model is not grid scale. Here, data points are grouped into ocean biomes as used in the version 2021 of MPI-SOM-FFN product (Landschützer et al., 2020) and training is done at each biome. These biomes are acquired by a self organizing map that divides the ocean into 16 regions based on statistical similarities in the seasonal cycles of SST, SSS, mixed layer depth and surface partial pressure of CO_2. The details of the SOM-FFN method can be found in (Landschützer et al., 2016). This choice was made because grid scale resolution does not provide enough data point for the complex NN model and would end up in large overfitting. On biome scale resolution, training with monthly timeseries was very costly in terms of computational resources. Hence, annual means were used. The output of the NN model is comparable with the simple linear model both over the 1990-2019 period and for forecasts (refer to the manuscript). Finally, the method is not limited to the choice of biomes. For instance, we used (Fay & McKinley, 2014) biomes and trained the network using MPI-SOM-FFN as the target (not shown here). The results showed similar skill of reconstruction on the global scale, while differences were more detectable on regional scales. Lastly, to avoid sharp changes over the edges of the biomes, a 3-by-3 lat-lon moving window spatial smoothing was applied to the NN outputs after biomes were combined (Landschützer et al., 2016).

S2. Preprocessing of CanESM5 predictors

Except for the atmospheric CO_2 concentrations that is the same xCO_2 as seen by CanESM, when making historical, assimilation, hindcast, and forecast simulations using the statistical models, ensemble means of CanESM5 predictors from the corresponding model runs where selected. These predictors were regridded into normal one-by-one degree resolution for compatibility. The CHL obsearvational data used for training (table S1), only extends back to 1998. To acquire estimates prior to this date (1982-1998), the time series are extended using the mean seasonal cycle of the observed period (Landschützer et al., 2016). To maintain consistency between the data that is used for training the statistical models and predictions using CanESM5 predictors, the same procedure is applied to CanESM5 CHL predictors.

Studies with ESMs have shown that initialized hindcasts simulations have biases and systematic errors when compared to the observations as a function of lead time (Kharin et al., 2012). Consequently, post processing bias correction is common practice for seasonal to decadal predictions. For each of the physical predictors and as a function of the lead time (number of years between the initialization year and prediction year), we perform a grid wise mean and trend adjustment to the corresponding observational data. The mean adjustment corrects for the mismatch between the mean over the period of the prediction at each grid cell with the mean of observations. Additionally, ESM hindcasts drift towards the preferred state of the model as represented in the historical simulation (Kharin et al., 2012). To counter this, trend adjustment based on the lead time is done to adjust for the systematic drifts of the predictors as a function of lead time. Please refer to (Kharin et al., 2012) for further details on the bias correction scheme. For CHL, only mean adjustment to the observation is applied as CHL does not exhibit a clear trend.

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Table S1. Observational products used for training

Variable	Source
Sea surface temperature	(Reynolds et al., 2002)
Sea surface salinity	*Hadley centre* EN4[a]
Surface Chlorophyll − a concentration	*GlobColour project*
Surface wind speed	*ERA5* [b]
Atmospheric CO_2 *concentrations*	*NOAA ESRL*

[a] (Good et al., 2013)

[b] (Copernicus Climate Change Service (C3S), 2017)

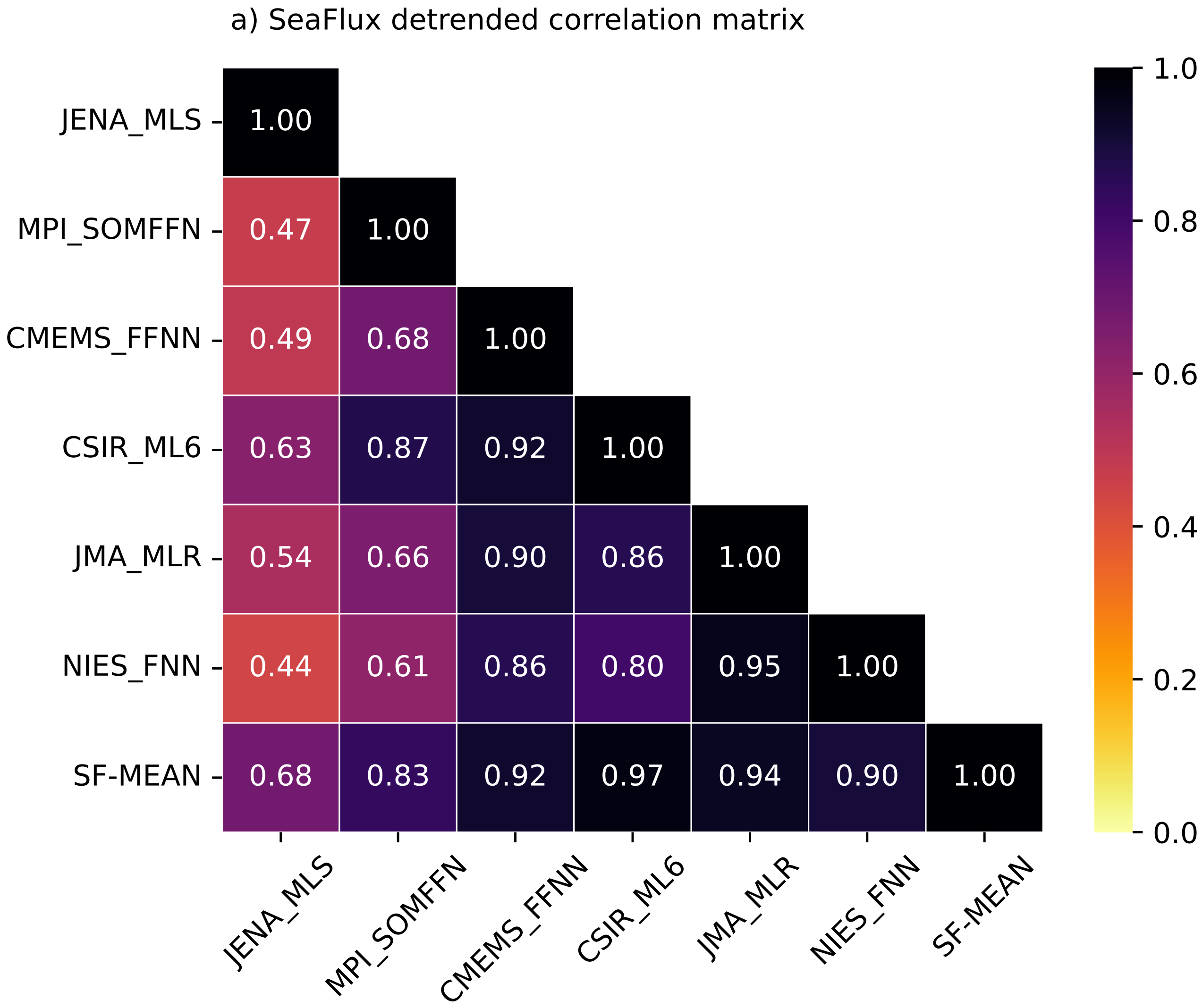

Figure S1. Cross-correlation matrix for detrended global SeaFlux observation-based ocean carbon flux products using ERA5 wind product.

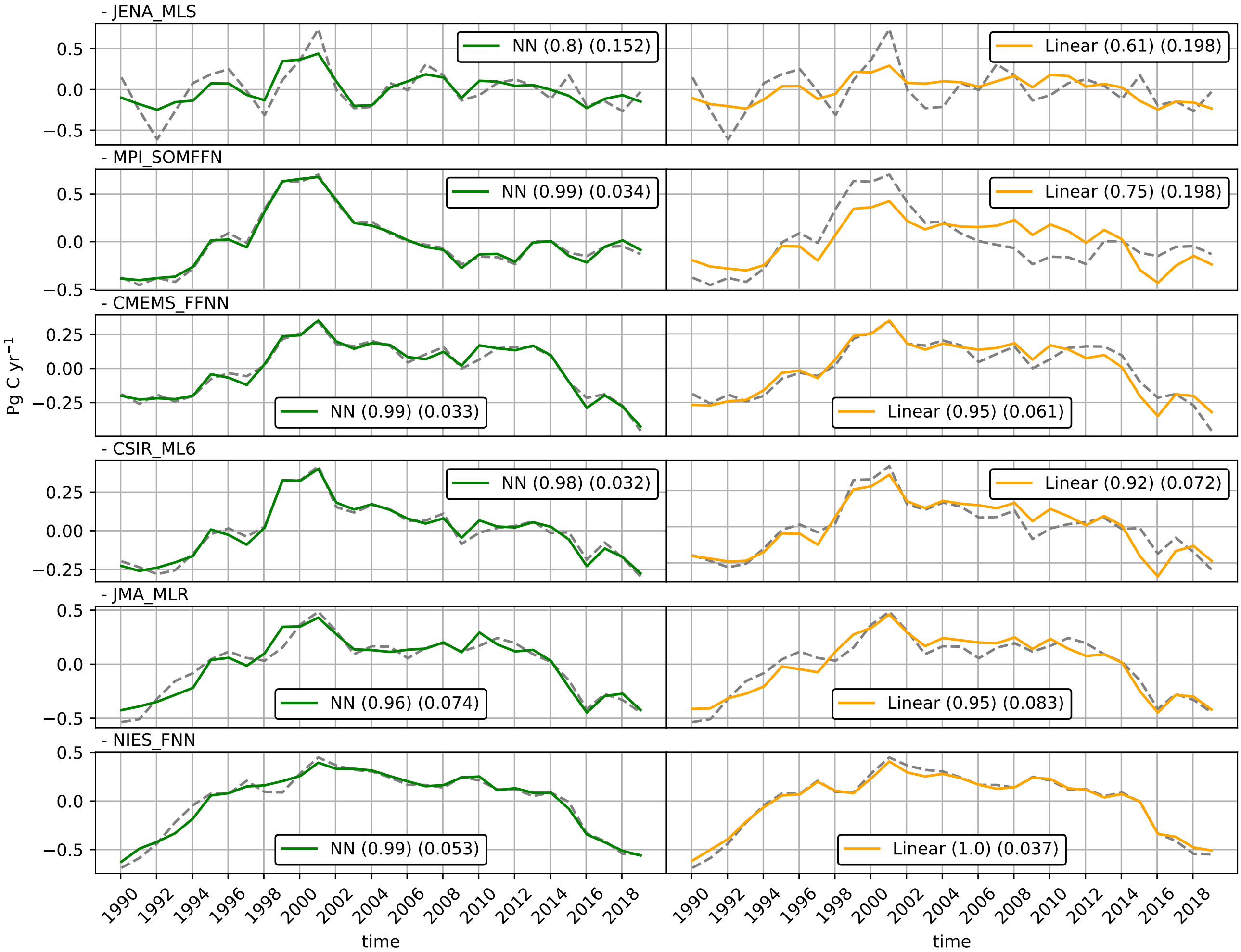

Figure S2. Time series of the detrended global ocean carbon flux reconstruction using observational predictors. Columns represent NN and linear models trained on individual products. Numbers in the legends are correlation (first number) skills versus the same product as used for training (dashed black lines), and root mean square error for the same time series (second number).

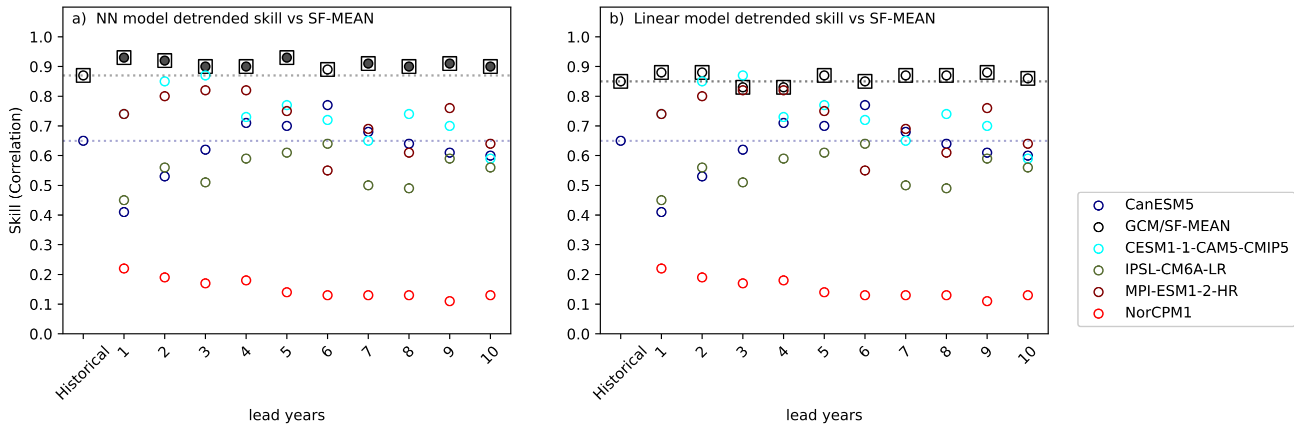

Figure S3. Detrended global ocean carbon flux skills based on bias corrected historical/hindcast predictors from CanESM5 (black dots) as well as raw CanESM5 scores (blue dots) for the hybrid model trained and evaluated using SF-MEAN. The scores that are statistically better than the raw CanESM5 score based on 1000 iteration bootstrap tests are shown with black boxes and the lead years where scores are significantly better than the historical score are filled. Colored dots are hidncast skills from ensemble means of all available CMIP6 models. The time period of this analysis is 1990-2017 as this is the common time period to all available CMIP6 models and our hybrid models.

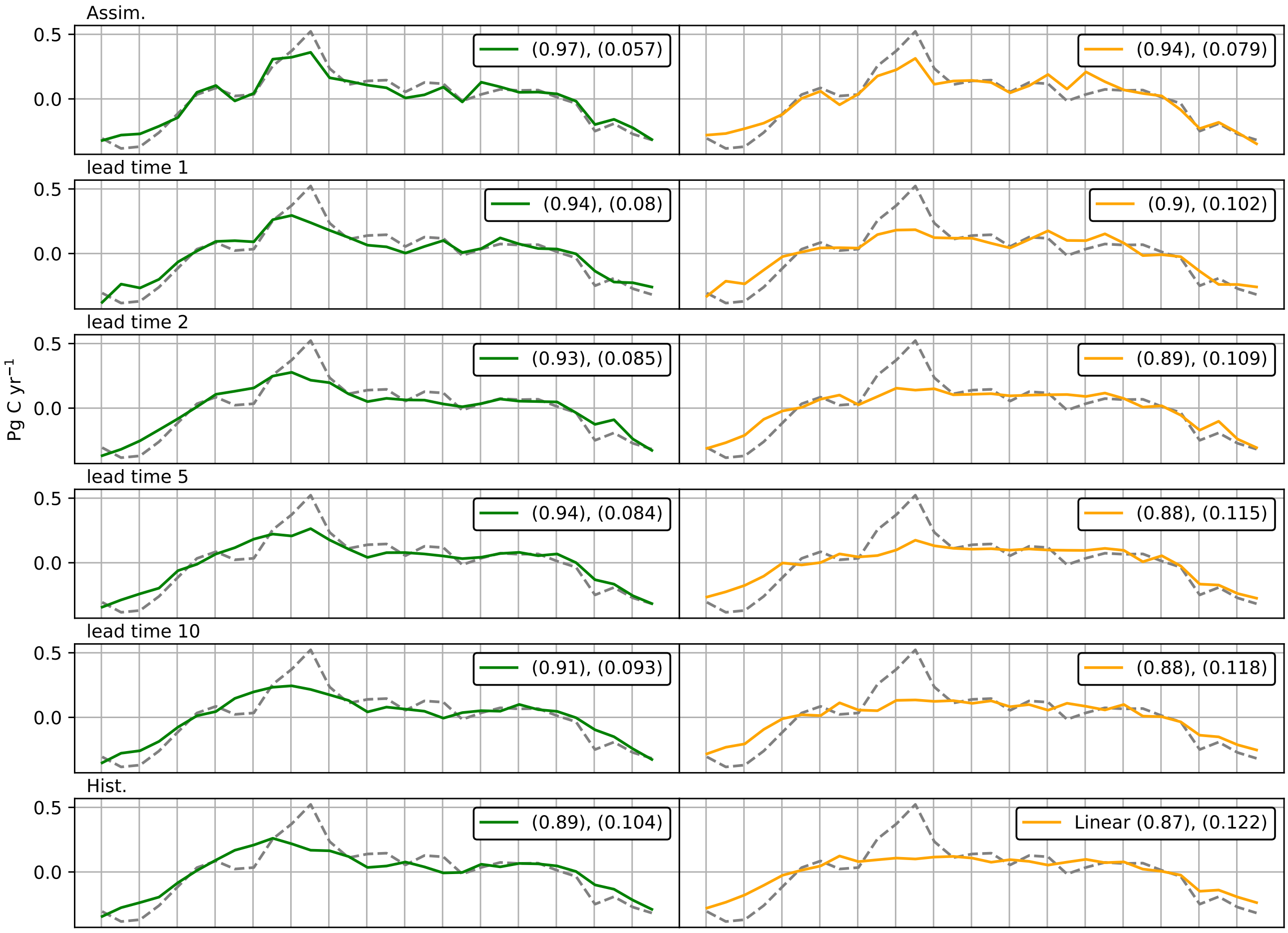

Figure S4. Detrended global ocean carbon flux time series for assimilation, hindcast years 1, 2, 5, 10, and historical simulations from NN (left column) and Linear (right column) models trained on SF-MEAN. The dashed line in the background is the detrended SF-MEAN and numbers in legends are correlation coefficients (first number) and root mean square error of the time series (second number). The plot shows how on longer lead times, the time series grow smoother and more similar to the historical time-series. They indicate less year to year variability, and are closer to the smooth decadal scale signal.

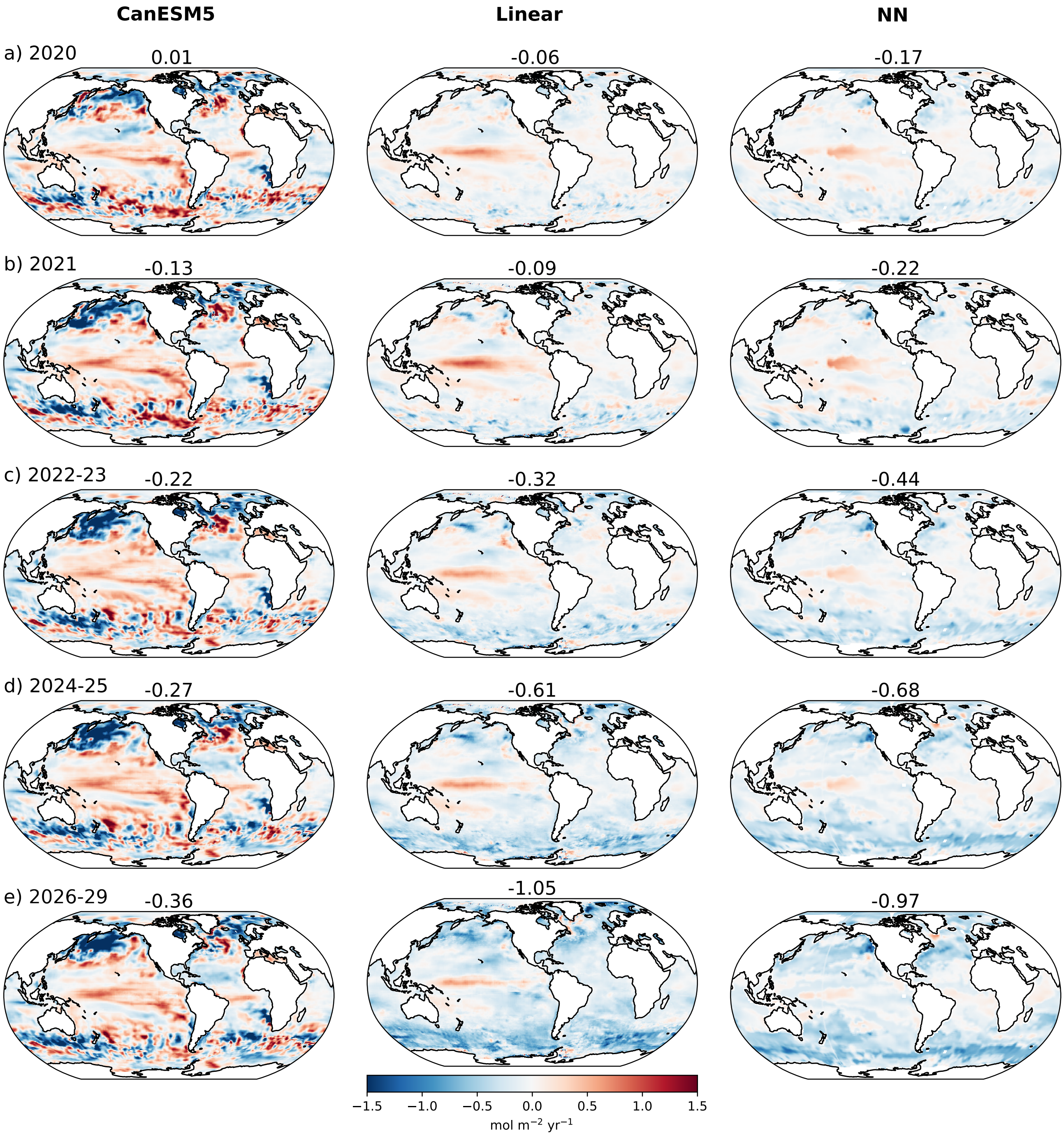

Figure S5. Regional patterns of forecasted changes in the ocean carbon flux for bias corrected CanESM5 (left column), hybrid NN model trained on SF-MEAN (middle column), and hybrid linear model trained on SF-MEAN (right column), relative to each product's 2019 projection. Numbers above each panel are global ocean carbon flux anomaly relative each product's 2019 in Pg C yr^{-1} over the same time periods of the maps.