Project:
GEOCARBON

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Operational Global Carbon Observing System

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1 Introduction

1.1 Short summary
Air-sea CO_2 fluxes for specific years with reasonable observational data coverage were carried out with 3 different Carbon Cycle Data Assimilation Systems (CCDASs) (CarbonTracker system, CMCC-PELAGOS system, MICOM-HAMOCC system). While CarbonTracker uses mainly a two-dimensional view, CMCC-PELAGOS and MICOM-HAMOCC are based on global three-dimensional biogeochemical ocean general circulation models (BOGCMs) for which data assimilation procedures have been applied to bring the modelled tracer distributions as close as possible to the respective measurements. Mainly the results are shown for the last decade or years thereof, depending on data availability. So far mainly sea surface pCO_2 data were used. The assimilation procedures result generally in an improved fit of the modelled pCO_2 field to the observations. Results for oceanic uptake still differ from model system to model system. Output data of the analysis are available upon request from the data originators.

1.2 Rationale for this deliverable
Importance: Employment of several CCDAS based on different state-of-the-art ocean models is crucial to properly quantify the uncertainties on global to regional carbon balances. Inter-comparisons of air-sea carbon fluxes from ocean models (Le Quéré et al. 2009; Roy et al., 2011; Arora et al., 2013), as well as from atmospheric inversion (Baker et al. 2006, Rödenbeck et al.,

2013) have revealed significantly different results. *Issue addressed:* So far, computation of seasonally and interannually changing air-sea CO_2 fluxes has been mostly carried out with forward models, that predict these fluxes and associated biogeochemical tracer distributions in the ocean. We aim here at systematically combine models with observations to achieve more realistic air-sea carbon fluxes than with less constrained models. *Fitting overall frame of project:* The tasks summarised here are synthesising the results from data collection/collation and modelling in combining them. The results would be the best so far achievable air-sea CO_2 flux for real years which are available at this stage. As it can well be assumed that net ocean-atmosphere fluxes (upward/downward) can be more accurately quantified, the results are also important for estimating the land-atmosphere fluxes as a residual from atmospheric observations and optimally reconstructed air-sea fluxes. This deliverable contributes to the following overall goals of GEOCARBON: (a) Develop improved Carbon Cycle Data Assimilation Systems (CCDAS). (b) Provide comprehensive and synthetic information on the annual sources and sinks of CO_2 for the globe and for large ocean and land regions.

1.3 Problems encountered and envisaged solution

The results were somewhat delayed due to some difficulties in synchronising the observed data streams and the technical set-ups for the CCDASs. Also some logistical problems due to lack of person power (people leaving partner institutions to accept permanent employment elsewhere) had to be solved. We could meanwhile overcome these difficulties by redistributing workloads ad hoc. Scientific difficulties/challenges are described – if applicable – in section 2.

2 Full description

2.1 Short introduction:

We describe below briefly the methodologies and main results for the different approaches to quantify annually varying air-sea carbon fluxes, and if possible also carbon stock changes, with different methodologies. First, a basically two-dimensional ocean approach using the CarbonTracker model is outlined. This model also includes a land biogeochemistry component, but no fully fledged ocean model. Two approaches based coupled three-dimensional physical-biogeochemical ocean general circulation models follow: The CMCC-PELAGOS model together with the adjoint data assimilation method (variational method), and the MICOM-HAMOCC model together with Ensemble Kalman Filter (EnkF, sequential method). The three methods together, provide a broad spectrum of approaches and hence also should provide a good overview on the current state-of-the-art in the field of marine carbon cycle data assimilation. This is a quite new field, and also yet imperfect studies should be welcomed as a means for paving the way towards further improvements.

2.2 The CarbonTracker approach:

Here the model *CarbonTracker Europe (CTE2013)* is employed. The CarbonTracker Data Assimilation System (CTDAS) estimates the global sources and sinks for CO_2 (Peters et al., 2010). It uses atmospheric observations of CO_2 to optimize prior estimates of the biospheric and oceanic fluxes, using a global atmospheric transport model TM5. CTDAS uses an ensemble Kalman filter scheme to estimate weekly scaling factors multiplying prior-model net carbon exchange over different land and ocean regions covering the globe. Flask and quasi-continuous CO_2 observations from ObsPack (version: obspack_CO_2_1_PROTOTYPE_v1.0.3_2013-01-29**,**) are assimilated to produce optimal surface flux estimates. A relatively short assimilation window of five weeks is used to determine adjustments to surface fluxes. Model-data mismatch errors assigned to observations range from 0.75 to 7.5 ppm. Atmospheric transport is simulated with the nested-grid TM5 model described in Krol et al. (2005), using winds from the European Centre for Medium-

Range Weather Forecasts. The horizontal resolution of the transport model is 3x2 degrees globally with 1x1 degree zoom regions over Europe and North America. CarbonTracker simulates four types of CO_2 exchange with the atmosphere. Fossil-fuel and biomass burning estimates are imposed without modification, and ocean and land exchange are subject to optimization.

For GEOCARBON we have performed 2 simulations with different setups (OD-CASA-GFED2-ecoregion and EI-SiBCASA-GFED4-gridded). The details described above hold for both versions. Furthermore the prior ocean fluxes were equal for both, they used the ocean inversion fluxes (OIF) by Jacobson et al. (2007). We optimize 30 ocean regions as defined by the OIF model. The other differences are included in Table 2.2.1 below. Global ocean fluxes are given in Fig 2.2.1.

Table 2.2.1:

	OD-CASA-GFED2-ecoregion	**EI-SiBCASA-GFED4-gridded**
Biosphere fluxes	CASA model	SiBCASA model
Fire emissions	GFED2 burned area	GFED4 burned area
Fossil fuel emissions	“Miller” product	“GEOCARBON” product
Meteorology	Operational data	Era interim reanalysis
Statevector	209 land ecoregions	Gridded Northern Hemisphere regions (9835 parameters)

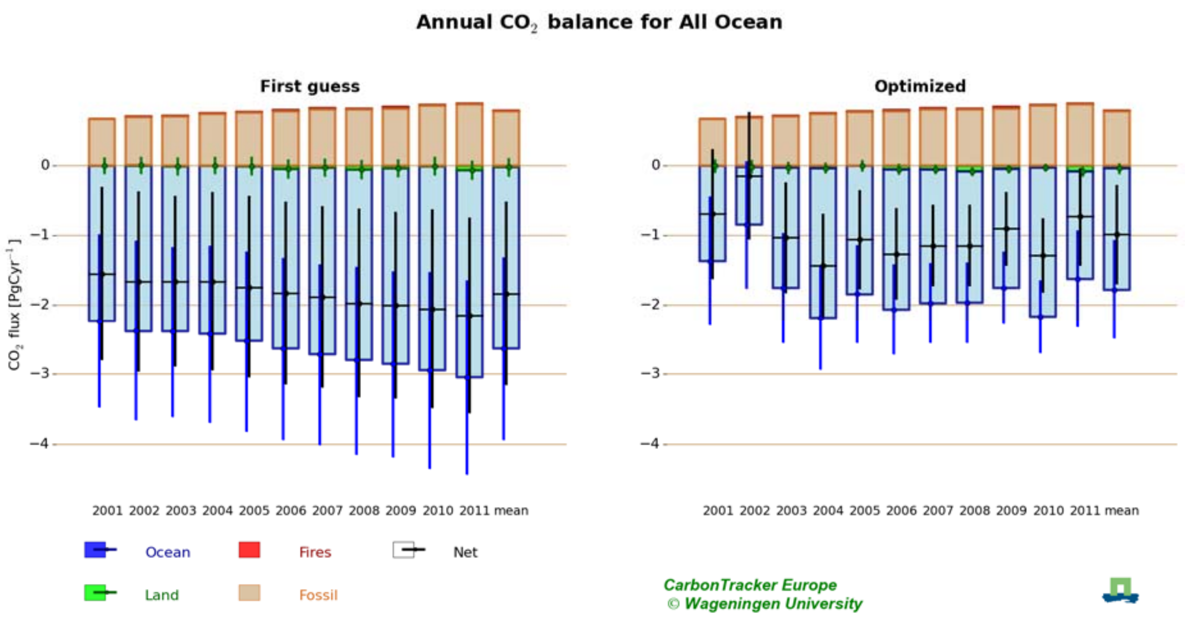

Figure 2.2.1: Global annual CO_2 carbon fluxes according to the CarbonTracker re-analysis (Source: https://carbontracker.eu).

2.3 The CMCC-PELAGOS approach:

For the CMCC-PELAGOS Ocean Carbon Data Assimilation System, a coupled physical-biogeochemical OGCM is used which is linked online to an ODAS for assimilating the physical components. At this stage, carbon components or other biogeochemical variables are not assimilated. However, the velocity field of the ocean is also one of the key parameters controlling the oceanic carbon cycle. Although the CCMC biogeochemical OGCM describes various chemical and biological cycles, for the purpose of this work the CCMC group mainly focused on the carbonate system variables.

The temperature and salinity reanalysis run (REAN) starts from the rest ocean on 01 January 1988, ending on 31 December 2010. This period is divided into an initial spin-up of five years, after which the analysis lasts from 01 January 1993 to the end of the run. In order to assess the impact of the data assimilation, we have produced a control run (CTRL), where no assimilation is included, starting from the same initial conditions.

The ocean model is forced with the atmospheric fields from ECMWF ERA-INTERIM reanalysis (Dee et al., 2011). The reanalysis data consist of 3-hourly forcing for wind velocity components, air temperature and humidity at two meters, together with the daily rates of snowfall, total precipitation, and incoming shortwave and long wave radiations.

The OGCM is the Nucleus for European Modelling of the Ocean (NEMO) 3.4, in the ORCA2 configuration (Madec and Imbar, 1996), coupled with the Louvain-La-Neuve sea-ice model (Fichefet et al., 1997). The number of ocean vertical levels is 30, 20 of which located in the top 500 meters. The river runoff input is a monthly climatology derived from the dataset of Dai and Trenberth (2002). Initial conditions for the temperature and salinity fields are derived from the Locarniniet al. (2010) data set, whereas the zonal and the meridional components of the velocity fields start from rest.

The ODAS for physical variables is the global implementation of a three-dimensional variational scheme [OceanVar] (Dobricic and Pinardi, 2008; Sorto et al., 2011). In the OceanVar scheme, the background error covariance of the model state is separated into a sequence of operators, accounting for the statistical estimation of the horizontal and vertical error covariances of temperature and salinity with bivariate corrections. Observational errors are derived from the profiles by Ingleby and Huddleston (2007) of instrumental errors, which are subsequently inflated to account for large representativeness errors in correspondence of areas of strong variability. The OceanVar system performs several data quality check, among which a check against the climatology and a check against background fields that rejects observations with a too large departure from the model fields.

The Biogeochemical Flux Model (BFM, Vichi et al., 2007a,b) describes the dynamics of major biogeochemical processes occurring in the marine systems. The model is based on a set of differential equations describing the interactions between the fluxes of various nutrients and specific biological functional groups.

The carbonate flux at the ocean surface is forced by using the atmospheric pCO_2 provided in the CMIP5 climate model intercomparison (http://cmip-pcmdi.llnl.gov/cmip5/). In the BFM, the net flux of CO_2 is proportional to the difference between the partial pressure of CO_2 at the sea surface and in the atmosphere, using the parameterisation of Wanninkhof (1992).

The time series for the global ocean carbon uptake fluxes are given in Figure 2.3.1.

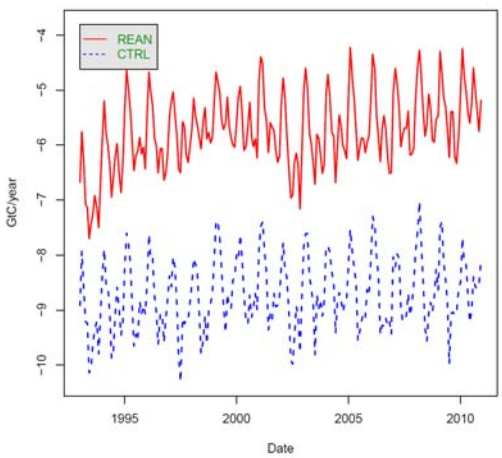

Figure 2.3.1: Global air-sea carbon flux with (REAN) and without (CTRL) data assimilation for the CMCC system.

2.4 The MICOM-HAMOCC approach:

This approach is based on the low-resolution (100x116 horizontal grid points, 32 vertical layers) version of MICOM-HAMOCC5 (Miami Isopycnic Coordinate Ocean Model and Hamburg Oceanic Carbon Cycle) model, which is the ocean component of the Norwegian Earth System Model (NorESM) (Aβmann et al., 2010; Tjiputra et al., 2013). The model was integrated offline into quasi-equilibrium, forced by the observed atmospheric forcing fields from the National Center for Environmental Prediction (NCEP) reanalysis product. The monthly atmospheric CO_2 concentration was taken from the Global Carbon Project (Le Quéré et al., 2013). For the observations, we employed the surface underway pCO_2 data collection from the Surface Ocean CO_2 Atlas (SOCAT, Pfeil et al., 2013). We use the monthly gridded monthly SOCAT product, and more specifically, the unweighted observations and their prescribed uncertainties. In Figure 2.4.1 the observational coverage is given along with the number of available monthly observations from the gridded SOCAT product. Most places have no observation at all and in most of the places where observations are present, one should expect the place to be observed only once per year, which raises issues for the temporal sampling of the annual cycle. The assimilation is carried out only in the biogeochemical component of the coupled model. Therefore, the physical dynamical fields are not corrected by the assimilation of pCO_2 observations. We choose as a first step two model parameters to be varied and which both yield reactions in the ocean model system and the respective pCO_2 simulation on short time scales (i.e., without requiring long-integration times): 1. The gas transfer velocity (physic-chemical parameter), 2. the nutrient uptake velocity of phytoplankton (biological parameter).
The data assimilation method used is a Gaussian anamorphosis extension of the deterministic ensemble Kalman filter (Simon and Bertino, 2012). This method is based on the deterministic ensemble Kalman filter (DEnKF, Sakov and Oke, 2008) and consists in introducing changes of variables, called Gaussian anamorphosis functions, in order to realize the analysis step with Gaussian distributed transformed variables (Bertino et al., 2003). This method has been demonstrated to be applicable in large systems (Simon and Bertino, 2009) and to efficiently estimate model parameters in nonlinear frameworks (Doron et al., 2011; Simon and Bertino, 2012).

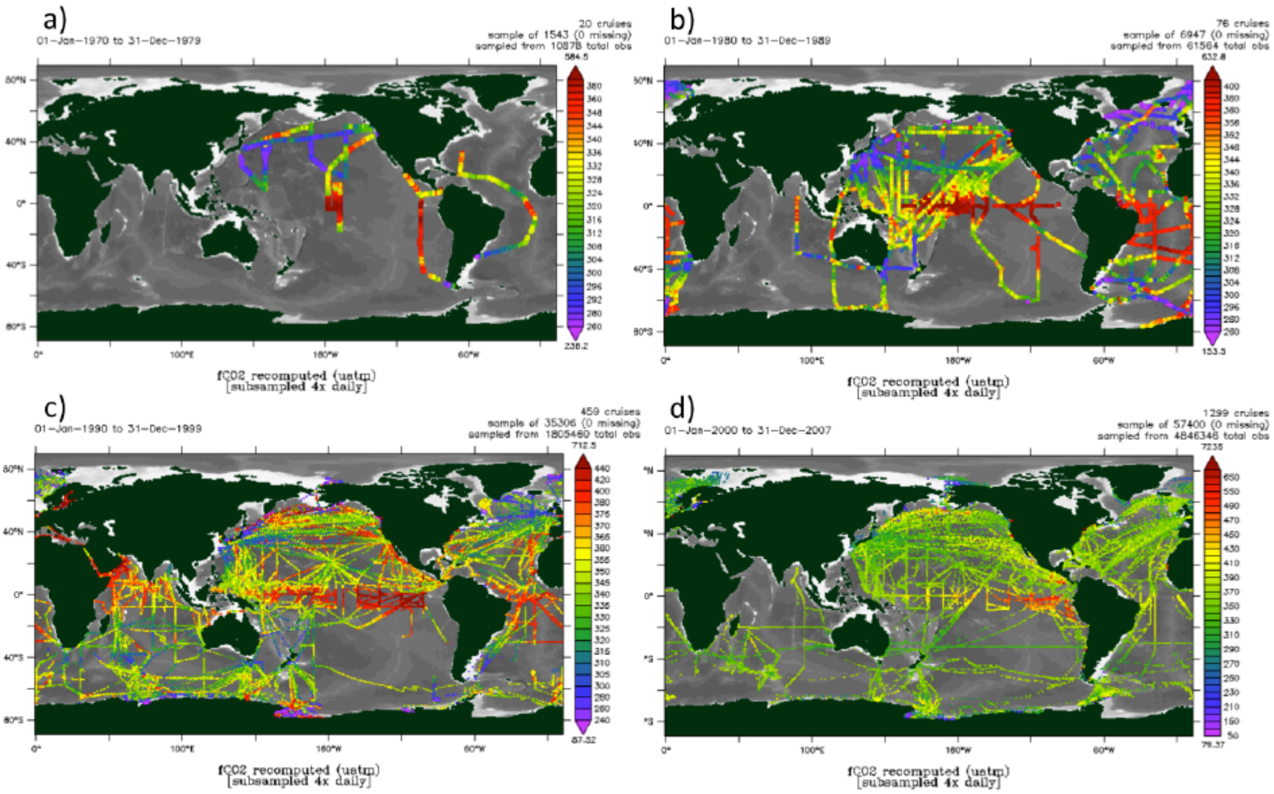

Figure 2.4.1: Data coverage for the sea surface pCO_2 data set SOCAT as used for the MICOM-HAMOCC data assimilation system (per decade: (a) 1970s, (b) 1980s, (c) 1990s and (d) 2000s) (Source: Pfeil et al., 2013, *Earth Syst. Sci. Data*, 5, 125–143).

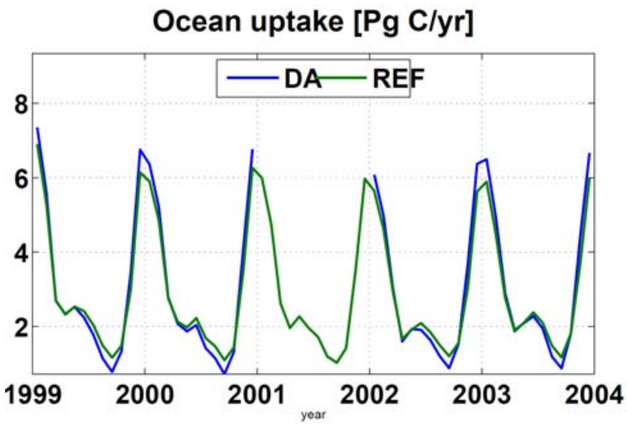

Figure 2.4.2: Global CO_2 air-sea fluxes into the ocean over the assimilation period (blue line is the run with data assimilation as compared to the control run marked in green).

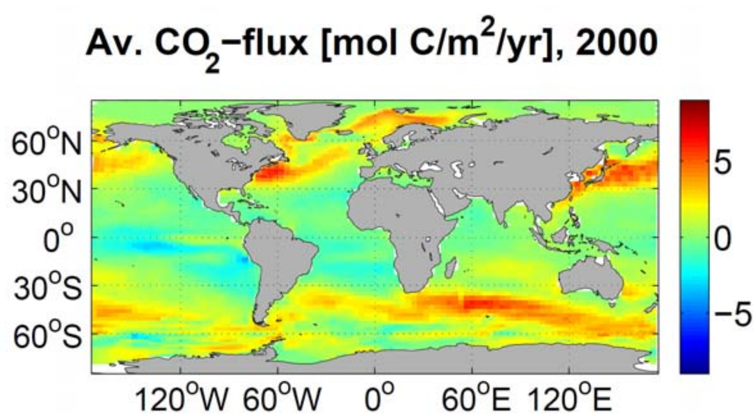

Figure 2.4.2: Global ocean-atmosphere fluxes of CO_2 for year 2000.

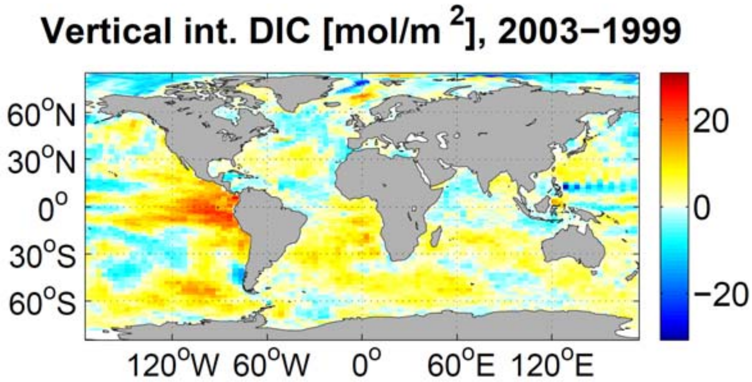

Figure 2.4.3: Additional carbon stocks which entered the ocean over the assimilation period (MICOM-HAMOCC).

The combined state parameter estimation is done by augmenting the state vector with the parameters to estimate (Evensen, 2009): the phytoplankton growth rate and the gas transfer velocity. We consider both parameters as 2D random variables with a Beta distribution (range [0.2 2.]). The ensemble is made of 96 members generated in January 1988 (drawing of the parameters). An ensemble simulation (no assimilation) is then run during 10 years in order the spin up the assimilation. The assimilation of the SOCAT data starts on 1 February 1998 and stops on 1 January 2004, both in twin experiments (synthetic observations) and with the real SOCAT data. In order to prevent too strong corrections during the first months, the observation error is multiplied by 8 on 1 February 1998, then by 4 on 1 July 1998, by 2 on 1 January 1999 and we use the SOCAT estimates from 1 July 1999. The localization radius is equal to 100 km, resulting in the assimilation of observations that belong to the grid point. Finally, there is no inflation and the parameters remain constant during the forecast step.
The global net CO_2 fluxes across the air-sea interface are given in Figure 2.4.2 and an example for a global net CO_2 air-sea flux map is shown in Figure 2.4.3. Finally in Figure 2.4.4, the change in carbon storage (carbon stocks) over the assimilation period is presented in order to illustrate where the additionally taken up carbon ends up within the ocean.

2.5 The OCVR model (LSCE)

A statistical model has been developed at LSCE and CLIMMOD (partly within the CARBONES project) to estimate the spatial and temporal variations of the ocean surface CO_2 partial pressure (pCO_2^{SW}), and from that the air-sea fluxes, using satellite, in-situ measurements and model outputs. The computation of pCO_2^{SW} is performed using an artificial neural network (Multi Layer Perceptron (MLP), Rosenblatt 1958) in a first step of the Ocean Carbon Variational

Reanalyzer (OCVR) system described briefly below and in more detail in an upcoming paper (Kane et al.).

The air-sea CO_2 fluxes can be defined from the following equation:

$$F_{CO2} = K_{ex} * (pCO_2^{SW} - pCO_2^{ATM}) \qquad \text{(X)}$$

where pCO2 is the partial pressure in the sea surface water (SW) and the atmosphere at the interface to the water (ATM) respectively, K_{ex} the exchange coefficient and F_{CO2} the CO_2 flux from the sea surface water to the atmosphere. pCO_2^{ATM} are taken from the surface pressure of the ERA-Interim reanalyses and corrected by the saturation vapour pressure at the water temperature.

K_{ex} is defined as the product of *k*, the gas transfer velocity, and *s*, the solubility of CO_2. In this study the Weiss formulation (Weiss, 1974) was chosen to estimate the solubility dependence on temperature and salinity. Many formulations of *k* are available in the scientific community (e.g. Liss and Merlivat, 1986; Wanninkhof, 1992; Nightingale et al., 2000, Takahashi et al., 2009). Typically they define *k* as a function of the wind speed at 10m above sea level (u) and of the water state (T, S). Here the Wanninkhof (1992) formulation is chosen

The pCO_2^{SW} is calculated using the artificial neural network (ANN) designed for the OCVR system, whose inputs are the variables that control the spatial and temporal evolution of pCO_2^{SW}: i) sea surface temperature (SST), ii) sea surface salinity (SSS), iii) mixed layer depth (MLD) and iv) chlorophyll content, as a proxy of the biogeochemistry (CHL).

The data used to train the ANN comprise 20685 "8-points vectors" composed of LAT, LON, MONTH, SST, SSS, MLD, CHL, pCO_2^{SW}. This database is further divided into two parts; 75% is used for the learning phase of the ANN, while the remaining data are used for the validation phase. The MLP network comprises elementary cells with non-linear transfer functions and a scaling coefficient, the weight of the cell. The number of cells (neurons) is 200 and the activation function is the hyperbolic tangent. The learning phase consists in the adjustment of all weights of the network in order to produce a non-linear multiple regression of the outputs (pCO_2^{SW}) against the explanatory variables (inputs), i.e:

$$pCO_2^{SW} = \text{MLP (LAT, LON, MONTH, SST, SSS, MLD, CHL)} \qquad \text{(X)}$$

The overall performance of the network is relatively good with a correlation coefficient between the estimated pCO_2^{SW} and the independent observations from the Takahashi database (Takahashi et al., 2009) of 0.80 (Kane et al., et al., in preparation).

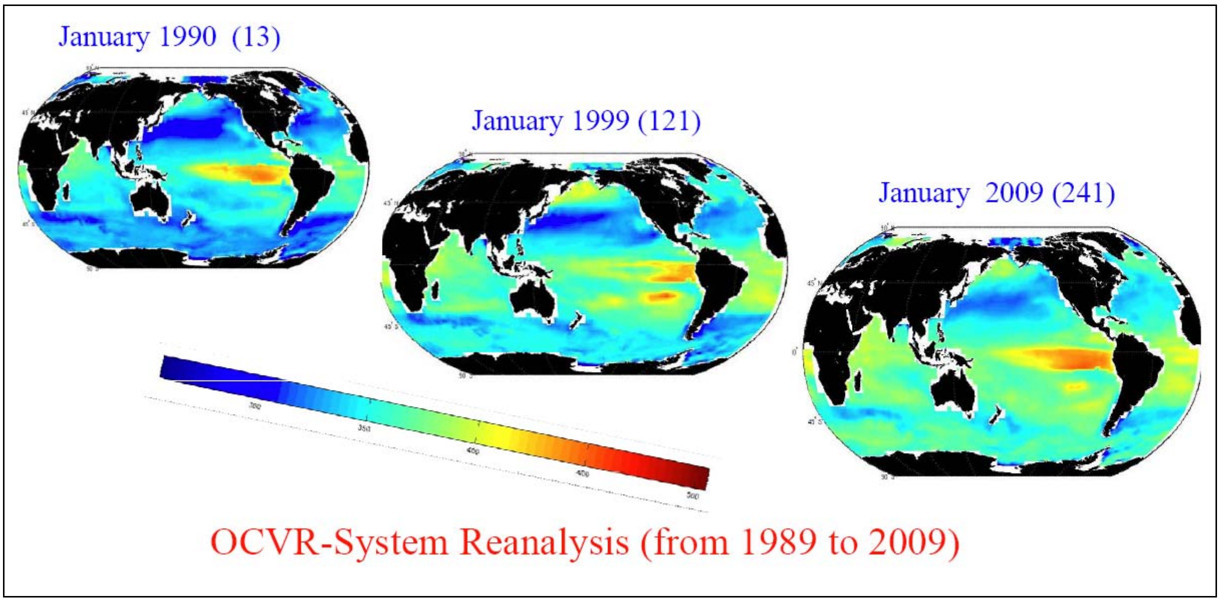

Figure 2.5.1: Global pCO2sw (in micro-atmosphere) maps from OCVR are shown and for simulations relevant for January 1990, 2000, and 2009.

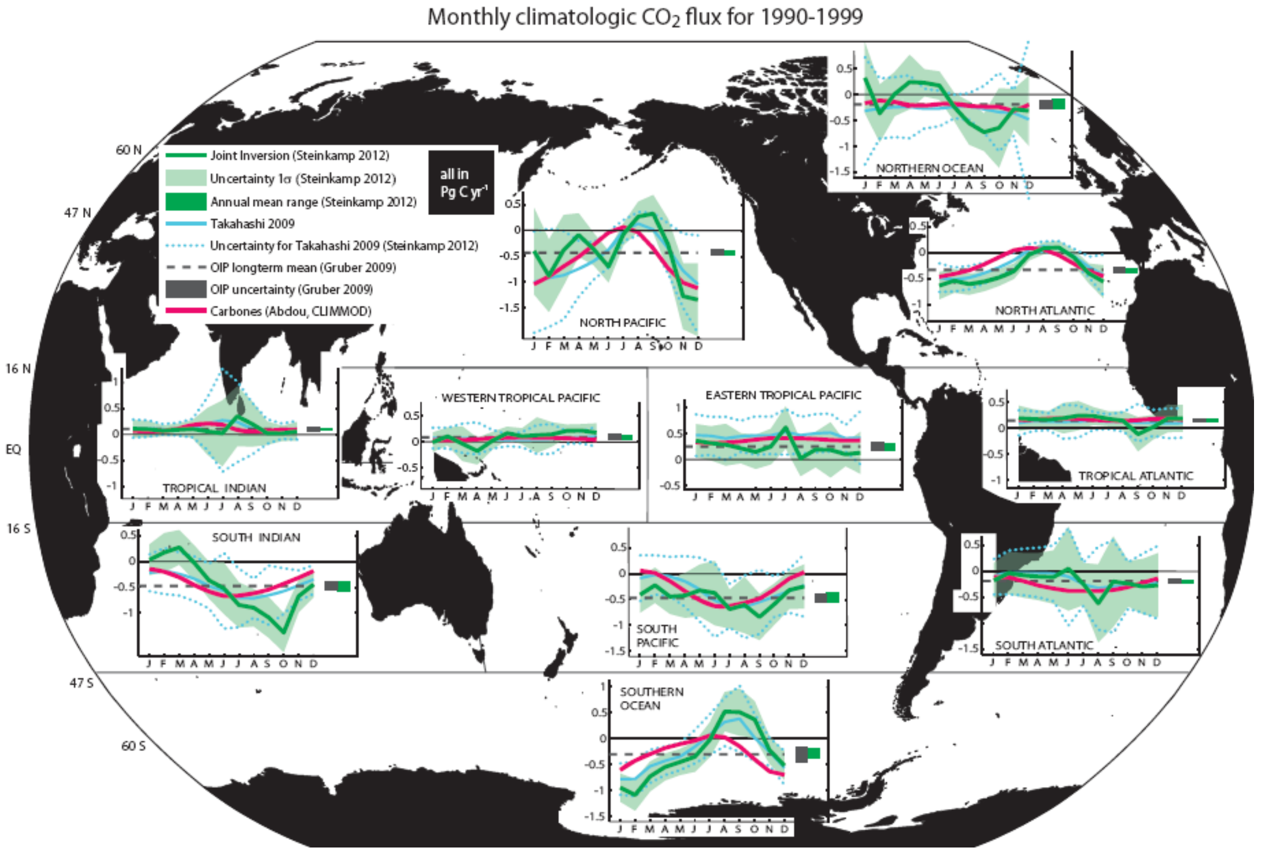

Figure 2.5.2: Mean seasonal air-sea flux estimates from OCVR for the period 1990-1999, for 11 regions, compared with independent estimates (see legend in the figure).

2.6 Synthetic appraisal:

In general, marine data assimilation to achieve an optimal interpolation of observations over time (best state estimate or re-analysis) in combination with a correction of model parameters for improving marine carbon cycle quantifications is still in its initial state. Progress could be made here using different approaches, namely (a) atmospheric inversion, (b) variational assimilation (physical fields, adjoint method), (c) and sequential assimilation (biogeochemical parameters/pCO_2, DEnkF). In general in all runs the fit of the simulated fields to the observations (sea surface pCO_2 data) could be improved. The assimilation procedures give different results as opposed to the respective uncorrected control runs. The differences in the temporally varying air-sea fluxes are smallest in the case of the MICOM-HAMOCC model. This may indicate that further parameters (including the ocean circulation) have to be changed in order to achieve larger changes. In the case of the CarbonTracker and CMCC-PELAGOS systems, the initially large fluxes in to the ocean have been corrected downward by the data assimilation period. The marine CO_2 uptake rates for the CMCC-PELAGOS model seem to be too high, which possibly can be attributed to a problem in the North Atlantic circulation field used in this particular set-up (it is interesting to see, that the data assimilation system tries to remove the deficiency which can be viewed on as a good result, especially when taking the difficulties in running adjoint models is taken into account). The CarbonTracker and MICOM-HAMOCC estimates for global oceanic net CO_2 uptake from the atmosphere are in about the same range.

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