MIT Joint Program on the Science and Policy of Global Change

Uncertainty in Atmospheric CO_2 Concentrations from a Parametric Uncertainty Analysis of a Global Ocean Carbon Cycle Model

Gary L. Holian

Report No. 39
October 1998

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To inform processes of policy development and implementation, climate change research needs to focus on improving the prediction of those variables that are most relevant to economic, social, and environmental effects. In turn, the greenhouse gas and atmospheric aerosol assumptions underlying climate analysis need to be related to the economic, technological, and political forces that drive emissions, and to the results of international agreements and mitigation. Further, assessments of possible societal and ecosystem impacts, and analysis of mitigation strategies, need to be based on realistic evaluation of the uncertainties of climate science.

This report is one of a series intended to communicate research results and improve public understanding of climate issues, thereby contributing to informed debate about the climate issue, the uncertainties, and the economic and social implications of policy alternatives.

Henry D. Jacoby and Ronald G. Prinn,
Program Co-Directors

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Submitted to the Department of Earth, Atmospheric, and Planetary Sciences
in partial fulfillment of the requirements for the degree of

MASTER of SCIENCE in ATMOSPHERIC SCIENCE

at the

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

September, 1998

Abstract

Key uncertainties in the global carbon cycle are reviewed and a simple model for the oceanic carbon sink is developed and described. This model for the solubility sink of excess atmospheric CO_2 has many enhancements over the more simple 0-D and 1-D box-diffusion models upon which it is based, including latitudinal extension of mixed-layer inorganic carbon chemistry, climate-dependent air-sea exchange rates, and mixing of dissolved inorganic carbon into the deep ocean that is parameterized by 2-D eddy diffusion. By calibrating the key parameters of this ocean carbon sink model to various “best guess” reference values, it produces an average oceanic carbon sink during the 1980s of 1.7 Pg yr^{-1}, consistent with the range estimated by the IPCC of 2.0 Pg yr^{-1} ± 0.8 Pg (1992; 1994; 1995). The range cited in the IPCC study and widely reported elsewhere is principally the product of the structural uncertainty implied by an amalgamation of the results of several ocean carbon sink models of varying degrees of complexity. This range does not take into account the parametric uncertainty in these models and does not address how this uncertainty will impact on future atmospheric CO_2 concentrations.

A sensitivity analysis of the parameter values used as inputs to the 2-D ocean carbon sink model developed for this study, however, shows that the oceanic carbon sink range of 1.2 to 2.8 Pg/yr for the 1980s is consistent with a broad range of parameter values. By applying the Probabilistic Collocation Method (Tatang, *et al.*, 1997) to this simple ocean carbon sink model, the uncertainty of the magnitude of the oceanic sink for carbon and hence atmospheric CO_2 concentrations is quantitatively examined. This uncertainty is found to be larger than that implied by the structural differences examined in the IPCC study alone with an average 1980s oceanic carbon sink estimated at 1.8 ± 1.3 Pg/yr (with 95% confidence). It is observed that the range of parameter values needed to balance the contemporary carbon cycle yield correspondingly large differences in future atmospheric CO_2 concentrations when driven by a prescribed anthropogenic CO_2 emissions scenario over the next century. For anthropogenic CO_2 emissions equivalent to the IS92a scenario of the IPCC (1992), the uncertainty is found to be 705 ppm ± 47 ppm (one standard deviation) in 2100. This range is solely due to uncertainty in the "solubility pump" sink mechanism in the ocean and is only one of the many large uncertainties left to explore in the global carbon cycle. Such uncertainties have implications for the predictability of atmospheric CO_2 levels, a necessity for gauging the impact of different rates of anthropogenic CO_2 emissions on climate for policy-making purposes. Since atmospheric CO_2 levels are one of the primary drivers of changes in radiative forcing this result impacts on the uncertainty in the degree of climate change that might be expected in the next century.

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TEPCO Professor of Atmospheric Chemistry

CONTENTS

LIST OF FIGURES AND TABLES

1. INTRODUCTION

Recent concerns about increasing anthropogenic emissions of greenhouse gases over the course of the last century have given impetus to studies of the global carbon cycle, focusing particularly on the existence and magnitude of natural sinks for atmospheric CO_2. This radiatively important gas, second only to water vapor in the atmosphere, has seen its mixing ratio increase from an average value of about 280 ppmv in pre-industrial times to nearly 360 ppmv today, as measured directly since 1957 (Keeling, *et al.* 1989) and as estimated by ice-core data prior to that (**Figure 1-1**). Future anthropogenic emissions of carbon, chiefly due to the combustion of fossil fuels, are predicted to double or even quadruple the concentration of CO_2 in the atmosphere over the next century, with potentially adverse consequences for regional and global climate. However, the ability to predict higher atmospheric CO_2 levels rests crucially on our ability to accurately model the natural carbon cycle and its response to anthropogenic emissions of CO_2 and perturbations of global climate.

Of the two primary surface sinks for atmospheric CO_2, the ocean has been widely studied for its potential to be the dominant sink of carbon owing to its large capacity to take up CO_2 through dissolution. Such studies have resulted in models of the oceanic carbon sink that vary in complexity from simple box models to complete global biogeochemical models that include full dynamical simulations of the ocean general circulation. As important as these models are as tools for understanding the behavior of the contemporary global carbon cycle, they are also widely used to forecast atmospheric CO_2 concentrations in the face of rising anthropogenic emissions of carbon in both climate change investigations and for policy-making purposes.

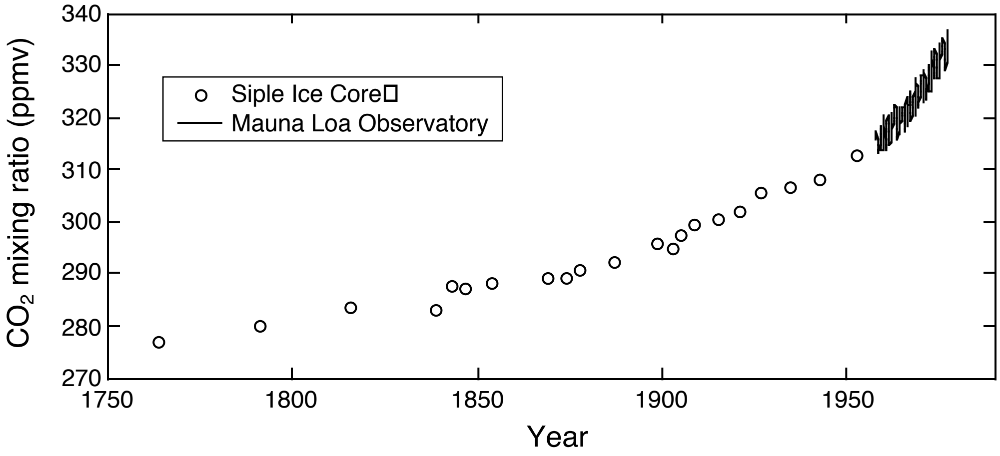


Figure 1-1 The Historical Atmospheric CO_2 Record

1.1 Thesis Statement

In order to assess the likelihood of various changes in global climate that may arise from increases in the concentration of atmospheric greenhouse gases such as CO_2 over the next century, it is necessary to be able to combine emissions forecasts for anthropogenically produced CO_2 with models of the surface sinks for carbon in order to compute a global carbon budget as a function of time. While the magnitude of anthropogenic emissions of CO_2 are fairly quantifiable or can at least be prescribed for emissions scenarios into the next century, the various processes which determine the magnitude of the natural sink for CO_2 in the two main reservoirs, the terrestrial biosphere and the oceans cannot since both sinks are themselves dependent on the atmospheric CO_2 concentration.

Uncertainties in the results of present models of these two natural carbon sinks are large, primarily since the currently estimated global values for these two sinks are difficult to observe directly. Parameters used in ocean carbon sink models are inevitably chosen to be in good agreement with "best guess" or "middle of the range" values of various independent observations, most notably isotopically measured gas transfer rates or tracer distributions in the ocean such as bomb-produced radiocarbon. The currently quoted uncertainty in the oceanic sink for atmospheric CO_2 is largely structural, primarily owing differences between independently constructed models of differing complexity that are driven with similar data and assumptions. However, the reasonableness of using of a global carbon cycle model that does a good job of representing current carbon budget in order to forecast future atmospheric CO_2 concentrations, rests on the certainty of the input parameters used to calibrate and run that model. Not much attention has been given in the literature to parametric uncertainty within ocean carbon sink models and the impact that uncertainty has on the ability to forecast atmospheric CO_2 concentrations with any confidence.

The purpose of this study, therefore, is to create a parameterized model of the oceanic sink for excess atmospheric carbon that can be used for forecasting future atmospheric CO_2 concentrations in climate change studies that also allows for a simultaneous examination of the parametric uncertainty inherent in calibrating it to agree with current observations. The 2-D Ocean Carbon Sink Model (OCSM) developed in this study determines the global sink for CO_2 in the ocean by a parameterization of the so-called "solubility pump," as described in IPCC (1994) to include:

1) Transfer of CO_2 gas across the air-sea interface.
2) Chemical interactions with dissolved inorganic carbon in the ocean.
3) Transport of additional dissolved carbon into the thermocline and deep waters by means of water mass transport and mixing processes.

This parameterized oceanic carbon sink model captures the essential mechanisms of the uptake of atmospheric CO_2 by the ocean through a limited set of easy to understand parameters. Since they have some measured or otherwise quantifiable uncertainty, it is possible to determine which are most important in contributing to the variance of the carbon sink and rank them accordingly. It is likewise possible to gauge the uncertainty in the desired output, namely the size of the oceanic sink for carbon and therefore the projected atmospheric concentration of CO_2. Instead of projecting a single concentration path for atmospheric CO_2 for a given anthropogenic emissions scenario based on "best guess" assumptions, it is possible to produce probability distributions for atmospheric CO_2 concentrations as a function of time due to the quantifiable uncertainties in the oceanic carbon sink. Such distributions of future atmospheric CO_2 concentrations can then be run through models of the global climate in order to propagate the CO_2 concentration uncertainty through key variables of climatic interest, such as global temperature, precipitation, and sea-level rise. These outputs, as the products of an uncertain input would consequently display a distribution that is broader than that demonstrated by uncertainty in emissions or the physical climate system alone.

1.2 Research Background

1.2.1 The Global Carbon Cycle

The global carbon cycle, on time scales of years to centuries, is composed primarily of three exchanging reservoirs: the atmosphere, the land biosphere, and the oceans. CO_2 is readily transferred between all three reservoirs through the atmosphere, such that for small perturbations in the system, a steady-state is restored through an exchange of excess carbon between these three sinks which is dominated by the buffering action of the oceans. Seasonal oscillations in atmospheric CO_2 concentration about this stable value are primarily the effect of the natural cycle of photosynthesis and respiration of land biota that is dominant in the Northern Hemisphere. In pre-industrial times, it is typically assumed that these three reservoirs were in steady-state, with fixed amounts of carbon partitioned between them and zero net annual exchange around a constant atmospheric concentration estimated to be about 280 ppmv (Fig. 1-1). However, the ice core record going back many thousands of years shows a large range of natural variability that is independent of anthropogenic perturbation (**Figure 1-2**), implying that natural mechanisms affect the steady-state concentration of CO_2 in the atmosphere in ways that are not yet completely understood. Over the last 200,000 years, atmospheric CO_2 levels appear to have been strongly correlated with surface temperature levels. The current atmospheric CO_2 concentration is without recent precedent: the concentration exceeds that of the last interglacial maximum, over 130,000 years ago. Future emissions of CO_2 are forecast to increase that concentration significantly beyond that maximum in the next few decades (IPCC, 1994; 1995).

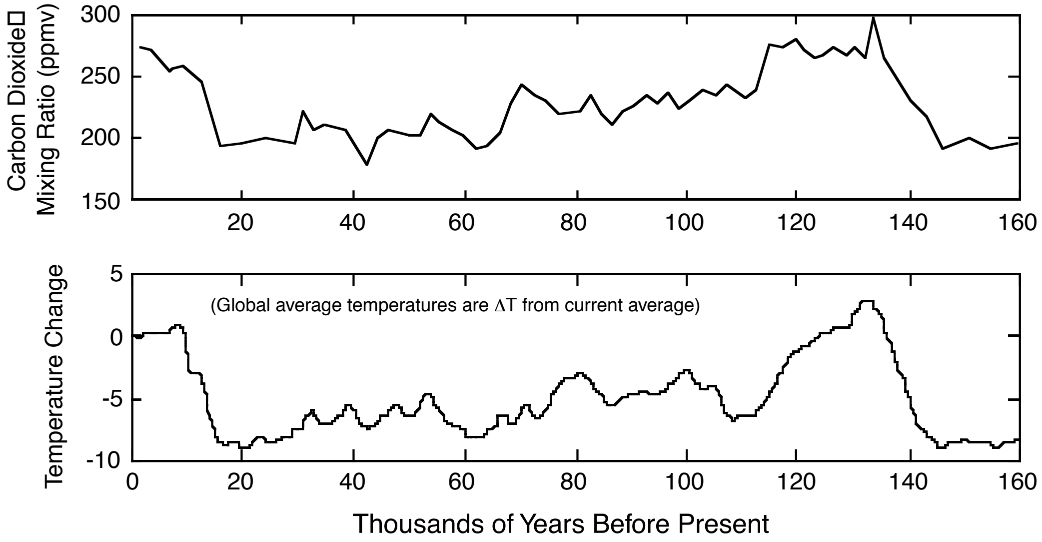


Figure 1-2 The Vostok Ice Core Record

Though atmospheric CO_2 levels have varied in the distant past, they have been remarkably stable for the last 10,000 years, with the often cited pre-industrial concentration of 280 ppmv being fairly representative (Fig. 1-2). While CO_2 levels can change quickly in terms of geologic time, there is little precedent for the approximately 0.4%/yr increase that is recently observed (Fig. 1-1). It is only within the last century, that a strong rising trend in atmospheric CO_2 (a current concentration that is 25% greater than the pre-industrial level) appears to have been superimposed on the natural carbon cycle. Despite such long-term observations, there are still large uncertainties in the strengths of the components that define the current global carbon budget, including the drivers of changes atmospheric CO_2 concentrations in the past.

1.2.2 Anthropogenic CO_2 Emissions

The recent increasing trend in atmospheric CO_2 is undoubtedly largely linked to the well documented emission of CO_2 from the surface by anthropogenic activity (Marland and Rotty, 1984). Average annual emissions of CO_2 during the 1980s amounted to 7.1 ± 1.1 petagrams (Pg, 10^{15} grams) of carbon with the majority, 5.5 ± 0.5 Pg/yr, coming from fossil fuel emissions. The remainder is due to deforestation, primarily from biomass burning, the extent of which is not as well documented and is the primary source of the uncertainty in emissions. The long-term trend of anthropogenic fossil fuel emissions have been calculated annually, summed up by country and fuel type, and are found to have grown at an average rate of 0.7%/yr over the last half century (**Figure 1-3**).

This rate of increase is much faster than the rate of increase of carbon in the atmosphere, implying the existence of large sinks for CO_2, either in the oceans or the land biosphere. During the 1980s, the annual rate of accumulation in the atmosphere amounted to only 3.2 petagrams of carbon per year (IPCC, 1994), implying a sink of nearly 4 Pg/yr. Only about 45% of the CO_2 released remains in the atmosphere and this represents the airborne fraction, while the rest is taken up elsewhere. Determining the location and mechanisms for these sinks has been the primary focus of much recent carbon cycle research, requiring an understanding of the behavior of the natural carbon cycle.

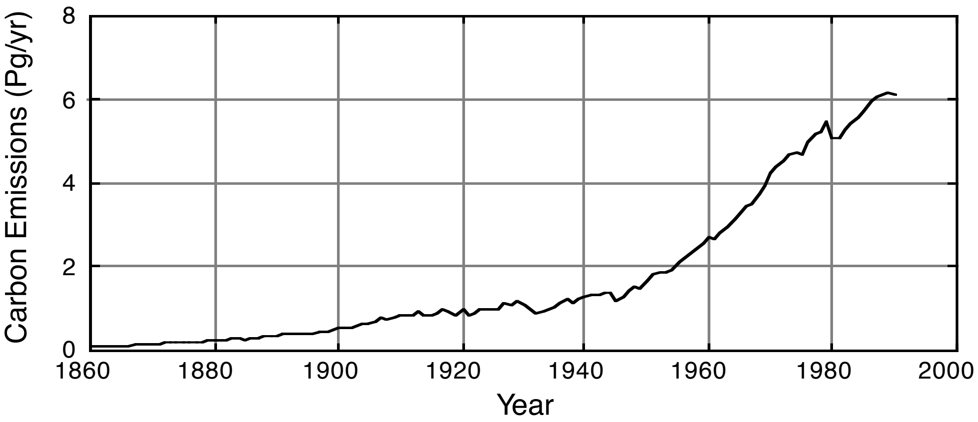


Figure 1-3 Historical Fossil Fuel Emissions of Carbon: 1860-1990 (in Pg/yr)

1.2.3 The Oceanic Carbon Sink

Because CO_2 is readily soluble in water and because the ocean is the largest rapidly exchanging reservoir of carbon, early research focused on its ability to take up the additional carbon. However, several different investigations have shown that the upper limit of the carbon uptake of the oceans during the 1980s to be between 2.0–3.0 Pg/yr of carbon, well short of the nearly 4.0 Pg/yr required to close the carbon budget. Half a dozen widely cited modeling efforts, most of which are validated by tracer studies of the rates of oceanic mixing, have calculated an average sink of about 2.0 Pg/yr with an uncertainty of about ± 0.8 Pg/yr (IPCC, 1994). In a careful analysis of atmospheric oxygen levels (Keeling and Shertz, 1992) which attempted to separate the impact of the ocean and land biosphere, an ocean sink was estimated at 3.0 ± 2.0 Pg. Another study, based on observed $^{13}C/^{12}C$ ratios in dissolved inorganic carbon in the ocean (Quay, *et al*., 1992), found a value of 2.1 ± 0.8 Pg/yr for the mean oceanic sink in the 1980s, in agreement with modeling efforts. On the low end of the spectrum, in an observational study of the spatial distributions of ΔpCO_2 across the ocean's surface, Tans, *et al*. (1990), found that the observed concentration differences between the atmosphere and ocean which drive the ocean uptake only supported a sink in the 1980s of order 1.0 Pg/yr (as high as 1.6 Pg/yr in a later correction). Their conclusion was that a large CO_2 sink must exist in the terrestrial biosphere. Most oceanographers concur that the oceans could not have taken up all of the missing carbon from the atmosphere.

The apparent inability of the oceans to take up all of the additional CO_2 required to close the contemporary carbon budget, is conjectured as indirect evidence of a significant sink in the terrestrial biosphere. One of the primary mechanisms proposed for the sink is the "CO_2 fertilization" effect, essentially an increase in photosynthesis by plants in response to rising atmospheric CO_2 concentrations. From the widely cited value of the oceanic sink during the 1980s of 2.0 Pg of C/yr, we estimate an average land sink of 2.0 Pg/yr. Inverse modeling of the latitudinal gradient of atmospheric CO_2 (Tans, *et al*., 1990), using a spatial distribution of oceanic sinks and land emissions suggests that a large land sink exists primarily in the Northern Hemisphere. From these studies, we have the widely disseminated picture of the current global carbon cycle acknowledged in many studies (**Figure 1-4**), in which roughly half of the CO_2 emitted to the atmosphere goes into the oceans and land, equally. Though up to half of the carbon may be disappearing into the land biosphere, part of this sink is being created by anthropogenic activity, changes in land use that are actively increasing carbon storage. Therefore, the truly natural component of the land sink is likely to be less than 2.0 Pg/yr. Since it is estimated to grow at a much lesser rate than the oceanic sink, the latter is considered to be the dominant sink for now and into the future.

1.2.4 Ocean Carbon Sink Models

As noted before, models of the oceanic carbon sink, range widely in complexity, they include the following:

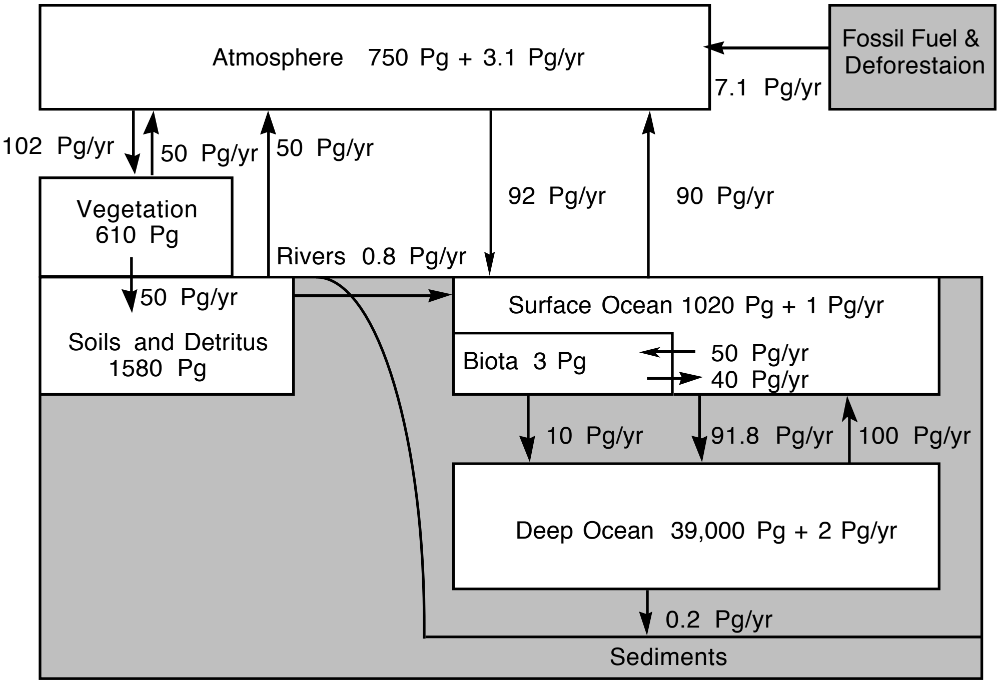


Figure 1-4 The Current Global Carbon Budget (Source: IPCC, 1995)

a) Revelle and Suess

One of the first models of anthropogenic carbon uptake was presented by Revelle and Suess in 1957. It consisted of three well-mixed reservoirs, an atmospheric box and two oceanic boxes. Exchange rates between the boxes were determined through calibration with radiocarbon measurements to determine an estimated exchange rate for anthropogenic carbon. This simple approach pointed towards a potentially important sink for anthropogenic carbon dioxide emissions and inaugurated the current research into quantifying how strong that sink might be. It identified the concept of the buffer factor for CO_2 exchange. Called the Revelle number, it is defined as:

$$R = \left. \frac{pCO_2 - pCO_{2,o}}{pCO_{2,o}} \middle/ \frac{DIC - DIC_o}{DIC_o} \right. \tag{1.1}$$

and it is a measure of the equilibrium capacity of oceans to take up carbon (through increases in dissolved inorganic carbon) from a increase in the atmospheric concentration of CO_2. Globally-averaged, the Revelle number of the current ocean is about 10. However, considering a reservoir a well-mixed box tends to be valid only when the internal mixing time of the box is short compared to the time scale of the process that is being modeled. In actuality, the ocean has lagged behind the rising levels of CO_2 in the atmosphere and an equilibrium cannot be assumed. The study excluded entirely the specific chemistry of oceanic inorganic carbon and the dynamics of oceanic mixing, in favor of capturing the equilibrium behavior of these exchanging reservoirs.

b) Simple and Complicated Box Models

Oeschger, *et al*. (1975), presented the first ocean carbon sink model to include time-dependent dynamics. The ocean was represented by a single oceanic mixed layer of 75m depth, connected to a well-mixed atmospheric layer above and deep ocean box below that simulated the mixing of carbon by a 1-D diffusion equation. The diffusion coefficient was assumed to be constant (in time and depth) and chosen to simulate the idealized profile of natural ^{14}C in the ocean. Air to sea transfer of carbon was calculated with a constant buffer factor, set to be the mean value observed for the current climate noted above. As a diagnostic, rather than prognostic model, the simple box-diffusion model was easily calibrated to achieve the desired result: large-scale agreement with tracer distributions and a large sink for anthropogenic CO_2 in the ocean.

The weaknesses of the 1-D box-diffusion model quickly became apparent and numerous researchers have attempted to improve upon the basic model by either increasing the number of boxes or improving the parameterizations that exchange carbon between the reservoirs in order to better capture the physics and chemistry of the processes involved. Improvements have included the addition of warm and cold surface boxes, advective terms, intermediate depth layers, multiple basins, the additions of realistic inorganic carbon chemistry, air-to-sea transfer rates, and biological cycles for organic carbon. The Outcrop-Diffusion model, for instance adds to a diffusive ocean, a pair vertically well-mixed regions at high latitudes to simulate deep convection from the rapid sinking of cold, dense water masses to great depth. The HILDA model (Shaffer and Sarmiento, 1992), adds to high-latitude exchange, advection in the ocean interior to better model the latitudinal differences between the exchange of water masses. Interestingly, this model is chosen as a reference by the IPCC for its sensitivity runs of atmospheric CO_2 concentrations.

c) Ocean General Circulation Models (OGCMs)

More recent attempts at oceanic carbon cycle modeling have employed general circulation models of the ocean’s dynamics that operate on a higher degree of geographical realism. Examples of such models include the Hamburg Ocean Carbon Cycle Model (Maier-Reimer, 1993), the GFDL Ocean GCM (Sarmiento, *et al*., 1992), and the LODYC OGCM (Orr, 1993). These models are based on the equations of motion of fluid dynamics and are developed to reproduce various scales of motion in the oceans as well as the observed distributions of temperature and salinity. Though these models still have trouble in resolving numerous high-resolution features, they capture large-scale behavior well enough to be considered a significant improvement over 1-D and 2-D models of the ocean circulation since they also allow for feedbacks from climate change to impact upon ocean circulation. They are considered superior for climate change simulations that seek to delve into uncertainty on longer time scales.

The ability of these models to reproduce the major features associated with the penetration of transient tracers into the ocean constitutes a significant validity test for the use of these OGCMs in simulating the oceanic uptake of carbon, since these models are not primarily tuned to do so, but rather to simulate the more frequently observed quantities such as temperature and salinity. Unfortunately, these models have not often been developed with the intention of simulating carbon uptake and therefore often suffer from simple parameterizations of carbonate chemistry, ocean biology, and other CO_2-specific processes, making a full treatment of the ocean's role in the carbon cycle difficult. Further, because of the computational costs of running even a limited number of simulations of such complex models and the difficulty of isolating a small number of parameters useful for capturing the full range of behavior of the model, it is difficult to analyze the parametric uncertainty of such models.

1.3 Thesis Outline

In the balance of this paper is a detailed description of the oceanic carbon sink model developed for this investigation, a discussion of the uncertainty methods applied to study its behavior, and the conclusions that might be drawn from the results. This thesis is organized into six sections:

The ocean carbon sink model is described in Section 2. It is a 2-D model of the inorganic carbon cycle in the ocean and incorporates the principle mechanisms of carbon sequestration that characterize the "solubility pump" in the ocean. It is calibrated with various "best guess" values for its reference parameters, driven by the historical CO_2 record, and is shown to determine a contemporary carbon sink well within the range of other ocean carbon sink models.

In Section 3, the 2-D OCSM is used for integrated global carbon cycle simulations where the atmospheric CO_2 concentration is endogenously determined by the oceanic carbon sink of the model. An emissions scenario for fossil fuel emissions is combined with an assumption for deforestation and a parameterization of the results of a terrestrial ecosystem model (TEM) in order to forecast atmospheric CO_2 concentrations to 2100. Sensitivity runs are then performed, where individual parameters of the model are varied to demonstrate the impact of changes in the input parameters on the oceanic carbon sink.

In Section 4 is a general discussion of uncertainty in models, both parametric and structural uncertainty. This is followed by a description of the Monte Carlo method for addressing parametric uncertainty in models and an explanation for why it is generally unfeasible for climate studies. A description of the Probabilistic Collocation Method (PCM) is then presented along with a justification for its use in lieu of other methods in this study.

The PCM is applied to the 2-D OCSM model in this study in Section 5. Key uncertain parameters in the model are chosen in order to be run through the uncertainty procedure presented in Section 4.4. Probability distributions are chosen for the uncertain inputs and the resultant uncertainty (mean values and variances) in the two main outputs: the oceanic carbon sink and the atmospheric CO_2 concentration, are determined as a function of time. The relative contribution of each uncertain parameter to the total variance in the outputs is examined. The accuracy of the collocation method is then investigated and alternative input distributions for the parameters are tested and compared to the initial results.

Section 6 summarizes the primary accomplishments of this thesis and the consequences of uncertainty in the global carbon cycle for current climate research and policy-making. Future work that is a natural outgrowth of this study is also addressed.

2. 2-D OCEAN CARBON SINK MODEL

2.1 Model Description

2.1.1 Structure

The 2-D ocean carbon sink model designed for this study, operates on the same horizontal grid scale as the MIT Joint Program on the Science and Policy of Climate Change's 2-D Climate-Chemistry model (Wang, Prinn, and Sokolov, 1998; Sokolov and Stone, 1997; Prinn, *et al.*, 1998), duplicating that model's simplified oceanic structure. The 2-D OCSM is therefore a multiple box-diffusion model, composed of a surface ocean mixed-layer of varying depth with latitude underlying a zonally-averaged atmospheric boundary layer. Mixed layer depths are kept constant, equivalent to annual average values, as shown in **Figure 2-1**.

The mixed layer is attached to an eddy-diffusive deep ocean in 10 vertical layers of increasing depth. The model extends meridionally over 24 latitude zones that are centered 7.826 degrees apart. It has may similarities to other box-diffusion models (Oeschger, *et al.*, 1975; Siegenthaler and Joos, 1991) and zonal models of the ocean (Stocker, *et al.*, 1994) upon which it based.

Each latitude zone in the model is divided into a land and sea fraction, preserving the real world distribution of oceanic surface area as a function of latitude (shown in **Figure 2-2**), but treating all

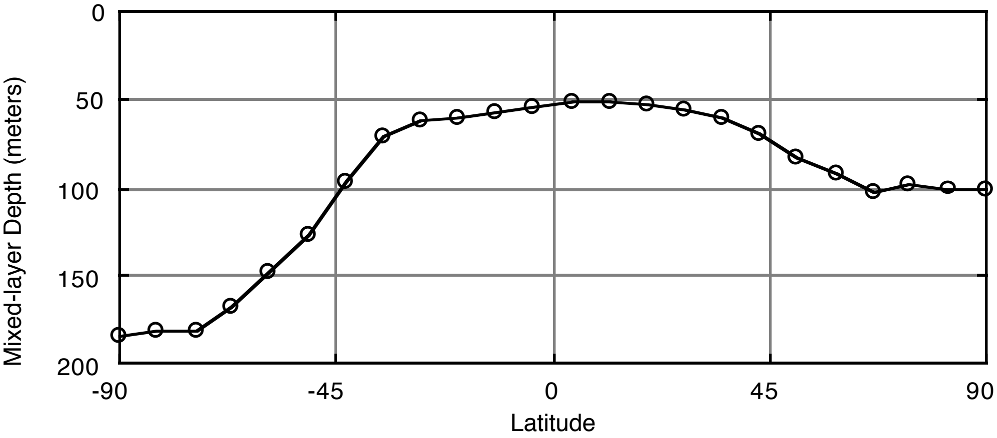


Figure 2-1 Mixed-layer Depth as a Function of Latitude in the 2-D OCSM

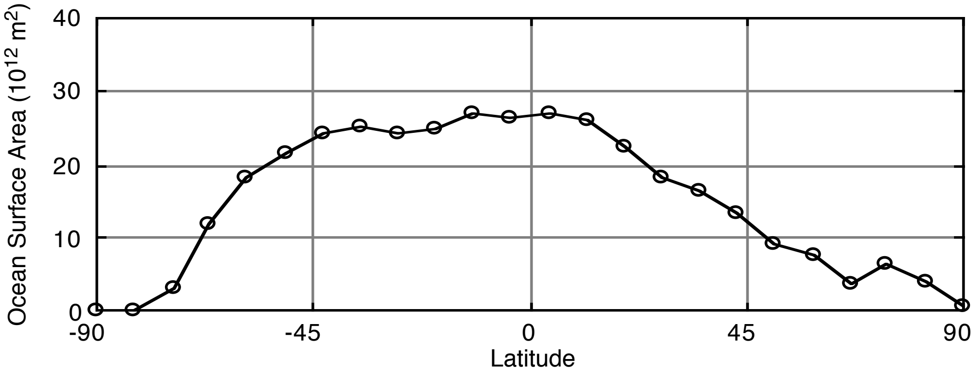


Figure 2-2 Average Ocean Surface Area as a Function of Latitude in the 2-D OCSM

basins in the same latitude zone similarly (*i.e.* as a zonal average). Open ocean, for the purposes of air-to-sea transfer of gaseous CO_2 in each latitude, is the total open ocean area minus the amount covered in sea-ice.

The first of the interactive feature of the model, it is dependent on the seasonality of sea-ice coverage, though such changes are not typically large enough to greatly impact on global CO_2 exchange. Note that the two southernmost latitude zones contain no open ocean and are composed perpetually of land, the Antarctic continent, while the northernmost zone is covered perpetually in ice. Bottom ocean topography is not considered and depth is assumed to extend to a constant 3750 meters, the approximate average depth of the world's oceans. The model is designed to be run either interactively with the 2-D Climate Model of Wang, Prinn, and Sokolov (1998), or as a standalone, taking its various inputs exogenously. The basic 2-D structure of the model is depicted in **Figure 2-3**.

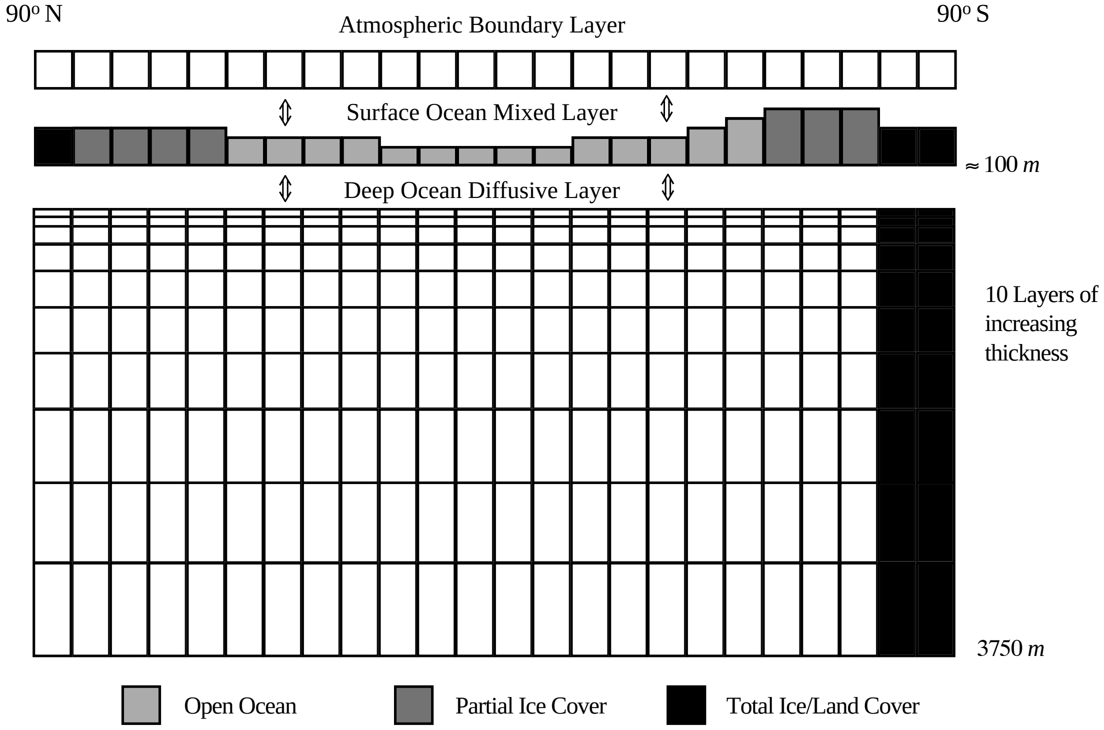


Figure 2-3 Structure of the 2-D OCSM

2.1.2 Air-to-Sea Flux

In the 2-D OCSM, the calculated air-to-sea flux of carbon is proportional to the CO_2 concentration gradient between the atmosphere and the oceanic surface layer for each of the 24 surface zones, multiplied by a calculated piston (*i.e.* transfer) velocity:

$$\mathrm{CO_2\,Flux} = V_p\left(pCO_2^{air} - pCO_2^{sea}\right) \tag{2.1}$$

The partial pressure of CO_2 in the atmosphere is supplied exogenously, either from the mean atmospheric CO_2 concentration under the reasonable assumption of a well-mixed atmosphere or is calculated by models of atmospheric chemistry and transport as the lowest layer of the model over the ocean, after anthropogenic input, previous biospheric and oceanic sinks, and the effects of atmospheric transport have been applied. In the surface ocean, the Henry's Law relation allows for the conversion from concentration of CO_2 in the mixed layer (as calculated in the chemistry Section below) to a partial pressure:

$$\left[\mathrm{CO}_2\right]^{\mathrm{sea}} = a_{sol}\ pCO_2^{sea} \tag{2.2}$$

where a_{sol} is the coefficient of solubility of CO_2 gas in seawater at the temperature, alkalinity, and salinity of the oceanic surface layer, the so-called "Henry's coefficient." a_{sol} is variable as a of latitude and time, primarily because of its strong dependence on temperature.

The greater the concentration gradient between air and sea (defined positive into the ocean), the greater the CO_2 flux into the ocean at any given latitude, attenuated by the variable transfer velocity. A negative gradient indicates a source of CO_2 in the ocean in that latitude zone, and the flux is added to the carbon budget of the atmospheric boundary layer as though it were any other source of CO_2. The piston velocity, to which the carbon flux is directly proportional, is calculated as a function of the magnitude of the external surface wind speed at each latitude (as shown in **Figure 2-4**), which is independent of the air-to-sea CO_2 gradient.

For this model, it was decided to use as a reference, the results of a study by Liss and Merlivat (1986) which empirically measured the rate of CO_2 entering the water as a function of increasing wind speed, primarily through laboratory experiments in wind tunnels. It was found that as the wind speed increases, the onset of turbulence, breaking waves, *etc.*, increased the dependence of the transfer rate on the wind speed, splitting into roughly three regimes (see Fig. 2-2). This, combined with surface air CO_2 concentrations, represents the second dynamic input into the model. Climate models output surface wind speed as a function of latitude, longitude, and time which allows for the direct calculation of the piston velocity and therefore the magnitude of the sink (or source) of CO_2 at that latitude zone.

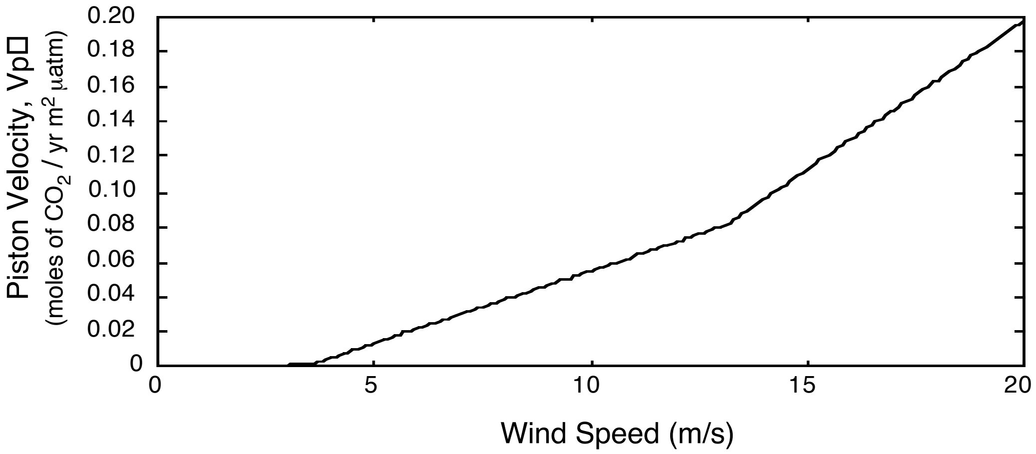


Figure 2-4 Dependence of the Piston Velocity on Wind Speed

2.1.3 Inorganic Mixed-layer Carbonate Chemistry

The buffering capacity of the mixed-layer of the ocean, *i.e*. its ability to uptake gaseous CO_2, is a direct consequence of aquatic carbon chemistry. Invading gaseous CO_2 must enter into a chemical equilibrium with dissolved carbonate and bicarbonate ions in the surface ocean, which is dependent on temperature, alkalinity, and the concentrations of boric, silicic, phosphoric and other acids. Together, total dissolved inorganic carbon in the ocean is defined as the sum of the concentrations of these three carbon species:

$$DIC = \left[CO_2^{\ *}\right] + \left[HCO_3^-\right] + \left[CO_3^{2-}\right] \tag{2.3}$$

Less than 1% of total DIC in the oceans (averaging about 2.05 mol/m^3) is actually dissolved CO_2 gas. Over 89% is present as HCO_3^- and 10% as CO_3^{2-} and while total DIC is preserved for changes in temperature and pressure, the relative proportions of these three species is not, affecting the concentration of dissolved CO_2, and therefore the partial pressure of CO_2 in the mixed layer through Henry's Law (Eq. 2.2). Carbonate and bicarbonate therefore play a direct role in determining the size of the concentration gradient between the atmosphere and sea: this is the buffering capacity of the ocean captured in equilibrium, by the Revelle number (Eq. 1.1). The temperature dependence of these reactions is primarily responsible for the natural seasonal cycle and distribution of pCO_2 in the surface ocean. In the 2-D OCSM, this translates into a latitudinal gradient in the surface partial pressure of CO_2 and a flux that will consequently depend on latitude.

Determination of the magnitude of the partial pressure of CO_2 in the mixed layer is paramount for gauging the sign and the magnitude of the air-sea flux of CO_2 in the ocean carbon sink model. These acid-base reactions have the effect of allowing more CO_2 to enter the mixed-layer than would be possible by simple dissolution alone. The specific formulation of the carbon system used in the 2-D OCSM is based primarily on that of Peng, *et al.* (1987), and other similar inorganic carbon chemistry models, which include the effects of temperature, dilute acids and tritation alkalinity on carbonate chemistry. The fundamental chemical equations governing the interaction of gaseous CO_2 from the atmosphere and the carbon species of the ocean are:

$$\begin{gathered} CO_2(g) + H_2O \Leftrightarrow CO_2(aq) \\ CO_2(aq) + H_2O \Leftrightarrow H_2CO_3 \\ H_2CO_3 \Leftrightarrow H^+ + HCO_3^- \\ HCO_3^- \Leftrightarrow H^+ + CO_3^{2-} \end{gathered} \tag{2.4}$$

Since in practice, it is very difficult to distinguish between the species CO_2(aq) and H_2CO_3, the sum of these two species is expressed as the combined pseudo-species, $CO_2^{\ *}$(aq).

In equilibrium, the concentrations of these species must obey the following relations that are obtained from the resultant three equations that define the inorganic oceanic carbon system:

$$
\begin{aligned}
K_0 &= \alpha_{sol} = \frac{[CO_2^*(aq)]}{pCO_2^{sea}} \\
K_1 &= \frac{[H^+][HCO_3^-]}{[CO_2^*(aq)]} \\
K_2 &= \frac{[H^+][CO_3^{2-}]}{[HCO_3^-]}
\end{aligned}
\tag{2.5}
$$

where the reaction rates K_1 and K_2 are the first and second apparent dissociation constants for each of the last two reactions involving carbonic acid. Note that the coefficient of the first reaction is simply the Henry's Law coefficient from above. The values are all strongly dependent on the temperature, alkalinity, and salinity of the ocean and have been studied empirically (Weiss, 1974; Mehrbach, *et al*., 1973). Reference for the constants follow the inorganic carbon chemistry described in Peng, *et al*. (1987), and include temperature and salinity dependence for K_1 and K_2. Their values are therefore a function of time and latitude in the model because of their dependence on temperature. Lower temperatures favor a higher concentration of dissolved inorganic carbon (DIC) for a given partial pressure of CO_2 in equilibrium with the atmosphere. Note that the concentrations are also dependent on the concentration of the hydrogen ion, $\left[H^+\right]$, namely the $\mathrm{pH} = (-\log_{10}[H^+])$ of the water. In turn, the pH is dependent on the alkalinity of the ocean which is a function of the concentrations of carbonate, bicarbonate, borate, silicate, and phosphorus ions, yielding non-linearity, since some of the constituents of DIC, indirectly serve to determine the partitioning of DIC. To solve these equations, we need a statement of charge balance, where equivalent acidity per unit volume is balanced by the sum of the major acids:

$$Alk_T = Alk_{water} + Alk_{carbonate} + Alk_{borate} + Alk_{silicate} + Alk_{phosphate} \tag{2.6}$$

where:

Alk_T = Total (titration) Alkalinty in eq L^{-1}

$Alk_{water} = [OH^-] - [H^+]$

$Alk_{carbonate} = [HCO_3^-] + 2[CO_3^{2-}]$

$Alk_{borate} = [H_2BO_3^-]$

$Alk_{silicate} = [H_3SiO_4^-]$

$Alk_{phosphate} = [H_2PO_4^-] + 2[HPO_4^{2-}] + 3[PO_4^{3-}]$

The vast majority of total alkalinity (at average ocean temperatures in equilibrium with the current atmospheric CO_2 concentration) is due to the two carbonate species (97%). The next largest contribution is from borate (2%) with the remainder comprising a small, but non-negligible residual. Depending on the focus and the need for accuracy of the particular carbon chemistry model, terms after borate are often dropped, or are lumped into the latter to balance total alkalinity. This model calculates values for these alkalinities in each latitude, as functions of temperature, pH, and the carbonate alkalinity. The non-carbonate alkalinities are determined pseudo-independently of inorganic CO_2 chemistry, but are linked through their dependence on temperature and pH (which is strongly dependent on carbonate chemistry), allowing one to write seven equations in seven unknowns. By exogenously supplying known observed quantities for each of the latitude zones of the model: Alk_T , DIC, Total Borate, Total Silicate, and Total Phosphorus, the seven equations are reduced into a single higher order equation in $\left[H^+\right]$, DIC, and Alk_{carb} which determines $(\mathrm{CO}_2)^{sea}$ (and equivalently pCO_2^{sea} by Henry's law):

$$
\begin{aligned}
[H^+] = \frac{K_1}{2 \cdot Alk_{carb}} \{ & (DIC - Alk_{carb}) + ((DIC - Alk_{carb})^2 \\
& + 4(Alk_{carb} \cdot \frac{K_2}{K_1})(2 \cdot DIC - Alk_{carb}))^{\frac{1}{2}} \}
\end{aligned}
\tag{2.7}
$$

This equation cannot be solved analytically, but by an iterative method that attempts to solve for a value of $\left[H^+\right]$ that is consistent with the carbonate alkalinity which it determines and which serve to determine it. Once this consistent value is known, the pCO_2^{sea} and all other concentrations consistent with that pH are determined in the model for that latitude and time step.

All of the above relations (Eqs. 2.3–2.7) are used to calculate CO_2 concentrations in the mixed layer in the 2-D OCSM. The result is the desired quantity, pCO_2^{sea} which together with the atmospheric concentration, drives a carbon flux into the ocean. **Figures 2-5** and **2-6** shows the other two major observed quantities supplied to the model to solve the equations, titration alkalinity (AlkT) assumed to be constant with time but a function of latitude, and likewise salinity, to which total borate (TB) is also proportional.

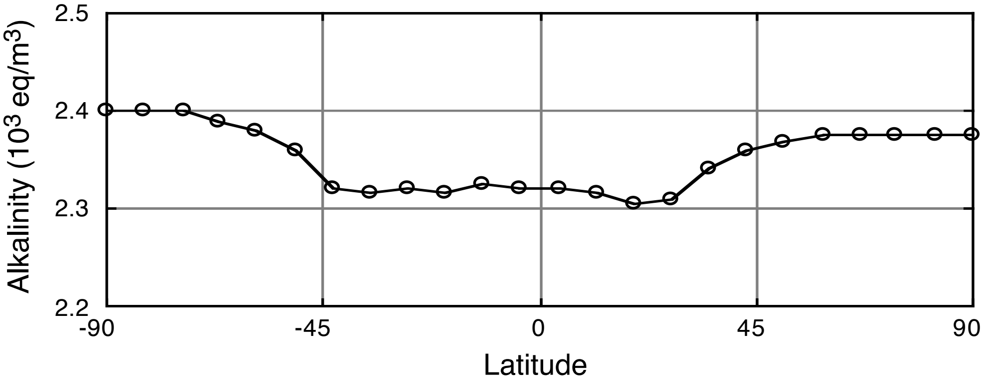


Figure 2-5 Total (Titration) Alkalinity as a Function of Latitude

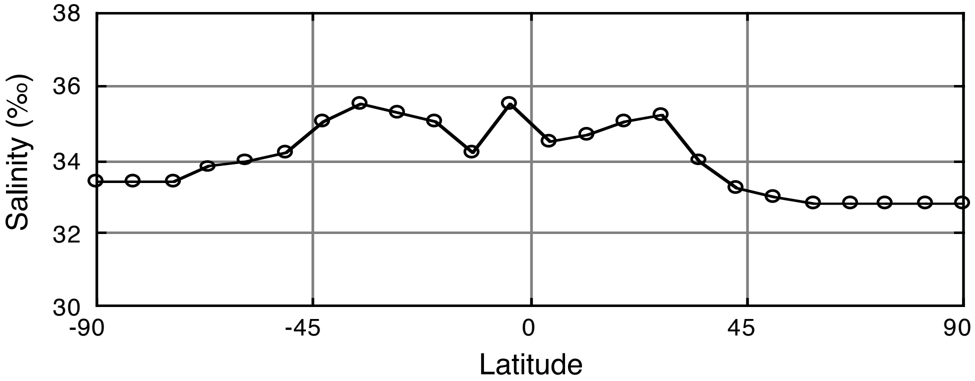


Figure 2-6 Salinity as a Function of Latitude

The surface flux from air-to-sea is not the only boundary of exchange in the mixed-layer. Additionally, total dissolved inorganic carbon in the mixed-layer is modified by the amount exported to the deep ocean by diffusion in each latitude zone in the model. This flux to the deep ocean reduces the concentration of DIC in the mixed-layer, therefore decreasing the partial pressure of CO_2 at the surface. This has the effect of delaying surface saturation with respect to dissolved CO_2 and increasing the air-to-sea gradient which allows more carbon to enter the ocean than gets in by buffering alone.

2.1.4 Deep-Ocean Mixing

The deep oceanic mixing processes that carry away excess carbon at the surface to sequestration at depth are parameterized in a way similar to that for heat in the 2-D Climate Model of Sokolov and Stone (1997). As noted above, dissolved CO_2, carbonate, and bicarbonate comprise dissolved inorganic carbon, DIC, which the 2-D Ocean Carbon Sink Model treats as a single inert tracer for the purposes of mixing and transport by oceanic circulation. A common simple parameterization for the effect provided by deep ocean mixing (which includes numerous dynamical processes such as ekman pumping, thermohaline circulation, and physical diffusion) is the assumption of diffusive-only transport in the vertical. In a diffusive-only model applied to a conserved quantity such as DIC, the transport equation depends solely on one parameter: K_v, the vertical eddy diffusion coefficient:

$$\frac{dDIC}{dt} = K_V \frac{d^2 DIC}{dz^2} \tag{2.8}$$

The vertical profile of DIC, is therefore determined by an apparent diffusivity. These values are chosen to reproduce the vertical structure of tracers whose spatial and temporal introduction into the ocean are relatively well known. Tracers that are commonly used for model calibration in order to validate the mixing provided by the model include the species radiocarbon (^{14}C), tritium (^{3}H), and CFCs. Here we use as reference values, a set of vertical diffusion coefficients (shown in **Figure 2-7**) that are computed to reproduce the zonally-averaged tritium profile in the ocean as a function of latitude. They are drawn from the 2-D Climate Model of Sokolov and Stone (1997) and are used in Hansen, *et al.* (1984). The former model is a modified version of the zonal mean statistical-dynamical model developed at GISS, based on parameterizations of physical processes of the GISS 3-D GCM.

These values agree with observations of the distribution of vertical mixing in the ocean, with strong sinking motion at high latitudes compared to equatorial waters due primarily to high-latitude deep water formation as a consequence of thermohaline circulation. When averaged and weighted by area, the mean value of the diffusion coefficients in Fig. 2-7 is only 2.5 cm^2/s, owing to the distribution of area in the surface ocean that biases towards low latitudes (Fig. 2-2). Additionally, to account for the effects of wind-driven gyres that tend to account for the effects of meridional mixing, the 2-D OCSM assumes horizontal mixing in the form of diffusion coefficients that are a function of depth (decreasing with the latter) but constant at as a function latitude (**Figure 2-8**).

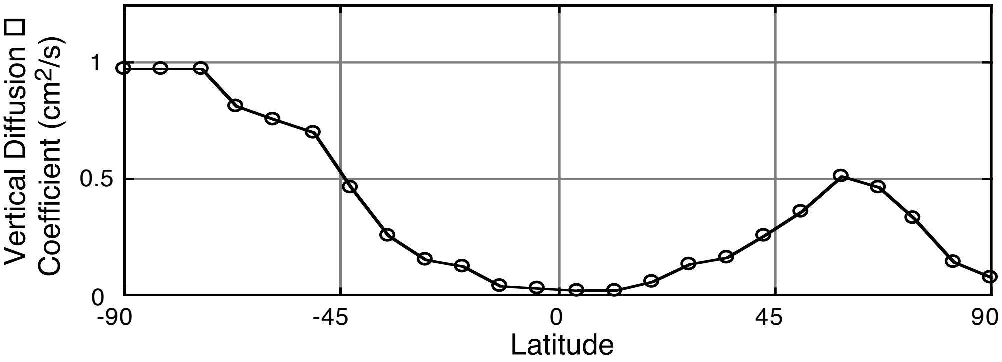


Figure 2-7 Vertical Diffusion Coefficients as a Function of Latitude

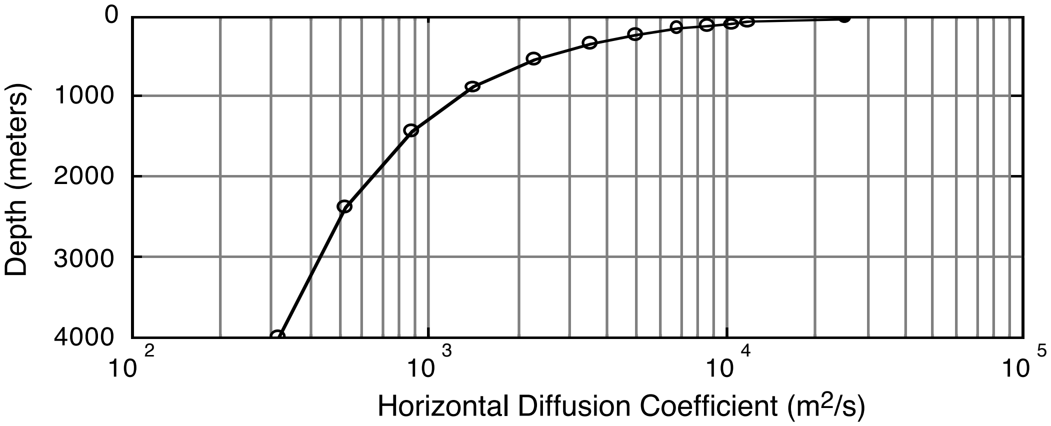


Figure 2-8 Horizontal Diffusion Coefficients as a Function of Depth in the 2-D OCSM

They represent the large-scale north-to-south transport of water masses that tend to smooth out the latitudinal gradients of DIC to better agree with observations. The coefficients have mixing time scales running from 25 years near the surface to over 500 years at depth.

Therefore, the total change in DIC (a quantity integral to computing the CO_2 concentration in the mixed-layer according to Eq. 2.7) in the mixed-layer from diffusive processes is solved according to Eq. 2.9 at each monthly time step:

$$\frac{dDIC}{dt} = K_V \frac{d^2\,DIC}{dz^2} + K_H \frac{d^2\,DIC}{dy^2} \qquad (2.9)$$

with explicit vertical and horizontal mixing (K_V a function of latitude and K_H a function of depth) across the grid of the 2-D ocean.

2.2 Model Calibration

2.2.1 Initialization

Once all the reference values for the parameters in the model have been set, the first requirement is to spin up the 2-D OCSM to a pre-industrial steady-state, consistent with our assumption of a pre-industrial atmospheric concentration of 280 ppmv and zero net exchange between all the major carbon reservoirs.

That assumption requires running the ocean carbon sink model beneath a well-mixed atmosphere with the CO_2 concentration given, until the net exchange across the latitude zones falls to zero, and net transport across any layer of depth in the ocean is also zero. Because the time step of the model is one month, such a run requires average monthly data for temperature as a function of latitude, and monthly zonally-average wind speed. This data was obtained for one year and was repeated yearly until a steady-state was achieved.

Due to the extremely long time it takes carbon to reach the deepest layers of the ocean, owing to the slowness of the diffusion process, a satisfactory equilibrium was only achieved after many thousands of years of calculation. After 10,000 years, starting from an ocean devoid of carbon to one in steady-state with the atmosphere at 277 ppmv, the result was a true steady-state, with carbon sources and sinks in the 2-D ocean model distributed latitudinally to produce a zero net annual sink into the ocean averaged over the globe. Since by assumption, the land biosphere was also in steady-state at this time, no model or dynamic assumption for terrestrial exchange is required. Because of the temperature dependence of carbonate chemistry, the distribution of sources and sinks, shown in **Figure 2-9**, is much as we expect.

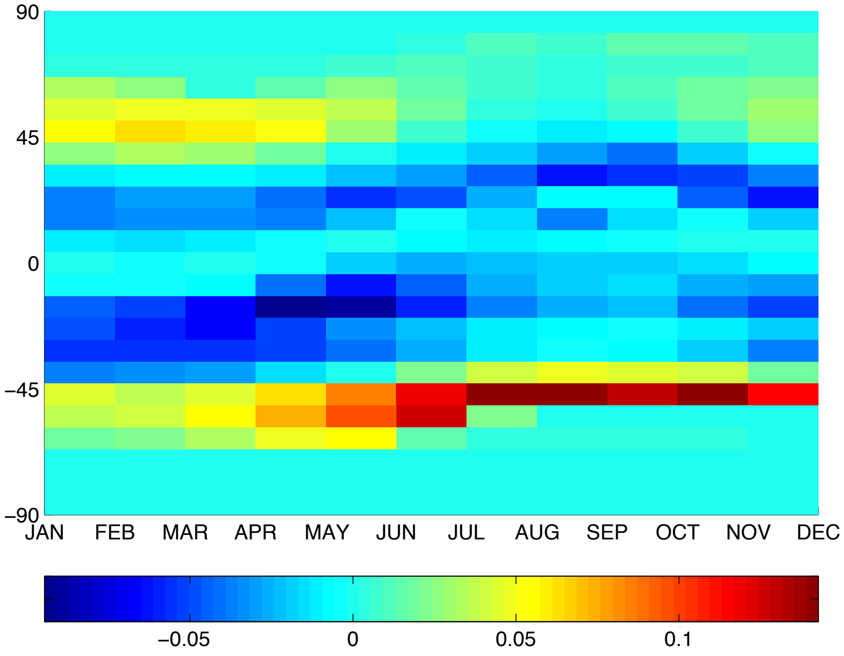


Figure 2-9 Distribution of Sources and Sinks in the Steady-State 2-D OCSM (in Pg/month; Regions of Sources are Negative)

Spatially, high latitude sinks in both hemispheres balance out equatorial sources of CO_2 to the atmosphere. Temporally, high latitude sinks are dominant in the southern and northern oceans in the southern and northern winters, respectively as would be expected from considerations of the temperature dependence of carbonate chemistry in conjunction with the distribution of diffusion coefficients.

Average concentrations of dissolved inorganic carbon in the steady-state ocean are in good agreement with globally observed values of 2.06 mol/m^3. A north-to-south gradient is observed in this steady-state, consistent with inorganic carbonate chemistry favoring higher DIC (lower pCO_2) concentrations at lower temperatures and lower DIC (higher pCO_2) at higher temperatures. However, the vertical gradient in DIC is weaker than that of the observed quantity in the oceans, due to the lack of a marine biological cycle in the model which tends to deplete the surface of carbon with respect to the deep ocean. However, this is generally considered a "fly-wheel" effect, since it is not transferring net carbon to depth. Because of nutrient limitations that cause the marine biological cycle to be insensitive to rising DIC, this is not thought a prohibitive assumption in the 2-D OCSM. The model is constructed to simulate the uptake of CO_2 perturbations in the atmosphere, and not the observed distribution of carbon in the oceans upon for which the imposition of an additional cycling of carbon by marine biota in the oceans is required.

2.2.2 Transient Spin-up, 1765-1990

In order to spin up the 2-D OCSM from the equilibrium established above (which must be re-established for any changes of the chemical parameters or diffusion coefficients), it must be driven from this steady-state to the present day by the historical atmospheric CO_2 record (from Fig. 1-1). It is arbitrarily assumed that a steady-state prevailed in 1765 and since atmospheric CO_2 levels increased imperceptibly before the early 1800s, this is not an assumption to which the result is particularly sensitive. An atmospheric CO_2 mixing ratio time series is estimated (**Figure 2-10**) from the historical CO_2 record compiled from ice-cores and direct observations at the South Pole and Mauna Loa (Fig. 1-1). As with the spin-ups of most ocean carbon sink models, the seasonality of atmospheric CO_2 is not imposed on the historical record used to drive the model to the present.

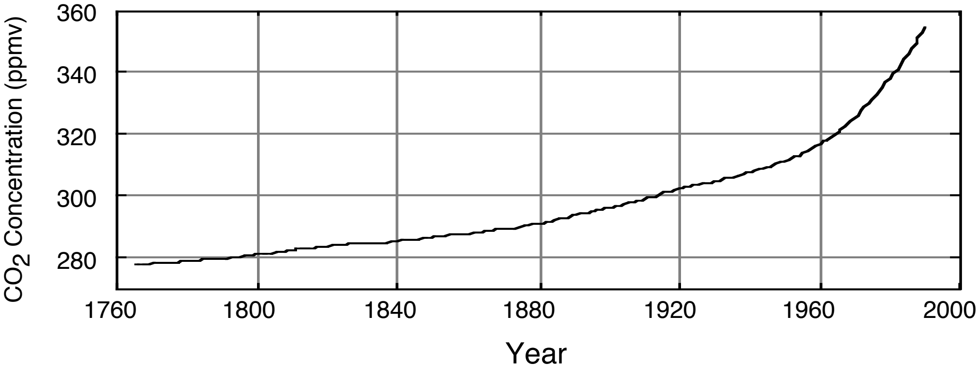


Figure 2-10 Historical CO_2 Concentrations for the Transient Spin-up

The oceanic carbon sink model also needs to be driven with zonally-averaged climatic data, including sea surface temperatures and surface wind speeds over the same period to spin it up to the present. This input can be either provided endogenously if it is run coupled with a climate model, or as exogenously supplied data otherwise.

2.3 Reference Ocean Carbon Sink

By setting reference values for all the parameters of the 2-D OCSM and spinning up the model using the historical CO_2 record as an input (Fig. 2-10), a net carbon flux is driven into the ocean that grows with time between 1765 and 1990. The net monthly CO_2 flux produced by the model is summed up globally is displayed in the **Figure 2-11**.

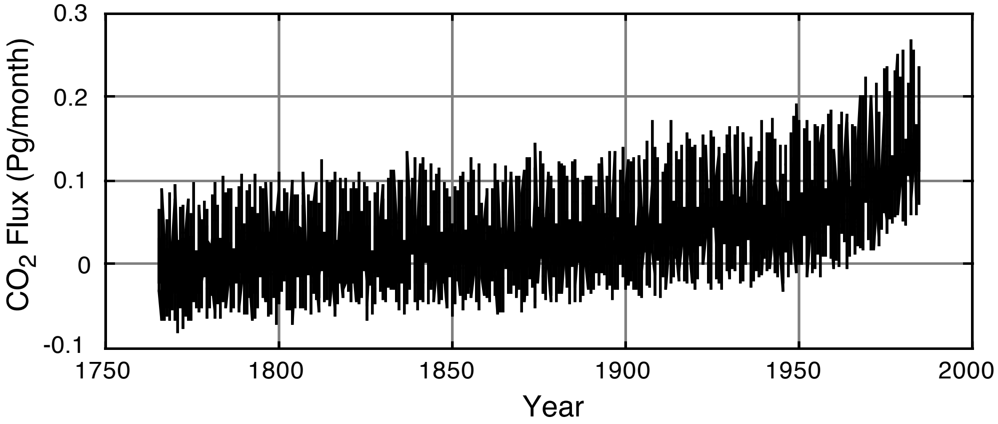


Figure 2-11 Monthly CO_2 Flux into the Ocean for the Transient Spin-up

Clearly visible in this time series is the strong seasonal cycle that is characteristic of the CO_2 exchange between the atmosphere and the ocean. In this model, it is produced by the strong seasonality of surface temperature, particularly at high latitudes. The noise in the time series is primarily caused by the noise in the wind speed data used to drive the flux, which exhibits a lot of inter-annual variability. It is difficult to ascertain the magnitude of the net carbon flux into the ocean for most of the period plotted in this figure, therefore it is necessary to sum up the monthly carbon fluxes to compute the annual exchange as a function of time. The annual carbon uptake of the 2-D OCSM from the period 1765-1989 in Pg/yr is plotted in **Figure 2-12**.

The average annual global flux in the 2-D OCSM rises from zero in the steady-state at 1765, to almost 1.8 Pg/yr in the late 1980s. Most of the increase in the oceanic carbon sink comes in the last 90 years of the run, when atmospheric CO_2 has been rising the fastest (Fig. 2-10). The average value of the uptake during the 1980s in this run is 1.71 Pg/yr, well within the range of uncertainty of 1.2–2.8 Pg/yr specified by the IPCC study (1994) for the oceanic carbon sink.

An examination of the change in the distribution of DIC in the ocean from the steady-state in 1765 to 1985 indicates where all the carbon is being taken up by the ocean as a function of latitude.

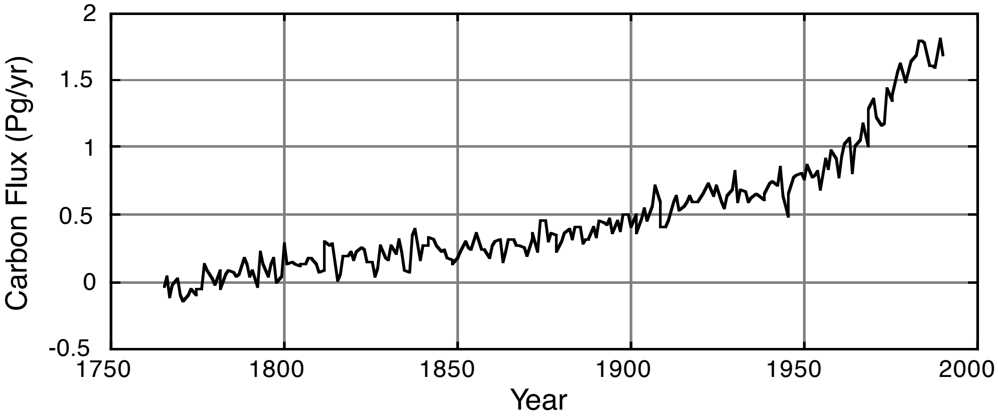


Figure 2-12 Annual Carbon Flux into the Ocean for the Transient Spin-up

Figure 2-13 shows the distribution of the additional dissolved inorganic carbon, DIC, added to the ocean as a function of latitude and depth for the top 2000 meters of the ocean. Units are in moles of DIC per cubic meter and quantities represent on order 1% of the surface concentration of background DIC. As we expect, most of the carbon taken up by the model remains near the surface, with decreasing amounts penetrating the ocean as a function of depth. Most of the increase in DIC by the 2-D OCSM is confined to the top 500 meters of the ocean near the surface.

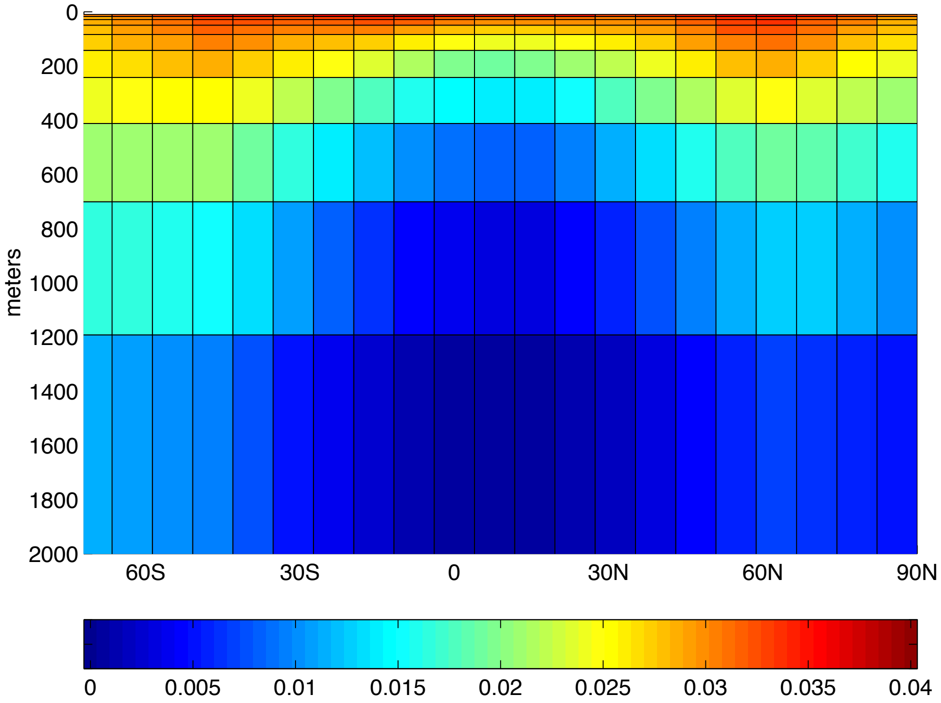


Figure 2-13 Distribution of Additional Total DIC in the Ocean, between 1765-1985 (in moles of DIC m^{-3})

Not surprisingly, the carbon is being taken up at high latitudes, where lower temperatures, larger mixed layer depths (Fig. 2-1), and faster vertical diffusion rates (Fig. 2-7) favor a larger sink. There is also an hemispheric imbalance, favoring the southern oceans, which might be expected due to the greater area of exchange, deeper mixed layer depths, and somewhat stronger diffusion in the southern oceans than the northern (Fig. 2-7). It is also noteworthy, that almost no carbon penetrates below the 500 meter mark in the equatorial part of the oceans, where slower mixing and higher temperatures do not favor a strong carbon sink. When the results are compared to the observations of ∆DIC from the GEOSECS Survey (1975), there is reasonable agreement with the depth of mixing (which for the period between 1825 and 1975 in the survey, has also been restricted to approximately the top 500–1000 meters of the Atlantic and Pacific oceans with deeper penetration at high latitudes). The observations show somewhat higher values of ∆DIC near the surface than in the 2-D OCSM. These maximal concentrations near the surface are closer to 0.05 mol/m^3 compared to 0.04 mol/m^3 in the 2-D OCSM. Those differences are owing to the influence of marine biological activity near the surface which deepens vertical gradients without transferring net carbon and weaker horizontal mixing rates than are assumed in the ocean carbon sink model. Additionally, the effect of bottom topography is important in determining the distribution of carbon at depth at high latitudes, since a shallower bottom that is assumed in the model limits the extent of carbon penetration, forcing meridional transport at lesser depths than are accounted for in the model.

A comparison of the output of the oceanic carbon sink model in this study with a group of the most commonly referenced models in the literature and by the IPCC (1994) is shown in **Table 2-1**. The reference response of the 2-D OCSM that is spun up to the present with the historical CO_2 record falls within the range of other models of the global oceanic carbon sink, both more and less complex than it. It takes up an average amount of carbon during the 1980s and a total amount between 1770 and 1980 that is consistent with other simulations.

Table 2-1 A Comparison of the 2-D OCSM Carbon Uptake to Other Models

Model:	2-D OCSM	Box-Diffusion	Princeton OGCM	HILDA	Hamburg HAMOCC-3	Stocker 2-D OGCM
Author:	(This Paper)	Oeschger *et al.*	Sarmiento *et al.*	Siegenthaler and Joos	Maier-Reimer	Stocker *et al.*
Mean Ocean Carbon Sink for 1980s (Pg/yr)	1.71	2.32	1.67	2.15	1.47	2.10
Cumulative Carbon Sink 1770–1980 (Pg)	98.6	123	92	107	X	100

3. FORECASTING ATMOSPHERIC CO_2 CONCENTRATIONS

3.1 Closing the Carbon Cycle

Having constructed a satisfactory model of the oceanic carbon sink that seems to be in good agreement with other models and observations of the currently estimated carbon flux, it can now be used to compute atmospheric CO_2 concentrations endogenously, under the conditions of a changing carbon budget.

In order to forecast atmospheric CO_2 concentrations into the future, the goal of which has been a primary focus of considerable recent climate research, it is necessary to include more than just the oceanic sink for carbon. On time scales of the current anthropogenic interest, increases in the atmospheric concentration of CO_2 are the net result of the difference between emissions of carbon from fossil fuel combustion and releases of carbon from land-use changes such as biomass burning, minus the natural sinks produced by the terrestrial biosphere and the ocean as represented in Eq. 3.1:

$$\frac{d[CO_2]^{atm}}{dt} = F_t - O_t + L_t - B_t \tag{3.1}$$

where F_t is the rate of fossil fuel emissions, O_t is the oceanic carbon sink, L_t is the anthropogenic carbon emission from land-use, and B_t is the terrestrial sink for carbon in the biosphere. This calculation can be most easily visualized, by applying it to the historical CO_2 data to extrapolate the carbon budget since the beginning of the industrial age. Such studies have been done by other researchers (Craig, *et al*., 1997; Siegenthaler and Joos, 1992; Keeling, *et al*., 1989) in the form of a model deconvolution using the historical CO_2 record in the atmosphere (Fig. 2-10) to calculate the continuous rate of carbon accumulation in the atmosphere in Pg per year. Using the historical fossil fuel emissions of carbon and the results of an ocean carbon sink model, the residual of the calculation is inferred to be the activity of terrestrial ecosystems.

For this study, using the data of Marland and Rotty (1984) for fossil fuel emissions (Fig. 1-4) and the newly acquired results of the 2-D oceanic carbon sink model driven by the historical CO_2 record (Fig. 2-12), a residual is obtained which is conjectured to be the net biospheric sink for atmospheric carbon, as shown in **Figure 3-1**.

The net biospheric sink for carbon is defined as $NB_t = L_t – B_t$, the difference between the man-made emission of CO_2 from the terrestrial biosphere and the amount taken up by ecosystems over the same period of time. Looking at Fig. 3-1, it is easy to see that the biosphere as a whole has been acting as a significant net sink for carbon over the last 50 years, increasing in size with time. It is comparable in size to the oceanic carbon sink (within the uncertainty of the latter) and in good agreement with the general observations of Tans, *et al*. (1990). This is the so-called “missing sink,” that is necessary to balance the carbon cycle. Clearly, the implication of this result is that in addition to anthropogenic emissions of CO_2, atmospheric CO_2 concentrations cannot be reliably forecast without an additional representation of the terrestrial sink for carbon.

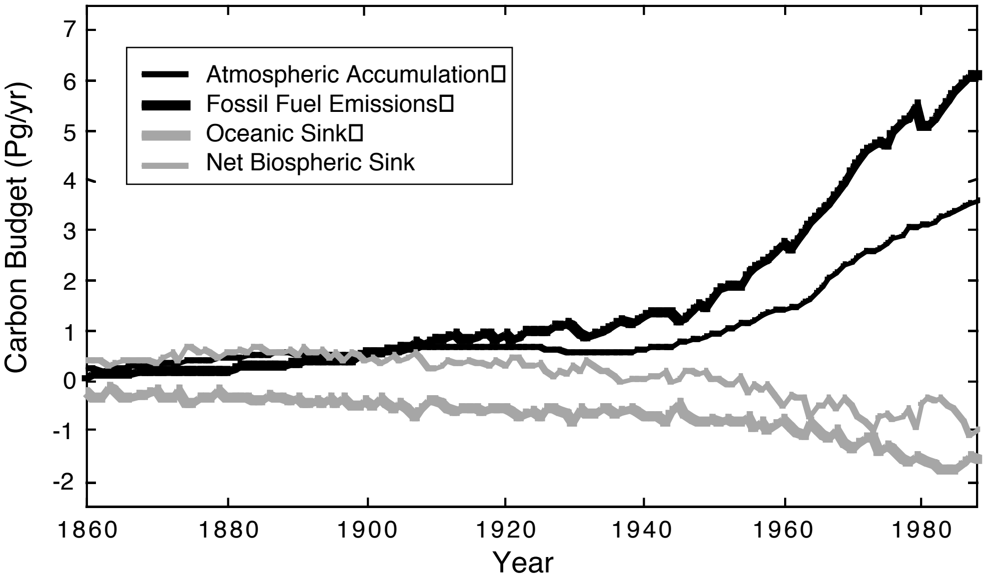


Figure 3-1 Deconvolution of the Historical Carbon Budget Inferred by the 2-D OCSM

3.1.1 Anthropogenic Fossil Fuel Emissions

The primary driver of the increase in atmospheric CO_2 concentrations has been and will continue to be the emissions of CO_2 from fossil fuel combustion. CO_2 emissions are expected to continue to grow rapidly for the foreseeable future and many forecasts for the rate of this increase have been made in recent times. However, the most widely publicized emissions forecasts for the purposes of climate studies are those of the Intergovernmental Panel on Climate Change’s 1992 report in which six scenarios were constructed which included variations in assumptions about economic activity, demographics, and policies to produce a broad range of possible CO_2 emissions paths out to the year 2100 (Leggett, *et al.*, in IPCC, 1992).

In this study, the carbon emissions scenario that is used to forecast atmospheric CO_2 concentrations is roughly equivalent to the IS92a scenario of the IPCC (1992) report. IS92a represents a middle of the road assumption, sometimes described as a “Business-as-Usual” scenario, in which little or no action is taken to curb the economic activities which are producing CO_2 emissions. These emissions are plotted in **Figure 3-2** for the period 1990-2100. All of the further forecasts in this study will be performed using this emissions scenario. This emissions path is not chosen because of any belief in the likelihood of its realization, but because it represents a frame of reference from which to compare the behavior of the 2-D Ocean Carbon Sink Model in this study with other models that are also driven by such carbon emissions.

Uncertainty in fossil fuel emissions are not considered in this paper because this is a study of uncertainty in the physical processes which produce or feedback on carbon sinks in the ocean and their contribution to uncertainty in atmospheric CO_2 concentrations. It is not a study of the total uncertainty in future atmospheric CO_2 concentrations which must necessarily include the impacts of various policies on emissions in conjunction with uncertainty in rates of demographic change or economic activity which are not considered here.

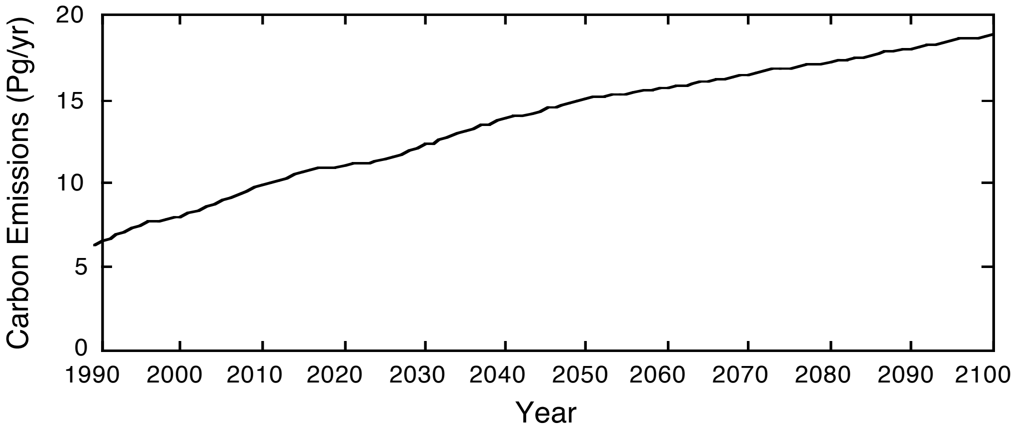


Figure 3-2 Reference Fossil Fuel Emissions Scenario, 1990-2100

3.1.2 Deforestation

A highly uncertain component of anthropogenic CO_2 emissions that is included in the land-use term of the carbon budget (L_t) and therefore is necessary for forecasting atmospheric CO_2 concentrations is the contribution from deforestation (primarily due to biomass burning). The IPCC (1992) establishes the average 1980s size of this emissions source at 1.6 ± 1.0 Pg/yr, though a more current estimate places it at 1.0 Pg/yr. The uncertainty in the size of this activity, however remains large and little has been done to constrain it.

In this study, a rather simple scenario is assumed (**Figure 3-3**), in which the current source is kept constant at 1.0 Pg/yr until 2025 and linearly decreased to zero by 2050 under the assumption that the opportunities and inclination to contribute to the deforestation source of carbon will decline with time and eventually disappear. As can be gauged by their relative sizes, the contribution of this source of carbon emissions relative to the total anthropogenic emission (fossil fuel and deforestation) quickly becomes negligible. Its primary importance is in partitioning the 1980's carbon budget, since the size of the natural land sink depends on the total sources and sinks assumed elsewhere.

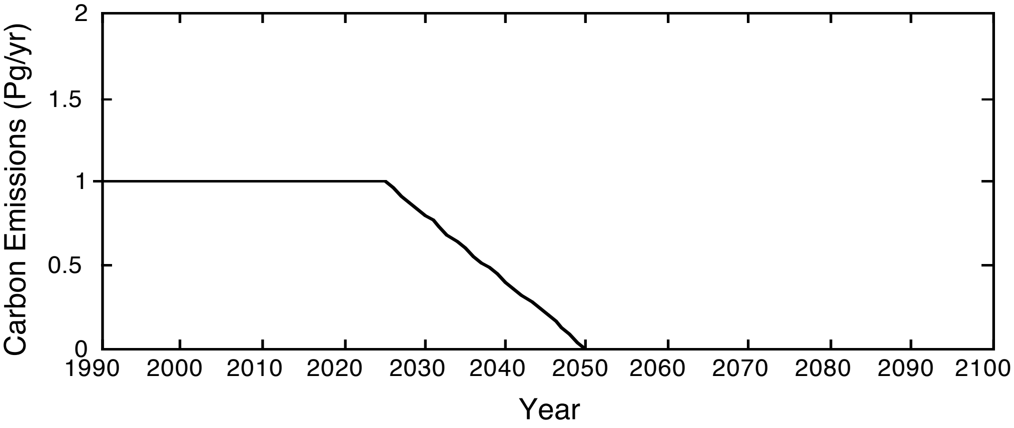


Figure 3-3 Deforestation Emissions Assumption for the Reference Carbon Run

3.1.3 Terrestrial Carbon Sink

Finally, a model of the terrestrial sink of carbon is required to balance the carbon budget. For that purpose one of a handful of current global ecosystems models is consulted to construct a forecast for the terrestrial carbon sink. The Terrestrial Ecosystems Model (TEM) of the Marine Biological Laboratory at WHOI Version 4.0 and 4.1 (Raich, *et al*., 1992; McGuire, *et al*., 1992, 1993, 1995, 1997; Melillo, *et al*., 1993, 1995; VEMAP Members, 1995; Pan, *et al*., 1996; Xiao, *et al*., 1997) is a process-oriented model of the terrestrial biosphere that can simulate either the equilibrium or transient response of surface land biota and soils to rising CO_2 levels in the atmosphere as well as to changes in climate, encompassing variations in temperature, precipitation, and cloudiness as well as the availability of limiting nutrients.

The TEM model includes 18 distinct ecosystems, called “biomes,” which are defined on a grid of the world, $^1/_2$° by $^1/_2$° in size that contains 62,483 land grid cells (about 25% of the globe), including 3,059 ice grid cells, and 1,525 wetland grid cells, ranging between 83°N and 56°S. Each grid cell is characterized by a combination of exchanging carbon and nitrogen pools, divided into vegetation and soils components that characterize a particular ecosystems type in interaction with atmospheric CO_2 and climate on a monthly timestep. The model uses data on long-term average climate (Leemans and Cramer, 1991; Cramer and Leemans, 1993), potential natural vegetation (Melillo, *et al*., 1993), soil texture (FAO/CSRC/MBL, 1974), and elevation (NCAR/Navy, 1984) are incorporated. It uses the water balance model of Vorosmarty, *et al*. (1988), to generate its hydrological input, including potential evaporation and soil moisture.

Higher CO_2 levels stimulate photosynthesis and cause vegetation to grow and hold more carbon. This is the primary dynamical response that the TEM model has been constructed to reproduce. Net Primary Productivity (NPP) is calculated in the TEM in each grid cell by biome type, as the difference between gross primary production (GPP) and autotrophic respiration, Rs(a). GPP in each grid cell of the model is calculated at a monthly timestep according to the following equation:

$$\mathrm{GPP} = \mathrm{C}_{\max} f(PAR)\, f(LEAF)\, f(T)\, f(\mathrm{CO}_2, \mathrm{H}_2\mathrm{O})\, f(NA) \qquad (3.2)$$

where C_{max} is the maximum rate of carbon assimilation, multiplied by functions of: PAR (photosynthetically active radiation), LEAF (the leaf area relative to its annual maximum), T (temperature), the atmospheric CO_2 concentration, H_2O (available water), and NA (the available nitrogen). Autotrophic respiration, R_A includes both maintenance respiration, R_M and construction respiration, R_C. R_M is a logarithmic function of temperature and R_C has been determined empirically to be 20% of the difference between GPP and R_M. NPP, the difference between GPP and R_A is:

$$\mathrm{NPP} = \mathrm{GPP} - \mathrm{R_M(T)} - 0.20[\mathrm{GPP} - \mathrm{R_M(T)}] \qquad (3.3)$$

Heterotrophic respiration, R_H, represents additional decomposition of organic matter in each ecosystem by organisms and decay. In the TEM, it depends directly on changes in temperature and precipitation as follows (an increasing function of temperature):

$$\mathrm{R_H} = k_d(C_S)e^{0.0693T}MOIST \tag{3.4}$$

with k_d equal to the gram-specific decomposition constant, C_S is the amount of soil carbon, and MOIST is a parabolic function of volumetric soil moisture. This allows for the computation of NEP (the carbon uptake of the particular grid cell in question at this timestep) as follows (with the expression for GPP taken from above):

$$\mathrm{NEP = GPP - R_M(T) - .20\ [GPP - R_M(T)]} — k_d(C_S)e^{0.0693T}MOIST \tag{3.5}$$

As is apparent, temperature and hydrology play an important role in most of the terms of this equation, in addition to atmospheric CO_2. However, CO_2 only plays a direct role in determining GPP, as indicated above, not in the respiratory terms. Currently, the model is only able to account for the effects of CO_2 fertilization and feedbacks from climate change (reflected in changes in temperature, precipitation, and cloudiness changes) on ecosystems production. Future plans for the model include the addition of the effects on carbon uptake of nitrogen deposition.

For the Terrestrial Ecosystems Model, a steady-state is presumed in pre-industrial times when the annual atmospheric concentration of CO_2 was relatively constant at 277 ppmv. The TEM has been spun-up in a transient run much like the 2-D OCSM, driven by the historical CO_2 record to the present day to produce a net sink for carbon as a function of time that is as large as 0.8–0.9 Pg/yr by the late 1980s. This sink is primarily due to the effects of CO_2 fertilization and is considered the dominant sink of carbon into the land biosphere. Net Ecosystems Production, or NEP, as calculated above is the total annual biospheric sink for carbon and whether NEP is positive, negative, or zero is dependent on the relationship between GPP and total respiration, Rs(a) + Rs(h), all of which are sensitive to climatic variables in addition to the atmospheric level of CO_2, in slightly different ways for each of the biomes of the model. Such sensitivities to climate change have already been explored with this model (Melillo, *et al*., 1993; Xiao, *et al*., 1996), but are not addressed here.

The TEM is currently too computationally intensive to be run concurrently with the 2-D OCSM in order to close the global carbon budget in this uncertainty study. Therefore, to provide a carbon sink to balance the anthropogenic emissions of carbon in a way that is consistent with the observed atmospheric increase, a terrestrial sink is estimated from the output of the TEM and parameterized in the form of a time-dependent lifetime for atmospheric CO_2 into the land biosphere. By using various atmospheric CO_2 concentration scenarios to the drive TEM carbon sink (calculated by the model as NEP in Eq. 3.5) it is possible to take the forecasts of NEP and construct a parameterization for the biospheric sink of carbon between 1990 and 2100 that is driven by atmospheric CO_2 concentrations. A constant term that incorporates additional sinks that are not as yet incorporated into the model is also added to close the carbon budget in the 1980s. The following equation for the total biospheric sink for carbon is assumed:

$$B_t = NEP_t^{TEM} + \overline{B} \tag{3.7}$$

The constant $\overline{B}$ is determined as the residual flux needed to balance the carbon budget in the 1980s, after applying oceanic carbon sink and the parameterized carbon sink from the TEM:

$$NEP_t^{TEM} = \frac{[CO_2]_t - 277}{T_t^B} \tag{3.8}$$

where T_t^B is the atmospheric lifetime of CO_2 due to the "CO_2 Fertilization" effect estimated from runs of the TEM driven by different forecasts of atmospheric CO_2 increase and computed as:

$$T_t^B = 187.8 + 1.639(t - 1985) \text{ for } t > 1985 \tag{3.9}$$

Simulations in which the Terrestrial Ecosystems Model is driven with prescribed atmospheric CO_2 concentrations between 1990-2100 cause it to generate a carbon sink (NEP) as a function of time that is approximated by Eq. 3.8 for the parameterization. The response of NEP to increases in atmospheric concentrations that rise from 352ppm in 1990 to 936, 740, and 592 ppmv at the end of the next century are plotted in **Figure 3-4**.

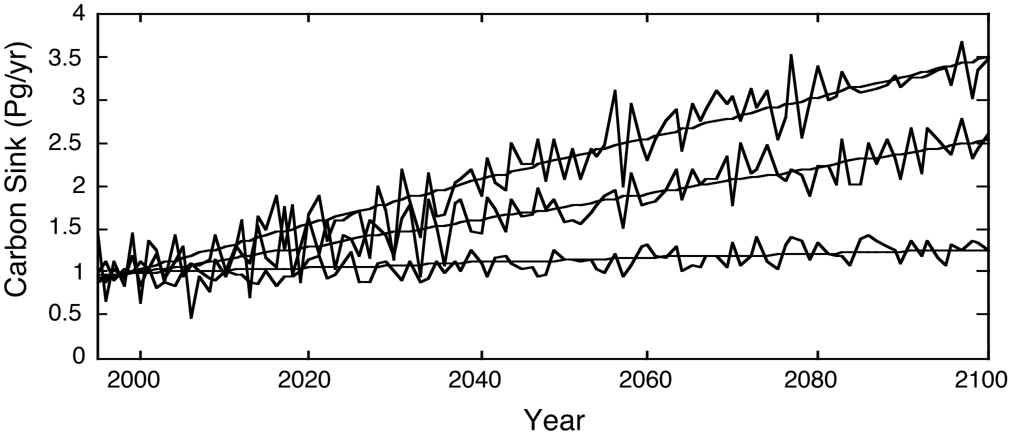


Figure 3-4 Reference TEM Carbon Sinks (NEP) and their Approximations

The terrestrial carbon sink grows from 0.9 Pg/yr in 1990 to almost 3.4, 2.6, and 1.3 Pg/yr in 2100 in the three curves, respectively for the three rates of atmospheric CO_2 increase. Included in the simulations are the effects of increasing global average temperature levels that are a component of the climatic response to rising atmospheric CO_2 concentrations (positively correlated) and act as a negative feedback to the terrestrial carbon sink (Prinn, *et al*. 1998; Xiao, *et al*. 1997). From these estimates, the lifetime for biospheric carbon is found to increase with time primarily due to a "saturation effect" analogous to that in the surface ocean where higher CO_2 levels, changes in precipitation, and higher temperature decrease the effectiveness of the terrestrial sink for carbon as a function of time. This parameterization is found to be valid for atmospheric CO_2 concentrations increasing to the range 600–900 ppm (well within the range of uncertainty that is estimated for the atmospheric CO_2 with the 2-D OCSM in Section 5) by the end of the next century, predicting a carbon sink that grows with time and increasing CO_2 concentrations.

3.2 Reference Atmospheric CO_2 Forecast

Taking the fossil fuel emissions scenario, terrestrial source and sink assumptions, and coupling them dynamically to the output of the 2-D OCSM, atmospheric CO_2 concentrations are forecast by the couple system for the period, 1990–2100, as shown in **Figure 3-5**.

Atmospheric CO_2 concentrations under the reference scenario increase from 352.7 ppm in 1990 to 715.5 ppm in 2100. The reference forecast calculated by the IPCC (1995) using the HILDA Model of Seigenthaler and Joos (1992) under the IS92a emissions scenario, forecasts atmospheric CO_2 concentrations to rise to just over 700 ppm. The range of results for all of the models tested in the IPCC survey, was about ± 20 ppm, so that the forecast of the 2-D OCSM falls within the range predicted by other models.

Beyond differences in individual budget calculations and terrestrial carbon sink assumptions assumed across all the models, the results of all these models rely on our assumptions of parameter values which are themselves not certain. The reasonableness of the forecast of the 2-D OCSM, for instance, in the light of those uncertainties is the key unanswered question for this particular ocean carbon sink model. Numerous other models which also purport to do a reasonable job of forecasting atmospheric CO_2 concentrations ignore the degree to which assumptions made in the construction of the model, inherently affect its predictive power. The sensitivity of the carbon sink to uncertainty in its parameters must be explored to gauge the robustness of the results.

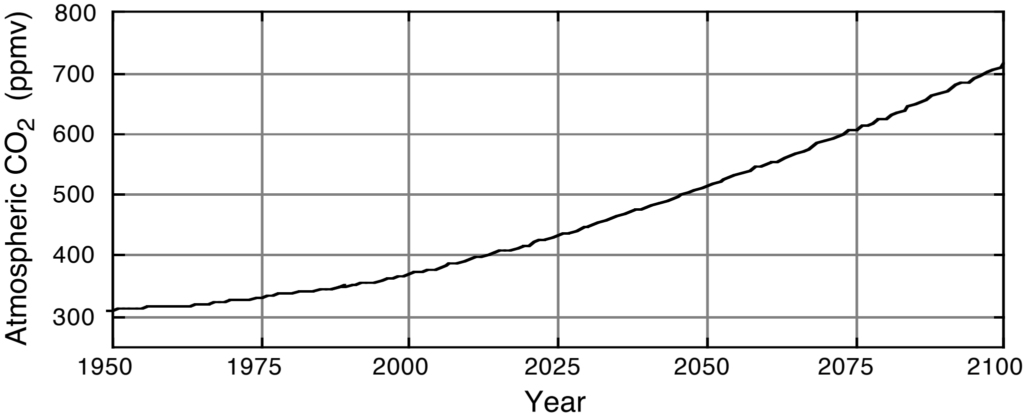


Figure 3-5 Reference Atmospheric CO_2 Concentrations Forecast, 1990–2100

3.3 Sensitivity of the Oceanic Carbon Sink

3.3.1 Choice of Parameters

From Section 2, it is recalled that the major transport mechanisms for the removal of atmospheric CO_2 by the oceans are: 1) the air-to-sea transfer across the surface, 2) the buffering by the oceanic mixed-layer, and 3) the mixing of dissolved carbon into the deep sea. The 2-D OCSM addresses the three “solubility pump” CO_2 sink mechanisms in the following way:
1) a wind-speed dependent piston velocity that drives the air-sea exchange over the interface;
2) explicit inorganic carbon chemistry in the oceanic mixed layer that converts additional dissolved

CO_2 into dissolved inorganic carbon; 3) the diffusion of dissolved inorganic carbon from the mixed layer to depth.

As noted in Section 2, the air-to-sea transfer rate depends on the relationship of the piston velocity to the wind speed, a single variable (Fig. 2-4). So it is chosen as an obvious parameter to test the sensitivity of the carbon sink to mechanism 1), above. The buffering capacity of the ocean is primarily the function of the particular chemical formulation of the inorganic carbonate system that is used, through its sensitivity to temperature. Therefore the equilibrium constants K_0, K_1, and K_2 from Eq. 2.7 as the three parameters by which mechanism 2) are primarily determined are chosen as three additional parameters for the sensitivity examination. Finally, in this model the uptake of carbon by the deep ocean by mechanism 3) is simply the function of the magnitude and distribution of the diffusion coefficients that are assumed: vertical and horizontal. Here, the globally averaged vertical diffusion coefficient and the vertically averaged horizontal diffusion coefficient are chosen as additional parameters for sensitivity testing.

3.3.2 Sensitivity to the Parameter Values

Taking the six parameters chosen above to represent the important mechanisms incorporated into the model, a test for the change in the contemporary carbon sink (average for the 1980s in Pg/yr) that would result from a factor 2 uncertainty in the reference values of these parameters was conducted. It is important to note that choosing twice and one-half the reference values of these six parameters to test the sensitivity of the oceanic carbon sink does not represent a pre-supposition of the likelihood of the parameters being in that range, but rather a normalization for the purposes of comparison so that the percent change in the output with respect to the same percent change in each of the input parameters can be examined.

Because the rate at which carbon is taken up into the deep ocean is well known to be strongly determinative of the size of the carbon flux into the ocean, let us examine in more detail the impact of choosing a fast (factor 2 times the reference) and slow (factor $^1/_2$ times the reference) rate of vertical diffusion for the 2-D OCSM. In **Figure 3-6**, the oceanic carbon sink calculated by the 2-D OCSM under the cases of faster and slower diffusion are plotted along side the reference value.

Clearly from this figure, a higher global rate of vertical diffusion increased the carbon flux into the ocean with respect to the reference. From an average of 1.71 Pg/yr in the reference, the average carbon sink in the 1980s was increased to over 2.2 Pg/yr in the fast diffusion case. In the situation of slow diffusion, the oceanic carbon sink was decreased from the reference by nearly the same percentage that it was increased, from 1.71 Pg/yr to under 1.3 Pg/yr. Interestingly, these carbon sinks still fall within the range estimated by the IPCC (1994) for the oceanic carbon sink during the 1980s.

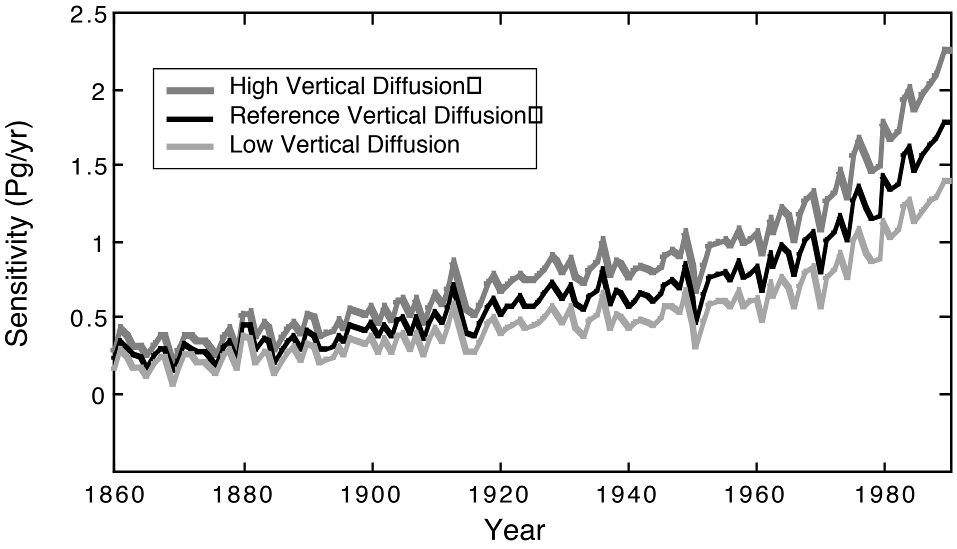


Figure 3-6 Sensitivity of the Oceanic Carbon Sink to the Vertical Diffusion Parameter

The difference in penetration of carbon into the deep ocean in the two scenarios and the reference is displayed in the following two figures. As the diffusion coefficient is varied in the fast and slow ocean cases, more carbon is taken up in the former and less in the latter, than in the reference (Fig. 2-13). **Figures 3-7** and **3-8** show the distribution of the additional carbon gained over and above the steady-state as a function of latitude and depth, which we can reference back to Fig. 2-13. It is noticeable that in the fast diffusion case, carbon penetration is deeper and near surface concentrations are lower than in the reference (less saturated) while in the slow diffusion case, penetration is shallower than in the reference and surface concentrations are higher (more saturated) because more carbon becomes trapped near the surface since it isn't dragged down out of the mixed-layer as quickly as in the reference. It is very clear that the level of vertical diffusion has a strong effect on the rate of carbon uptake by the model.

Similar pairs of runs were completed for the other five parameters chosen and tabulated below for all six parameters.

Table 3-1 Sensitivity of Average 1980s Carbon Sink to Variations in Parameters

Parameter	Values of Input Parameters (Relative to Reference Values)		% Impact on Mean Oceanic Carbon for 1980s Sink Relative to the Reference: 1.71 Pg/yr	
	High	Low	High	Low
Coefficient of Vertical Diffusion (Global Average)	5 cm^2/s	1.25 cm^2/s	+31.52%	–27.03%
Coefficient of Horizontal Diffusion (Surface Value)	$5x10^4$ m^2/s	$1.25x10^4$ cm^2/s	+5.84%	–5.61%
Piston Velocity (x Factor)	2	0.5	+9.5%	–12.1%
K_0 (at 20° C)	$6.5x10^{-2}$ M/atm	$1.6x10^{-2}$ M/atm	+2.65%	–3.12%
K_1 (at 20° C, 35 $^{o}/_{oo}$)	$1.9x10^{-6}$ M	$4.7x10^{-7}$ M	–22.79%	+15.3%
K_2 (at 20° C, 35 $^{o}/_{oo}$)	$1.31x10^{-9}$ M	$3.29x10^{-10}$ M	+12.68%	–18.6%

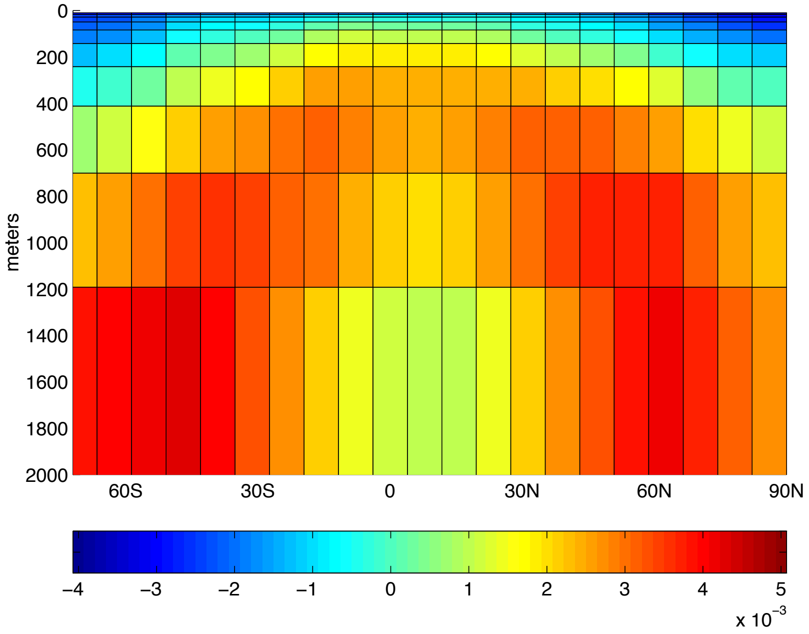


Figure 3-7 Difference of ΔDIC in Ocean, Between Fast Diffusion and Reference Case (1985-1765) (in moles of DIC m^{-3})

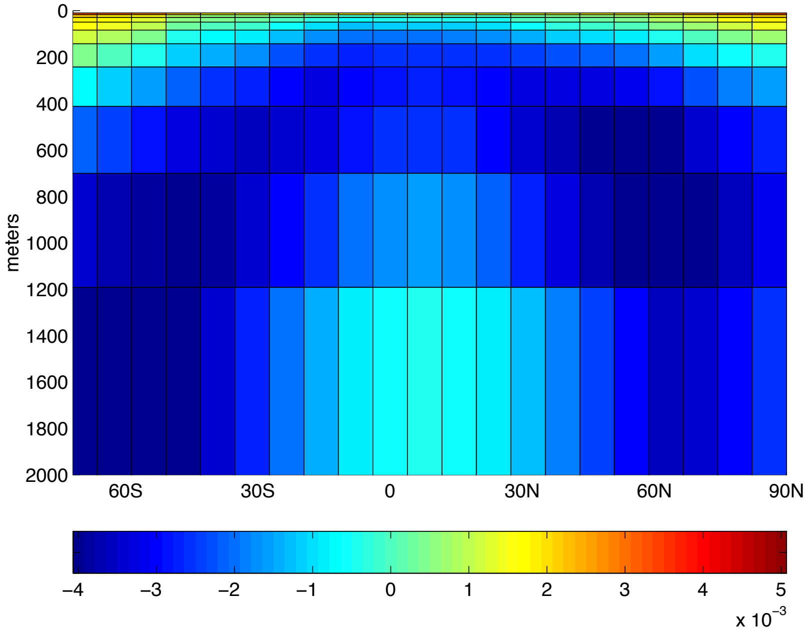


Figure 3-8 Difference of ΔDIC in Ocean, Between Slow Diffusion and Reference Case (1985-1765) (in moles of DIC m^{-3})

Once again, focusing on the average 1980s carbon sink reported by the model as a benchmark for the sensitivity test, it is clear that all of these parameters have non-negligible impacts on the output for the same percentage change in the value of the input parameter. Some of the parameters, clearly, are more important for determining the change in the output than others, particularly the coefficient of vertical diffusion and the first and second disassociation constants of carbonic acid. However, it is interesting to note that K_1 and K_2 have opposite effects on the size of the carbon sink. Increasing K_1, decreases the oceanic carbon sink, in opposite direction of all the other parameters. Such sensitivities in all these parameters might point to potentially large effects on the uncertainty of the oceanic carbon sink, depending on how uncertain the parameters are. Addressing this uncertainty is the subject of the balance of this paper.

4. UNCERTAINTY ANALYSIS

4.1 Sources of Uncertainty in Complex Models

There are two primary types of uncertainty which can impact upon assessing the validity of the response of a large, complex model: 1) structural uncertainty and 2) parametric uncertainty. Structural uncertainty arises from incomplete or incorrect knowledge about the form or design of the process that is being modeled. Considerations such as dimensionality, model resolution, missing or poorly understood processes, and parameterized dynamics all contribute to structural uncertainty in models. Parametric uncertainty, on the other hand, is attributable to imperfect knowledge of the values of the parameters used to calibrate the behavior of a model given a particular model formulation. Since the output of the model is dependent on particular parameter values, the results will be uncertain if values of the parameters are not known with a great deal of confidence.

While both sources of uncertainty are widely considered in assessments of current climate research, the primary focus of such studies has been structural uncertainty, since the dynamical equations involved are well understood, but the limitations of computational power have required less than ideal formulations that demand serious compromises for the sake of feasibility and efficiency. However, in the case of global biogeochemical models, the dominant uncertainty is not often considered structural, but parametric since the quantities necessary to calibrate these models such as global sources and sinks of constituent species are typically observed with large uncertainties.

4.2 Structural Uncertainty and Parametric in Oceanic Carbon Cycle Models

As noted in Section 1.2.4, models of the oceanic carbon cycle range widely in complexity. The differences in the dimension and resolution of the various ocean carbon sink models represents a source structural uncertainty that is evident in the different results produced by such models (Table 2-1). More serious, perhaps is the possible uncertainty owing to the exclusion or inclusion of a dynamical ocean and the marine organic carbon cycle. While the role of these uncertainties is more fully discussed in Section 6.1, it is clear that they represent important limitations on the ability of ocean carbon cycle models to forecast atmospheric CO_2 concentrations very far into the future. The IPCC study (1995) is a simple quantitative examination of structural uncertainty, taking the output of independently constructed models of the oceanic carbon sink to estimate the widely disseminated uncertainty in the ocean carbon sink for the 1980s of 1.2–2.8 Pg/yr. There is also an Ocean Carbon-Cycle Model Intercomparison Project (OCMIP), analogous to the Atmospheric Model Intercomparison Project (AMIP) which seeks to formally document the results of various contemporary ocean carbon cycle models. Naturally, these models have been tuned to be in good agreement with current observations so that their results show parametric convergence. On the other hand, it is arguably more straightforward to analyze the uncertainty in how the response of a particular ocean carbon sink model is dependent on the choice of parameters used to calibrate the model. The choice of diffusive parameters, for instance, common to both box models and dynamical models controls the amount of carbon entering the deep ocean and influences the carbon flux determined by the model.

4.3 Methods of Parametric Uncertainty Analysis

The basic question we want to answer with an examination of parametric uncertainty in complex models is how sensitive the outputs are to a given uncertainty in the inputs. Mechanisms and methods for assessing parametric uncertainty in models, such as the 2-D Oceanic Carbon Sink Model developed in this study, are numerous. Perturbation methods, Spectral methods, Neumann expansion methods, and moment methods are all existing procedures for addressing parametric uncertainty. However, these methods are hampered by the necessity that the model's equations be restructured to perform the analysis. The requirement that the dynamics of the model be essentially treated as a so-called "black box," constrains the number of viable methods available for performing uncertainty analysis on a complex model.

A general procedure for performing uncertainty analysis on a model may be summarized as follows:

1) Obtain or Develop a Model of a System
2) Decide on Uncertain Parameters in the Model
3) Specify the Probability Distributions of the Uncertain Variables
4) Promulgate the Uncertainty of the Parameters through the Model
5) Analyze the results, focusing on the contributions relative of the parameters to uncertainty in the outputs.

4.3.1 Monte Carlo Methods

One the most commonly cited method for addressing parametric uncertainty in complex models is the so-called Monte Carlo simulation. The method relies on choosing a random set of samples from the probability distributions of each of the input parameters that are deemed uncertain and running the model with that sample to calculate and record the resultant output. This procedure is repeated for a sufficiently large number of samples until a histogram of the outputs generates a discrete representation of the probability distribution function. It is asserted that this distribution approximates that of the true output variable in question. The Monte Carlo simulation is quickly revealed as highly impractical for studies of models requiring significant computational effort. This is inefficiency occurs because the number of runs necessary for a successful analysis of the model's outputs can typically run into the thousands. For climate studies, where even simple representations of the systems involved can require hours of computational time, the proposition of performing thousands of runs becomes unfeasible.

4.3.2 Probabilistic Collocation Method

Because of the computational impediment of using a traditional Monte Carlo method on complex and costly to run models such as those typically constructed for climate studies, an alternative method is required to perform an uncertainty analysis of the 2-D OCSM in this paper. The Probabilistic Collocation Method (sometimes called the Deterministically Equivalent Modeling Method or DEMM) which is described fully in Tatang, *et al.* (1997) is chosen for its inherent efficiency in analyzing large and sufficiently complex models.

The Probabilistic Collocation Method (PCM) allows for expansion into orthogonal polynomials, the probabilistic response of the examined model's uncertain outputs from uncertainty in its parametric inputs. The resultant polynomials, constitute a reduced-form version of the original model to which traditional uncertainty methods such as the Monte Carlo method can be applied with efficiency. To explain how the PCM operates, suppose we have a deterministic model *f*, where *y* is the output of the model obtained at the values of the *N* parameters of the model, *p*:

$$y = f(p_1, \ldots, p_n, \ldots, p_N) \tag{4.1}$$

Since the parameters of the real model are presumed to be known with some uncertainty, we treat these parameters as variable. By characterizing this uncertainty and assigning them with individual probability distributions, the parameters can be treated as random variables, $p_n(x)$ where *x* is the probability space of the distribution. Being a function of random variables, the model's output *y* also becomes a random variable, $y(x)$. This output variable can be seen as having a complex response surface that is *N*-dimensional which we want to approximate with polynomial functions of the parameters of the model: $H_n(p_n)$. For the PCM, we want these polynomials to be orthogonal functions of the parameters whose weighting functions are the probability distribution functions (PDFs) of the parameters. We therefore define the orthogonal polynomials (implementing a procedure called ORTHPOL outlined in Gautschi (1994):

$$H_n^{-1}(p_n) = 0$$
$$H_n^{0}(p_n) = 1$$

and

$$\int_{p_n} g_n(p_n) H_n^i(p_n) H_n^j(p_n)\, dp_n = \mathrm{C}\ \delta_{\mathrm{ij}} \qquad \text{for } i, j \tag{4.2}$$

where $g_n(p_n)$ is the probability distribution of the parameter, p_n and C is a constant, and δ_{ij} is the Kronecker Delta Function. For C=1 the orthogonal functions are also orthonormal. With these polynomials the independent random variables that represent the parameter inputs may be written as:

$$p_n = p_n^0 + p_n^1 H_n^1(p_n) \quad (\text{for } n = 1 \text{ to } N) \tag{4.3}$$

The dependent output y is approximated by a polynomial chaos expansion:

$$y = y_0 + \sum_{i_1}^{1\le i_1+\ldots+i_N\le M} \cdots \sum_{i_n}^{1\le i_1+\ldots+i_N\le M} \cdots \sum_{i_N}^{1\le i_1+\ldots+i_N\le M} y^{i_1 i_2\ldots i_N} H_1^{i_1}(p_1) H_2^{i_2}(p_2)\ldots H_N^{i_N}(p_N) \tag{4.4}$$

where M is the order of the expansion in $H_n(p_n)$. By running the model a sufficient number of times at selected values of the N parameters, p_n and obtaining the outputs y, the coefficients, y_0, $y^{i_1}, y^{i_2}, \ldots y^{i_N}$ of the polynomials are estimated. The polynomials are a reduced-form representation of the behavior of the model. Every output chosen for examination, $y_1 \ldots y_T$, will have its own polynomial chaos expansion in the form of Eq. 4.4.

If this expansion remains sufficiently accurate (*i.e.*, reproduces with acceptable error, the output of the model with the same parameter inputs), then a Monte Carlo approach can be applied to the resultant “meta-model” in a highly economical fashion (since the reduced models are simply polynomials) to determine the probability distribution of the model’s uncertain outputs, effectively by proxy.

4.4 Application of the PCM

Applying the PCM requires choosing probability distributions of the inputs and then calculating sets of N values (one for each parameter) from the PDFs of the parameters in order to solve the approximation. The polynomials used in the chaos expansion of the model (Eq. 4.2) are also used to generate the sets of parameter values that are used as inputs to runs of the original model to fit the coefficients of the orthogonal polynomials. The M+1 roots of the orthogonal polynomial of order M+1 that correspond to each of the parameters, p_n, are chosen as these points.

These parameter values used to estimate the polynomials are also called the “collocation points” and because they are chosen within the high probability region of each input parameter, the approximation of the outputs y_t is particularly good within this range. The error of the approximation is estimated by choosing another set of collocation points from the roots of the polynomials of next order M+2, repeating the approximation, and comparing it to the original. By iteratively increasing the order of the polynomial chaos expansions, M, the accuracy of the PCM approximation can be tested until the error of the approximation is sufficiently small to consider it a successful reduced-form model of the original model. The higher the order of the approximation, the more runs that are required to perform the analysis so there is a natural trade-off. Such an approximation must be made for every output examined for the model, y_t, but can be performed with the same sets of model runs and collocation points so that the number of outputs chosen is not prohibitive to the examination.

DEMMUCOM (Tatang, 1994) is a program written to automate the performance of the PCM approximation on a model with a given set of uncertain parameters and probability distributions. DEMMUCOM calculates the collocation points that will be used as inputs to the model runs from the probability distributions of the parameters provided to it as well as the order of the approximation that is desired. By inputing the resultant outputs from the runs to DEMMUCOM and running it a second time, it calculates the coefficients of the polynomial expansions (from Eq. 4.4), creating a so-called "meta-model" of the original, while reporting statistics of the accuracy of the approximation that can be used to evaluate the effectiveness of the results. Traditional uncertainty methods such as the Monte Carlo simulation described above, can then be applied to the meta-model as if it were the original model, itself.

5. APPLICATION OF UNCERTAINTY ANALYSIS TO THE 2-D OCSM

5.1 Preparing the Model for Uncertainty Analysis

A model developed to be analyzed with the Probabilistic Collocation Method needs to be adapted to be run recursively with new parameter values read in as inputs that will change with every run necessary to make the approximation. The number of runs of the original model that is necessary is dependent on the order of polynomial fit chosen to approximate the model's outputs (as indicated in Section 4.4). Since the initial conditions of the model differ slightly for any changes in the input parameters, the ocean carbon sink model needs to be driven to a new pre-industrial steady-state with an atmospheric CO_2 concentration of 277 ppm and spun-up to the present state with the historical CO_2 record for each set of parameters values before a new atmospheric CO_2 forecast can be calculated.

After choosing the uncertain parameters that are considered important to the outputs of the model, the probability distribution functions for the uncertain parameters chosen in this study need to be specified. The DEMMUCOM program requires not only specifying the distributions of these inputs, but also choosing the individual outputs for which an approximation is going to be made and the order of the polynomial model that will describe each of these outputs. Provision must be made to save the chosen outputs separately (and concatenated for all the runs) in order to be fed back to the DEMMUCOM program to produce the desired approximation. The outputs selected for approximation by the probabilistic collocation method in this study are the oceanic carbon sink at five year intervals between 1765 and 1990, at five year intervals between 1990 and 2100, and the atmospheric CO_2 concentrations forecast between 1900 and 2100 by the ocean carbon sink model under a fixed emissions scenario (Section 3.1.1) and constrained by the observed carbon budget described in Section 3. Finally, the original model must also be available to test the performance of the polynomial approximations, by performing additional runs with different parameters values than the ones chosen for the approximation and comparing the outputs.

5.2 Uncertain Parameters in the 2-D OCSM

The first step required to perform the uncertainty analysis on the 2-D Ocean Carbon Sink Model is to determine the uncertain input parameters to which the model's outputs are most sensitive. Because the number of runs required to perform the analysis grows quickly with the number of parameters, a trade-off is inherently involved for sufficiently complex models. The sensitivity study performed in Section 3.3, makes it reasonable to assume that all six of the parameters chosen there should be retained for the uncertainty analysis. These uncertain parameters are treated as random variables with probability distribution functions that are known, or must be approximated.

In Section 3.3.1, the importance of the mechanisms that determine the "solubility pump" for carbon were addressed, and the following six parameters were chosen as potentially important in the processes that determine the size of the global oceanic carbon sink. Because these quantities have not up until now been frequently or very well observed, empirical estimates of their probability distributions are not possible and their distributions must be qualitatively specified. Such specification is made based on a combination of the current state of knowledge and the judgment of the author. The principle chosen to guide the specification of these distributions is that they are designed to be broad and to capture as much of the uncertainty supported by the observations so that the maximal reasonable parametric uncertainty can be examined. The probability distribution of the six uncertain parameters are specified below:

a) K_V - The Coefficient of Vertical Diffusion

The coefficient of vertical diffusion controls the amount dissolved inorganic carbon that is drawn out of the mixed layer, effectively delaying surface saturation with respect to CO_2 and drawing more carbon into the ocean. The global average value of the diffusion vertical coefficients determined for tritium mixing and weighted by ocean area are approximately 2.5 cm^2/s (Fig. 2-7) and this is consistent with the global rate of vertical mixing used by 1-D models estimated from bomb-produced radiocarbon (Oeschger, *et al*. 1975; Broecker and Peng, 1994). These are the reference values used in the 2-D OCSM and they are larger than the diffusion coefficients used in dynamical ocean general circulation models because these coefficients must account for all vertical transport by apparent diffusion alone. It is found that the range of 0.5 cm^2/s (one-fifth) to approximately 12.5 cm^2/s (factor five) is what is needed to match the range of uncertainty in the delay of warming by the ocean produced by the uptake of heat perturbations (when treated as a conserved tracer) by various AOGCMs (Sokolov and Stone, 1997) by this same diffusion scheme. These uncertainties are probably due to different assumptions about sub-grid scale mixing in these models and the relative sensitivity of the mixing rate to these parameterizations. But these observations provides a broad range around which to gauge an estimate of the uncertainty in the diffusion parameter that is also consistent with the still large uncertainties extant in the various tracer inventories and distributions (IPCC, 1995).

The beta distribution is chosen to characterize the probability distribution of the coefficient of vertical diffusion because it allows for specification of the probability range of the variable while constraining it within a specified interval: 0 and c > 0:

$$f(x)=\frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}\left(\frac{x}{c}\right)^{\alpha-1}\left(1-\frac{x}{c}\right)^{\beta-1}\left(\frac{1}{c}\right)$$

it has the following properties: symmetric if $\alpha = \beta$, asymmetric otherwise, the mean is $\alpha/(\alpha+\beta)$, the variance is $\alpha\beta/(\alpha+\beta)^2$ and it can be transformed linearly. For vertical diffusion (a quantity which is restricted to be positive), it is subjectively estimated that the median of the distribution will remain at the reference value of 2.5 cm^2/s with a 50% probability that it is either greater or lesser. Using the range needed to fit the mixing of various AOGCMS, it is decided that the probability is only 5% that it is smaller than 0.5 cm^2/s and 95% that is smaller than 12.5 cm^2/s, giving a beta distribution with parameters $\alpha = 2.72$ and $\beta = 12.2$, which is depicted in Fig. 5-1.

b) K_H - The Coefficient of Horizontal Diffusion

Due to latitudinal gradients in DIC carbon created largely by gradients in surface temperature and the differential flux of carbon into the ocean, the rate of horizontal diffusion is important in controlling the amount of downwelling dissolved inorganic carbon that is drawn equatorward. Various processes forced by the wind-driven circulation that are strongest near the surface effect this transport. As a rough estimate, assume a gyre circulation of about 35 Sv in a latitude zone between 20° and 40° that is 60 degrees wide and 500 meters deep, which gives a recirculation time of about 5 years. Meridional mixing with an equivalent horizontal diffusivity of about $2.5 \times 10^4\ m^2s^{-1}$ is needed to explain the latitudinal transport which provides an estimate for horizontal mixing in the ocean. By further assuming that this rate falls off exponentially as a function of depth as indicated in Fig. 2-8, a rough measure of the reference strength of the horizontal mixing in the ocean can be conservatively estimated. This estimate can be subjectively estimated to be in error by a factor of two. So a beta distribution for this parameter is chosen, spanning the range 0 to 2 times the reference value set above, with parameters $\alpha = 3.5$ and $\beta = 3.5$. This gives a symmetric distribution with a 50% probability that diffusion parameter is within 0.5 and 1.5 times the reference value.

c) V_p - The Piston Velocity

The piston velocity parameter determines how much CO_2 is transferred across the air-sea interface for a given wind speed. It is an increasing function of the wind speed and acts on the concentration gradient between air and sea to drive a flux. The current global mean transfer rate should be consistent with the empirically measured rate of 20 ± 3 moles of $CO_2/m^2/yr$. Tans, *et al.* (1990), point out that the factor calculated by Liss and Merlivat (1986) and multiplied by the wind speed to calculate the transfer velocity for a given difference in partial between the atmosphere and ocean is easily uncertain to within a factor of two. Since the Liss and Merlivat specification is used in this model as a reference value, a factor 2 and 0.5 times the standard formulation is assumed to contain about one standard deviation of the probability (approximately 67%). Because the coefficient of transport cannot be negative, the beta distribution is also chosen and constructed assuming a mode of 1 (the reference value). The asymmetry assumed above indicates that the probability that the piston velocity factor is less than 1 is $^{1}/_{3}$ and greater than it $^{2}/_{3}$. It is assumed to range between 0 and 5, with a 95% probability that it is less 3 times the reference.

d) K_0 - The Henry's Law Coefficient

The Henry's law coefficient determines the amount of dissolved carbon dioxide necessary to balance a given partial pressure of CO_2 in equilibrium. It is highly temperature dependent and determines the air-to-sea gradient of CO_2 by computing the partial pressure of the dissolved gas based on its concentration. The normal distribution is chosen to characterize the uncertainty in the Henry's law coefficient, with properties μ = mean and σ^2 = variance:

$$f(x|\mu,\sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-(x-\mu)^2 / 2\sigma^2}$$

Reference values are taken from Weiss (1974), which at 20° C and 35 $^{o}/_{oo}$ salinity gives a value of pK_0 ($-\log10(K_0)$) approximately 3.2. A standard deviation of ± 0.1 pK is assumed normally distributed from this reference.

e and f) K_1 and K_2- The First and Second Disassociation Constants of Carbonic Acid

The first and second disassociation constants for carbonic acid determine the partitioning of dissolved CO_2, dissolved carbonate and bicarbonate in the surface ocean and therefore affect the air-to-sea gradient in CO_2. Strongly temperature dependent, as well as dependent on salinity and pressure, these parameters in conjunction with the Henry's law constant control the magnitude of the "Revelle Factor," an empirical measure of the effective amount of dissolved CO_2 that can be taken up by the ocean in equilibrium with other dissolved carbon species (from Eq. 1.1).

The values for these parameters have been measured empirically in a handful of studies (Mehrbach, 1973; Hansson, 1979; Goyet and Poisson, 1989; Roy, *et al*. 1993; Lee and Millero, 1995). A study of the uncertainty in these coefficients performed by Lee and Millero (1995) show that most of these measurements do a reasonable job of fitting the observations of quantities such as dissolved inorganic carbon, alkalinity, and pH with standard deviations in the range of .01–.04 pK units. Because of that uncertainty, the values of these coefficients in this study are assumed normally distributed. The parameters are assumed to have a mean in the middle of the observations of $pK_1 = 5.89$, $pK_2 = 9.04$ at 20° C and 35 $^{o}/_{oo}$ with standard deviations of ± 0.05 pK units, slightly larger than the estimates that focused on data from the North Atlantic so to account for the accumulation of errors when zonally-averaged temperature values used to determine the coefficients. The probability distributions of the six input parameters are displayed in **Figure 5-1**.

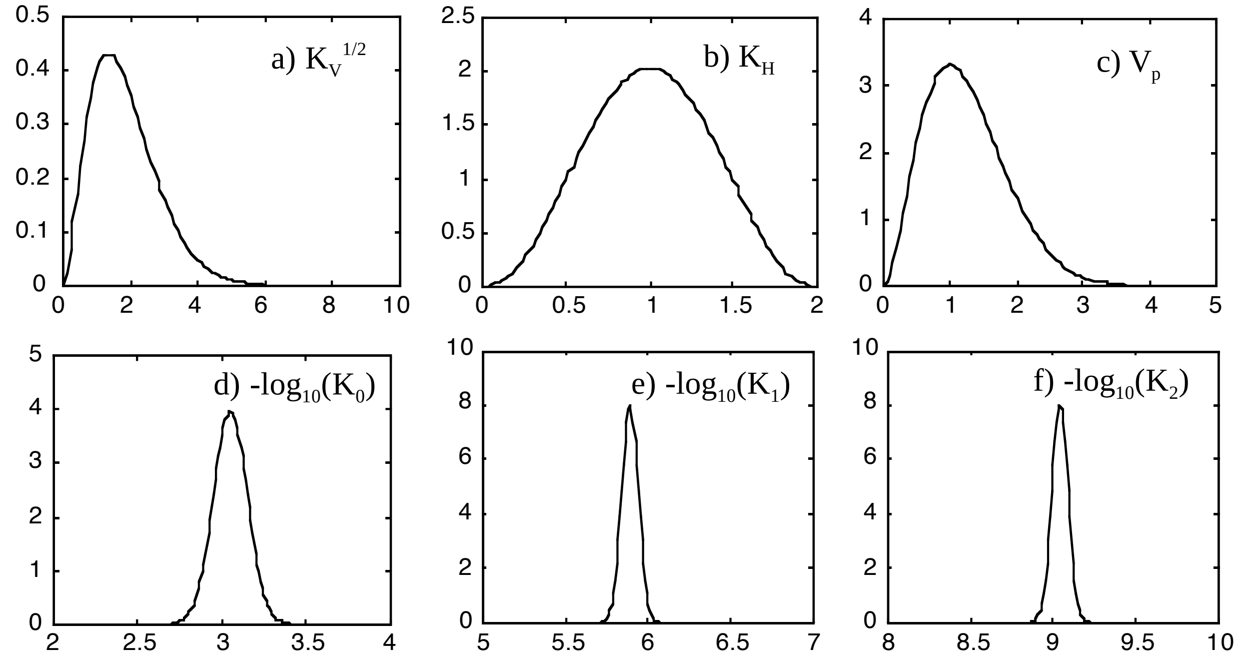


Figure 5-1 Probability Distributions of the Uncertain Parameters in the 2-D OCSM

5.3 Uncertain Response of the 2-D OCSM

After the probability distribution functions for the six uncertain parameters are chosen and DEMMUCOM is called to generate the collocation points for the uncertainty run, the procedure outlined in Section 4.4 is followed to generate the approximation of the outputs. A third-order fit with cross-terms in all six of the parameters is chosen to approximate the model's outputs, requiring a total of 74 runs of the 2-D OCSM to complete. The historical oceanic carbon sink calculated by the 2-D OCSM is approximated by the PCM at five year intervals between 1765 and 1990 and the results between 1860 and 1990 are displayed in **Figure 5-2**. Plotted is the mean and error bars that represent one standard deviation of the ocean carbon sink approximation calculated by the model as a function of time.

The trend in the mean ocean carbon sink determined by the approximation is qualitative similar to the result that was obtained when the model was spun up with the reference parameter values (Fig. 2-12) with an increasing oceanic sink from pre-industrial times to 1990. Most of the increase in the oceanic carbon sink has come in the last 90 years of the run when atmospheric CO_2 has been rising the fastest. However, the mean oceanic carbon sink in the 1980s estimated by the approximation is 1.84 Pg/yr, about 7.6% higher than in the reference run with 1.71 Pg/yr. The standard deviation of the result which grows with time over the course of the approximation, averages about 0.68 Pg/yr in the 1980s, giving a range of values for the oceanic carbon sink of 1.16–2.52 Pg/yr (with 67% confidence). The IPCC (1994) range for the 1980s oceanic carbon sink from structural uncertainty is only slightly smaller and is estimated at 1.4–2.6 Pg/yr, however with a subjective estimate in confidence of 90% (Siegenthaler and Sarmiento, 1993).

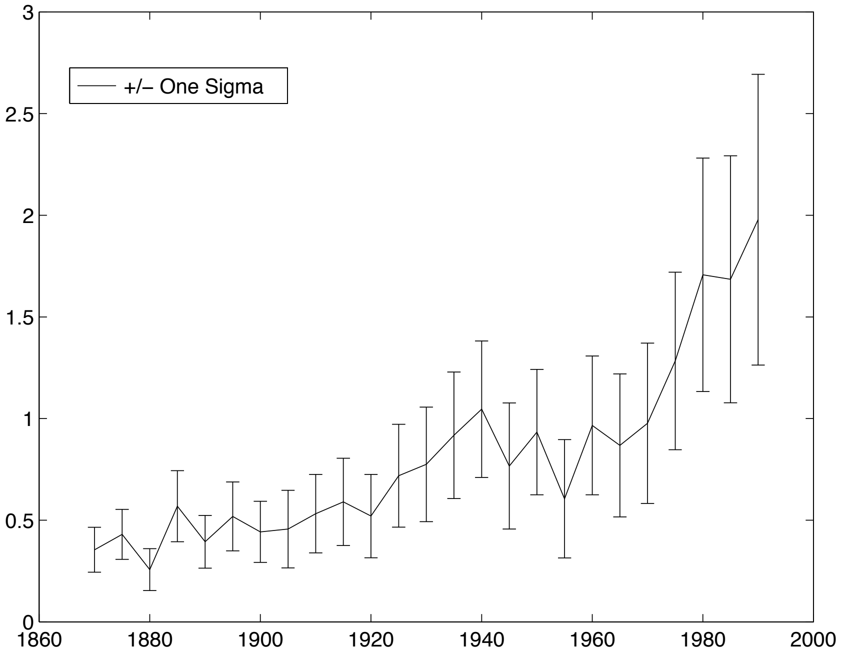


Figure 5-2 Mean and Standard Deviation of the PCM Approximation of the Historical Oceanic Carbon Sink (in Pg/yr)

Looking more closely at the approximation for the mean 1980s ocean carbon sink, the reduced-form model of the 2-D OCSM for the sink by the PCM is subjected to a 10,000 run Monte Carlo simulation to generate a discrete representation of the probability distribution of the output in the form of a histogram shown in **Figure 5-3**. The probability distribution of the output: the mean oceanic carbon sink for the 1980s, covers a broad range of values with over 90% of the probability contained between 0.0 and 4.0 Pg/yr, indicating that the uncertainty in the carbon sink derived from the uncertainty in the input parameters for this model has exceeded that of the IPCC (1994) range from structural uncertainty alone.

5.3.1 Forecasting Atmospheric CO_2 Concentrations Under Uncertainty

Using the same emissions (fossil fuel + deforestation) scenario as for the reference forecast in Section 3.2, the atmospheric CO_2 concentration is forecast under the uncertainty in the input parameters described in Section 5.2. The PCM is used to approximate the atmospheric CO_2 concentration at 5 year intervals between 1990 and 2100. The mean of the approximation and the standard deviation is plotted in **Figure 5-4** along with the reference calculation (dotted-line) from Fig. 3-5 in Section 3.

The mean atmospheric CO_2 forecast predicts slightly lower atmospheric CO_2 concentrations than the reference run, though the latter clearly falls well within the uncertainty of the approximation. The atmospheric CO_2 concentration forecast in 2100 is 705.1 ppm compared to 715.5 ppm in the reference (about 1.5% smaller), implying that the mean oceanic carbon sink as a function of time is higher in the approximation than in the reference. As one might expect, the uncertainty in the atmospheric CO_2 concentration forecast by the model grows with time and the standard deviation is 47.2 ppm by 2100. That indicates an uncertain range of nearly 100 ppm (with 67% confidence) in the forecast atmospheric CO_2 concentration in 2100 from the solubility sink in the ocean alone.

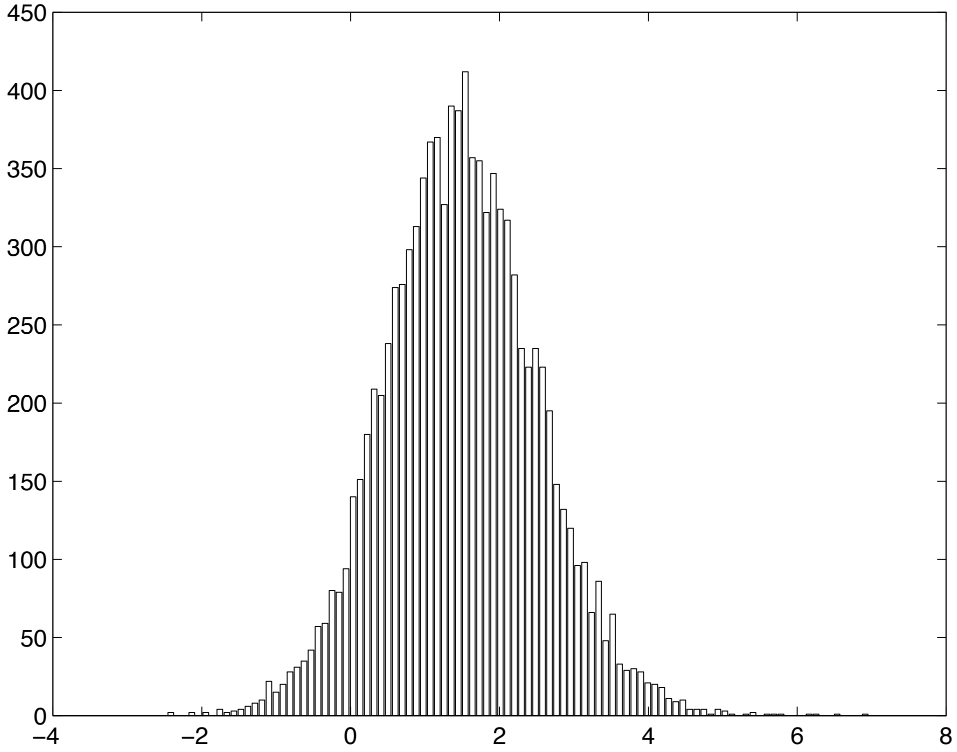


Figure 5-3 Histogram of 10,000 Monte Carlo Runs for the Approximation for the mean 1980s Oceanic Carbon Sink (in Pg/yr)

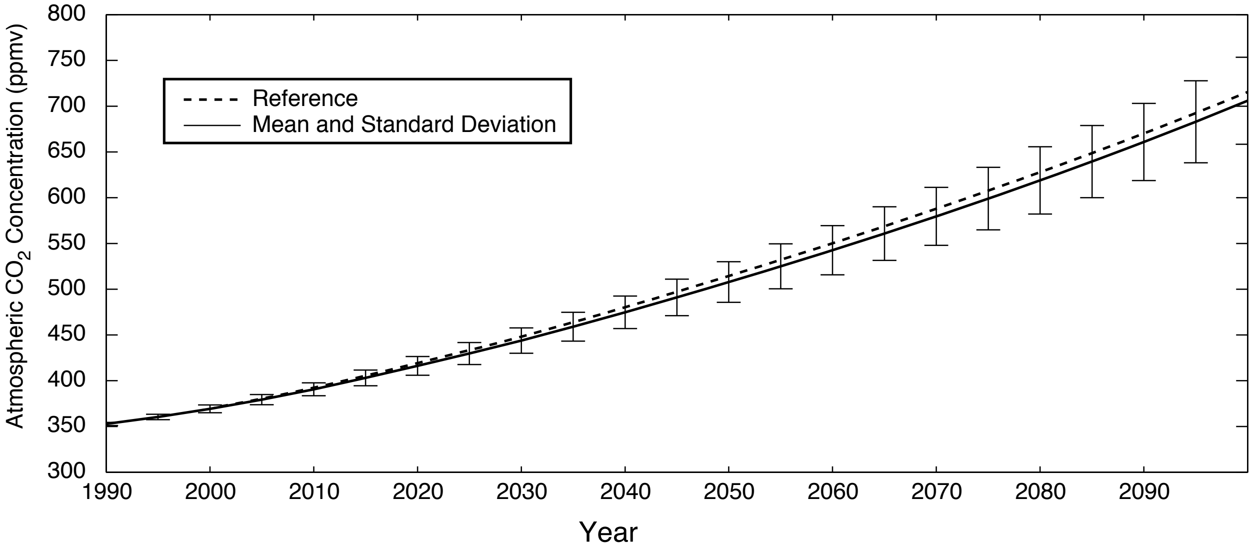


Figure 5-4 Mean and Standard Deviation of PCM Approximation of the Atmospheric CO_2 Forecast: 1990-2100

Looking specifically at the forecasts made in 2000, 2050, and 2100 by the model and the polynomial fits to the atmospheric CO_2 concentration in those years created by the PCM, a Monte Carlo simulation of 10,000 runs is calculated to produce discrete probability distributions of the outputs, as shown in **Figure 5-5**.

As expected, the probability distribution of the outputs broaden as a function of time due to an accumulation of uncertainty. The extent of the uncertainty in atmospheric CO_2 concentrations is dependent on the character of the uncertainty asserted in the input parameters. For the uncertainty asserted in Section 5.2, the range covered by two standard deviations in the atmospheric CO_2 concentration by 2100 is almost 200 ppm.

The range of the uncertainty in atmospheric CO_2 concentrations is actually smaller than it might have been absent the assumption of an atmospheric CO_2-depedent terrestrial sink (described in Section 3.1.3). Looking at the uncertainty in the variable component of the B_t term in the carbon budget (Eq. 3.1), NEP, which depends on the atmospheric CO_2 concentration, the PCM can be used to estimate the uncertainty in the terrestrial ecosystems (TEM) sink, which is plotted in **Figure 5-6**.

By 2100, the mean terrestrial carbon sink grows to over 3.9 Pg/yr and the variable component has an uncertainty of 0.25 Pg/yr (with 67% confidence) due to the uncertainty of the oceanic sink for carbon. Because the size terrestrial carbon sink is positively dependent on atmospheric CO_2

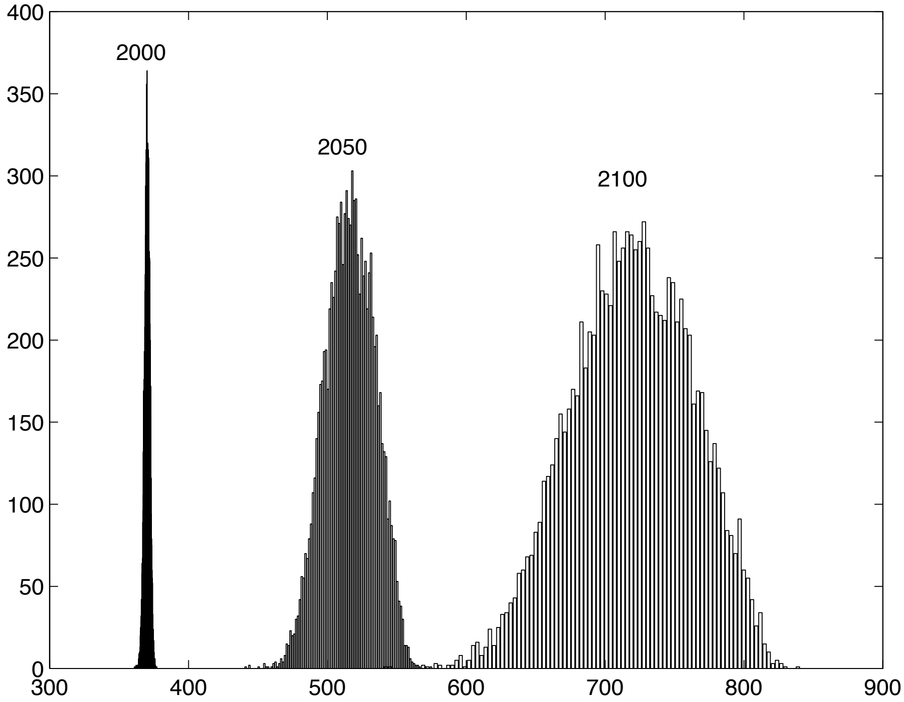


Figure 5-5 Histograms of 10,000 Monte Carlo Runs of the Approximation of Atmospheric Concentrations in 2000, 2050, and 2100

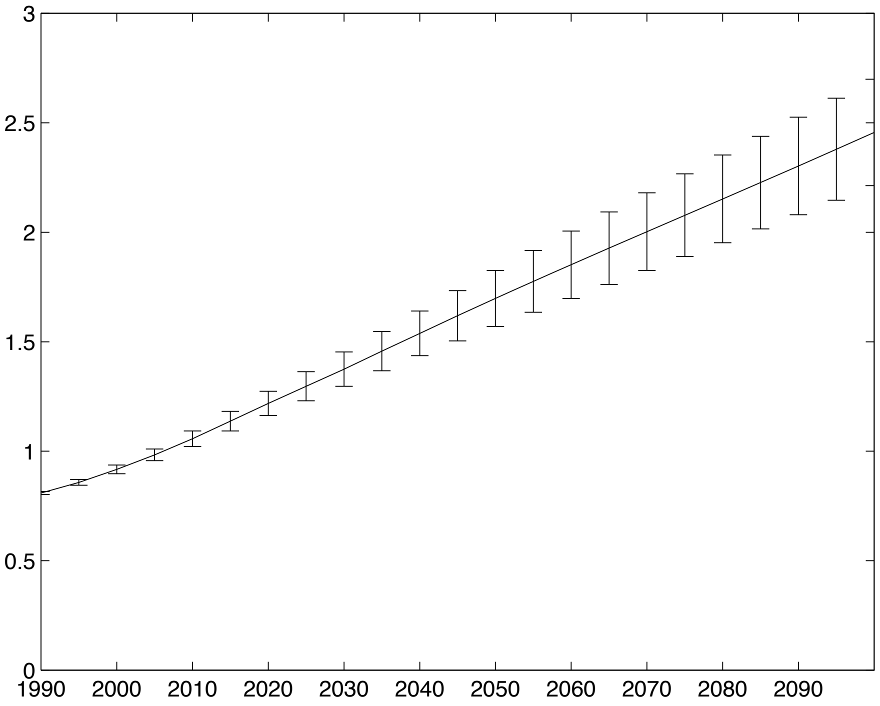


Figure 5-6 Uncertainty in the TEM Sink Implied by Uncertainty in the 2-D OCSM (in Pg/yr)

concentrations it acts as a negative feedback to atmospheric CO_2 concentrations. When atmospheric CO_2 concentrations rise faster (because of a smaller oceanic sink driven by changes in its parameters) the terrestrial sink increases faster which slows the increase in atmospheric CO_2 concentrations. Conversely, when atmospheric CO_2 concentrations rise slowly because of a fast growing ocean sink, the terrestrial sink rise slowly, increasing atmospheric CO_2 concentrations. This represents a decrease in the uncertainty in atmospheric CO_2 concentrations relative to an assumption of a fixed terrestrial sink for carbon because of interactions between the two sinks. More such interactivity is discussed in Section 6.1 and expanded to include the contribution of parametric uncertainty in the terrestrial sink.

5.3.2 Relative Importance of the Uncertain Parameters

The uncertainty in the six parameters chosen for this study is directly responsible for the uncertainty in the oceanic carbon sink (Fig. 5-2) and the atmospheric CO_2 concentration (Fig. 5-4) seen above. However, not all of the chosen parameters contribute to this uncertainty equally and neither is their relative impact the same as a function of time. The DEMMUCOM program reports not only the mean and standard deviation of the output variables it approximates, but the relative contribution of each parameter to the variance of the output variable. For example, looking at the value of the mean oceanic carbon sink for the 1980s, the relative contribution of each parameter to the total variance is noted in **Table 5-1**.

Table 5-1 Contributions of the Parameters to the Variance in the Average 1980s Carbon Sink

Parameter	% Contribution to Standard Deviation
K_V	51.91
K_H	5.26
V_p	18.97
K_0	0.01
K_1	6.57
K_2	2.80

The coefficient of vertical diffusion clearly dominates all of the other parameters in terms of its importance to the uncertainty in the output, contributing more than half of the variance. This is undoubtedly owing to the fact that the surface ocean is usually close to equilibrium with the atmosphere and that the major control on whether more carbon can be taken up in the sea is the amount exported to depth from the mixed-layer. The only other large factor appears to be the piston velocity which controls the air-to-sea exchange rate. For positive gradients into the ocean, this factor determines the size of the oceanic carbon sink that drives the ocean back to a steady-state with the atmosphere. The effects of uncertainty in the three chemical parameters are small.

Plotting the contribution to the variance in the forecast atmospheric CO_2 concentration between 1990 and 2100 for all six of the input parameters, it is found that their relative contributions change as a function of time, as shown in **Figure 5-7**.

The major trends that are evident in this graph include the fact that the importance of the coefficient of vertical diffusion increases from 50% to 75% of the total variance. The relative importance of the piston velocity collapses from under 20% in 1990 to 1% of the total variance in 2100 implying that the large gradient between the atmosphere and ocean and not the surface exchange rate is controlling the carbon flux in the future. The importance of all three of the chemical parameters, K_0, K_1, and K_2 steadily increases as a function of time from a combined

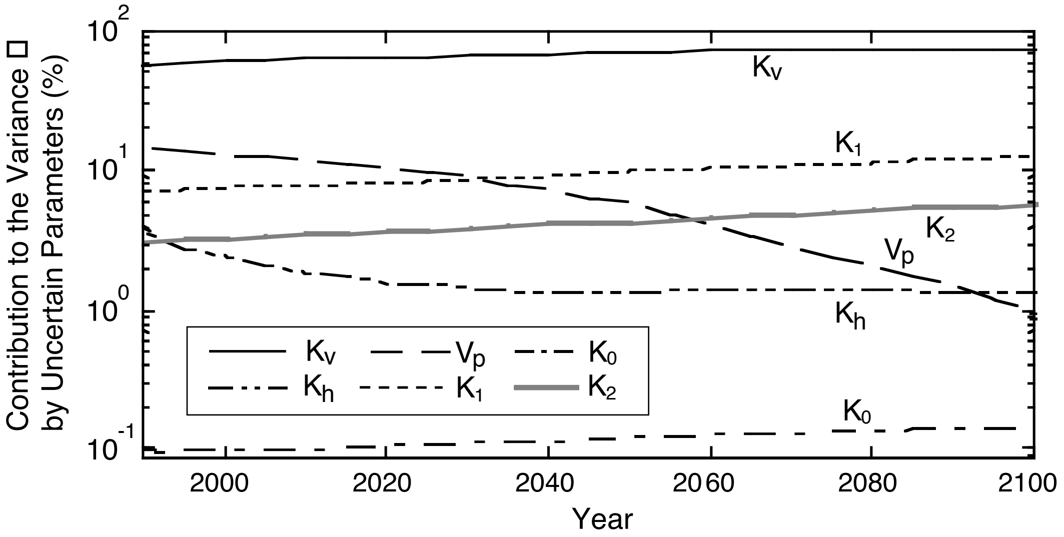


Figure 5-7 Percentage Contribution to the Variance by the Uncertain Parameters

9.5% in 1990, doubling to nearly 19% in 2100. This can be speculated to occur because of the effect of a changing effective “Revelle Factor” as the carbon sink becomes increasingly sensitive to the chemistry of the surface water due to near-surface saturation as more of the dissolved carbon is held as dissolved CO_2.

5.3.3 Accuracy of the Uncertainty Estimates

A third order approximation with cross-terms appears to do a very good job of fitting the output of the 2-D OCSM. However, there are quantitative means of checking the performance of PCM in approximating the behavior of the oceanic carbon sink model. One such variable is the index of agreement, d (Wilmott, 1982), which measures the quality of the approximation to the performance of the actual model by summarizing such normally calculated indexes such as the root mean square error, the mean absolute error, the intercept and the slope of the least-squares regression among others:

$$d = 1 - \left(\frac{\sum_{i=1}^{N} (y_M^i - y_A^i)^2}{\sum_{i=1}^{N} \left(\left| y_A^i - \bar{y}_M \right| + \left| y_M^i - \bar{y}_M \right| \right)^2} \right)$$

where N is the number of runs used to check the error, y_M is the true model result and y_A is the approximated model result. The closer to unity that d is, the better the approximation. d is calculated for each of the output variables that is fit by the polynomials with 50 runs of the model using randomly chosen parameters and found to range between 0.9977 and 0.9963 for the atmospheric CO_2 concentration between 1990 and 2100 and 0.9951 and 0.9989 for the oceanic carbon sink between 1860 and 2100. These are very good agreements and indicate that the reduced-models do a very effective job of capturing the variability of the real model.

Figure 5-8 shows the accuracy of the fit of atmospheric CO_2 concentrations in the year 2000 by plotting the results obtained from runs by the full 2-D OCSM model and the polynomial fit to the model obtained from the PCM approximation for the same 30 randomly chosen sets of parametric inputs.

The results should fall along the diagonal line to be considered good and indeed they show that the approximations by the “meta-model” and the original model are in very good agreement. Looking beyond the year 2000, knowing that the uncertainty in the outputs is increasing as a function of time, the same experiment is conducted in the years 2050 and 2100 and the comparisons are plotted in **Figure 5-9**.

The reduced-form model does a reasonably good job at approximating the output of the real model as a function of time. However, it becomes more evident in Fig. 5-9 that the reduced-form models produced by the PCM do a better job of approximating the real model in the regions of high probability for the uncertain parameters than further out in the tails of the distributions. As pointed out in Section 4.3 this is an artifact of the way the PCM is constructed as it meant to be most effective in the high probability regions of the input parameters and output variables.

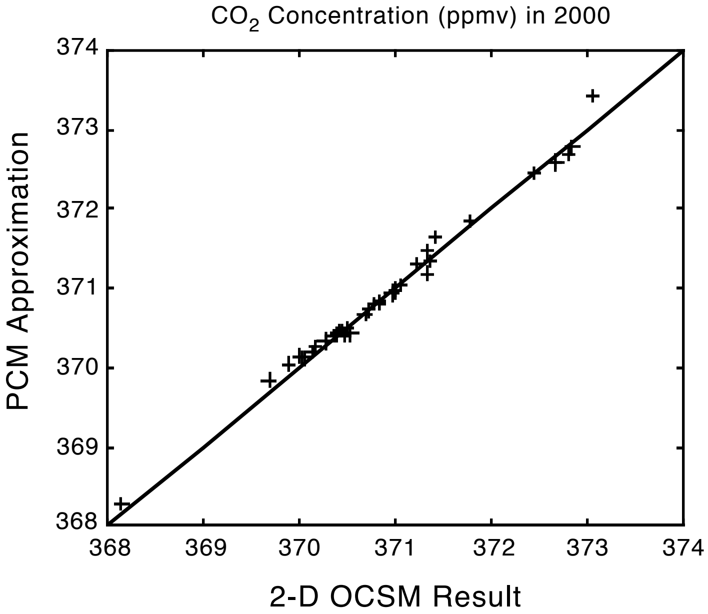


Figure 5-8 Accuracy of the Forecasts of Atmospheric CO_2 Concentrations in 2000

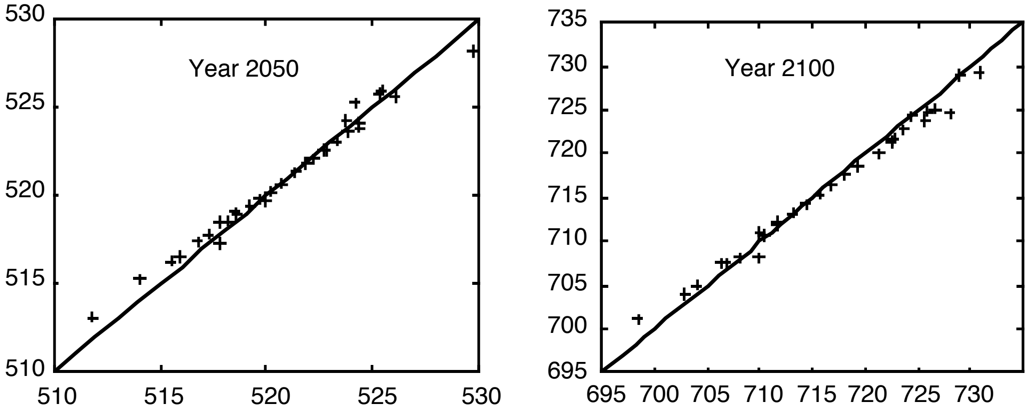


Figure 5-9 Accuracy of the Forecast of Atmospheric CO_2 Concentrations in 2050 and 2100

5.3.4 Sensitivity of the Results to Parametric Specification

Applying the probabilistic collocation method to a model allows you to characterize the uncertainty in a model's outputs to its parametric inputs. In the case of this study, because the accuracy of the "meta-model" approximation to the real model is very good as is demonstrated in Section 5.3.3, uncertainty in the results of the results of the uncertainty in the oceanic carbon sink approximated for the 2-D OCSM are not so much dependent on failures of the PCM, but rather on the quality of the input parameter probability distributions (Fig. 5-1) used to perform the analysis. Assuming the model of the system being examined is well-constructed and if the probability distributions of the input parameters are known with certainty, then the uncertainty in the outputs could be regarded as very good estimates of the true uncertainty in the behavior of the modeled system. As noted in Section 5.2, however, the probability distributions of the six inputs chosen for this study are not very well known, so we must test for the possibility that the results are going to be sensitive to the PDFs that were chosen to produce them.

Therefore, for the six parameters chosen in Section 5.2 the PCM approximation was performed again with uniform probability distributions that span a range of probability equivalent to two standard deviations from the reference values chosen to drive the model in Section 2. This requires computing new collocation points for the estimation followed by new runs of the 2-D OCSM to re-estimate the polynomials fits to the outputs. The new distributions are plotted in **Figure 5-10**.

Performing the approximation once again using the PCM with the new input parameter distributions and calculating the mean oceanic carbon sink for the 1980s, we can compare its probability distribution to the previous result by constructing a histogram of the contemporary carbon sink estimated by the model, as shown in **Figure 5-11**.

The distribution of the new oceanic carbon sink has a slightly higher mean and somewhat larger standard deviation than the previous result, with a new mean sink of 1.92 ± 0.93 Pg/yr. This indicates that changes in the input parameter distributions do have direct and quantifiable impacts on the estimates of the outputs of the model. The new input parameter specifications have scarcely changed the mean oceanic sink upwards by 6%, but have increased the standard deviation by almost 37%, increasing significantly the parametric uncertainty of the contemporary carbon sink.

Using the new probability distributions to forecast atmospheric CO_2 concentrations it is found that the mean concentration path is not significantly different from the previous result. The mean and standard deviation of the approximation are plotted in **Figure 5-12**.

The mean atmospheric CO_2 concentration forecast in 2100 is 698.7 ppmv which is only 1% smaller than the prior estimate using the initial parameter distributions and only 2.3% smaller than

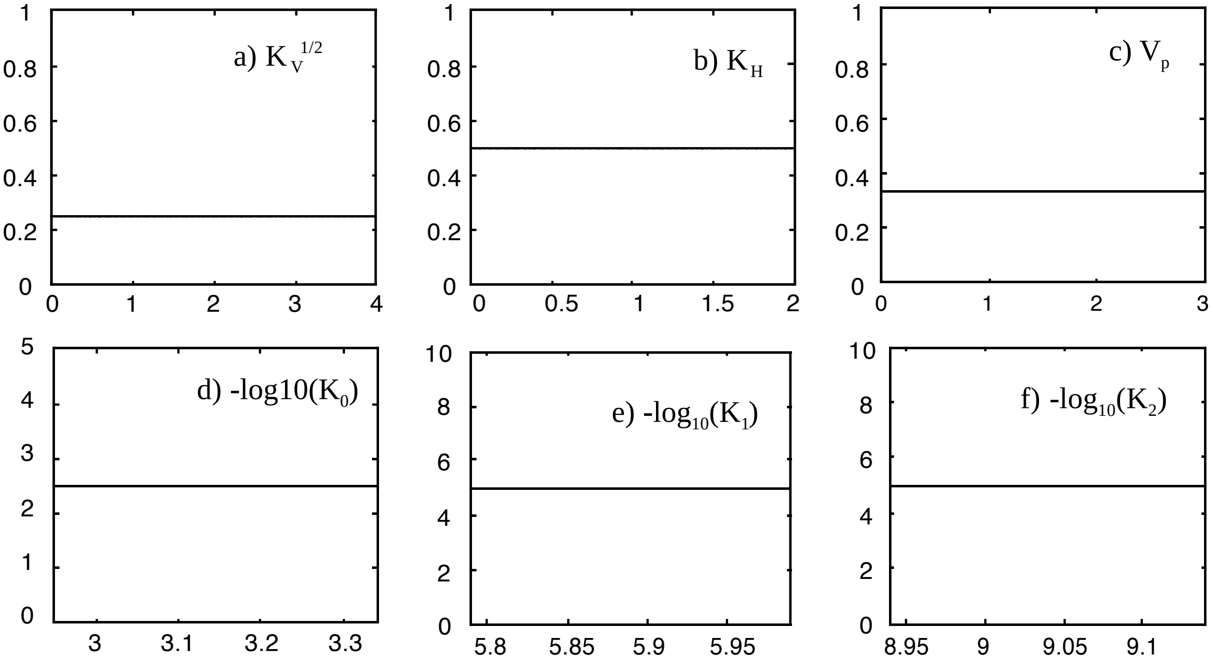
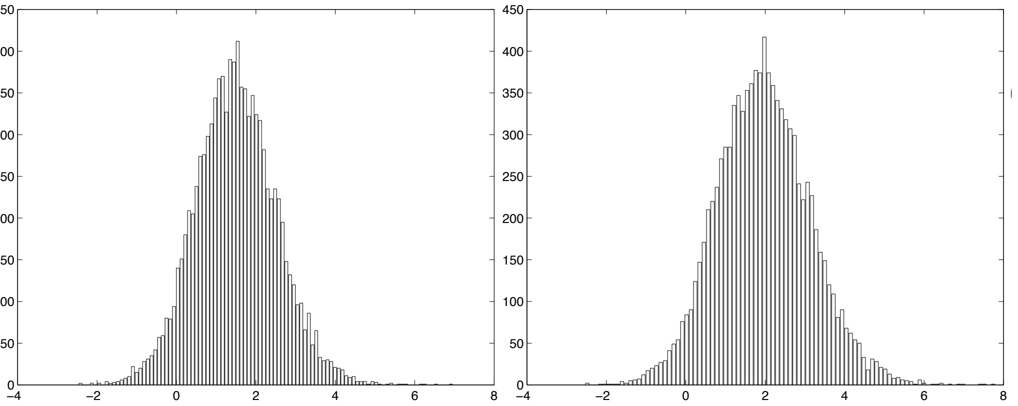


Figure 5-10 Uniform Probability Distributions for the Uncertain Parameters



Previous Parameter Distributions

Alternate Parameter Distributions

Figure 5-11 A Comparison of the PDFs of the Average 1980s Oceanic Carbon Sink Between the Two Parameter Specifications (in Pg/yr)

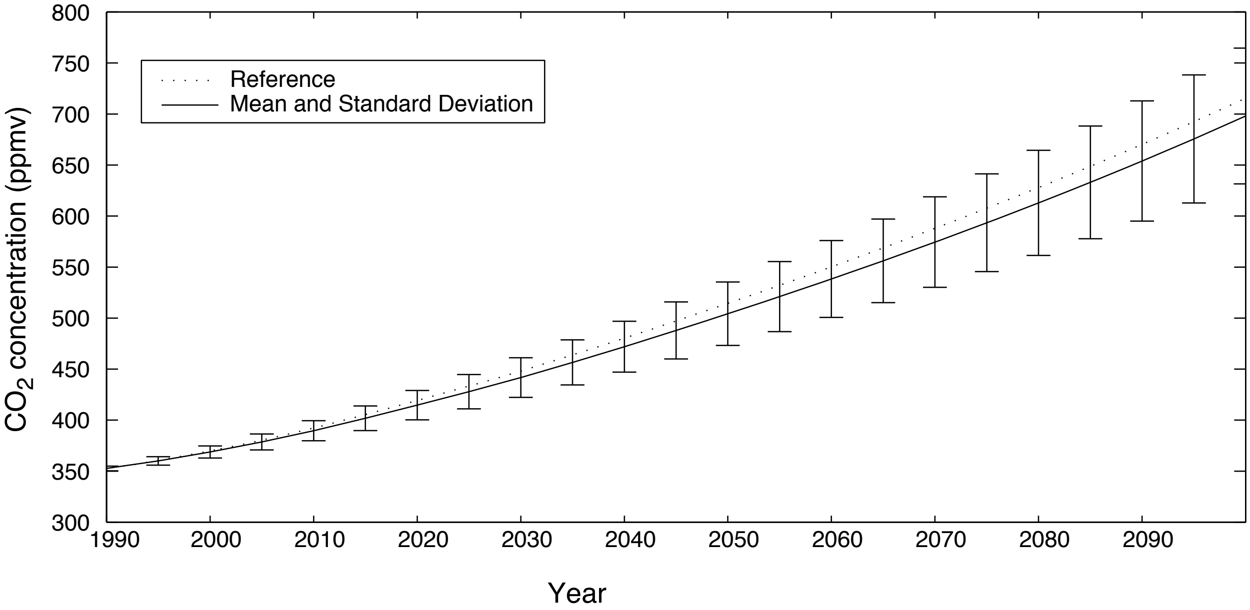


Figure 5-12 Uncertainty in Atmospheric CO_2 Concentrations from Alternate Parameter Distributions

the reference value of 715.5 ppmv. On the other hand, the standard deviation of this approximation is much larger, increasing from 47.2 ppmv in 2100 in Section 5.3.1 to 66.8 ppmv here. Since for each of the new probability distributions, no particular parameter value is favored among the others over a broad range of values, the mean oceanic carbon sink and hence mean atmospheric CO_2 concentration is a fairly robust result for this model and is not very sensitive to the particular shapes of the PDFs that are specified. However, the increase in parametric uncertainty (as indicated by the large change in variance) is a direct result of the change in input parameter distributions. As expected, the range of uncertainty in the outputs is shown to be directly keyed to the assumptions of uncertainty in the parametric inputs.

6. CONCLUSION

6.1 Summary and Observations

In this thesis a parameterized model of the oceanic sink for carbon has been constructed for use in studies of the contemporary global carbon budget and for forecasting future atmospheric CO_2 concentrations in climate change simulations. The 2-D Ocean Carbon Sink Model (2-D OCSM) described in Section 2 determines the global sink for CO_2 in the ocean by means of the so-called “solubility pump” mechanism including air-to-sea exchange, dissolution in the surface mixed-layer, and diffusive mixing of dissolved carbon to sequestration at depth. The marine organic carbon cycle is assumed to be nutrient limited and not a net sink of carbon. It is therefore not included in this simple model. Using reference parameter values, the model is initialized by being driven to a steady-state with a pre-industrial atmospheric CO_2 concentration of 277 ppmv before being spun up to the present using the historical atmospheric CO_2 record to generate a current oceanic carbon sink of 1.7 Pg/yr, consistent with the results of other oceanic carbon sink models. The model is used to forecast atmospheric CO_2 concentrations into the next century by closing the current global carbon budget with the addition of an atmospheric CO_2 concentration-dependent parameterization of the land sink for carbon estimated from the Terrestrial Ecosystems Model (Xiao, *et al.*, 1997) in Section 3.1.3 and driving it into the future with an anthropogenic emissions scenario equivalent to the IS92a scenario of the IPCC (1992).

The 2-D OCSM has been developed with an acknowledgment of the parametric uncertainty inherent in calibrating the model to agree with current observations. This study explores that uncertainty quantitatively by examining the uncertainty in the outputs from specified uncertainty in the input parameters through the application of the Probabilistic Collocation Method (Tatang, *et al.*, 1997) described in Sections 4.3-4.4. The PCM makes it possible to efficiently quantify the uncertainty in the model’s most important outputs: the global oceanic carbon sink and future atmospheric CO_2 concentrations. The method requires specifying the probability distributions of the input parameters and the order of the polynomial approximation of the model’s outputs. For the 2-D OCSM, the air-to-sea piston velocity, the Henry’s Law coefficient, the first and second dissociation constants for carbonic acid, and the vertical and horizontal diffusion rates are the parameters chosen to represent the uncertainty in the model’s primary carbon sink mechanisms.

For a reasonable range of uncertainty in these six parameters, the mean oceanic carbon sink for the 1980s is calculated to be 1.8 ± 1.3 Pg yr^{-1} (with 95% confidence). When compared to the IPCC range for the uncertainty of the oceanic carbon sink of 2.0 Pg yr^{-1} ± 0.8 Pg (1992; 1994; 1995), it is demonstrated that the parametric uncertainty in this oceanic carbon sink model is more than sufficient to span this range. The IPCC range is due primarily to structural uncertainties between various oceanic carbon sink models, while the uncertainty in the output of the 2-D OCSM is strictly parametric. Since the calculated uncertain range of 0.5–3.1 Pg yr^{-1} is less than the average 3.9 Pg yr^{-1} required to close the contemporary carbon budget, this implies a positive terrestrial carbon sink over the range of 0.8–3.4 Pg yr^{-1} for the 1980s which is consistent with the observations (IPCC, 1994). The parametric uncertainty in the 2-D OCSM can also be propagated through forecasts of anthropogenic CO_2 emissions to calculate uncertainty in future atmospheric CO_2 concentrations. For anthropogenic CO_2 emissions equivalent to the IS92a scenario of the IPCC (1992), the uncertainty in atmospheric CO_2 concentrations is found to be 705 ± 93 ppmv in 2100 (with 95% confidence). Like the mean oceanic carbon sink for the 1980s, the range of atmospheric CO_2 concentrations of 612–798 ppmv by the end of the next century is much larger than that implied by the structural uncertainty in the IPCC study (1994; 1995).

Because it has been well established that atmospheric CO_2 levels are a strong driver of radiative forcing in the atmosphere, this result has implications for quantifying uncertainty in studies of future climate change. A range of atmospheric CO_2 concentrations of nearly 200 ppmv in 2100 is expected to produce discernible differences in global surface temperatures that may dwarf the impacts of certain modest policies to reduce or stabilize forecast CO_2 concentrations. The ability to produce probability distributions for atmospheric CO_2 concentrations as a function of time from quantifiable uncertainties in the oceanic carbon sink allows for the testing of anthropogenic carbon emissions paths and scenarios for the stabilization of atmospheric CO_2 concentration with some estimate of the likelihood that they can be achieved. Distributions of future atmospheric CO_2 concentrations can then be run through global climate models in order to propagate the uncertainty in atmospheric CO_2 concentrations through the climatic system to quantify impacts on key outputs of interest such as global temperature, precipitation, and sea-level rise. However, the relative quality of such results depends on the quality of the estimates of uncertainty in the input parameters, since the uncertainty in the oceanic carbon sink is directly keyed to the assumptions of uncertainty in the parametric inputs as is noted in Section 5.

Improving the quality of the probability distributions of the six input parameters is therefore paramount for decreasing the uncertainty in size of the oceanic carbon sink. The “solubility pump” is a well recognized process in the ocean, though it has been difficult to quantify by observation since net fluxes are small compared to gross exchanges. By examining the contribution of the uncertainty in the parameters of the model in this study to the variance in the outputs, it has been possible to rank their relative importance in Section 5.3.2. The three chemical parameters and the coefficient of horizontal diffusion appear to have relatively small impacts on the uncertainty of the oceanic carbon sink relative to the coefficient of vertical diffusion which accounts for 50% or more of the uncertainty. The rate of vertical mixing into the deep ocean is determined to have the greatest effect on the uncertainty of the oceanic carbon sink, which agrees with the observation that the surface ocean and atmosphere remain close to equilibrium and that the rate of export of dissolved carbon to the deep ocean should control the size of the sink. This study also indicates that the importance of such transport increases with time (Fig. 5-7). Much of the recent work into inferring the vertical mixing rate from tracer distributions such as bomb-produced radiocarbon appears to be well justified (Broecker, *et al*., 1985; 1995) since reductions in the uncertainty of the mixing rate will have the greatest impact on the total uncertainty of the oceanic carbon sink. The strength of the oceanic carbon sink can be expected to be strongly sensitive to the strength and nature of the mixing assumed in a particular oceanic carbon sink model, which might be parameterized as in this model, or dynamical as in various 3-D Ocean GCMs. These uncertainties caution the interpretation of the results of individual models of the oceanic carbon sink as they exist now, since critical gaps in knowledge and a disparity in the degree of complication make the effectiveness of such models difficult to compare without doing so in conjunction with an analysis of the parametric uncertainty of each model.

6.2 Future Work

The large parametric uncertainty evident in the 2-D OCSM which spans the observed range of uncertainty indicates that current models have done little to quantitatively narrow the uncertainty in the oceanic carbon sink. One obvious improvement is to produce more accurate observations of tracer distributions in the ocean in order to improve the calibration of the mixing of such models since this appears to be their most sensitive parameterization. In the process, parametric uncertainty is reduced and the models will provide a less uncertain estimate for the contemporary oceanic carbon sink. However, the strong sensitivity of the 2-D OCSM to the choice of vertical diffusion parameter points up a major problem with the reasonableness of using a simple 2-D ocean carbon sink model to predict future carbon concentrations since this factor is fixed in time and calibrated only to reproduce the current rate of mixing into the ocean.

A robust feature of many climate models is disproportionate warming at high latitudes in scenarios involving a doubling of atmospheric CO_2. In a pair of studies, Maier-Reimer, *et al*. (1996), and Sarmiento and Le Quere (1996) looked at the impact of these global warming scenarios on the uptake of the carbon by the ocean, both with and without ocean biology as well as with and without a feedback from changes in the physical climate system upon the oceanic circulation. High latitude warming had the effect of weakening the thermohaline in both of these models, strongly decreasing the carbon sink when ocean biology is excluded and only mildly decreasing the oceanic carbon sink when ocean biology was included (versus the carbon sink that would have prevailed without the change in circulation). Diffusion is very limited in its utility for understanding the impact of changes in oceanic circulation on the carbon uptake compared to a dynamical ocean model. Of course, this is simply an acknowledgment of the fact that structural and parametric uncertainty are both in operation at the same time and must ultimately be considered in conjunction. As has been observed by Wigley (1993) the nature of the contemporary global carbon balance assumed by the particular model (oceanic *vs*. terrestrial sinks), impacts quantitatively on the future carbon budgets forecast by the model. This dependence represents another form of structural uncertainty which must be broached in order to further reduce total uncertainty in the global carbon cycle. It is therefore difficult to see how uncertainties in the oceanic carbon sink will be reduced in isolation from the uncertainty in the terrestrial carbon sink.

The development of a coupled global carbon cycle model, comprising the two rapidly exchanging systems: the oceans and the land biosphere, with consistent and detailed representations of the major sink and source mechanisms for carbon (and secondary species such as nitrogen) is increasingly necessary if further uncertainty in the global carbon cycle is going to be explored with any degree of success. Such a model must allow for an exploration of parametric uncertainty in the two sub-models as well as the role of changing climate in the evolution of the global carbon cycle. The elements of a coupled-model that are needed to address these goals and the experiments that could be performed with such a model are described below.

The coupled model proposed above requires process-based models of the global oceanic and terrestrial cycles of carbon and not box models or simple one-dimensional parameterizations based on commonly accepted simplifications of the mechanisms of carbon sequestration in the land and sea in order to reduce structural uncertainty. Such simple models cannot be reasonably used to forecast changes in the global carbon budget into the next few centuries or to model changes in the carbon sinks brought about by feedbacks and interactions with the physical climate system. Individual models of the terrestrial and oceanic carbon exchange vary in their degree of complexity and their objectives. Since complex, process-based models of these individual systems have rarely been developed with a comprehensive consideration of each other we are left with detailed, but isolated studies of each system with which to create a coupled system. In the ocean, is required a sub-model for the air-to-sea exchange of CO_2 as well as the inorganic and organic cycles of carbon that includes a dynamical model for the oceanic circulation. Changes in chemistry and the physical climate system are combined to form a complete response from oceanic carbon cycle. In the case of the land biosphere, there are numerous expert studies of the important biotic processes involved, including some few models of the effect of rising atmospheric CO_2 concentrations, nitrogen deposition, and changing climate on primary productivity. One such model was described earlier in this study, the Terrestrial Ecosystems Model of the Marine Biological Laboratory, located in Woods Hole, Massachusetts. It is a global model of the natural land exchanges of carbon and nitrogen that is driven by climatic variables. A terrestrial ecosystems model of at least as much complexity is required for the land carbon sink sub-model.

It is important to construct a coupled model of the global cycle of carbon that allows for an exploration of the primary interactions between the source and sink mechanisms for CO_2 and their feedbacks from changing climate. Variables that affect carbon storage include, but are not limited to temperature, precipitation, sunlight, the strength of the oceanic circulation, the flow of nutrients, and changes in the chemical composition of the principal reservoirs. The coupled-model can rank the effectiveness of the individual exchange mechanisms for carbon as well study and order the relative roles of interactions of the closely linked carbon and nitrogen cycles in the land and ocean. The temporal and spatial dimensions of these changes are expected to be important and should be included, which implies the use of 3-D models of sufficiently high resolution. However, for studies of uncertainty which require numerous long-term simulations, the computational burden of coupling 3-D AOGCMs to coupled-carbon cycle models would be prohibitive. Therefore, tools like the Probabilistic Collocation Method (Sections 4.3–4.4) would be invaluable as a means to assess parametric uncertainty by allowing the response of the coupled-model to be simulated by reduced-form representations that attempt to capture the complex behavior of the sub-models.

Feedbacks in both systems that play a role in determining atmospheric CO_2 on various time scales which vary from the seasonal to the millennial should be a part of the study of such a coupled model. As an example are the changes in oceanic circulation that can feedback on terrestrial carbon storage by drawing CO_2 out of the atmosphere and lowering the atmospheric concentration or the simultaneous effects of rising surface temperature on the biotic systems of the land as well as the ocean. These systems need to be examined both inside and outside of the context of the anthropogenic CO_2 problem, this includes trying to explain the paleo-CO_2 record that we see in the Vostok ice core (Fig. 1-2) which represents a kind of climatological *Rosetta Stone* for the interaction of the global carbon cycle with the rest of the physical climate system. If we can understand why CO_2 and temperature have been so strongly correlated in the past, we may be better able to understand how future anthropogenic emissions will impact on atmospheric CO_2 concentrations and therein reduce the uncertainty in the climate change that might result from these changes.

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