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I. G. Enting and G. I. Pearman

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ABSTRACT

The analysis of the DAP one-dimensional carbon cycle model is refined in a number of ways. Minor modifications to the model and a recalibration based on constrained inversion techniques are described.

Contents

1. Introduction

This report documents a number of refinements to the one-dimensional carbon cycle model developed within the Division of Atmospheric Research (formerly Division of Atmospheric Physics), CSIRO Australia. The modelling program involving the one-dimensional model was developed with the following aims;

(i) to provide a basis for interpreting the results of the Division's observational programs, particularly those involving ^{13}C

(ii) to ensure that the air-sea exchange formalism that is used in the Division's two-dimensional atmosphere-ocean-surface model (Hyson et al., 1980; Pearman and Hyson, 1980) does not lead to inconsistencies when incorporated into a full global carbon cycle model. This aspect of the model has been extended, with the aim of avoiding the use of any arbitrary rate constants so that all processes are characterised by physical constants that can be determined independently of carbon cycle models.

A preliminary description of the model was given by Pearman (1980). A detailed technical description is given by Enting and Pearman (1982) and a general account of the model together with a description of studies of temperature-dependent effects has been given by Enting and Pearman (1984).

The refinements described in this report involve a number of minor modifications to the model structure. The main refinement is in the calibration techniques. The calibration technique is based on techniques of constrained inversion (see for example Twomey, 1977; Jackson, 1972). The use of constrained inversion in calibrating box models has been recommended by Wunsch and Minster (1982). Enting (1984) has pointed out that the selective parameter fitting used by Enting and Pearman (1982) can be regarded as a first approximation to a constrained inversion technique.

The outline of the remainder of this report is as follows: Section 2 gives a general description of the model. Section 3 specifically describes the changes that have been made to the form described by Enting and Pearman (1982). Section 4 outlines the constrained inversion techniques. Section 5 lists the prior estimates of the parameters that are modified by fitting the carbon cycle data which is listed in Section 6. Section 7 quotes some of the main results of applying the formalism from Section 4 to the parameter estimates and carbon cycle data listed in Sections 5 and 6.

2. Model Structure

The model has been described by Enting and Pearman (1982). The general structure is similar to a number of other global carbon cycle models. References to descriptions of other carbon cycle models have been given by Allison and Talmage (1982). The most distinctive feature of the model is not the particular structure but the extent to which the model incorporates additional geophysical information. It is this aspect that naturally leads to the use of constrained inversion techniques for model calibration as described in Section 4.

The processes modelled are

(i) release of fossil carbon into the atmosphere
(ii) production of carbon-14 by cosmic rays
(iii) production of carbon-14 by nuclear tests

(iv) exchange of carbon between the atmosphere and the terrestrial biosphere

(v) exchange of carbon between the atmosphere and the ocean surface

(vi) circulation of carbon within the oceans by large scale advection with smaller scale processes modelled by an eddy diffusion formalism

(vii) detrital settling of carbon from the ocean surface to deeper layers.

Figure 2.1 gives a schematic representation of the model structure.

The various processes are characterised by a number of geophysical parameters. Some of the processes involve functions of time. The various functions are

(i) $F(t)$, the rate of fossil carbon release. This is known on the basis of data from Rotty (1979)

(ii) $r(t)$, the $^{13}C:^{12}C$ ratio in fossil fuel. In earlier studies this was set as a constant. In Section 3 a time dependent form is described, based on data from Tans (1981a)

(iii) $Y(t)$, the rate of energy release from nuclear weapons tests. This is used in the form $\Lambda Y(t)$ to describe the rate of carbon-14 production from weapons tests, so that in these studies all of the uncertainties are absorbed into the parameter Λ which defines the relation between the energy yield and carbon-14 production

(iv) $C(t)$, which gives the net transfer of carbon from the biosphere to the atmosphere due to forest clearing. The low resolution parameterization is described in Section 3

(v) $T_c(t)$, $T_w(t)$ which describe the time dependence of the ocean surface temperature. Most studies have used constant temperatures but Enting and Pearman (1984) have described a group of studies involving varying temperatures

(vi) $\omega(t)$, the rate of carbon-14 production by cosmic-rays. Again most studies have used constant ω, but it is possible to estimate the variation of ω on short time scales on the basis of sun-spot activity with larger long-time variations due to changes in the geomagnetic field.

In principle the model could be run with any of the parameters varying and the program structure makes explicit provision for such optional modifications. In practice most studies use fixed values of the parameters assigned as either the prior values from Section 5 or on the basis of the calibration procedure described in Section 4.

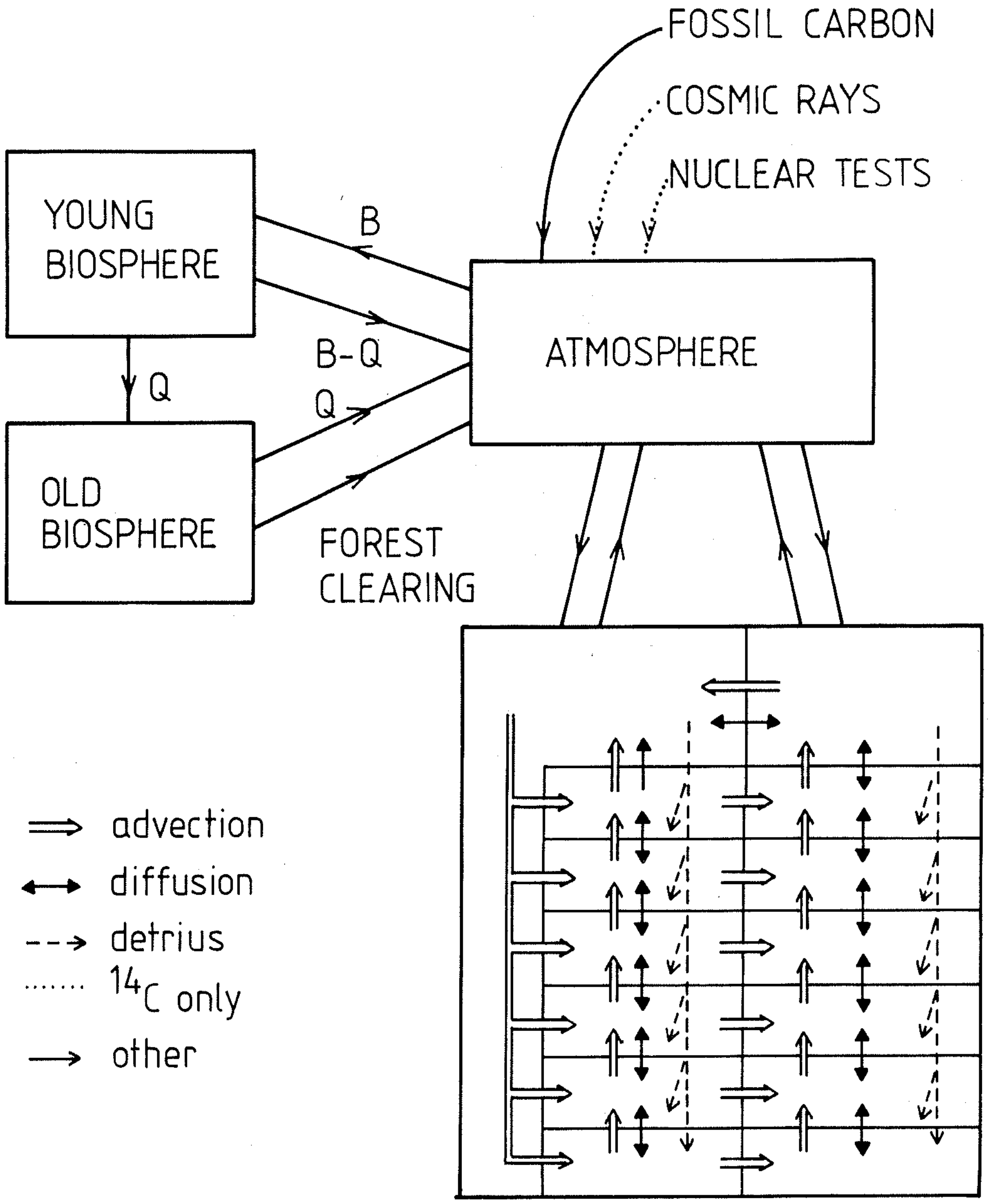

Figure 2.1 Schematic representation of the model structure showing the division of the biosphere into two reservoirs and the division of the oceans into warm and cold regions each of which has a surface reservoir and a number of subsurface reservoirs. The model describes the behaviour of the amounts of each of the three isotopes ^{12}C, ^{13}C and ^{14}C in each reservoir.

3. Modifications from Earlier Versions

The modifications made to the model defined by Enting and Pearman (1982) are

(i) use of time dependent δ_{13} for fossil fuel

(ii) inclusion of more general forest clearing histories

(iii) allowing the biospheric flux to vary with the size of the biosphere

(iv) changes to the advection to allow the direct formation of intermediate ocean waters from surface waters

(v) modifying the detrital rainout to include re-dissolution at intermediate depths.

In each case except the fossil fuel δ_{13}, the modification is made in such a way that the version of the model described by Enting and Pearman (1982) can be recovered by using an appropriate set of parameters. The version of the model with the δ_{13} of fossil fuel fixed could be recovered by using the facility for optional changes to the library as described above.

3.1 Carbon-13 in fossil fuel

The initial testing of the model (Enting and Pearman, 1982) used a fixed fossil fuel $^{13}C:^{12}C$ ratio corresponding to a δ_{13} value of -25‰. While this is an adequate approximation for most purposes, for detailed studies and interpretation of carbon-13 observations a more precise specification is desirable. Tans (1981a) has estimated the δ_{13} of fossil fuel. The estimates are shown in Figure 3.1, together with the approximation used in the refined version of the model. The approximation corresponds to linearly interpolating between the values given in Table 3.1.

Date	δ_{13} (‰)
1800	-24·00
1870	-24·00
1914	-24·32
1941	-25·06
1953	-25·86
1958	-25·97
1971	-27·28
1980	-27·28

Table 3.1

Values of fossil fuel δ_{13} used in approximating the data given by Tans (1981a). Values at intermediate times are obtained by linear interpolation.

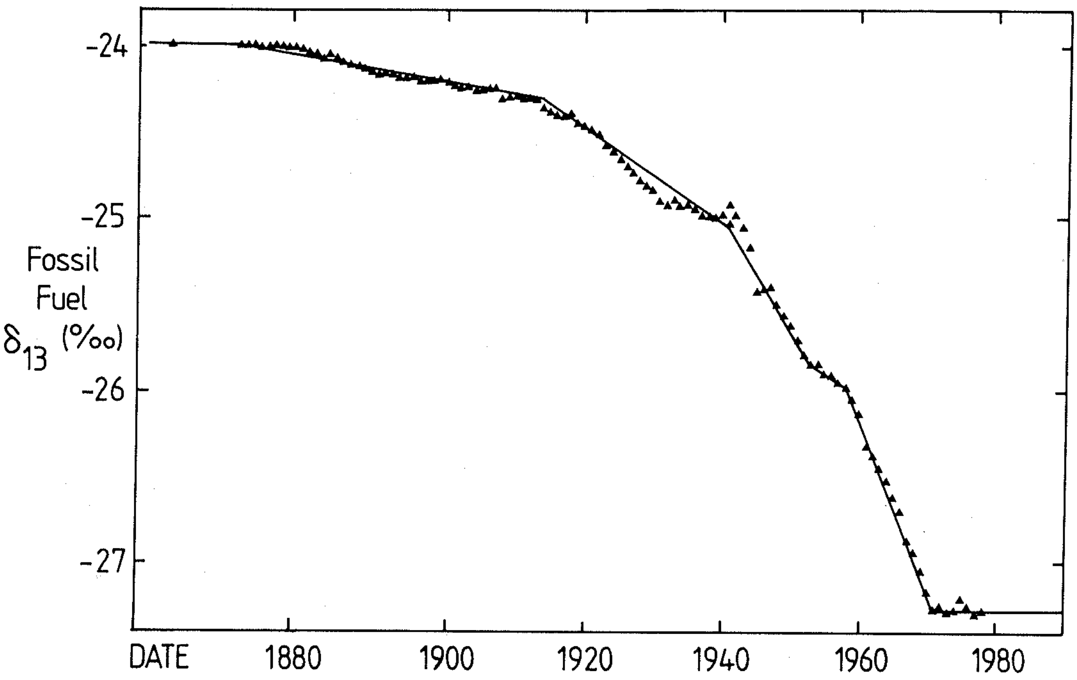

Figure 3.1 Approximation to fossil fuel δ_{13}. The triangles show the data given by Tans (1981a). The line shows the approximation used in the refined form of the model, linearly interpolating between the values given in Table 3.1.

3.2 Generalised forest clearing functions

The revised form of the forest clearing is a quadratic spline that has nodes at 25-year intervals from 1815 onwards. This spline is expressed as a sum of 8 B-splines. Each B-spline, $b_i(t)$ is non-zero only in the range $t_0^{(i)} \leq t \leq t_3^{(i)}$. The four nodes defining the non-zero region of each $b_i(t)$ are listed in Table 3.2.

n	1	2	3	4	5	6	7	8
$t_0^{(n)}$	1815	1840	1865	1890	1915	1940	1965	1990
$t_1^{(n)}$	1840	1865	1890	1915	1940	1965	1990	2015
$t_2^{(n)}$	1865	1890	1915	1940	1965	1990	2015	2040
$t_3^{(n)}$	1890	1915	1940	1965	1990	2015	2040	2065

Table 3.2 Nodes of B-splines b_n

The mathematical expression for the release rate C is

$$C(t) = \Sigma q_i b_i(t) \tag{3.1}$$

where

$$b_i(t) = (t - t_0^{(i)})^2/31250\ , \qquad t_0^{(i)} \leq t \leq t_1^{(i)} \tag{3.2a}$$

$$= (1875 - (2t - t_1^{(i)} - t_2^{(i)})^2)/62500, \qquad t_1^{(i)} \leq t \leq t_2^{(i)} \tag{3.2b}$$

$$= (t_3^{(i)} - t)^2/31250\ , \qquad t_2^{(i)} \leq t \leq t_3^{(i)} \tag{3.2c}$$

$$= 0 \quad \text{otherwise} . \tag{3.2d}$$

The B-splines are defined so that

$$\int_{t_0^{(i)}}^{t_3^{(i)}} b_i(t)\, dt = 1 \tag{3.3}$$

so that the q_i in equation (3.1) represent the total amount of carbon released by the corresponding B-spline component.

This formulation of the release functions cannot describe all the possible release functions encompassed by the formalism given by Enting and Pearman (1982) but it can include the case used in the standard calibration by setting q_i, i = 1, 8 to 20, 60, 60, 20, 0, 0, 0, and 0 Gt respectively.

This form of biospheric release could include the possibility of negative values of the q_i so that regrowth is allowed, without having to specify whether it is due to a change in agricultural practices or to growth enhanced by increased CO_2 concentrations, i.e. the so-called β-effect (Keeling, 1973).

3.3 Biospheric exchanges

The structure of the biosphere-atmosphere exchange system is shown in Figure 3.2. The biosphere is divided into two reservoirs, denoted young and old biosphere. Enting and Pearman (1982) have shown how, with an appropriate choice of transfer rates, the combined biosphere will have exactly the same age distribution as the form, used by Keeling (1973), which has 'short-lived' and 'long-lived' biospheric reservoirs that do not exchange carbon with each other. In Figure 3.2 the quantities B and Q detail natural exchange rates and C denotes the rate of release of biospheric carbon due to forest clearing; this function is described in the previous subsection.

The refinement that has been added to this formalism is to realise that once C is included, the size of the old biosphere changes and the rate of transfer through the old biosphere can be expected to change.

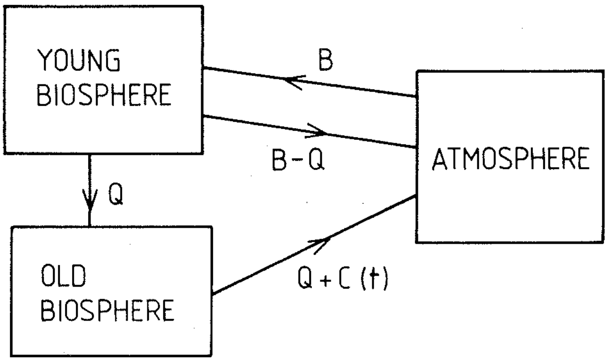

Figure 3.2

Exchange processes used in modelling the biosphere.

This form is modelled by putting

$$Q = Q_o + N_b/\tau_b \qquad (3.4)$$

where N_b is the size of the old biosphere. The case considered by Enting and Pearman (1982) corresponds to the limit $\tau_b \to \infty$ while in the case $Q_o = 0$, the exchange rate would be proportional to the size of the old biosphere and τ_b would represent a turnover time.

The isotopic fractionation is carried out using the formalism described by Enting and Pearman (1982). Appropriate values for the biosphere parameters are discussed in Section 5.

3.4 Changes to ocean advection

In the earlier forms of the model, the advective flow consisted of an upwelling over all of the warm ocean regions and 90% of the cold ocean regions. The upwelling velocity was taken as being constant in both regions and at all depths. Return flows were required for mass balance with horizontal transports in the top and bottom layers and a downflow from the cold surface to cold bottom layers.

The modified form of advection injects cold surface water into each of the cold ocean layers with additional horizontal transport into the warm ocean layers. The corresponding upwelling velocities are taken as being equal in each region at any given level and increasing in proportion to the height above the ocean bottom.

For compatibility with earlier work, the generalised form of the model uses two upwelling parameters, v_{up} and v_{top}. The amplitude of the advective flux that was used in the earlier studies is proportional to v_{up} while an additional component with injection of equal amounts of water into each layer is described by the parameter v_{top}, so that earlier work corresponds to $v_{top} = 0$. Since the corresponding water mass fluxes are of the form velocity times area and have to be multiplied by concentrations of the form content divided by (thickness times area), most of the area factors cancel and the expressions can be written in terms of reduced concentrations $Q_{r,m}$ which represent reservoir contents divided by layer thicknesses, as was done by Enting and Pearman (1982). Each of the concentrations involved in vertical transports is the mean concentration of the source and destination reservoirs except for the downflow and injection where the concentration is that of the cold surface water. Because of numerical instabilities encountered with the 'centred' concentrations, all horizontal transports use 'upstream' concentrations. In the following list of rates of carbon transport, v represents v_{up}, the uniform part of the advective velocity, n represents the number of layers and u represents the change in the vertical advective velocity between two successive layers

$$\text{i.e. } u = v_{top}/(n - 1) \quad . \tag{3.5}$$

The rates of carbon transport are

(i) horizontal flux, cold to warm, layer m

$$F = u\ Q_{c,m}\ A_w/A_c \qquad m = 2,n \tag{3.6}$$

with an additional flux

$$F = v\ Q_{c,m}\ A_w/A_c \quad \text{in layer } n \tag{3.7}$$

(ii) the return horizontal flux in the surface layer is

$$F = (v + (n - 1)u)\ Q_{w,1} \tag{3.8}$$

(iii) the horizontal injection into cold layer m is

$$\begin{aligned} F &= u(0.9A_c + A_w)\ (Q_{c,1}/A_c) \\ &= Q_{c,1}u(0.9 + A_w/A_c) \quad \text{for } m = 2,n \end{aligned} \tag{3.9}$$

with an additional injection

$$\begin{aligned} F &= v(0.9A_c + A_w)\ (Q_{c,1}/A_c) \\ &= v\ Q_{c,1}\ (0.9 + A_w/A_c) \quad \text{into layer } n. \end{aligned} \tag{3.10}$$

(iv) In the warm region the upwelling from layer m + 1 to layer m is

$$F = (v + u(n - m))\ A_w(Q_{w,m}/A_w + Q_{w,m+1}/A_w)/2$$

$$= (v + u(n - m))\ (Q_{w,m} + Q_{w,m+1})/2 \quad , \quad m = 1, n - 1 \qquad (3.11)$$

(v) In the cold region the upwelling from layer m + 1 to layer m transports with rate

$$F = (v + u(n - m))\ 0.9\ A_c\ (Q_{c,m}/A_c + Q_{c,m+1}/A_c)/2$$

$$= 0.45\ (v + u(n - m))\ (Q_{c,m} + Q_{c,m+1}) \quad , \quad m = 1, n - 1\ . \qquad (3.12)$$

3.5 Changes to the detrital flux

The form of the detrital flux was generalised from that described by Enting and Pearman (1982) by allowing an additional flux that transports equal amounts of carbon into each of the subsurface boxes in each region, r

i.e. $$F_{det}(1,r \rightarrow m,r) = (D^*/(n - 1) + D\delta_{m,n})A_r/(A_w + A_c) \qquad (3.13)$$

where D is the global rate for detrital transport from surface to bottom D^* is the global rate for detrital transport from surface to subsurface layers, and n is the number of ocean layers and $\delta_{m,n}$ is the Kroenecker delta. The form used by Enting and Pearman (1982) corresponds to $D^* = 0$.

The isotopic ratios in the detrital flux are obtained by applying a fractionation Δ_{13} to the $^{13}C:^{12}C$ ratio in the surface box and $2\Delta\delta_{13}$ to the $^{14}C:^{12}C$ ratio, as was done by Enting and Pearman (1982).

4. Model Calibration Based on Constrained Inversion

In the initial calibration of the model, Enting and Pearman (1982) encountered considerable numerical difficulty due to the fact that the carbon cycle data did not adequately determine the model parameters. There are however a variety of techniques for working with underdetermined problems and these have been applied in several geophysical contexts (Wunsch, 1978; Twomey,1977; Anderssen,1968 for example). The techniques are generally referred to as 'constrained inversion techniques' or less specifically 'inverse methods'. Some of the reasons for applying such techniques to carbon cycle model calibrations are

(i) As mentioned above, carbon cycle data are inadequate for complete model calibration.

(ii) As described by Wunsch (1978) indirect methods based on inversion of tracer data are not adequate for determining the global movement of ocean waters. To the extent that the carbon cycle depends on the general circulation of the oceans, the incomplete description of the ocean circulation implies an incomplete description of the carbon cycle.

(iii) If carbon-13 levels in tree-rings are used in an attempt to reconstruct the history of biospheric changes the reconstruction becomes an underdetermined deconvolution problem.

(iv) The fact that the release of fossil carbon has increased in a nearly exponential manner means that, in so far as the system is linear, the atmospheric response gives no information about the natural response rates of the system. Even if the source did have major departures from exponential behaviour, the problem of inverting the atmospheric response data to determine the response function of the system would still be similar to the well-known ill-posed problem of numerically inverting Laplace transforms.

(v) The constrained inversion techniques can provide a systematic way of using additional geophysical information, particularly if these techniques are interpreted in terms of Bayesian inference.

The form of constrained inversion used here has been described by Enting (1983, 1984). The formalism makes use of J measurements m_j with standard deviations v_j. The model predictions for the m_j are denoted y_j. The y_j are functions of K parameters x_k, and the functional relation is expressed as $y_j(\underset{\sim}{x})$. The constrained inversion requires some independent prior estimates of the x_k. These prior estimates are denoted q_k, and the standard deviations of these prior values are u_k.

The constrained inversion formalism obtains estimates of the parameters by choosing as estimates of x_k, the values $\hat{x}_k$ that minimise

$$\theta = \sum_{j=1}^{J} (m_j - y_j(\underset{\sim}{x}))^2/v_j^2 + \gamma \sum_{k=1}^{K} (x_k - q_k)^2/u_k^2 \quad . \qquad (4.1)$$

In constrained inversion methods the quantity γ determines the relative contribution of the two types of information. The desirable situation is to have the final estimates relatively insensitive to the value of γ that is chosen. If the results depend strongly on γ it can be an indication that the observations m_j are inconsistent with the prior parameter estimates q_k, at least within the context of the given model. Such inconsistency would require a re-assessment of either the model, the way in which it is parameterised or the type of data that is used to fit it.

An interesting interpretation of the role of the quantity γ can be obtained by extending the ideas of Karplus (1977). Karplus compared different approaches to modelling and described a spectrum of models ranging from purely black-box or curve fitting models through to completely determined, or white-box, models for which no calibration is needed. The spectrum ranges through intermediate or 'grey-box' models. In these terms, different γ values in expression (4.1) would correspond to assuming that the model lies in different parts of the model spectrum - large values of γ mean that it is assumed that the prior geophysical information embodied in the q_k is sufficient to determine the behaviour of the carbon cycle - small values of γ mean that the prior information is discarded as being inapplicable and only the carbon cycle measurements contribute to the calibration.

Enting (1983) has shown how the minimisation of (4.1) can correspond to a Bayesian inference procedure if the probability distributions are assumed to be multivariate normal. The advantage of this approach is that it gives a more complete treatment of the uncertainties in the parameter estimates unlike the conventional approaches used in constrained inversion (Jackson, 1972) or the equivalent formalism of ridge regression (Hoerl and Kennard, 1970a,b) which only deal with a restricted class of variations.

The major advantage of the analysis described below is that it describes the combined effects of uncertainties that would, in a conventional calibration technique, be associated with either the uncertainties in the carbon cycle data or with the uncertainties in the predetermined parameters i.e. between those uncertainties associated with the 'statistical' estimation and those uncertainties that are outside the estimation procedure. Any complete analysis must, of course, consider both classes of uncertainty. In a conventional calibration this would require estimating a subset of parameters using the carbon cycle data and then repeating this estimation procedure using slightly different values for those parameters that are regarded as pre-determined but which are not precisely known. This approach rapidly becomes impractical when it becomes necessary to consider a range of possible variations in several pre-determined parameters.

The constrained inversion formalism combines both classes of uncertainty into one formalism. The value of each parameter is estimated from a combination of the prior estimate and the fit to the carbon cycle data, thus emphasising that the question of whether parameter values should be pre-determined or estimated from the carbon cycle is a matter of degree rather than an absolute distinction.

The analysis of uncertainties in the model predictions (the sensitivity analysis) has been described by Enting (1983, 1984). A form that is convenient for numerical calculations determines the uncertainties in some arbitrary model prediction (denoted Z) by minimising

$$\phi = \theta - 2\alpha Z \tag{4.2}$$

with respect to the parameters x_k where α is an arbitrary small number that acts like a Lagrange multiplier. If the prediction for Z from the best fit parameters $\hat{x}_k$ is denoted $\hat{Z}$ and if $Z'(\alpha)$ is the value of Z corresponding to the minimum of ϕ then in terms of the statistical interpretation described by Enting (1983),

$$\mathrm{Var}\ (Z) = \frac{\gamma}{\alpha}\ (\hat{Z} - Z(\alpha)) \quad . \tag{4.3}$$

Two other procedures commonly associated with constrained inversion formalisms concern the marginal utility of data and the model resolution specified appropriate to the data.

The marginal utility of the data (Jackson, 1972) or the information content of the data (Twomey, 1977) involve the question of the extent to which various data items assist in the determination of the model parameters, reducing the extent to which the model is underdetermined. An appropriate form of this type of study for carbon cycle modelling would be to repeat an initial calibration with additional data included and determine the extent to which uncertainties (as determined by equation 4.3) are reduced.

The use of constrained inversion techniques in studying the appropriate resolution is based on consideration of the role of γ in equation 4.1. If the resolution (i.e. the number of parameters or independent degrees of freedom in the model) is too high then the model will be underdetermined (by the data) and relatively large values of γ will be required to obtain stable parameter estimates by constraining the excessive degrees of freedom. In the context of carbon cycle modelling, resolution involves both temporal (and possibly spatial) resolution (e.g. the density of nodes in the splines described in Section 3.2), and the distinction between alternative ocean mixing processes. Questions of resolution can even include the distinction between processes that are quite different physically but which have similar effects on the carbon cycle, at least over the period of current observations.

5. Parameter Values

The modified form of the model has 39 parameters which are used in the computer program. In the constrained inversion calibration considered here, only 31 parameters are considered. The parameters that are not directly adjusted by this procedure are

(i) all four carbon-14 fractionation factors since these are assumed to be determined by the carbon-13 fractionation,

(ii) the carbon-13 fractionation factor for transfer from the biosphere to the atmosphere. This is taken as exactly 1,

(iii) the term Q_o in the biosphere flux equation (3.4); this is set to zero, giving a flux that is proportional to the amount of carbon in the reservoir,

(iv) the 8th B-spline amplitude, because the spline is 0 until 1990 and so cannot influence any current data,

(v) the transfer of detrital fallout directly to only the lowest reservoir is set to zero, leaving only the contribution which distributes the detrital material uniformly with depth.

Each of the remaining 31 parameters must be assigned a prior value and a standard deviation which measures the uncertainty of the prior estimate. In the analysis used by Enting and Pearman (1982) the initial parameter estimates served merely as starting points for an iterative fitting procedure but in the present analysis the initial (prior) values contribute to the final estimates and so the values must be chosen more carefully. The rest of this Section considers each parameter in turn.

5.1 Pre-industrial CO_2 concentration in the atmosphere

For many years, it was widely believed that the preindustrial CO_2 concentration in the atmosphere was about 290 ppmv (see for example Keeling, 1978). This belief was based mainly on the review by Callender (1938) of earlier CO_2 measurements. There is, however, an increasing body of evidence which suggests that concentrations early last century may have been nearer to 260 ppmv with an increase late last century due to clearing of forests for agricultural purposes. In a recent review Wigley (1983) has summarised the evidence as

(i) carbon-13 measurements on tree rings,

(ii) ocean chemistry,

(iii) direct measurements of CO_2 in ice-cores,

(iv) CO_2 modelling studies - the so-called 'missing-carbon' problem,

(v) direct estimates of changes in the biosphere, and

(vi) early CO_2 observations, particularly those in the southern hemisphere.

In order to avoid circularity in the calibration procedure it is necessary to ignore the results of other modelling studies in determining a prior estimate of the concentration. Similarly, the connection between biospheric inventories and the pre-industrial concentrations involves the use of some sort of model. The biospheric inventories are used to determine prior estimates of the amount of clearing but to avoid circularity they cannot be used to determine prior estimates of the atmospheric CO_2 concentration.

The ocean chemistry data is most readily taken as part of the data set used to calibrate the model, as is the data on carbon-13 in tree-rings although it should be noted that recent work (Francey and Farquhar, 1982) has cast some doubt on the possibility of using tree-ring data to determine changes in atmospheric carbon-13 levels. The direct estimates of CO_2 from either the atmosphere or from bubbles trapped in ice-cores could also be regarded as carbon cycle data to be fitted, leaving no independent prior estimates of the initial CO_2 concentration. Most of the prior estimates involve geophysical information that is independent of the carbon cycle but of course this will never be possible for CO_2 concentrations. For reasons of mathematical convenience we use the directly observed values as our prior estimates and regard the ocean chemistry data (and in some studies, tree ring data) as observations to be fitted by the model.

The most recent measurements of CO_2 in air bubbles from ice-cores (Neftel et al., 1982) give values in the range 260-300 ppmv. The measurements from the coldest-sites (i.e. those with the least effect from remelting) give 271 ppmv with a standard deviation of 9 ppmv.

The direct atmospheric observations quoted by Wigley (1983) are those of Muntz and Aubin (1886). Wigley notes that the observed very low concentrations (around 270 ppmv) at southern hemisphere sites, suggest that the higher northern hemisphere values used by Callender (1938) were affected by local contamination. The observations need to be treated with caution because they show a degree of day to day variability that would not be expected from modern experience in the southern hemisphere. In addition, it is not clear whether the date of the measurements is sufficiently early to precede the bulk of the forest clearing.

As a prior estimate of the atmospheric CO_2 concentration we use 270±50 ppmv. The relatively large uncertainty assigned to this estimate will ensure that the final (posterior) estimate is determined mainly by contemporary observations.

5.2 Preindustrial atmospheric δ_{13}

This is one parameter for which there is virtually no independent information although carbon cycle studies indicate that it would be about -6‰. Since the parameter value must be determined by the model we use, as prior estimates

$$\delta_{13}\big|_o = -6 \pm 3‰ .$$

The very large uncertainties mean that the parameter value will be determined by the data. This corresponds, roughly, to the 'non-informative prior distributions' described by Box and Tiao (1973).

5.3 Atmosphere-ocean fractionation factors

The most recent study of isotopic fractionation factors for gas exchange between the atmosphere and the ocean is that of Siegenthaler and Münnich (1981). They calculated fractionation factors on the assumption that diffusion was the rate-limiting process and then assessed the uncertainties that could arise from the effects of CO_2 hydration. We have used their values for the carbon-13 fractionation factors which were

$$f_{ao} = 0{\cdot}99795 \pm 0{\cdot}00025$$

$$f_{oa} = 0{\cdot}99005 \pm 0{\cdot}00025 .$$

The carbon-14 fractionation factors are taken as

$$f_{ao}^{*} = 2f_{ao} - 1$$

$$f_{oa}^{*} = 2_{foa} - 1 .$$

5.4 Ocean-surface alkalinity

Alkalinity measurements from the GEOSECS program have been described by Takahashi et al. (1981). The mean values for the various surface regions are given in Table 5.1, together with the weighted global mean. To cover most of the range of values an uncertainty of ±30 μeq/kg is assigned, giving 2311 ± 30 μeq/kg for the normalised alkalinity at the surface. (For the global mean, the difference between normalised and unnormalised alkalinities is small compared to the regional variations that we averaged).

To convert to the volumetric units used in the model, the mean density of sea-water of 1·025 g/cm^3 is used, giving

$$A = 2{\cdot}369 \pm 0{\cdot}021 \text{ mol/m}^3.$$

Ocean	Range	A_s μeq/kg
N. Atl.	0-35N	2287
S. Atl.	0-45S	2295
N. Pac.	0-50N	2310
S. Pac.	0-45S	2307
N. Ind.	0-20N	2283
S. Ind.	0-45S	2282
Ant.	45S-90S	2354
Average		2311

Table 5.1 Normalised alkalinities for the top 50 m of the oceans, from GEOSECS observations, Takahasi et al. (1981).

5.5 Friction velocities

The friction velocities u_* are required for both warm and cold regions. In the model they are used in the formalism of Deacon (1977) in which the CO_2 flux densities are given by

$$F = 48\ (1 + 0{\cdot}007T)\ u_*^{\text{eff}}\ (C_a - p_{CO_2})$$

in picograms per square metre per second, where T is the temperature (°C), C_a is the atmospheric CO_2 concentration (in ppmv) and pCO_2 is the partial pressure of dissolved CO_2. Deacon (1977) used the actual friction velocities directly. Enting and Pearman (1982) described an elaborate procedure for obtaining more appropriate effective u_* values by taking wind stress data from Hellerman (1967, 1968) and applying corrections for apparent non-linearities in the dependence of gas exchange on wind speed. This approach suffered from the limitation that Hellerman only quoted mean values of the components of wind stress and covariance effects mean that mean magnitudes of the wind stress cannot be recovered from this data. A simpler approach is based on Figure 5 of Liss (1983) which suggests that a quadratic dependence of flux on u_* is a much better approximation than the linear form used by Deacon (1977) and is comparable to the bilinear form described by Enting and Pearman (1982). In the units used by Liss, the Deacon relation gives a piston velocity (transfer velocity, V_L) in cm/hr

$$V_L = 10u_* \quad \text{(Deacon)}$$

while the bulk of the observations considered by Liss suggest

$$V_L \simeq 100u_*^2 \quad \text{(Experiments)}.$$

On this basis the appropriate way to use the Deacon formalism is with an effective u_* given by the time average

$$u_*^{\mathrm{eff}} = \overline{10u_*^2}$$

with all the u_* values in m/sec. From the definition of u_*, it is related to the wind stress τ by

$$u_*^2 = \tau/\rho$$

so

$$\overline{u_*^2} = \bar{\tau}/\rho ,$$

where ρ is the density of air which is taken as 1•2 kg/m^3. As mentioned above, the data given by Hellerman (1967, 1968) refer to mean components of the wind stress τ since it is the mean components that define the momentum transfer from air to sea. Mean wind stress charts for the Atlantic are given by Hellerman (1965) and suggest

$$\bar{\tau}_{\mathrm{cold}} = 2 \text{ dyne/cm}^2 = 0{\cdot}2 \text{ N/m}^2$$

$$\bar{\tau}_{\mathrm{warm}} = 1 \text{ dyne/cm}^2 = 0{\cdot}1 \text{ N/m}^2$$

whence

$$u^*_{\mathrm{eff}} = 1{\cdot}7 \pm 1{\cdot}2 \text{ m/s} \quad \text{(cold)}$$

$$= 0{\cdot}8 \pm 0{\cdot}5 \text{ m/s} \quad \text{(warm)}.$$

The uncertainties reflect both the uncertainties in the determination of the mean wind stresses and the uncertainties in the u_* dependence of the gas exchange rate.

5.6 Ocean surface temperatures

The ocean surface temperatures were obtained by taking area-weighted averages of the temperatures for 10° latitudinal bands as given in Table 65 of Defant (1961). The values were taken as 10•3 ± 5°C for the cold regions and 25•2 ± 2°C for the warm regions. These uncertainties represent the spatial variability of the temperatures without taking into account the seasonal variability.

In calculating the averages, the regions corresponding to the mean sea-ice cover were excluded.

5.7 Ocean mixing parameters

The model uses five parameters to describe the mixing of the ocean waters

(i) v_{up}, an upwelling, uniform both horizontally and vertically, and resulting from injection of cold surface waters into the lowest layer

(ii) v_{top} an additional upwelling through the bottom of the mixed layer resulting from cold surface waters injected in equal amounts into each subsurface layer

(iii) K_v, an eddy diffusion coefficient for vertical mixing

(iv) K_v', a rate of change of vertical eddy mixing

(v) K_h, an eddy diffusion coefficient for horizontal mixing.

These five parameters give only a crude representation of the complexities of the general circulation of the ocean, which is itself only poorly known. As prior estimates we use the following

$$v_{up} = 1{\cdot}80 \pm 1{\cdot}35 \text{ m/yr.}$$

This is based on the use of rates of formation of Antarctic bottom water (AABW) of 20 ± 15 svedrup. (1 svedrup = 10^6 m^3/sec). Carmack and Foster (1975) estimate a rate of formation of new AABW of 2 to 5 sv in the Wedell Sea. This range represents 12 to 30% of their estimated outflow of AABW, the remainder being bottom waters entrained in the circulation. Gordon and Taylor (1975) suggest rates of production of 30 to 40 sv on the basis of heat and salt balance considerations. As suggested by Broecker (1979) the older estimate of 20 sv (Stommel and Arons, 1960) represents a reasonable compromise. Stommel and Arons also estimates a sinking rate of 20 sv in the North Atlantic (see Pritchard et al., 1971, for a review). The situation in the North Atlantic is more complicated since the source of North Atlantic Deep water is intermediate waters rather than surface water (possibly with entrained AABW, Broecker, 1979). A detailed study of the North Atlantic circulation (Worthington, 1976) estimates the rate of dense water production from the Norwegian sea as 6 Sv with an additional 2 to 4 Sv from the Labrador sea.

Alternative estimates can be obtained from modelling studies such as that of Kuo and Veronis (1973) which suggest an upwelling velocity of 4•7 m/yr immediately below the thermocline on the basis of studies of oxygen concentrations. (The estimate of 4•4 m/yr, Munk (1966), used as an initial estimate by Enting and Pearman (1982) is based in part on carbon-14 data and so is not an independent prior estimate.)

On the basis of these estimates we use

$$v_{top} = 2{\cdot}5 \pm 2 \text{ m/yr.}$$

For vertical eddy diffusion we use

$$K_v = 3500 \pm 2000 \text{ m}^2\text{/yr}, \quad (1{\cdot}1 \pm 0{\cdot}6 \text{ cm}^2\text{/sec}).$$

The first of the various estimates on which we base this value is $1{\cdot}7\ \mathrm{cm}^2/\mathrm{s}$ (Broecker et al., 1980; on the basis of tritium penetration but no advection). In addition, analysis of the temperature salinity profiles in the Pacific indicates $K_v/v = 1{\cdot}1$ km so that the mean upwelling of 2 m/yr would give $K_v = 2200\ \mathrm{m}^2/\mathrm{yr}\ (0{\cdot}7\ \mathrm{cm}^2/\mathrm{s})$. Veronis (1975) has reviewed a number of studies involving K_v, using similar techniques and giving similar ranges of values.

The parameter K_v' cannot be assigned any detailed geophysical significance, indeed Munk (1966) comments on the difficulty of assigning a significance to K_v itself. The introduction of K_v' can serve to represent some of the more complex aspects of the mixing, for example the role of the intermediate water circulation. In order to allow a significant range for $K_v(z)$ if required by the data, we use

$$K_v' \quad = \quad 0 \pm 1\ \mathrm{m/yr}.$$

For the horizontal diffusion coefficient between the two surface layers we use

$$K_h \quad = \quad 2{\cdot}5 \times 10^4 \pm 2 \times 10^4\ \ \mathrm{m}^2/\mathrm{sec}.$$

This is the same value as was used by Enting and Pearman (1982) and is based on the work of Okubo and Ozmidov (1970) who studied the scale dependence of horizontal diffusion coefficients. The main uncertainties involve the choice of the most appropriate length scale selected as being representative of the model structure and so a very large uncertainty is assigned.

5.8 Detrital rainout rates

The most direct methods of determining the rate of detrital rainout rely on measurements of carbon gradients between the ocean surface and the deep layers, combined with estimates of the mixing rate. In the present study this procedure is part of the overall calibration. One way of obtaining an independent prior estimate is to use measurements of carbonate sedimentation rates.

Broecker (1974) quotes an accumulation rate of $0{\cdot}8$ g $\mathrm{CaCO_3/cm^2/10^3}$ years in dated cores. All cores contained only calcite (rhombohedral $CaCO_3$) and no aragonite (orthorhombic $CaCO_3$) so that the total $CaCO_3$ flux would be about $1{\cdot}6\ \mathrm{gm/cm^2/10^3}$ years. If this flux is globally representative then the global average rate of $CaCO_3$ falling and then redissolving would be $0{\cdot}9 \times 1{\cdot}6\ \mathrm{gm/cm^2/10^3}$ years on the basis of 50% (the calcite) not redissolving in 20% of the ocean floor (in which calcite sediments occur). This gives carbon transfer of $0{\cdot}6$ Gt carbon/year as $CaCO_3$. On the basis of alkalinity changes Broecker (1974) estimates the ratio of organic carbon to $CaCO_3$ as 2:1 so the total carbon flux is $0{\cdot}6\ (1 + 2/0{\cdot}9) = 1{\cdot}9$ Gt carbon/year. (The $0{\cdot}9$ reduction allowing for 10% sedimentation does not apply to organic material.)

Because of the crudeness of the calculation we use a rate of 2 ± 3 Gt/year where the large uncertainty means that the fallout rate will be determined by the carbon cycle measurements. It is meant to imply a 'flat' prior distribution rather than suggesting that negative values are acceptable. If the prior distribution of this parameter was found to influence the final estimates to any significant degree and in particular if negative values occurred in the analysis then it would be necessary to transform the parameters to force only realistic values to be considered by using $\log (D^*)$ for example.

For the present study the entire detrital flux is assigned to the term in equation 3.13 involving D^* which has the carbon dissolving equally in each subsurface layer. More realistic depth distributions could be used but are probably not justified in any model that does not distinguish between the Atlantic and Pacific Oceans.

Sackett et al. (1965) quote values of marine organic δ_{13} in the range -20‰ to - 30‰, but inorganic detritus would have a δ_{13} of approximately zero. Using the 2:1 ratio of organic to inorganic detritus suggests a relative depletion of -20 ± 10‰.

5.9 Mixed layer depth

The depth of the mixed layer shows considerable latitudinal and seasonal variation. Monin et al. (1977) have given examples showing seasonal variations over the range 20-170 m at 50N, 20-80 m at 45N, 20-160 m at 30N and 60-20 m at 20N. In order to cover this variability we use

$$d_m = 100 \pm 60 \text{ m.}$$

5.10 Parameterising the biosphere

In the model, the biosphere is described in terms of two reservoirs, denoted 'young' and 'old', with carbon from the atmosphere passing through the 'young' reservoir before being returned to the atmosphere or being transferred to the 'old' reservoir. In the model, the representation of the biosphere has to fulfil two main requirements. It must contain the correct total amount of carbon for ages up to thousands of year so as to give an appropriate sized reservoir for carbon-14. It must also have the correct distribution of transit times (see Bolin and Rodhe, 1973) since this distribution determines the extent to which the biosphere 'damps out' fluctuations in the isotopic composition of the atmosphere.

On the basis of the values shown in Table 5.2 we parameterise the biosphere in terms of:

Size of young biosphere, N_s = 140 ± 70 Gt/carbon
NPP = flux into young biosphere = 100 ± 50 Gt C/yr.
Size of old biosphere, N_b = 1400 ± 700 Gt (pre-clearing)
Flux into old biosphere, Q = N_b/τ_b
Turnover time of old biosphere, τ_b = 60 ± 30 years.

The main changes from the values used by Enting and Pearman (1982) are the use of a 'natural' flux into and out of the old biosphere that varies in proportion to the amount of material present (i.e. the Q_o term in equation 3.4 is set to zero), and an increase in the flux into the young biosphere in line with more recent estimates. Table 5.2 shows a number of recent estimates that were used in assigning the values and uncertainties given above. Earlier estimates are listed by Atjay et al. (1979).

<table>
<tr><th>Total
Gt</th><th>NPP
Gt/yr</th><th>Young
Gt</th><th>Old
Gt</th><th>Dead
Gt</th><th>Reference</th></tr>
<tr><td></td><td>52•8</td><td colspan="2">827</td><td></td><td>Woodwell et al. (1978), based on Whittaker and Likens (1973)</td></tr>
<tr><td>1760</td><td>113</td><td>106</td><td>452</td><td>1202</td><td>Emanuel et al. (1981) (Dead = litter + 'active' soil carbon)</td></tr>
<tr><td></td><td>110±10</td><td colspan="2">560±100</td><td></td><td>Olson (1982)</td></tr>
<tr><td></td><td></td><td></td><td></td><td>1456</td><td>Schlesinger (1977)</td></tr>
<tr><td></td><td>60</td><td colspan="2">559</td><td>1800±200</td><td>Atjay et al. (1979)</td></tr>
<tr><td></td><td>100±50</td><td>140±70</td><td colspan="2">1400±700</td><td>Present</td></tr>
</table>

Table 5.2 Estimates of amounts of carbon in the biosphere in various categories and rates of net primary production (NPP).

5.11 Rate of forest clearing

The most appropriate scenario for forest clearing, at least for prior estimates would seem to be the reference scenario proposed by Moore et al. (1981). In terms of the quadratic B-spline amplitudes defined in Section (3.2) the release can be characterised by the 7 amplitudes 0, 15, 32•5, 37•5, 57•5, 102•5, 87•5, Gt where the 8th B-spline is zero before 1990 and so does not contribute to the past releases.

The reference scenario corresponds to a loss of 148 Gt of carbon over 1860-1970 and a loss of 3 Gt in 1970.

In comparison it should be noted that estimates of the total release range from 70 to 195 Gt on the basis of carbon-13 studies and estimates of the 1970 release range from 0•4 to 18 Gt/yr (see Moore et al., 1981).

A recent review by Olson (1982) suggests a biospheric decrease of 0•5 to 2 Gt carbon per year in 1980 with more extreme bounds of -2 to +4 Gt/yr. In view of these very considerable uncertainties, it seems appropriate to use, as estimates of the standard deviations, values that are comparable to the quantities in question and so we use 10, 20, 40, 60, 80, 100, 100, uncertainties on the first seven amplitudes.

5.12 ^{13}C fractionation factor for the terrestrial biosphere

The ^{13}C content of biological material varies considerably both between species and, within a species, with changes in environmental conditions. A recent study by Francey and Farquhar (1982) proposes a possible model for some of this variability. This work poses an important problem in carbon cycle modelling involving carbon-13 because it suggests that atmospheric CO_2 concentrations may, at least in some species, be one of the factors that systematically affects the isotopic fractionation.

As described by Enting and Pearman (1982) the one-dimensional model allows a choice of fractionation formalisms for the transfer of carbon from the atmosphere to the biosphere. The fractionation can be either fixed or made to respond to atmospheric CO_2, and comprehensive studies of isotopic changes should involve tests using both forms.

For the fixed fractionation we use, (following Keeling et al., 1980)

$$f_{ab} = 0{\cdot}982 \pm 0{\cdot}004$$

corresponding to a contempory biospheric δ_{13} in the range -21‰ to -29‰, which is typical of the majority of C-3 plants.

5.13 Carbon-14 production by cosmic rays

O'Brien (1979) calculated the rate of production of carbon-14 from cosmic rays by taking observed mean alpha-particle and proton fluxes, and applying modulation effects due to variations in solar particle production and geomagnetic field strength. The calculations gave values ranging from $1{\cdot}91$ atoms/cm^2/s (1965) to $1{\cdot}60$ atoms/cm^2/s (1969), with the integrated effective production rate (i.e. the constant production rate that would give the same total current inventory as the time dependent values) being $1{\cdot}75$ atoms/cm^2/s. He quotes earlier calculations (Light et al., 1973) as being 25% higher.

Converting to a total production rate with a 25% uncertainty gives $\omega = 1{\cdot}482 \pm 0{\cdot}370 \times 10^{-5}$ mol/s.

5.14 Carbon production rate from nuclear detonations

As in our previous studies the carbon-14 production from nuclear weapons is based on a list of detonations and the carbon-14 production is calculated from the yield. Enting (1982) pointed out that this approach is essential in two-dimensional models because the atmospheric carbon-14 history is not known with sufficient spatial resolution for it to be used to define the amount of carbon-14 released. As with the air-sea exchange formalism, use of the more detailed parameterisation in the one-dimensional model can help validate the use of the same formalism in two-dimensional modelling studies.

As a first approximation all of the uncertainties are associated with a single parameter Λ which represents the number of carbon-14 atoms produced for each megaton of energy yield. Machta et al. (1963) give $\Lambda = 2 \times 10^{26}$ carbon-14 atoms per megaton, independently of whether fission or fusion energy is involved. Enting (1982) shows how this figure can be obtained from basic fission data but the wide variety of fusion reactions prevents this calculation being extended to that case. Glasstone and Dolan (1977) give results that are consistent with equal neuton production rates for fission and fusion detonations but the uncertainties are very large.

Since the parameter Λ must also absorb the inaccuracies in the history of detonation yields, the value of $2 \times 10^{26} \pm 1 \times 10^{26}$ carbon-14 atoms per megaton is used so that the value is determined by the available carbon-14 observations.

6. Data Fitted

The data set that is fitted is essentially the same as the set used by Enting and Pearman (1982). Most of the refinements that we have made in obtaining information for calibrating the model have been made to the prior parameter estimates. In preparing the data set for the constrained inversion calibration, our main concern has been to check for consistency between the quantity that is actually measured and the way the quantity is modelled.

The present calibration is designed as a basic reference calibration and so that data set is similar to that used in the calibration of other carbon cycle models (see for example Oeschger et al., 1975).

The present data set excludes some of the data fitted by Enting and Pearman (1982). Future studies will investigate the extent to which such additional data can reduce the uncertainties in the calibration.

6.1 Atmospheric CO_2 concentrations

The CO_2 concentrations that are fitted are observations from Mauna Loa, Hawaii, corrected to approximate an average atmospheric concentration by subtracting 1·90 ppmv. This correction represents -2·9 ppmv correction to convert Mauna Loa values to South Pole averages and +1·0 ppmv to convert South Pole averages to atmospheric averages. The corrections are based on the two-dimensional modelling studies described by Fraser et al. (1983) and Pearman et al. (1983).

The choice of the most appropriate averages to fit will depend on the way in which the model is to be used. To justify our use of atmospheric averages we consider a two layer (stratosphere and troposphere) model of the atmosphere and construct equations for perturbations of the CO_2 concentration about some pre-existing equilibrium.

Let

M_S be the mass of air in the stratosphere,
M_T " " " " " " " troposphere,
C_S " " " " excess CO_2 in the stratosphere,
and C_T " " " " " " " " troposphere.

If the exchanges between the reservoirs and with the ocean surface are taken as being linear in the perturbations in concentration then the response to an exponential source can be described by the equations

$$\frac{d}{dt}C_S = k(C_T/M_T - C_S/M_S) \qquad (6.1a)$$

$$\frac{d}{dt}C_T = k(C_S/M_S - C_T/M_T) - \beta C_T + B\exp(\lambda t), \qquad (6.1b)$$

which has solutions

$$C_s = A_s \exp(\lambda t) \quad (6.2a)$$

$$C_T = A_T \exp(\lambda t) \quad (6.2b)$$

with

$$\lambda A_s = k(A_T/M_T - A_s/M_s) \quad (6.3a)$$

$$\lambda A_T = k(A_s/M_s - A_T/M_T) - \beta A_T + B \quad (6.3b)$$

whence

$$\beta A_T = B - \lambda(A_T + A_s). \quad (6.3c)$$

If we actually want to try and model the behaviour of this system using a single atmospheric reservoir with an amount C of excess CO_2 then the relevant equations will be

$$\frac{d}{dt} C = -\beta' C + B \exp(\lambda t) \quad (6.4)$$

so that

$$C = A \exp(\lambda t) \quad (6.5)$$

with

$$\beta' A = B - \lambda A \quad (6.6)$$

In each of equations (6.3c) and (6.6) the rate constants for transfer into the ocean i.e. β, β' respectively, are determined by fitting the observed atmospheric contents.

Comparing (6.6) to (6.3c) it will be seen that fitting the quantity A in (6.6) to $A_T + A_s$ in equation (6.3c) will produce an estimate of β' which differs from the value β appropriate for the more detailed two-layer model. The value β' will however have the property that $\beta' A$ which describes the rate of transfer of CO_2 into the ocean will agree with the rate of transfer of CO_2 into the ocean in the more detailed model.

Thus in working with a single atmospheric reservoir, fitting the model value of the atmospheric concentration to the mean concentration of a two-reservoir model will give the correct rate of total transfer of CO_2 into the ocean. (Note that this correspondence will still be preserved if the air-sea exchange terms are generalised to $\beta(A_T - p_m)$ and $\beta'(A - p_m)$ respectively with p_m being proportional to the partial pressure of CO_2 in the ocean surface.)

The observations at Mauna Loa have been made since 1958 but Keeling et al. (1982) have indicated problems with the data between May 1964 and January 1969 and so data from this period have been excluded. The data chosen is given in Table 6.1 with uncertainties of 0·3 ppmv in each case.

Date	Mauna Loa annual mean ppmv	Corrected ppmv
1959.5	315.66	313.76
1963.5	318.71	316.81
1970.5	325.51	323.61
1973.5	329.82	327.92
1977.5	333.63	331.73
1980.5	338.36	336.46

Table 6.1

Annual averages of CO_2 concentrations at Mauna Loa, Hawaii (Keeling et al. 1982) and corrected values obtained by subtracting 1•9 ppmv to obtain an approximate atmospheric average.

6.2 Atmospheric carbon-14

In the early studies with this model, Pearman (1980) used data from Telegardas (1971) as a check on the rate of ocean uptake of carbon-14 from nuclear tests. In later model calibrations, Enting and Pearman (1982) also used data from Nydal et al. (1980) and found that these data were more useful since the uncertainties were smaller and the period covered was longer. Tans (1981b) has assembled a more comprehensive set of observations but they only apply to the troposphere. It is only that later part of this data set that can be regarded as representing an atmospheric average. The longer data set would be appropriate for a model with separate stratospheric and tropospheric reservoirs.

Table 6.2 is the data taken from Nydal et al. (1980) but it is essentially equivalent to the values given by Tans (1981b). The decreasing uncertainties are chosen to reflect the decreasing differences between stratosphere and troposphere. (Tans assigned 10‰ uncertainties to his tropospheric values.)

Date	Δ-14,‰	Uncertainty,‰
1967.0	650	50
1969.0	580	50
1971.0	500	50
1973.0	450	30
1975.0	420	30
1977.0	350	30

Table 6.2

Atmospheric Δ-14 values used, together with uncertainties.

6.3 Atmospheric carbon-13

One of the original aims of the carbon cycle modelling program in the Division of Atmospheric Physics was to have a basis for interpreting the results of carbon isotope measurement program in the Division. Until this record is extended for a longer time and the calibration relative to other laboratories is established, it is necessary to rely on limited and somewhat indirect observations of atmospheric δ_{13}.

Keeling et al. (1979) estimated

$$\delta_{13}(a) = -6{\cdot}69 \pm 0{\cdot}13‰ \ (1956.25)$$

$$= -7{\cdot}24 \pm 0{\cdot}05‰ \ (1978)$$

In each case the δ_{13} value was obtained by establishing a mixing relation connecting δ_{13} to concentration and then selecting the δ_{13} appropriate to the CO_2 concentration representative of the time and location of samples used.

6.4 Ocean carbonate concentrations

The most detailed compilation of ocean carbonate measurements is given by Takahashi et al. (1981) from GEOSECS observations. The ΣCO_2 values are in µmol/kg and have been normalised to a constant salinity of 35‰.

In order to obtain values appropriate for the mixed layer (0 to 100 m in the model) and the lowest layer (above 3730 m in the model) two observations for each of these layers are given so as to indicate the range of observed values. In addition the standard deviation (column sd in Table 6.3) is given to indicate the spread of values at each depth.

Table 6.3 Dissolved inorganic carbonate measurements from the GEOSECS program, (Takahashi et al., 1981).

Latitude	Depth m	CO µmol/kg	sd µmol/kg	Table from Takahashi et al.
South of 50S	0-24	2198.1	35.02	S14
	75-99	2215.3	44.66	
	3000-3999	2281.1	9.08	
	5000-5999	2278.7	10.44	
50S to 10S	0-24	1979.5	60.19	S20
	75-99	2006.8	61.67	
	3000-3999	2287.4	48.56	
	5000-5999	2288.6	19.96	
10S to 10N	0-24	1947.5	22.06	S19
	75-99	2041.0	58.62	
	3000-3999	2308.2	67.93	
	5000-5999	2307.4	23.03	
North to 10N	0-24	1982.4	64.07	S18
	75-99	2012.5	80.80	
	3000-3999	2307.3	83.90	
	5000-5999	2304.0	54.83	

The assignment of values to the boxes in the model is complicated by the differences in the zones used. The values used are

$$\Sigma CO_2 = 2080 \pm 150\ \mu mol/kg = 2{\cdot}132 \pm {\cdot}102\ mol/m^3$$

cold surface

$$= 1960 \pm 40\ \mu mol/kg = 2{\cdot}009 \pm {\cdot}041\ mol/m^3$$

warm surface

$$= 2280 \pm 40\ \mu mol/kg = 2{\cdot}337 \pm {\cdot}041\ mol/m^3$$

cold deep

$$= 2300 \pm 60\ \mu mol/kg = 2{\cdot}358 \pm {\cdot}062\ mol/m^3$$

warm deep .

We have selectively biased our values towards the southern regions because of the greater area of ocean.

6.5 Ocean carbon-14

The most comprehensive set of ocean Δ-14 measurements is from the GEOSECS program and has been described by Stuiver and Ostlund (1980) and Ostlund and Stuiver (1980) who give, for the Atlantic and Pacific Oceans respectively, individual measured values and diagrams showing cross sections of the ocean. A summary with average profiles has been given by Stuiver et al. (1981), using the same zonal divisions as in Table 6.3 above. In addition data from other times is given by Broecker et al. (1960) and Nydal et al. (1980).

The GEOSECS data in Table 6.4 is obtained from the main profiles given by Stuiver et al. (1981) with the uncertainties representing the differences between the ocean regions. Because of the very great degree of variability between water masses, no attempt has been made to fit values of Δ-14 at intermediate depths.

Table 6.4 Carbon-14 in the oceans. GEOSECS data is from Stuiver et al. (1981)

Reservoir	Date	Δ-14‰	Source
Cold deep	1973.5	-150 ± 50	GEOSECS
Warm deep	1973.5	-150 ± 50	GEOSECS
Cold surface	1955.5	- 58 ± 10	Broecker et al. (1960)
	1973.5	120 ± 50	GEOSECS
Warm surface	1955.5	- 58 ± 10	Broecker et al. (1960)
	1968.5	150 ± 70	Nydal et al. (1980)
	1973.5	120 ± 50	GEOSECS
	1978.5	100 ± 50	Nydal et al. (1980)

6.6 Suess effect data

The Suess effect is the reduction in carbon-14 levels in the biosphere due to the atmospheric carbon dioxide having increasing amounts of input from fossil carbon which contains no carbon-14. The data used are taken from Lerman et al. (1970) (their Figure 2) and are

$$
\begin{aligned}
\Delta\text{-14 (tree rings)} &= 0 \pm 5‰,\ 1890 \\
&= -5 \pm 5‰,\ 1910 \\
&= -12 \pm 5‰,\ 1930 \\
&= -22 \pm 5‰,\ 1950
\end{aligned}
$$

The data represent a composite of a set of observations. In the model, tree-ring data are fitted to the young component of the biosphere, evaluated at the time at which the tree-ring was laid down.

7. Results of a Reference Calibration

This Section describes the results of two of our reference calculations. The first calibration was based on fitting 22 parameters, involving the set considered by Enting and Pearman (1982), including those that were dropped because stable estimates could not be obtained. The second calibration fitted 31 parameters. The main results are the parameter estimates given in Table 7.1.

The minimisation of θ (as defined by equation 4.1) was performed using a iterative sequence of linear approximations. The initial step used the prior parameter values as a starting point and used $\gamma = 1000$. For each of the γ values 100, 10 and 1, the solution from the previous γ value was used as a starting point. This procedure converged rapidly, only 3 iterations being required for each minimisation. As pointed out by Rodgers (1977) this rapid convergence provides a useful test of the adequacy of the linear assumptions made in the error analysis.

The values of θ, the sum of squares, are plotted against γ, the weighting factor, in Figure 7.1. The behaviour is smooth so that there is no indication of major inconsistencies in the information fitted. These calibrations were performed with the biospheric carbon-13 fractionation being determined by the formalism described by Francey and Farquhar (1982).

In order to assess the uncertainties in the predictions of the model, we analysed the errors in the model prediction for the atmospheric CO_2 concentration in the year 2050, assuming 2.25%/yr growth in fossil carbon release and no biospheric changes after 1985 (i.e. the spline curve was terminated discontinuously).

The uncertainties in this prediction were assessed using equations 4.2, 4.3. The first result obtained was

$$
\begin{aligned}
C_a(2050) &= 680.3 \pm 11.1 \text{ ppmv (fitting 22 parameters)} \\
&= 677.3 \pm 12.7 \text{ ppmv (fitting 31 parameters)}.
\end{aligned}
$$

The ranges shown correspond to θ one standard deviation. The range is slightly larger when the larger number of parameters is used as explained in Section 4. Including the additional parameters in the inversion formalism enables us to assess the effect that the uncertainties will have on model predictions, even though going through the process of fitting the parameters does not significantly reduce the initial uncertainties in the parameter values.

From the results given above it can be seen that the uncertainties in these additional parameters have no significant influence on either the accuracy or precision of the predictions of the model when it is calibrated using the data set described in Section 6. It is however quite possible that the uncertainties about biospheric parameters in particular may be extremely significant in limiting the extent to which ^{13}C observations from either atmospheric or biospheric sources can be used to improve the calibration of the model.

The smoothness of the curve in Figure 7.1 and the small values of θ that are obtained indicate that it is possible to fit the carbon cycle data using parameter values that are consistent with the prior information. The major discrepancies involve the biospheric release history.

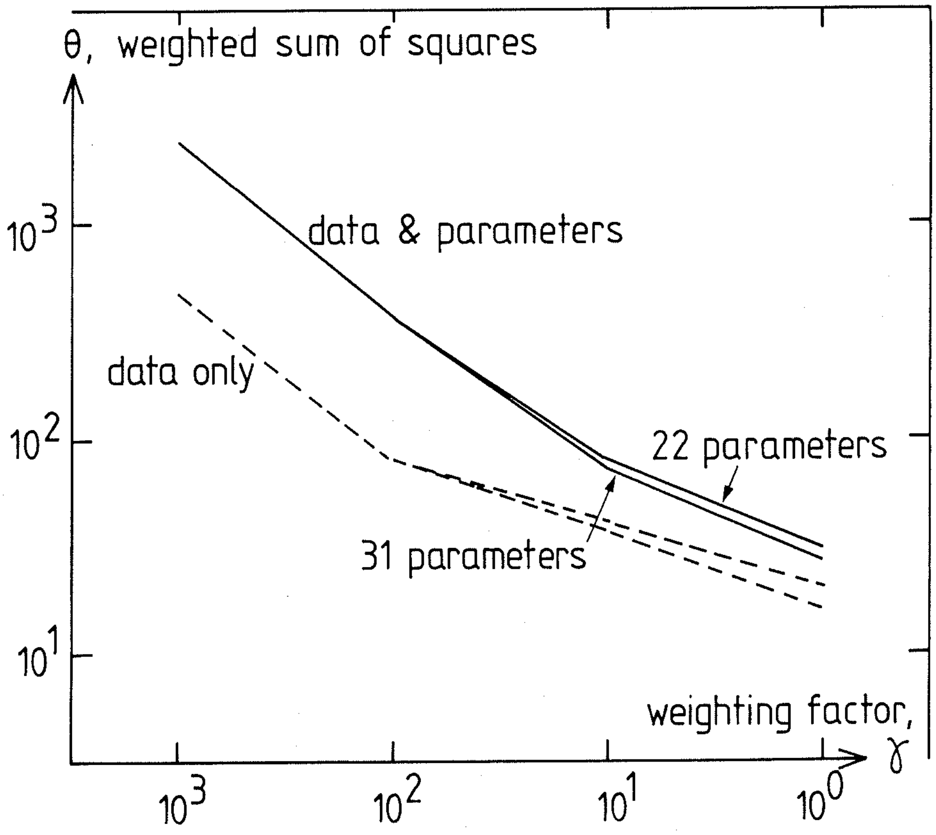

Figure 7.1 Variation of the weighted sum of squares, θ, and of the sum of squares of deviations from carbon cycle data only, plotted against the weighting factor γ. The smoothness of these plots is an indication of the absence of gross inconsistencies in the sets of information fitted.

Table 7.1 The results of two reference calibrations. Estimates 1 and 2 correspond to fitting 22 and 31 parameters respectively. For estimate 1, parameters 23 to 31 are fixed at the prior values.

No. k	Quantity		prior q_k	sd u_k	Estimate 1	Estimate 2
1	Preindustrial CO_2	ppmv	270	50	263	262
2	^{14}C from weapons × 10^{26}	atoms/ megaton	2·00	0·50	1·49	1·41
3	Preindustrial δ_{13}	‰	-6·00	3·0	-5·21	-5·24
4	Biospheric release coefficient	Gt	0·0	10·0	0·015	0·06
5		Gt	15·0	20·0	14·6	14·7
6		Gt	32·5	40·0	25·8	25·9
7		Gt	37·5	60·0	22·5	25·1
8		Gt	57·5	80·0	27·9	30·7
9		Gt	102·5	100·0	-35·7	-35·5
10		Gt	87·5	100·0	-22·0	-11·7
11	Cold ocean temp.	°C	10·3	5·0	10·6	10·6
12	Warm ocean temp.	°C	25·2	2·0	26·5	26·5
13	Alkalinity	mol/m^3	2·369	0·021	2·35	2·35
14	Uniform upwelling	m/yr	1·8	1·35	0·27	0·23
15	Varying upwelling	m/yr	2·5	2·0	0·43	0·53
16	Vertical diffusion	m^2/yr	3500	2000	4987	5255
17	$\frac{d}{dt}\left(\text{vertical diffusion}\right)$	m/yr	0	1·0	0·299	0·257
18	Horizontal diffusion	m^2/s	25000	20000	23736	23626
19	ω	mol/s	1·484·10^{-5}	3·7×10^{-6}	1·341×10^{-4}	1·339×10^{-4}
20	u^*_{cold}	m/s	1·7	1·2	1·57	1·54
21	u^*_{warm}	m/s	0·8	0·5	1·29	1·29
22	Detrital fallout	Gt/yr	2·0	3·0	3·42	3·57
23	Young biosphere	Gt	140	70		174
24	Old biosphere	Gt	1400	700		1145
25	NPP	Gt/yr	100	50		104
26	Old biosphere t.over	yr	60	30		65·8
27	δ_{13} depletion of detritus	‰	-20	10		-20·1
28	Mixed layer depth	m	100	60		104·1
29	f_{as}	-	·99795	·00025		·997949
30	f_{sa}	-	·99005	·00025		·990051
31	f_{ab}	-	·982	·004		·9796

8. Conclusions

The major conclusion of this report is that techniques based on constrained inversion can be a powerful way of calibrating carbon cycle models, particularly when the model is built around direct representations of geophysical processes. This is because the procedure was found to be numerically stable and rapidly convergent, unlike the process of fitting a smaller number of parameters to only the carbon cycle data, as described by Enting and Pearman (1982). In addition the constrained inversion formalism makes sensitivity analysis both simpler and more comprehensive than other formalisms. A secondary conclusion that follows from the consistency that is indicated in Table 7.1 is that our geophysical knowledge is generally consistent with current observations of the carbon cycle. This gives us considerable confidence in using the high-resolution description of such geophysical processes in high-resolution carbon cycle models.

As pointed out in Section 4, the constrained inversion formalism can be used as a basis for a number of sensitivity studies and studies of the utility of various types of data in adding to our understanding of the carbon cycle. Such studies will be described elsewhere.

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