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Principles of constrained inversion in the calibration of carbon cycle models

By I. G. ENTING, *CSIRO Division of Atmospheric Research, Private Bag No. 1, Mordialloc, Victoria, Australia, 3195*

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ABSTRACT

The calibration of carbon cycle models by using techniques of constrained inversion is described. These techniques provide a systematic means of assessing the uncertainties in the calibration. The specific calibration technique is analysed in terms of the requirements of carbon cycle studies, and the relation to other constrained inversion formalisms is discussed. As an example of the technique, a linearized version of the box-diffusion model is calibrated.

1. Introduction

This paper describes a technique for calibrating carbon cycle models (and similar models) that is based on techniques of constrained inversion. Such techniques have been used relatively frequently in geophysical problems but relatively seldom in geochemical studies. In general, constrained inversion techniques can be regarded as conventional parameter fitting procedures (such as least-squares parameter fitting) supplemented by constraints that ensure numerical stability of the computational procedures and, where necessary, uniqueness of the solution. The constraints should also be chosen to ensure that the solution is consistent with known physical laws.

The specific form of calibration described here uses geophysical (and biological) information as the additional constraint, requiring that the parameters of the carbon cycle model are consistent with this additional information as well as fitting the known aspects of the carbon cycle. There are thus two ways of regarding this calibration procedure.

(i) It can be considered as a constrained inversion technique. Observations of various aspects of the carbon cycle are used to deduce values of model parameters. This "inversion" of the carbon cycle data is "constrained" by the additional geophysical information.

(ii) Alternatively the calibration can be regarded as conventional parameter fitting using an extended data set, and no special significance is assigned to the division of this data set into a set of observations of the carbon cycle and a set of observations of other relevant geophysical quantities. The specific calibration procedure presented in the following sections can be described more precisely as being a weighted least-squares fit to the extended data set.

The description of the technique that is given in the following sections will make use of both of these interpretations at various times. The interpretation as a least-squares fit to an extended data set allows a direct use of a large body of standard theory concerning the uncertainties in the parameter estimates (see for example Bard, 1974). Rodgers (1977) has pointed out that the correct way to assess the uncertainties in any constrained inversion is to transform the formalism into one of fitting an extended data set. The interpretation of the calibration procedure as a constrained inversion is used because the literature of constrained inversion addresses a number of problems (such as determining unknown functions) that are relevant to carbon cycle modelling but which are

not commonly considered in "conventional" analyses of parameter fitting. In addition to the two interpretations given above, the calibration procedure can also be related to Bayesian estimation procedures (Box and Tiao, 1973) and the linearized form of the calibration can be related to an augmented matrix solution (see Lawson and Hanson (1974) Section 25.4). These various interpretations are described in more detail in Appendix C which also describes how the method relates to techniques using pseudo-inverses of matrices. Appendix C also compares the techniques to those used by Bolin et al. (1983) in one of the few applications of constrained inversion techniques to a geochemical problem.

There are three main reasons for proposing the present calibration technique in carbon cycle studies.

(i) The technique gives a unified and fairly general method for calibrating geochemical models. Frenkiel and Goodall (1978) have commented that "systematic methods of approaching model estimations and validations have not received much attention in the simulation literature". In the specific context of carbon cycle modelling, Bolin et al. (1979) have commented on the lack of systematic use of the available carbon cycle data in modelling studies; they cited the work of Oeschger et al. (1975) as a major exception.

(ii) The simple or "unconstrained" inversion of carbon cycle data can tend to be numerically unstable particularly when more than a few parameters have to be estimated simultaneously. A specific example of this difficulty is described by Enting and Pearman (1982). Allison (1979) has suggested that this situation is very general and that mathematical modelling is only reasonable in situations where the inverse problem is unstable. His argument is that the relatively crude approximations to the physical processes modelled must lead to small deviations in the outputs of the model if the modelling is to be valid. Consequently in the unconstrained inverse problem, relatively small errors in the data that is fitted to the model outputs can lead to relatively large errors in the estimates of the parameters describing the model processes.

Numerical instability in the calibration procedure is undesirable for the practical reason that it makes the "best-fit" parameters very difficult to determine. More importantly, numerical instability generally reflects the fact that the parameter estimates are very sensitive to the data that is fitted, i.e. that small errors in the data lead to large errors in the parameters. In such a case, even if very sophisticated numerical techniques were used to determine the "best-fit" parameters, the values that would be obtained would be subject to very large uncertainties. Therefore, whenever simple parameter fitting techniques become unstable, some form of constrained inversion is necessary.

(iii) Carbon cycle studies can require the determination of unknown functions. In particular, for many studies of the carbon cycle it is desirable to treat the net rate of change of the carbon content of the biosphere over the last century as being unknown. Since direct estimates of biospheric changes appear to be inconsistent with current carbon cycle models (see, for example, Broecker et al. (1980)) any comprehensive investigation of this discrepancy must be able to consider a range of possible biospheric release functions. The determination of unknown functions from limited amounts of data and the study of the extent to which the functions can be resolved is a problem that is addressed directly by constrained inversion, particularly in the fields of remote sensing and seismology.

The layout of the paper is as follows. Section 2 describes some of the key concepts in constrained inversion and discusses the type of results that can be expected from the technique. Section 3 gives a mathematical definition of the calibration technique. Sections 4 and 5 describe the application of the constrained inversion techniques to calibrating a linearized approximation to the box-diffusion model of Oeschger et al. (1975). In Section 6, the results are compared to the calibration used by Oeschger et al. and to the revised calibration described by Broecker et al. (1980).

There are three appendices that describe aspects of the present calculations that are peripheral to the general principles. Appendix A describes the numerical techniques that were used in the example quoted in Sections 4 and 5. Since the calibration is defined in terms of minimizing an objective function there are a variety of other techniques that could have been used. Extensive discussions of such problems are given by Kowalik and Osborne (1968) and Bard (1974). Appendix B defines the linearized approximation to the box-diffusion model. Appendix C describes a number

of different interpretations of the constrained inversion scheme presented here and compares this technique to other approaches, particularly that used by Bolin et al. (1983). Finally, Appendix D summarizes the notation that is used.

2. Concepts in constrained inversion

Constrained inversion techniques have been used to obtain solutions to underdetermined problems in fields such as remote sensing of the atmosphere (Twomey, 1977), seismology (Wiggins, 1972) and oceanography (Wunsch, 1978). Many of the basic concepts can be introduced in terms of the linear inversion problem; the description here follows the analysis of Chapter 2 of Lawson and Hanson (1974).

The general linear parameter estimation problem consists of determining a set of parameters, x_k, $k = 1, K$ (denoted $\boldsymbol{x}$) given a model that gives a set of predictions y_j, $j = 1, J$ (denoted $\boldsymbol{y}$) that depend linearly on the x_k. The y_j are fitted to a set of observations m_j, $j = 1, J$ (denoted $\boldsymbol{m}$). The linear model can be written in the form

$$\boldsymbol{y} = \boldsymbol{S}\boldsymbol{x}, \tag{2.1a}$$

i.e.

$$y_j = \sum_k S_{jk} x_k. \tag{2.1b}$$

The parameter estimation problem becomes that of obtaining the "best" possible solution to

$$\boldsymbol{m} = \boldsymbol{S}\boldsymbol{x}. \tag{2.2}$$

Lawson and Hanson (1974) show how the analysis of this problem is aided by taking the singular value decomposition of $\boldsymbol{S}$. They show that one can write

$$\boldsymbol{S} = \boldsymbol{U}\boldsymbol{R}\boldsymbol{W}^{\mathrm{T}}, \tag{2.3}$$

where $\boldsymbol{U}$ and $\boldsymbol{W}$ are orthogonal matrices of dimensions $J \times J$ and $K \times K$ respectively and $\boldsymbol{R}$ is a $J \times K$ matrix which is zero except for the first r elements of the leading diagonal which are positive and decrease along the diagonal. The number r is the rank of the matrix $\boldsymbol{S}$. The orthogonal transformation $\boldsymbol{U}^{\mathrm{T}}$ transforms the representation of vectors $\boldsymbol{y}$ and $\boldsymbol{m}$ into a new basis which displays an explicit subdivision of the vector space into two subspaces E_1 and E_2. E_1 is spanned by the first r of the new basis vectors and E_2 is spanned by the last $J - r$ of the new basis vectors.

Similarly $\boldsymbol{W}^{\mathrm{T}}$ transforms the components representing $\boldsymbol{x}$ vectors into a new basis which displays an explicit subdivision of the space of $\boldsymbol{x}$ vectors into two subspaces E_1' and E_2'. E_1' is spanned by the first r of the new basis vectors and E_2' is spanned by the last $K - r$ basis vectors. Vectors $\boldsymbol{m}$ and $\boldsymbol{x}$ are denoted $\tilde{\boldsymbol{m}}$, $\tilde{\boldsymbol{x}}$ when transformed to the new basis.

If $r < J$ then an exact solution to (2.2) is in general impossible and the best that can be obtained is the solution that minimizes $\|\boldsymbol{y} - \boldsymbol{m}\|$ where $\|\ \|$ denotes an appropriate vector norm. This section uses only the Euclidean norm which is invariant under orthogonal transformations such as $\boldsymbol{U}$ and $\boldsymbol{W}$. In later sections weighted norms are used.

When minimizing $\|\boldsymbol{y} - \boldsymbol{m}\|$ using the Euclidean norm (i.e. performing a least squares fit), the residual is given by

$$\|\boldsymbol{S}\boldsymbol{x} - \boldsymbol{m}\| = \|\tilde{\boldsymbol{m}}_2\|, \tag{2.4}$$

where

$$\boldsymbol{U}^{\mathrm{T}}\boldsymbol{m} = \tilde{\boldsymbol{m}} = \tilde{\boldsymbol{m}}_1 + \tilde{\boldsymbol{m}}_2, \tag{2.5}$$

with

$$\tilde{\boldsymbol{m}}_1 \in \mathrm{E}_1 \quad \text{and} \quad \tilde{\boldsymbol{m}}_2 \in \mathrm{E}_2.$$

If

$$\boldsymbol{W}^{\mathrm{T}}\boldsymbol{x} = \tilde{\boldsymbol{x}} = \tilde{\boldsymbol{x}}_1 + \tilde{\boldsymbol{x}}_2, \tag{2.6}$$

with $\tilde{\boldsymbol{x}}_1 \in \mathrm{E}_1'$ and $\tilde{\boldsymbol{x}}_2 \in \mathrm{E}_2'$ then the best fit vector $\boldsymbol{x}$ has $\tilde{\boldsymbol{x}}_1$ given by the unique solution of

$$\boldsymbol{R}\tilde{\boldsymbol{x}}_1 = \tilde{\boldsymbol{m}}_1, \tag{2.7}$$

and has $\tilde{\boldsymbol{x}}_2$ arbitrary. Thus whenever $r < K$ (i.e. E_2 is non-trivial) the least squares problem is underdetermined and the parameters can only be fixed within the r-dimensional subspace E_1'. Any parameter vector from the $K - r$ dimensional subspace, E_2', may be added to a least-squares solution to obtain an alternative least squares solution.

A central task of constrained inversion techniques when applied to underdetermined systems is to obtain unique solutions. This is achieved by adding additional information to the problem. Such additional information may be:

(a) based on analogies with past experience or related problems;

(b) entirely arbitrary;

or

(c) external to the original problem.

The use of analogies with past experience can often be appropriate in remote sensing applications (see Twomey, 1977). This approach of basing interpretations on prior results can be naturally interpreted in terms of Bayesian estimation (see Appendix C). Whitney (1977) has described a Bayesian formulation of remote sensing problems.

The use of arbitrary additional constraints merely provides the mathematical convenience of a single representative solution from a large range of equally acceptable solutions. As pointed out by Anderssen (1977) this can be useful if the solution is to be used merely as a step in calculating some secondary quantity that does not depend on which of the many solutions is chosen as the representative. Anderssen emphasized that the question of whether a system is underdetermined or not depends on what is being calculated. If the final requirement is for a quantity F that depends on $\boldsymbol{x}$ then for linear dependences a general function F can be written as

$$F = \boldsymbol{f}^{\mathrm{T}}\boldsymbol{x} = \boldsymbol{f}^{\mathrm{T}}\boldsymbol{W}^{\mathrm{T}}\boldsymbol{W}\boldsymbol{x}$$

If $\boldsymbol{W}\boldsymbol{f}$ (i.e. $(\boldsymbol{f}^{\mathrm{T}}\boldsymbol{W}^{\mathrm{T}})^{\mathrm{T}}$) lies within the r-dimensional subspace E_1' is then the value of F will be unchanged when an arbitrary $\tilde{\boldsymbol{x}}_2$ is added to the least-squares solution, and applying an arbitrary constraint to determine $\tilde{\boldsymbol{x}}_2$ will not affect F. A common form for the arbitrary constraint is to choose the smallest vector $\boldsymbol{x}$ that satisfies the least squares condition of minimizing $\|\boldsymbol{S}\boldsymbol{x} - \boldsymbol{m}\|$. The solutions can be obtained using the pseudo-inverse of matrix $\boldsymbol{S}$ as described in Appendix C (see also Deutsch (1965), Bard (1974), Lawson and Hanson (1974)).

This paper is concerned mainly with using external information for the constraint. The additional information is obtained by relating carbon cycle model parameters to geophysical quantities that can be estimated independently of the carbon cycle. In this context, the techniques of constrained inversion provide a systematic way of combining carbon cycle data with external geophysical information and, in particular, the techniques give a guide to the relative importance that should be applied to the two different types of information.

The results of such constrained inversion calibrations are:

(i) a set of parameter estimates based on the use of both prior information and carbon cycle data; an additional advantage is that the inclusion of the prior information should serve to reduce any numerical instability involved in obtaining parameter estimates;

(ii) estimates of the uncertainties in the parameters; this should be given as a covariance matrix since many parameter estimates may be highly correlated;

(iii) estimates of the uncertainties in the predictions of the model; As emphasized by Anderssen (1977), any specification of the extent to which a system is underdetermined only has a meaning when applied to some specific aspect of the system;

(iv) estimates of the extent to which various observations are effective in reducing the uncertainties in the model predictions; although such considerations can be applied in any statistical estimation, they can be particularly useful in underdetermined problems in which there are large uncertainties that could, in principle, be greatly reduced by particular types of observation; the concept has been described by Jackson (1972) as the "marginal utility of data".

3. Mathematical formalism

The general mathematical formalism for constrained inversion calibrations uses the following quantities

(i) model parameters x_k, $k = 1, K$;

(ii) prior estimates q_k of the parameters x_k. Ideally these estimates should be independent of the carbon cycle observations so as to avoid circularity in the parameter fitting procedure;

(iii) standard deviations w_k for the prior estimates q_k. These express the extent to which the x_k are known before fitting the model to the observations;

(iv) carbon cycle observations m_j, $j = 1, J$;

(v) standard deviations v_j for the m_j; these standard deviations should reflect not only experimental errors but also, following the suggestion of Bolin et al. (1981), the degree of spatial and temporal variability in the m_j;

(vi) model predictions y_j for the various m_j; these will be functions of the set of parameters; this dependence is denoted $y_j(\boldsymbol{x})$;

(vii) a weighting factor γ determines the relative weight that is given to the prior information as opposed to the carbon cycle data; since, as described by Twomey (1977), γ is arbitrary, one

criterion for choosing γ is that the parameter estimates should be relatively insensitive to the precise γ value chosen; in addition, in the present formalism, if the various uncertainties have been realistically assessed, then the appropriate value of γ would be of order 1;

(viii) a weighted sum of squares of deviations, θ, defined by

$$\theta = \sum_{j=1}^{J} (y_j(\boldsymbol{x}) - m_j)^2/v_j^2 + \gamma \sum_{k=1}^{K} (x_k - q_k)^2/w_k^2. \tag{3.1a}$$

The constrained inversion formalism obtains parameter estimates by taking the values that minimize θ.

It is possible to write

$$\theta = \|\boldsymbol{y} - \boldsymbol{m}\|^2 + \gamma \|\boldsymbol{x} - \boldsymbol{q}\|^2 \tag{3.1b}$$

so long as the norms of vectors in the two spaces are defined as including the weighting factors v_j^2 and w_k^2. The vector form of (3.1b) shows how this formalism is related to the forms described in Section 2. Firstly the vector norms (i.e. $\|\ldots\|$) are defined with a specific weighting so that the numerical values do not depend on such things as the units that are used for the various components of $\boldsymbol{x}$ and $\boldsymbol{m}$. Secondly the constraint on $\boldsymbol{x}$ is to force it to lie near $\boldsymbol{q}$ rather than necessarily near $\boldsymbol{0}$ as in pseudoinverse solutions. Thirdly, instead of minimizing $\|\boldsymbol{y} - \boldsymbol{m}\|$ and then using the remaining degrees of freedom to minimize $\|\boldsymbol{x} - \boldsymbol{q}\|$, subject to the condition that $\|\boldsymbol{y} - \boldsymbol{m}\|$ remain minimal, the "compromise" procedure of minimizing the combination (3.1b) is used. (The relation between these two types of minimization is discussed further in Appendix C.)

The choice of specific weighting factors removes one of the difficulties encountered by Bolin et al. (1983). The precise results obtained by their method depends on the relative scaling of the various parameters. The weights used in eq. (3.1) are chosen so that when $\gamma = 1$ the variances of the parameter estimates is smaller than would be obtained with any other set of weights (see Deutsch, 1965).

Enting (1983) has suggested that when the analysis indicates that $\gamma > 1$ is appropriate, this may be because either the estimates of the prior standard deviations were unreasonably large due to doubts about the applicability of certain prior information or that the errors in the carbon cycle data were not independent, effectively reducing the number of observations. If it is found that the parameter estimates vary rapidly with γ, a possible inconsistency in the information is indicated, i.e. there is no broad range of "compromise" solutions that fit both the prior information and the carbon cycle observations. Such inconsistency is of course occurring within the context of fitting a specific model and so what is most probably indicated by extreme sensitivity of the estimates of x_k to γ is some inadequacy in the model.

An important part in the analysis is played by the sensitivity matrix, $\boldsymbol{S}$, whose elements are defined by

$$S_{jk} = \frac{\partial y_j}{\partial x_k}, \quad j = 1, J, \quad k = 1, K. \tag{3.2}$$

If a particular parameter set x_k^* is taken, then a linear approximation about this point in the parameter space gives

$$y_j(\boldsymbol{x}) = y_j^* + \sum_{k=1}^{K} S_{jk}\,\Delta x_k, \tag{3.3a}$$

where

$$y_j^* = y_j(\boldsymbol{x}^*), \tag{3.3b}$$

$$\Delta x_k = x_k - x_k^*. \tag{3.3c}$$

Substituting into eq (3.1) gives

$$\theta \cong \theta^* + 2 \sum_{k=1}^{K} \Delta x_k (\gamma(x_k^* - q_k)/w_k^2 + \sum_{j=1}^{J} S_{jk}(y_j^* - m_j)/v_j^2) + \sum_{k=1}^{K} \sum_{k'=1}^{K} \Delta x_k\,\Delta x_{k'} \times \left(\gamma I_{kk'}/w_k^2 + \sum_{j=1}^{J} S_{jk}\,S_{jk'}/v_j^2\right), \tag{3.4a}$$

where

$$\theta^* = \sum_{j=1}^{J} (y_j^* - m_j)^2/v_j^2 + \gamma \sum_{k=1}^{K} (x_k^* - q_k)^2/w_k^2, \tag{3.4b}$$

and $I_{kk'}$ denotes the k, k' element of the $K \times K$ identity matrix.

If the values of x_k^* do not define a minimum for θ then an approximate (linear) estimate of the changes Δx_k required to minimize θ can be obtained by differentiating eq. (3.4a) with respect to each Δx_k. This leads to a set of equations

$$\sum_{k'=1}^{K} V_{kk'}(\gamma)\,\Delta x_{k'} = -b_k, \quad k = 1, K, \tag{3.5a}$$

where

$$b_k = \gamma(x_k^* - q_k)/w_k^2 + \sum_{j=1}^{J} S_{jk}(y_j^* - m_j)\,v_j^2, \tag{3.5b}$$

$$V_{kk'}(\gamma) = \gamma I_{kk'}/w_k^2 + \sum_{j=1}^{J} S_{jk}\,S_{jk'}\,v_j^2. \tag{3.5c}$$

In non-linear estimation problems this approach must be applied iteratively to produce a succession of estimates x_k^* with the matrix $\boldsymbol{S}$ being re-evaluated at each stage.

Once the minimum has been achieved, the terms in eq (3.4a) that are linear in the Δx_k will vanish identically for *all* possible parameter changes.

For $\gamma = 1$, if the standard deviations are correctly assigned and the errors are independently normally distributed then the matrix $\boldsymbol{C}(1)$ is the covariance matrix for the parameter estimates where in general $\boldsymbol{C}(\gamma)$ is the inverse of $\boldsymbol{V}(\gamma)$. This conclusion can be reached from either conventional estimation theory, regarding eq. (3.1) as giving a least squares fit to two sets of data (the m_j and the q_k) or equivalently from a Bayesian estimation procedure (see Appendix C and Enting, 1983) For $\gamma > 1$, Enting's interpretation based on lack of independence in the observations leads to a parameter covariance matrix $\gamma\boldsymbol{C}(\gamma)$. Somewhat different expressions are obtained if the minimization of expression (3.1) is regarded as a weighted least squares procedure with non-optimal weights.

In most theoretical treatments of constrained inversion (see for example Jackson (1972)) the treatment assumes that the constraints are arbitrary, at least to the extent that estimates of the accuracy of the constraints are not considered. This means that the estimate of parameter uncertainties in such treatments must of necessity be restricted to the uncertainties in locating the reference parameter set subject to the assumption that the constraints are exactly correct. In the formalism described above, which follows the approach of Rodgers (1977), the use of the uncertainties in the prior parameter estimates allows a more complete treatment of the uncertainties in the final estimates.

In order to consider uncertainties in the predictions of the model, we consider some arbitrary quantity Z predicted by the model as a function of the parameters. If the best-fit parameters x_k^* give a value Z^* then a linearized expansion about this value gives

$$Z(\boldsymbol{x}) \simeq Z^* + \sum_{k=1}^{K} T_k\,\Delta x_k, \tag{3.6a}$$

with

$$T_k = \frac{\partial Z}{\partial x_k}. \tag{3.6b}$$

The variance of Z is then given by

$$\begin{aligned}\mathrm{Var}(Z) &= E[(Z - Z^*)^2] \\ &= \gamma \sum_{k=1}^{K}\sum_{k'=1}^{K} T_k\,C_{kk'}(\gamma)T_{k'}\end{aligned} \tag{3.7}$$

since $\mathrm{Cov}(x_i, x_j) = \gamma C_{kj}$.

A convenient numerical technique for evaluating $\mathrm{Var}(Z)$ without explicit construction of the matrix $\boldsymbol{C}(\gamma)$ is based on minimizing the quantity

$$\phi = \theta - 2\alpha Z. \tag{3.8}$$

Expanding (3.8) about the best-fit point gives

$$\begin{aligned}\phi = \theta^* - 2\alpha Z^* &+ \sum_{k=1}^{K}\sum_{k'=1}^{K} \Delta x_k\,V_{kk'}(\gamma)\,\Delta x_{k'} \\ &- 2\alpha \sum_{k=1}^{K} T_k\,\Delta x_k.\end{aligned} \tag{3.9}$$

Minimizing with respect to the Δx_k gives

$$2\sum_{k'=1}^{K} V_{kk'}(\gamma)\,\Delta x_{k'} = 2\alpha T_k, \quad k = 1, K, \tag{3.10}$$

whence

$$\Delta x_k = \alpha \sum_{k'=1}^{K} C_{kk'}(\gamma)\,T_{k'}, \quad k = 1, K. \tag{3.11}$$

Multiplying (3.11) by γT_k and summing over k gives,

$$\gamma(Z(\alpha) - Z^*) = \alpha\,\mathrm{Var}(Z), \tag{3.12}$$

where $Z(\alpha)$ is the value of Z at the point at which ϕ is minimized.
Thus,

$$\mathrm{Var}(Z) = \frac{\gamma}{\alpha}(Z(\alpha) - Z^*). \tag{3.13}$$

The quantity α is arbitrary but should be small enough for the linear approximation to be valid.

Rodgers (1977) has pointed out that one good indication of the validity of the linear approximation in the error analysis is the rapidity of the convergence of the iterative minimization scheme that is based on the linear approximation.

Jackson (1972) has considered the concept of the "marginal utility of data" in the context of the reductions in overall uncertainties in the parameter estimates. (These uncertainties were characterized in terms of the eigenvalues of the parameter covariance matrix.) In the context of carbon cycle modelling, the most useful measures of the utility of data are likely to be given in terms of the reductions in the uncertainties in one or more model predictions and the formalism leading to eq. (3.13) seems to give the most appropriate technique for calculating such quantities.

This approach would involve assessing the utility of a particular data item by calibrating the model twice, once using the data item and a second time omitting that data from the calibration. The difference in the uncertainties of the predictions of a quantity Z will give a measure of the utility of the data item in determining these predictions. It is a "marginal" utility in that what is being determined is the utility of including the particular data item given that the rest of the data set remains unchanged.

An alternative technique for ranking the utility of various data items is to minimize $\theta - 2\alpha Z$ and compare the rates at which the residuals that contribute to θ increase with α. It is the quantities whose residuals increase most rapidly that will be most important in contraining the range of uncertainty of Z.

4. Calibrating the box-diffusion model by constrained inversion

This section describes the use of the techniques described in the previous section in calibrating a linearized approximation to the box-diffusion model of Oeschger et al. (1975). The reasons for choosing to study the calibration of this model are as follows.

(i) The model is familiar to most workers in the field of carbon cycle modelling.

(ii) The model has been very successful in describing the global carbon cycle. A demonstration of constrained inversion techniques using a less adequate model would probably give an example showing inconsistencies between the carbon cycle data and the prior information. In such a case many aspects of the techniques described in Section 3 could not be applied until the model has been refined.

(iii) There are two thorough studies of the calibration of the box-diffusion model by more conventional techniques (see Oeschger et al. (1975) and Broecker et al. (1980)) against which the results of the present calibration can be compared.

The box-diffusion model, as used in this study, characterizes the global carbon cycle in terms of A, the carbon content of the atmosphere, N the carbon content of the ocean surface mixed layer (of depth 100 m) and $C(z)$ the carbon content (per unit depth) of the deep oceans as a function of z, the height above the mean ocean bottom, with z = 3630 m at the bottom of the mixed layer. The corresponding amounts of ^{14}C in these regions are a, r and $c(z)$. The time evolution of these quantities is defined by the differential equations given in Appendix B.

That Appendix also gives the approximate solutions of these equations based on linearized approximations. These solutions are used to define the model predictions y_j that are fitted to the observations m_j. Table 1 lists the full set of data fitted. For each j it gives a description of the quantity, an algebraic expression of y_j and the numerical values of the observations $m_j \pm v_j$. This data set is essentially a subset of that used by Enting and Pearman (1983).

The model parameters are any quantities that have to be specified in order to obtain a set of numerical results from the model. This means that the parameter set will include any quantities that are required to define the initial state of the global carbon cycle. In the form of the box-diffusion model used here, it is assumed that there is a pre-industrial equilibrium and a constant rate of ^{14}C production from cosmic-rays and so only the

Table 1. *The carbon cycle observations used in the calibration of the linearized approximation to the box-diffusion model; the expressions for the y_i are in terms of quantities defined in Appendix B*

j	Description	Expression for y_j	$m_j \pm v_j$
1	deep ocean Δ-14	Δ_d	-160 ± 30
2	surface ocean carbon concentration	$\simeq N_0/358 \times 10^{16}$	2.10 ± 0.05 mol/m^3
3	atmospheric Δ-14 in 1950	$\Delta_a(1950)$	0 ± 5
4	ocean surface Δ-14 in 1950	$\Delta_n(1950)$	-50 ± 30
5	atmospheric Δ-14 in 1890	$\Delta_a(1890)$	22 ± 5
6	atmospheric CO_2 in 1958	$A(1958)/1.773 \times 10^{14}$	315.0 ± 0.3 ppmv
7	atmospheric CO_2 in 1960	$A(1960)/1.773 \times 10^{14}$	316.5 ± 0.3 ppmv
8	atmospheric CO_2 in 1964	$A(1964)/1.773 \times 10^{14}$	319.1 ± 0.3 ppmv
9	atmospheric CO_2 in 1968	$A(1968)/1.773 \times 10^{14}$	322.1 ± 0.3 ppmv
10	atmospheric CO_2 in 1972	$A(1972)/1.773 \times 10^{14}$	327.1 ± 0.3 ppmv
11	atmospheric CO_2 in 1976	$A(1976)/1.773 \times 10^{14}$	331.2 ± 0.3 ppmv
12	atmospheric CO_2 in 1980	$A(1980)/1.773 \times 10^{14}$	337.1 ± 0.3 ppmv
13	atmospheric Δ-14 in 1967	$\Delta_a(1967)$	650 ± 30
14	atmospheric Δ-14 in 1969	$\Delta_a(1969)$	580 ± 30
15	atmospheric Δ-14 in 1971	$\Delta_a(1971)$	500 ± 30
16	atmospheric Δ-14 in 1973	$\Delta_a(1973)$	450 ± 30
17	atmospheric Δ-14 in 1975	$\Delta_a(1975)$	420 ± 30
18	atmospheric Δ-14 in 1977	$\Delta_a(1977)$	350 ± 30
19	ocean surface Δ-14 in 1973	$\Delta_n(1973)$	95 ± 30

initial atmospheric CO_2 concentration is needed to define the initial state once the various rates are specified. As in any modelling study, certain quantities are regarded as being fixed by the structure of the model and are excluded from the calibration studies. For example, the mixed layer depth is taken as fixed in this study.

The constrained inversion formalism requires prior parameter estimates that are independent of carbon cycle data. In order to achieve this it becomes necessary to construct a model that can be related directly to the physical, chemical and biological processes that are involved in the carbon cycle. When selecting data for use in calibrating the model it is important to ensure that the data has not been "transformed" or "corrected" on the basis of some other carbon cycle model. If the data values are in part dependent on some other carbon cycle model, there is a danger of either circularity, leading to underestimates of the uncertainties, or inconsistency, leading to possible overestimates of the uncertainties. The simple form of the box-diffusion model makes it difficult to avoid all of these problems. For this reason, as well as all the restrictions listed below, the calculations presented here must be regarded as an illustration of the techniques rather than as a detailed assessment of the uncertainties in global carbon cycle models.

The various parameters used are as follows.

$x_1 = 1/k_1$, the atmospheric residence time with respect to exchange into the mixed layer. This is set at 7.7 ± 5.0 years. The value is that determined by Oeschger et al. (1975). This is one point at which a degree of circularity has been introduced into the present calibration. In order to reduce the extent to which this circularity affects the calibration, the prior uncertainty has been made relatively large so that the posterior estimate will be determined mainly by the carbon cycle data.

$x_2 = 1/k_2$, the effective (or differential) residence time for the mixed layer with respect to exchange with the atmosphere. This is set at 1.0 ± 0.5 years corresponding, approximately to the value used by Oeschger et al. (1975).

$x_3 = C_a$, the pre-industrial atmospheric CO_2 concentration. This parameter was not used directly in much of the original analysis by Oeschger et al. (1975) because the special structure of the model and the particular data set chosen enabled them to work solely with ratios and differences rather than absolute levels. The present analysis used a prior estimate of 290 ± 50 ppmv, based

on Keeling (1978). In order to make the analysis consistent with the model assumptions we have deliberately neglected recent evidence of lower concentrations representing a pre-agricultural-clearing level.

Imposing this artificial restriction on C_a for the purposes of avoiding inconsistency makes it impossible to use a realistic prior probability distribution for C_a. The very large range ± 50 ppmv serves to give a distribution that is essentially flat over the physically reasonable region. Thus in the calibration procedure C_a is restricted to reasonable values only by the observations of contemporary CO_2 concentrations. In the Bayesian terminology, C_a has been given a non-informative prior distribution (see Box and Tiao (1973), Section 1.3).

$x_4 = \kappa$, the deep-ocean eddy diffusion coefficient. We use 5400 ± 2000 m^2 yr^{-1}, based on the analysis by Broecker et al. (1980) of post-bomb tritium penetration. The uncertainty represents the difference between this value and that used by Oeschger et al.

$x_5 = \xi$, the buffer factor. The prior estimate is 9 ± 1. The value can be estimated from chemical equilibrium considerations (Broecker, 1974). Oeschger *et al.* (1975) considered a range of values from 8 to 10.

$x_6 = \Gamma$, the rate of ^{14}C production from cosmic-rays. On the basis of the analysis by O'Brien (1979), we used $\Gamma = 470 \pm 100$ moles yr^{-1} initially. The analysis described in Section 5 reveals an inconsistency that is interpreted as an incomplete description of the ^{14}C inventory by the box-diffusion model so that consistent estimates are only obtained when the prior uncertainty is arbitrarily increased to ± 500 moles yr^{-1} to reduce the influence of the prior estimate. Oeschger et al. (1975) avoided the use of Γ by only considering ratios.

$x_7 = \Lambda$, the rate of ^{14}C production from nuclear tests. This is set at 300 ± 80 moles/Megaton yield following Machta et al. (1963). This quantity is used in conjunction with estimates of the yields of test series so in this analysis, the uncertainties in the test yields must be formally treated as uncertainties in Λ.

$x_8 = F$, rate of carbon transfer into the biosphere. $(2100 \pm 1000) \times 10^{-2}$ moles yr^{-1} is the value used by Oeschger et al. (1975) with a 50% uncertainty applied.

$x_9 = \tau$, biospheric turn-over time. The value 60 ± 20 years is that used by Oeschger et al. (1975) with a 33% uncertainty.

$x_{10} = \varepsilon$, the biospheric enhancement factor. The value used was 0.2 ± 0.5.

For τ and ε, the uncertainties are set to relatively large but rather arbitrary values to reflect the lack of direct knowledge of these quantities.

With the set of initial parameter estimates $q_n \pm w_k$, and $m_j \pm v_j$ from Table 1 and the expressions for $y_j(\boldsymbol{x})$ obtained by substituting the solutions from Appendix B into the expressions in Table 1, we have enough information to apply the calibration formalism of Section 3. The objective function θ defined by eq (3.1) can be evaluated by direct substitution. Since $y_j(\boldsymbol{x})$ can be evaluated for any $\boldsymbol{x}$, numerical approximations for $S_{jk} = \partial y_j / \partial x_k$ can be obtained and used in expression (3.5a) which can be solved to give a set of corrections Δx_k that reduce θ towards its minimum.

5. Results of the constrained inversion calibration of the linearized box-diffusion model

The constrained inversion calibrations described here suffer from several limitations. Firstly, as in the original study by Oeschger et al. (1975), no forest clearing is allowed. Secondly, the solutions used are only approximate solutions of the original equations. Thirdly, the comments of Wunsch and Minster (1982) suggest that the models with many degrees of freedom that remain underdetermined are the most suitable for constrained inversion studies that aim at assessing model uncertainties while the box-diffusion model has, for example, only a single parameter describing ocean mixing. For these three reasons the present study can only represent an exploration of the techniques and an illustration of the procedures rather than a quantitative assessment of the uncertainties in our understanding of the carbon cycle.

The calibration procedure was applied with various data sets in order to illustrate the way in which choice of data set affects the results.

(i) An initial attempt to use similar data to that used by Oeschger et al. (1975)

The set of m_j was reduced to the first five items in Table 1. Most aspects of the calibration

appeared to be consistent and the sum of squares θ was reduced to 1.88 for $\gamma = 1$. Of this over 50% was contributed by the term $(x_6 - q_6)^2/w_6^2$ representing the residual of the cosmic ray production term. This suggests that there is some problem in the calibration but because of the small number of degrees of freedom the calibration was repeated using more data in order to check that the anomaly persisted.

(ii) Calibration including atmospheric CO_2 concentrations

The set of m_j was extended to include the first 12 items from Table 1. For $\gamma = 1$, this had $\theta = 8.73$ with $\|\boldsymbol{y} - \boldsymbol{m}\|^2 = 7.36$ and $\|\boldsymbol{x} - \boldsymbol{q}\|^2 = 1.37$. The main contributions to $\|\boldsymbol{y} - \boldsymbol{m}\|$ were the atmospheric CO_2 concentrations. The signs of the residuals were irregular, suggesting that this discrepancy is due to irregularities in the interannual variation of the concentration that cannot be described by this model. Over 60% of the contribution to $\|\boldsymbol{x} - \boldsymbol{q}\|^2$ came from the $(x_6 - q_6)^2/w_6^2$ term.

(iii) Relaxing the constraint on x_6

Because Γ (i.e. x_6) was anomalous the calibrations were repeated with the standard deviation on the prior value of Γ arbitrarily inflated so that the posterior value would be largely determined by the data. As an illustration of the effect of this change, Fig. 1 shows a plot of θ from (3.1) as determined using the original estimate ($\Gamma = 470 \pm 100$ moles yr^{-1}) and the modified value ($\Gamma = 470 \pm 500$ moles yr^{-1}). It will be seen that, over much of the range of γ, the effect of this change is equivalent to changing γ by about 10, i.e. increasing the s.d. of Γ by a factor of 5 improves the fit as much as increasing all parameter s.d.'s by a factor of about 3.

The reason for the value Γ being inappropriate for this model appears to be an underestimate of the ^{14}C reservoir and, since the model is calibrated using isotopic ratios, this implies that the total carbon reservoir is being underestimated. Part of this discrepancy may be associated with biospheric carbon although eq (8.1b) has the ^{14}C exchanging with an effective biospheric reservoir of about 1500 Gt of carbon. However, a large amount of ocean carbon is ignored in the box-diffusion model which assumes an equilibrium state with a uniform carbon distribution $C(z)$. In fact deep-

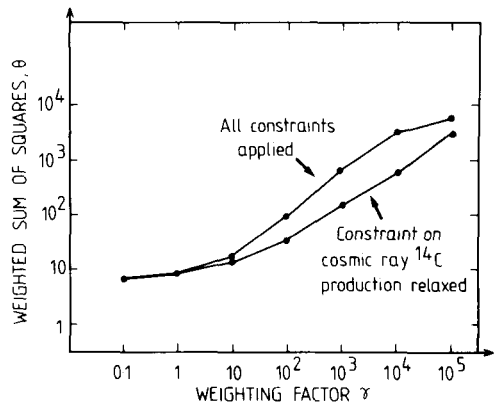

Fig. 1. Variation of the quantity θ (from eq. (3.1)) which measures the "goodness-of-fit", as a function of γ which determines the weighting given to the prior parameter estimates. The two plots differ in the uncertainties assigned to the cosmic-ray production rate. The upper curve uses 470 ± 100 moles yr^{-1}, the lower curve 470 ± 500 moles yr^{-1}.

ocean concentrations are typically 15% above surface concentrations (Li et al., 1969; Takahashi et al., 1981). The difference can represent as much as 3000–4000 Gt. of carbon, depending on how the concentration varies with depth. Changing the s.d. of Γ in this study is of course only a first stage—ultimately the discrepancy indicates a need for refinement of the model.

(iv) Inclusion of post-bomb ^{14}C data

The set of m_j was extended to include all 19 items in Table 1. For $\gamma \geqslant 50$, the results were similar to the previous case but for smaller γ the results appeared to indicate signs of instability. One of the more anomalous parameters was the biospheric uptake rate. In order to fit small discrepancies in the rate of change of ^{14}C in the atmosphere, the calibration technique reduces the biospheric uptake rate, reducing the extent to which the biosphere can act as a sink for ^{14}C. In the absence of precise direct estimates of this rate and in the absence of carbon cycle data that constrains this rate, the calibration technique must accept changing this rate as the best way of fitting the ^{14}C data. At $\gamma = 1$ the parameter estimation technique converged very slowly and for smaller γ values it apparently failed to converge. This behaviour is probably reflecting the fact that the variances in many of the q_k were made unreason-

ably large in a deliberate attempt to avoid circularity in the procedure.

Table 2 summarizes the results of cases (ii) (iii) and (iv), listing the actual parameter estimates obtained.

(*v*) *Sensitivity studies*

All of the parameter estimates given in Table 2 have uncertainties associated with them and the errors in the various parameters will be correlated. It is, however, not particularly illuminating to display the full covariance matrix for the parameters; what is of interest is the extent to which these uncertainties affect the predictions of the model. The quantity that we consider is the model prediction of the atmospheric CO_2 concentration in the year 2030. Two cases were considered using two alternative release scenarios:

$$R_2(t) = 1.5147 \times 10^{14} \exp(0.04118 \times (t - 1950)) \text{ moles yr}^{-1}; \quad (5.1a)$$

$$R_2'(t) = R_2(t) - 6.95 \times 10^{11} \exp(0.1 \times (t - 1950)) \text{ moles yr}^{-1}. \quad (5.1b)$$

The two release functions are plotted in Fig. 2. The first release represents a continuation of the exponential growth characteristic of the period 1950–1970. The second release is one which peaks early next century—the rapid decline after 2030 does not affect the present calculations. These functions were chosen for mathematical convenience because they can be integrated analytically in the approximate model described in Appendix B. The functions represent two extremes of possible behaviour and not predictions of what might occur.

For each of these releases the formalism defined by eq. (3.13) was applied with the quantity Z representing the atmospheric CO_2 concentration in the year 2030. The results of these calculations are shown in Fig. 3. The two solid curves represent the predictions obtained using the two different release functions shown in Fig. 3. The dashed lines show a range of uncertainties around these predictions and correspond to two standard deviations, i.e. the lines are $C_a(2030) \pm 2\sqrt{\text{Var}(C_a(2030))}$ with the variance determined numerically using eq. (3.13) and again using a quasi-Newton minimization of the type defined by eq. (3.6a) to obtain Z^* by minimizing expression (3.8).

For each release function, the calculation were performed both with and without the use of the

Table 2. *Parameter estimates obtained at various stages of the constrained inversion*

		Prior q_k	sd w_k	Without post-bomb data $\gamma = 1$	$\gamma = 1$	$\gamma = 10$
	number of data points	—	—	12	19	19
	γ	—	—	1	1	10
	ssq data dev.	—	—	7.28	18.1	54.7
	ssq param dev.	—	—	0.678	13.6	2.4
1	C_a (ppmv)	290	50	300	300	299
2	$1/k_1$ (yr)	7.7	5.0	8.5	12.1	8.0
3	$1/k_2$ (yr)	1.0	0.5	1.22	1.8	1.28
4	κ ($m^2 yr^{-1}$)	5400	2000	5314	6612	5948
5	ξ	9	1	9.06	8.87	8.95
6	Γ (moles yr^{-1})	470	500	380	367	379
7	Λ (moles/megaton)	350	80	na	202	270
8	F (10^{12} moles yr^{-1})	2100	1000	2240	659	1140
9	τ (yr)	60	20	60.4	68.4	61.8
10	ε	0.2	0.5	0.5	1.42	0.67

The fit to 12 items involves a data set similar to that originally used by Oeschger et al. (1975). The 19 data items used in the last two columns include ^{14}C data from the period following nuclear testing. Comparison of $\gamma = 1$ and $\gamma = 10$ indicates that the stability of the calibration is reduced when the data is extended in this way.

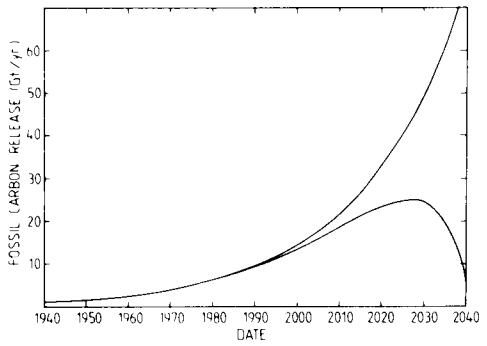

Fig. 2. The two release functions for fossil carbon used in this study, representing widely differing patterns of future fossil fuel use. The upper curve (from eq. (5.1)) represents a continuation of historical trends. The lower curve (from eq. (5.1)) represents a reduction in the growth of fossil fuel use.

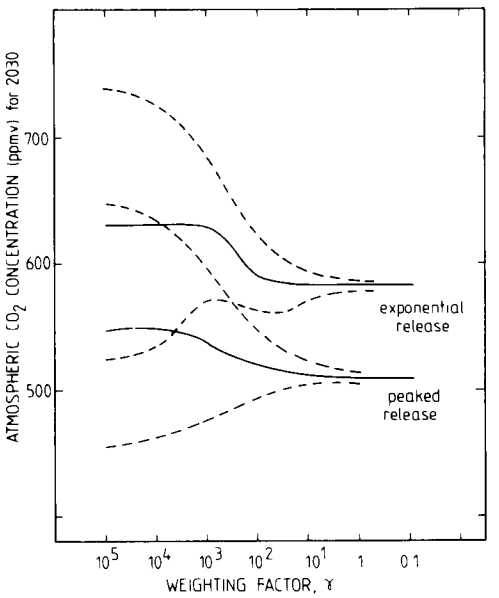

Fig. 3. Estimates of the uncertainties in predictions of future atmospheric CO_2 concentrations for the two release scenarios from Fig. 2. These uncertainties are evaluated in the limited context of the model and in particular biospheric effects other than those proportional to the CO_2 concentration are excluded.

post-bomb atmospheric carbon-14 data. The results were the same to within 1%. This indicates that the post-bomb carbon-14 data are relatively unimportant for constraining the future CO_2 concentrations. It is possible to determine which data is important by performing the sensitivity calculations defined by minimizing (3.8) and examining the residuals that make up the sum. The variations in Z will be constrained by those quantities that have large residuals. In the present case it is the atmospheric CO_2 data that are most important in providing constraints on the CO_2 concentrations that can arise from particular release scenarios.

6. Comparison of techniques

In order to assess the value of the techniques presented here, the calibration procedure from the preceding sections is compared to the procedure used by Oeschger et al. (1975). Their stated procedure was to use independent parameter estimates wherever possible, thus reducing the number of parameters that had to be estimated from the data. In addition, their equations were structured so that a number of important observable quantities depended on only a small number of parameters. Much of the calibration concerns only two parameters, the eddy diffusion coefficient, κ, and the air–sea gas exchange rate (effectively the k_1 of Appendix B). The eddy diffusion coefficient is estimated from the pre-industrial distribution of ^{14}C in the oceans because the expressions do not involve any of the other unknown parameters. Once κ is known, the air–sea gas exchange rate can be estimated from the preindustrial distribution of ^{14}C between the atmosphere and oceans. Oeschger et al. then check that these parameter values lead to a reasonable description of the dilution of atmospheric ^{14}C due to the Suess effect. The results of the Suess effect depend on the parameters describing the biosphere (F and τ in the notation of Appendix B), as well as on κ and k_1. Oeschger et al. do not attempt to estimate the biospheric parameters. They use independent estimates and check that, when combined with the model estimates of k_1 and κ, they are consistent with the Suess effect. Oeschger et al. then consider the behaviour of the atmospheric CO_2 concentration. Even in the simplified case of an exponential release of fossil carbon, two new parameters, ε and ξ, appear in the expressions. They consider a range of ξ values based on ocean observations and obtain a range of estimates of ε that are consistent with the CO_2 data. The final parameter set which is based on

analytic solutions was then used in a numerical version of the model. Using this model the responses to the actual fossil carbon release and to the ^{14}C from nuclear tests were determined and found to be in good agreement with the observations. Fitting the increase of CO_2 due to release of fossil carbon involved estimating C_a, the pre-industrial CO_2 concentration of the atmosphere.

The analysis of the box-diffusion model by Broecker et al. (1980) follows a sequence similar to that used by Oeschger et al. Both studies start from a consideration of the same two parameters, κ and k_1. Broecker et al. give independent estimates that differ slightly from those used by Oeschger et al. κ is estimated from the penetration of tritium into the oceans and k_1 is estimated from the radon-deficit method of determining air–sea gas exchange rates. They then check that the Suess effect and the ocean uptake of ^{14}C from nuclear testing are given consistently by using these parameters. However, agreement with the behaviour of the atmospheric CO_2 requires an additional sink of CO_2. Thus Broecker et al. are identifying a biospheric sink of carbon more definitely than was done by Oeschger et al. In terms of the basic model used by Oeschger et al. this biospheric sink would correspond to a non-zero value of ε. Essentially the study of the box-diffusion model by Broecker et al. is more of a model validation study than a calibration of the type performed by Oeschger et al.

These two extensive studies of the box-diffusion model give a good basis for assessing the constrained inversion calibration formalism described in this paper.

(i) The constrained inversion formalism does not require any special structure of the model because the parameters are estimated simultaneously rather than sequentially.

(ii) The constrained inversion formalism does not impose an arbitrary distinction between those parameters for which prior estimates are used and those which are estimated from the carbon cycle data. Any available prior estimates are used and are refined by using the carbon cycle data.

(iii) The sensitivity analysis is simplified because all parameters are treated in the same way rather than having to consider the two distinct cases of sensitivity to the parameters based on prior estimates and sensitivity to the uncertainties in the calibration.

(iv) The use of a broadly-based data set including as many independent prior parameter estimates as possible minimizes the effects of the inclusion of anomalous or inconsistent data. It also increases the chances of detecting anomalies due to inappropriate data or model inadequacies.

One very considerable advantage of the constrained inversion technique that is not illustrated by the simple example presented in this paper is the ability to handle relatively large numbers of parameters. Enting and Pearman (1982) encountered numerical instability when estimating 12 parameters in a one-dimensional carbon cycle model. After refining the model to remove some anomalous aspects, Enting and Pearman (1983) were able to "estimate" 31 parameters using the constrained inversion technique described in Section 3. Of course many of the final parameter estimates were found to be essentially unchanged from the prior estimates and could have been omitted from the calibration—the point is that it is not necessary to identify such parameters before calibrating the model.

The other feature of the constrained inversion study described by Enting and Pearman (1983) was the attempt to deduce the unknown function describing the net exchange of carbon between the atmosphere and the biosphere. (The prior estimate for this function was obtained from the work of Moore et al. (1981).) The determination of this biospheric release function and an assessment of its uncertainty is essential in order to check existing carbon cycle models and in order to determine the accuracy with which future CO_2 concentrations can be predicted. Because the box-diffusion model considers only a possible class of biospheric uptake function, i.e. those functions where the uptake rate is proportional to the CO_2 concentration, the uncertainties in the magnitude of this function do not adequately represent the uncertainties in the net exchange between the atmosphere and the biosphere. Oeschger and Heimann (1983) have shown that the interpretation of current changes in CO_2 concentration involves weighted integrals over the biospheric release functions so that restricted classes of function restrict the possible interpretations of current changes. For this reason the sensitivity study leading to Fig. 3 does not represent the full uncertainties in the calibration and a similar restriction will apply to any modelling study that restricts the biosphere to being fixed or to varying in a special manner. Since con-

strained inversion techniques are commonly used in the determination of unknown functions they would be particularly appropriate for carbon cycle modelling even without the other advantages that have been explicitly considered in this paper.

7. Acknowledgement

The author wishes to express his appreciation of the work of the un-named referees of this paper. Their comments and suggestions have played an important part in shaping the descriptive material in the introductory sections.

8. Appendix A. Computational techniques for constrained inversion calculations

The constrained inversion procedure was defined in Section 3 as determining the set of parameters (described by vector $\boldsymbol{x}$) that minimized the quantity

$$\theta = \sum_{j=1}^{J} (y_j(\boldsymbol{x}) - m_j)^2/v_j^2 + \gamma \sum_{k=1}^{K} (x_k - q_k)^2/w_k^2 \qquad (A.1)$$

given $\boldsymbol{m}$, $\boldsymbol{q}$, $\boldsymbol{v}$, $\boldsymbol{w}$, and γ.

This problem can be conveniently divided into two separate subproblems:

(i) given $\boldsymbol{x}$, determine $y(\boldsymbol{x})$;

(ii) determine the vector $\boldsymbol{x}$ that minimizes θ, assuming that $y(\boldsymbol{x})$ can be calculated for any arbitrary $\boldsymbol{x}$ that lies within some physically meaningful region.

A.1. Determining x

The vector $\boldsymbol{x}$ gives the set of model parameters such as air–sea exchange rates and $\boldsymbol{y}$ gives the set of model outputs that are to be compared to the observed data. For example in the calibration presented in Sections 4 and 5, y_1, y_2 and y_3 represented the box-diffusion models prediction of the deep ocean Δ-14, the surface ocean carbon concentration, and the atmospheric Δ-14 in 1950 respectively. This type of quantity is obtained by integrating the differential equations describing the model. For simple models the integration can be performed analytically (as for example in Appendix B). In such cases, subproblem (i) of evaluating $\boldsymbol{y}(\boldsymbol{x})$ simply involves a set of explicit evaluations of the formulae that define these analytical solutions. In more complex models, analytic solutions are not possible and the $\boldsymbol{y}(\boldsymbol{x})$ must be determined by numerical integration of the model equations. In this case it can be convenient to order the y_j (and corresponding m_j and v_j) according to the times t_j at which the measurements m_j were made. Thus the model equations are integrated from the initial state t_1 at which time y_1 is determined and then the model is integrated from t_1 to t_2 to determine y_2 and so on.

In all of the integrations, numerical or analytic, it is necessary to specify the initial state. In all the work presented here this state is specified as being an equilibrium state corresponding to a specified atmospheric CO_2 concentration. In general the specification will be in terms of such implicit requirements as equilibrium and explicit parameter values.

A.2. Minimizing θ

The second subproblem is that of minimizing θ, given the ability to calculate $\boldsymbol{y}(\boldsymbol{x})$. For small problems, the most appropriate technique may be to use a standard minimization procedure. Such procedures are readily available in many commercially distributed subroutine libraries. A typical procedure would require as inputs (a) an initial guess of $\boldsymbol{x}$ ($\boldsymbol{q}$ may be suitable in many inversion calibration studies), (b) the name of a function to calculate $\theta(\boldsymbol{x})$ (this would be an "EXTERNAL" function in Fortran), (c) usually some indication of the degree of precision required. The function to calculate $\theta(\boldsymbol{x})$ simply evaluates sum (A.1) using a procedure to evaluate $\boldsymbol{y}(\boldsymbol{x})$.

There are, however, a number of reasons for not using such a standard procedure for minimizing θ. In particular:

(a) attempting to minimize θ as though it was an arbitrary function rather than recognizing the special least-squares structure can be relatively inefficient;

(b) special procedures may be necessary on small computer systems;

(c) a special purpose routine can be easily adapted to perform both the basic minimization of θ and the sensitivity studies based on minimizing $\theta - 2\alpha Z$ (see eq. (3.8)); in particular, the final value of the matrix S_{jk} obtained when minimizing θ (see eq. 3.3a) can be used in the sensitivity studies if it is preserved;

Computational techniques for obtaining the parameter estimates by means of various least-squares procedures have been described by Bard (1974). For the least-squares sum (A.1) the "normal equations" defining the minimum are

$$\frac{\partial\theta}{\partial x_i} = 2\sum_{j=1}^{J}\frac{\partial y_j}{\partial x_i}(y_j(\boldsymbol{x}) - m_j)/v_j^2 + 2\gamma(x_i - q_i)/w_i^2 = 0, \tag{A.2}$$

and are to be solved for $\boldsymbol{x}$. The multivariate Newton–Raphson technique gives quadratic convergence near the optimum but requires $\partial^2\theta/\partial x_i\gamma x_k$ which, from (A.2), involves terms such as $\partial^2 y_j/\partial x_i\partial_k$ $(y_j(\boldsymbol{x}) - m_j)$ and $\partial y_j/\partial x_i\partial y_j/\partial x_k$ (see Bard (1974), Section 5.6). A simpler technique is to approximate the Newton–Raphson method by neglecting all the terms of the form $\partial^2 y_j/\partial x_i\partial x_k$, i.e. by using a linear approximation to the $y_j(\boldsymbol{x})$ as in equation (3.4a). Bard (1974, Section 5.9) refers to this as the Gauss method.

The minimization technique based on the linear approximation to the y_j is described by eq. (3.4a) and (3.5a–c). It was this technique that was used in the calculations presented in Section 5 and also in the more extensive calculations described by Enting and Pearman (1983).

9. Appendix B. The linearized approximation to the box-diffusion model

The box diffusion model represents the distribution of carbon in the atmosphere and ocean in terms of A, the number of moles of CO_2 in the atmosphere, N the number of moles of carbon in the ocean mixed layer and $C(z)$ the number of moles of carbon per unit depth in the deep oceans. The quantities a, n and $c(z)$ represent the corresponding amounts of ^{14}C.

The defining equations of the model are

$$\frac{dA}{dt} = -k_1 A + k_2(N - B) + \sum_{i=1}^{4} R_i(t), \tag{B.1a}$$

$$\frac{da}{dt} = -k_1 a + k_2(N - B)\, n/N - \lambda a - F(a(t)/A(t) - a(t-\tau)/A(t-\tau)) + \sum_{i=1}^{4} r_i(t), \tag{B.1b}$$

$$\frac{dN}{dt} = k_1 a - k_2(N - B) - \kappa\left.\frac{\partial C}{\partial z}\right|_{z=3630}, \tag{B.2a}$$

$$\frac{dn}{dt} = k_1 a - k_2(N - B)\, n/N - \lambda n - \kappa\left.\frac{\partial c}{\partial z}\right|_{z=3630} \tag{B.2b}$$

$$\frac{\partial C}{\partial t} = \kappa\frac{\partial^2 C}{\partial z^2}, \tag{B.3a}$$

$$\frac{\partial c}{\partial t} = \kappa\frac{\partial^2 c}{\partial z^2} - \lambda c, \tag{B.3b}$$

with the boundary conditions at bottom of mixed layer, i.e. ($z = 3630$ m)

$$C(3630) = N/d_m = N/100, \tag{B.4a}$$

$$c(3630) = n/d_m = n/100, \tag{B.4b}$$

$$\frac{\partial C}{\partial z} = 0, \quad \text{at } z = 0, \tag{B.5a}$$

$$\frac{\partial c}{\partial z} = 0, \quad \text{at } z = 0. \tag{B.5b}$$

The model involves parameters, k_1, k_2, C_a, κ, ξ, Γ, Λ, F, τ and ε that are defined (and assigned prior values) in Section 4. The rate of ^{14}C decay, λ, is $1/8627$ yr^{-1} and the quantity B is defined by

$$\xi = N_0/(N_0 - B), \tag{B.6a}$$

whence

$$B = (\xi - 1)\, A_0\, k_1/k_2, \tag{B.6b}$$

where A_0, N_0 denote the initial equilibrium values of A and N. A_0 is obtained from C_a by using an atmospheric "mass" of 1.773×10^{20} moles. d_m is the mixed layer depth and is taken as 100 m.

The R_i and r_i are the source functions for total carbon and ^{14}C respectively and are as follows.

(i) Cosmic ray production

For this study, the cosmic-ray production of ^{14}C is taken as constant:

$$r_1(t) = \Gamma, \tag{B.7a}$$

with no corresponding production of total carbon:

$$R_1(t) = 0. \tag{B.7b}$$

(ii) Fossil carbon release

The release of fossil carbon is approximated by a single exponential to give

$$R_2(t) = 1.5147 \times 10^{14} \exp \times (0.04118\,(t - 1950)) \text{ moles yr}^{-1}, \quad \text{(B.8a)}$$

$$r_2(t) = 0. \quad \text{(B.8b)}$$

A modified form that assumed a peak release rather than continual exponential growth was used in part of this study and was given by

$$R_2'(t) = 1.5147 \times 10^{14} \exp (0.04118(t - 1950) - 6.95 \times 10^{11} \exp (0.1\,(t - 1950)) \text{ moles yr}^{-1}. \quad \text{(B.9)}$$

The two alternative release functions are shown in Fig. 2.

(iii) Biospheric response to CO_2

The only biospheric change considered by Oeschger et al. (1975) was a response to increasing CO_2 given by

$$R_3(t) = -\varepsilon F(A(t) - A(t - \tau))/A_0, \quad \text{(B.10a)}$$

with the corresponding ^{14}C flux being

$$r_3(t) = -\varepsilon F(a(t) - a(t - \tau))/A_0. \quad \text{(B.10b)}$$

(iv) ^{14}C from nuclear tests

The injection of ^{14}C from nuclear tests was treated as a series of pulses corresponding to the major test series;

$$R_4(t) = 0,$$

$$r_4(t) = \sum_{k=1}^{9} Y_k \Lambda \delta(t - t_k), \quad \text{(B.11b)}$$

where Y_k is the yield in megatons (corrected for absorption of neutrons by the ground), Λ is the number of moles of ^{14}C per megaton, δ denotes the Dirac-delta and t_k is the time of the pulse. The 9 (Y_k, t_k) pairs used were (6.5, 1958.1), (13.6, 1958.4), (7.5, 1958.6), (20.6, 1958.8), (13.0, 1961.6), (98.0, 1961.8), (20.6, 1962.4), (154.0, 1962.6) and (45.9, 1962.8).

Formal analytic solutions for the amounts of total carbon can be obtained by using the standard techniques for linear equations. One approach is to take a finite difference representation of $C(z)$ and represent the eqs. (B.1a), (B.2a), (B.3a) in a vector form

$$\frac{\partial}{\partial t}\boldsymbol{p} = \boldsymbol{G}\boldsymbol{p} + \boldsymbol{H}\boldsymbol{p}(t - \tau) + \sum_i \boldsymbol{f}^{(i)} \exp(\gamma_i t), \quad \text{(B.12)}$$

where the first 2 components of $\boldsymbol{p}$ represent A and N and the remaining components represent $C(z)$. This has the solution

$$\boldsymbol{p} = \boldsymbol{p}^{(0)} + \sum_i \boldsymbol{p}^{(i)} \exp(\gamma_i t), \quad \text{(B.13)}$$

where $\boldsymbol{p}^{(0)}$ is determined by the initial atmospheric concentration C_a and the requirement that the system be in equilibrium, i.e.,

$$p_1^{(0)} = A_0 = C_a \times 1.773 \times 10^{14}, \quad \text{(B.14a)}$$

$$p_2^{(0)} = N_0 = \xi A_0 k_1/k_2. \quad \text{(B.14b)}$$

The $\boldsymbol{p}^{(i)}$ are given formally by

$$\boldsymbol{p}^{(i)} = [\gamma_i - \boldsymbol{G} - \boldsymbol{H} \exp(-\gamma_i \tau)]^{-1} \boldsymbol{f}^{(i)}. \quad \text{(B.15)}$$

These solutions can be used in a linearized approximation to the equations for ^{14}C.

The substitutions that are required are

$$k_2 nB/N \simeq k_2 nB/N_0 + k_2 n_0 B(1/N - 1/N_0) \simeq k_2 nB/N_0 - k_2 n_0 B(N - N_0)/N_0^2, \quad \text{(B.16)}$$

$$-F(a(t)/A(t) - a(t - \tau)/A(t - \tau)) \simeq -F(a(t)/A_0 - a(t - \tau)/A_0) + \sum_i Fa_0 A^{(i)} \times [1 - \exp(\tau\gamma_i)]/A_0^2, \quad \text{(B.17)}$$

where $A^{(i)}$ denotes $p_1^{(i)}$.

These approximations make it possible to write the ^{14}C equations in the form

$$\frac{\partial}{\partial t}\boldsymbol{p}^* = \boldsymbol{G}^*\boldsymbol{p}^* + \boldsymbol{H}^*\boldsymbol{p}^*(t - \tau) + \Gamma\boldsymbol{e} + \sum_i \boldsymbol{Q}\boldsymbol{p}^{(i)} \times \exp(\gamma_i t) + \boldsymbol{e} \sum_k Y_k \Lambda \delta(t - t_k), \quad \text{(B.18)}$$

where $\boldsymbol{e}$ is a vector with only the first component non-zero and $\boldsymbol{G}^*$, $\boldsymbol{H}^*$ and $\boldsymbol{Q}$ are matrices whose coefficients represent the original coefficients in eqs. (B.1b), (B.2b), (B.3b).

The solution is given by

$$\boldsymbol{p}^* = \boldsymbol{p}^{(0)*} \sum_i p^{(i)*} \exp(\gamma_i t) + \sum_{k\alpha} \boldsymbol{p}^{(k\alpha)*} \Theta(t - t_k) \times \exp(-\mu_\alpha(t - t_k)), \quad \text{(B.19)}$$

where Θ denotes a unit step function. $\boldsymbol{p}^{[0]}$ is given by

$$\boldsymbol{p}^{(0)*} = -[\boldsymbol{G} + \boldsymbol{H}]^{-1}\,\Gamma\boldsymbol{e}, \tag{B.20}$$

$$\boldsymbol{p}^{(i)*} = [\gamma_i \boldsymbol{I} - \boldsymbol{G} - \boldsymbol{H}]^{-1}\,\boldsymbol{Q}\boldsymbol{p}^{(i)}, \tag{B.21}$$

$$\boldsymbol{p}^{(k\alpha)*} = [\gamma_i \boldsymbol{I} - \boldsymbol{G} - \boldsymbol{H}]^{-1}\,\boldsymbol{Q}\boldsymbol{p}^{(i)}, \tag{B.21}$$

and $\boldsymbol{p}^{(k\alpha)*}$ is an eigenvector of $-\boldsymbol{G}$ with eigenvalue μ_α. For short times after the tests there will be no contribution to $\boldsymbol{p}^{(k\alpha)*}$ from the $\boldsymbol{H}\boldsymbol{p}^*(t-\tau)$ term). The $\boldsymbol{p}^{(k\alpha)*}$ are normalized by the requirement

$$\sum_\alpha \boldsymbol{p}^{(k\alpha)*} = \boldsymbol{e}\Lambda Y_k. \tag{B.22}$$

In practice these formal solutions can be simplified considerably by recognizing that the deep ocean contributions to $\boldsymbol{p}^{(i)}$ and $\boldsymbol{p}^{(i)*}$ will be of the form

$$C^{(i)}(z) \propto \cosh\,(z\sqrt{\gamma_i/K}), \tag{B.23a}$$

$$c^{(i)}(z) \propto \cosh\,(z\sqrt{(\gamma_i+\lambda)/K}). \tag{B.23b}$$

The validity of these two expressions extends to the equilibrium, i.e. the $\gamma_i = 0$ case.

Substituting these expressions into the full equations reduces the systems of equations represented by (B.12), (B.15), (B.20) and (B.21) to systems involving only two components. The remaining terms (i.e. those involving the response to nuclear testing) were evaluated by applying the formalism of eq. (B.19), (B.22) to a three reservoir model in which the mixed layer and the subsurface layer had equal volumes.

The y_i used in the calibration requred:
atmospheric CO_2 concentrations, i.e. $A(t)/1.773 \times 10^{14}$ where $A(t)$ is $p_1(t)$. The conversion is from moles to p.p.m.v.;
ocean surface concentration, this is approximated by the initial concentration, i.e. by $N_0/358 \times 10^{16}$ where the conversion is from moles to moles/m^3.

The ^{14}C levels are represented by Δ-14 values, i.e.

$$\Delta_a(t) = 1000\,(a(t)/R_s\,A(t) - 1), \tag{B.24a}$$

$$\Delta_n(t) = 1000\,(n(t)/R_s\,N(t) - 1), \tag{B.24b}$$

while the deep ocean levels are approximated by the pre-industrial value of

$$\Delta_a = 1000\,(c^0(z=0)\,d_m/N_0R_s - 1). \tag{B.24c}$$

R_s is the ^{14}C:C ratio of the standard and is 1.176×10^{-12}.

10. Appendix C. Relations between various inversion formalisms

C.1. *Weighted least squares*

The most straightforward interpretation of the calibration presented in Section 3 is to regard it as a least squares fitting procedure where the x_k are adjusted so that the set of m_j and q_k are fitted as well as possible. Setting $\gamma = 1$ in (3.1) gives a weighting that is optimal in the sense that the variances of the estimates of the x_k are minimized. In this interpretation, splitting the sum into two separate sums over terms involving the m_j are q_k, respectively, is of no special significance.

C.2. *Constrained inversion*

The parameter estimation procedure based on minimizing (3.1) can also be regarded as an example of the type of constrained inversion that is commonly required in geophysical problems. It is regarded as adjusting the x_k so that the $y_j(\boldsymbol{x})$ fit the m_j. Because a direct fit can tend to be unstable it is usually necessary to constrain the solutions. In eq. (3.1) the term $\gamma\sum\,(x_k - q_k)^2/\mathrm{w}_k^2$ acts as the constraint. Twomey (1977) has described a wide range of inversion formalisms, but Rodgers (1977) has suggested that the interpretation of the uncertainties in constrained inversions is best performed by relating the inversion formalism to an extended fit to two sets of data as in the previous subsection.

C.3. *Bayesian inference*

It is also possible to regard the calibration procedure as an example of Bayesian inference. In this interpretation one starts with a range of parameter estimates q_k. These are assigned prior probability distributions given by normal distributions. These prior distributions are refined by using the observations m_j to obtain an unnormalized posterior probability distribution by using

$$P(\boldsymbol{x}\,|\,\boldsymbol{m}) \propto P(\boldsymbol{m}|\,\boldsymbol{x})P(\boldsymbol{x}). \tag{C.1}$$

The distribution of the m_j given $\boldsymbol{x}$ is taken as being a normal distribution with means $y_j(\boldsymbol{x})$ and variances

$$\mathrm{Var}(m_j) = v_j^2.$$

Eq. C.1 becomes

$$P(\boldsymbol{x}\,|\,\boldsymbol{m}) \propto \prod_j [\exp\,(-(y_j - m_j)^2/2v_j^2))$$
$$\times \prod_k \exp\,(-(x_k - q_k)/2w_k^2)]. \tag{C.2}$$

The maximum posterior likelihood is thus given by maximizing $P(\boldsymbol{x}|\boldsymbol{m})$ or equivalently by minimizing θ as in Section 3.

C.4. Techniques using the pseudoinverse

The use of a pseudoinverse matrix is a way of formalizing the analysis described in Section 2. The aim is to construct solutions to

$$\boldsymbol{m} = \boldsymbol{S}\boldsymbol{x}. \tag{C.3}$$

The least squares solution was described in terms of the singular value decomposition of the $J \times K$ matrix $\boldsymbol{S}$

$$\boldsymbol{S} = \boldsymbol{U}\boldsymbol{R}\boldsymbol{W}^{\mathrm{T}}, \tag{C.4}$$

where $\boldsymbol{U}$ and $\boldsymbol{W}$ are orthogonal matrices and $\boldsymbol{R}$ is a matrix which is zero except for the first r elements of the main diagonal; which are λ_i, $i = 1, r$. The pseudoinverse of $\boldsymbol{R}$ is defined as the $K \times J$ matrix $\boldsymbol{R}^+$ which is zero except for the first r elements of the main diagonal which are given by λ_i^{-1}.

The matrix $\boldsymbol{R}^+$ is used to define $\boldsymbol{S}^+$, the pseudoinverse of $\boldsymbol{S}$ as

$$\boldsymbol{S}^+ = \boldsymbol{W}\boldsymbol{R}^+ \boldsymbol{U}^{\mathrm{T}}. \tag{C.5}$$

Thus, as described in Section 2, the solution

$$\boldsymbol{x} = \boldsymbol{S}^+ \boldsymbol{m}. \tag{C.6}$$

represents a solution of (C.3) that minimizes the residuals $\|\boldsymbol{S}\boldsymbol{x} - \boldsymbol{m}\|$ and, given that these residuals are minimized, then has the minimum possible $\|\boldsymbol{x}\|$.

The relation with the inversion formalism described in Section 3 is best described by noting that the pseudoinverse solution to (C.3) is also a least-squares solution to

$$\boldsymbol{S}^{\mathrm{T}} \boldsymbol{m} = \boldsymbol{V}\boldsymbol{x} = \boldsymbol{S}^{\mathrm{T}} \boldsymbol{S}\boldsymbol{x}. \tag{C.7}$$

For the case when the prior estimates are equal to zero, the linearized formalism described in Section 3 corresponds to solving

$$\boldsymbol{S}^{\mathrm{T}} \boldsymbol{m} = (\boldsymbol{V} + \gamma \boldsymbol{I})\, \boldsymbol{x}. \tag{C.8}$$

In terms of the singular value decomposition we can put

$$\boldsymbol{V} + \gamma \boldsymbol{I} = \boldsymbol{W}(\boldsymbol{R}^{\mathrm{T}}\boldsymbol{R} + \gamma \boldsymbol{I})\, \boldsymbol{W}^{\mathrm{T}} = \boldsymbol{W}\boldsymbol{R}_{\gamma}\boldsymbol{W}^{\mathrm{T}}, \tag{C.9}$$

where $\boldsymbol{R}_{\gamma}$ is a $K \times K$ with the diagonal elements given by $(\lambda_i^2 + \gamma)$, $i \leqslant r$, and γ for $r < i$.

Thus,

$$\boldsymbol{x} = (\boldsymbol{V} + \gamma \boldsymbol{I})^{-1}\, \boldsymbol{S}^{\mathrm{T}} \boldsymbol{m} = \boldsymbol{C}(\gamma)\, \boldsymbol{S}^{\mathrm{T}} \boldsymbol{m}, \tag{C.10}$$

where

$$\boldsymbol{C}(\gamma) = \boldsymbol{W}\boldsymbol{R}_{\gamma}^{-1}\, \boldsymbol{W}^{\mathrm{T}}. \tag{C.11}$$

Thus $\boldsymbol{C}(\gamma)$ has a structure similar to $\boldsymbol{V}^+$. The λ_i^{-2} are replaced by $1/(\lambda_i^2 + \gamma)$ and the zeroes on the diagonal of $(\boldsymbol{R}^{\mathrm{T}}\boldsymbol{R})^+$ are replaced by $1/\gamma$. The use of $\boldsymbol{C}(\gamma)$ avoids an abrupt change in the way the singular values are treated as they become small. It is also possible to describe the formalism of Section 3 as being directly related to the original pseudoinverse solution. Lawson and Hanson (1974, Section 25.4) show how adding K extra rows to $\boldsymbol{S}$ to constrain the $\boldsymbol{x}$ vectors to be small leads to a modified matrix whose singular values are $(\lambda_i^2 + \gamma)^{1/2}$, where γ is the weight of the constraint. They prove this explicitly by applying Givens rotations to the extended matrix.

C.5. The multi-box-ocean model inversion

Bolin et al. (1983) described an inversion calibration of a model of ocean geochemistry which can be expressed as

$$\frac{\partial}{\partial t}\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{0} \quad \text{for equilibrium.} \tag{C.12}$$

The y_i are the model values of the concentrations and the x_k are transport parameters in the model. We denote the observed values of the concentrations by m_i. Bolin et al. consider two cases. Both cases assume that the concentrations are fitted exactly, i.e.

$$\boldsymbol{y} = \boldsymbol{m}. \tag{C.13}$$

The first case is the indeterminate case which has

$$\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{m}) = \boldsymbol{0}, \tag{C.14}$$

and chooses $\boldsymbol{x}$ to minimize $\|\boldsymbol{x}\|$. The second case is when there is no exact solution to (C.14) and the solution that is taken is the $\boldsymbol{x}$ which minimizes $\|\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{m})\|$.

In each case linear inequality constraints are applied to the x_k. These are mainly positivity constraints on quantities such as diffusion coefficients but for many of the transport coefficients they were found to be unnecessary.

In contrast, the formalism of Section 3 would be to always have $\boldsymbol{y}$ defined by

$$\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{0}, \tag{C.15}$$

but to determine $\boldsymbol{x}$ by requiring that it minimizes

$\theta = |\boldsymbol{y} - \boldsymbol{m}||^2 + \gamma||\boldsymbol{x} - \boldsymbol{q}||^2$.

This overcomes some of the problems that Bolin et al. identified in their formalism. There is no need to make a distinction between indeterminate and inconsistent cases. While there is a problem with choosing the appropriate weights for the components of $\boldsymbol{f}$ when $||\boldsymbol{f}||$ is to be minimized there is a natural relative weighting once the constraints are related to specific prior information. The practical disadvantage of the inversion scheme based on minimizing θ is that it leads to non-linear equations.

11. Appendix D. Notation

Roman

a	atmospheric ^{14}C content in box-diffusion model (BDM)
A	total atmospheric carbon content in BDM
$\boldsymbol{b}$	"error" vector used in iterative solution of least-squares problem
B	intercept on the "N" axis of the linearized buffering relation, connecting mixed layer carbon (N) to CO_2 partial pressures
$c(z)$	^{14}C content (per unit depth) of deep ocean in BDM
$C(z)$	total carbon (per unit depth) of deep ocean in BDM
C_a, $C_a(t)$	atmospheric CO_2 concentration
$\boldsymbol{C}(\gamma)$	inverse of matrix $V(\gamma)$, $\gamma C(\gamma)$ can be interpreted as the covariance matrix for parameter estimates
$C_{kk'}(\gamma)$	element of $C(\gamma)$
$E\|\ \|$	statistical expectation, i.e. mean
E_1, E_1', E_2, E_2',	vector spaces used in describing pseudo-inverse solutions
F	rate of uptake of biospheric carbon in BDM
$\boldsymbol{G}, \boldsymbol{H}$	matrices used to represent BDM as a general linear system of ODE's
j	index of set of carbon cycle observations
J	number of carbon cycle observations fitted
k_1, k_2	rate constants for atmosphere–ocean exchange in BDM
k	index of set of parameters estimated in calibration procedure
K	number of parameters estimated
m_j	jth carbon cycle observation
n	^{14}C content of mixed layer in BDM
N	total carbon content of mixed layer in BDM
N_0	initial (strictly $t = -\infty$) equilibrium value of N
$\boldsymbol{p}$	vector used with matrices $\boldsymbol{G}$ and $\boldsymbol{H}$ to represent BDM as a general linear ODE's; p_1 corresponds to A and p_2 corresponds to N
$\boldsymbol{p}^{(i)}$	a contribution to $\boldsymbol{p}$ where $\boldsymbol{p}$ is represented as a sum of $\boldsymbol{p}^{(i)} \exp(\gamma_i t)$
$\boldsymbol{p}^*$	vector used to represent the ^{14}C contents in the form of a general ODE
$\boldsymbol{p}^{(i)*}$	component of $\boldsymbol{p}^*$ varying as $\exp(\gamma_i t)$
$\boldsymbol{p}^{(k\alpha)*}$	component of $\boldsymbol{p}^*$ representing response to nuclear testing and behaving as $\Theta(t - t_k) \exp(-\mu_\alpha(t - t_k))$
q_k	
$\boldsymbol{Q}$	matrix defining effective "source" terms in the ^{14}C equations of the BDM due to perturbations in total carbon
r	rank of matrix $\boldsymbol{S}$
r_i	source function for *ith* process producing ^{14}C
R_i	source function for ith process releasing carbon into the atmosphere
R_s	standard ^{14}C:C ratio used in defining Δ values
$\boldsymbol{S}$	sensitivity matrix for non-linear models and matrix defining linear models
S_{jk}	$\partial y_j/\partial x_k$, element of sensitivity matrix
t	time (years)
t_k	time of kth nuclear test series
T_k	$\partial Z/\partial x_k$, sensitivity of prediction Z to parameter x_k
$\boldsymbol{U}$	orthogonal matrix used in singular value decomposition of $\boldsymbol{S}$
v_j	uncertainty (expressed as a standard deviation) for carbon cycle observation m_j

$\boldsymbol{V}(\gamma)$	matrix defined by eq. (3.5c) used in locating best fit and describing covariances of parameter estimates
$V_{kk}(\gamma)$	element of $\boldsymbol{V}(\gamma)$
w_k	uncertainty (expressed as a standard deviation) for prior parameter estimate q_k; in Bayesian terms this would be the standard deviation of the prior distribution for x_k
$\boldsymbol{W}$	orthogonal matrix used in singular value decomposition of S
x_k	kth parameter
$\boldsymbol{x}$	set of K parameters, regarded as a vector
$\boldsymbol{x}^*$	set of best-fit parameters (or current approximation to best fit)
y_j	model prediction of quantity m_j
$y_j(\boldsymbol{x})$	y_j written to show functional dependence on parameters
$y_j^* =$	$y_j(\boldsymbol{x}^*)$
Y_k	yield (megatons) of nuclear test series at time t_k
z	height above ocean bottom in BDM
Z	any arbitrary quantity predicted by model.

Greek

α	Lagrange multiplier used in studying sensitivity of Z
γ	weighting factor used to determine the relative importance attached to prior information and carbon cycle observations
γ_i	time constant of an exponentially increasing component of the fossil carbon release
Γ	rate of ^{14}C production by cosmic rays in BDM
δ	dirac delta function
Δ	small differences
Δ-14	measure of isotopic ratio, treated as difference from standard (strictly including a normalization for ^{13}C)
ε	biospheric enhancement factor in BDM
θ	quantity defined by eq. (3.1), minimized in constrained inversion calibration
θ^*	minimum of θ.
Θ	unit step function
κ	eddy diffusion coefficient in BDM
λ	^{14}C decay factor = $1/8627$ yr^{-1} (used in BDM)
λ_i	ith singular value of S
Λ	rate of ^{14}C production for nuclear weapons (moles/megaton) used in BDM
μ_α	eigenvalue describing decay rates of response to pulse of ^{14}C from nuclear testing
ξ	buffer factor of oceans, used in BDM
τ	biospheric turnover time, used in BDM
ϕ	quantity defined by eq. (3.8), minimized in sensivity studies

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