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Data-Based Mechanistic Modelling, the Global Carbon Cycle and Global Warming

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Abstract

This Report first outlines our generic *Data-Based Mechanistic* (DBM) modelling philosophy, in which models are only deemed credible if, in addition to explaining the time series data in a statistically efficient, parsimonious manner, they also provide an acceptable physical interpretation of the system under study. It also contrasts this DBM approach to modelling, in which the model is inferred directly from measured data in an *inductive* manner, using the minimum of *a priori* assumptions, with the alternative *hypothetico-deductive* approach, where the model form is based strongly on the prior assumptions and paradigms of the scientist and model builder. The Report then goes on to consider the problem of modelling the global carbon cycle; a problem that has great relevance in the current debate about global warming. Using the DBM approach, we identify a simple stochastic differential equation model that includes a negative, temperature dependent, feedback effect. This not only affects the projected future levels of atmospheric CO_2, but it also provides an important independent validation of the significance of the observed increases in global average temperature measured over the last few decades and their effects on the global carbon cycle: namely, the likely existence of anthropogenically-induced global warming. The report continues by employing our DBM model to generate hypothetical forecasts of future CO_2 and Northern Hemisphere temperatures to the end of the 22^{nd} Century.

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1 Introduction

Natural systems are normally a complex assemblage of interacting physical, chemical, and biological processes, many of which are inherently nonlinear, with considerable uncertainty about both their nature and their interconnections. It is surprising, therefore, that stochastic dynamic models are the exception rather than the rule in research on natural systems. One reason for this anomaly lies in the very successful history of physical science over the last century. Modelling in deterministic terms has permeated scientific endeavour over this period and has led to a pattern of scientific investigation which is heavily reductionist in nature. When applied within an environmental context, such deterministic reductionism appears to be guided by a belief that environmental systems can be described very well, if not exactly, by deterministic mathematical equations based on well known scientific laws, provided only that sufficient detail can be included to describe all the physical processes that are *perceived* to be important by the scientists involved. This leads inexorably to large, nonlinear models reflecting the scientist's perception of the environment as an exceedingly complex dynamic system.

Although such deterministic reductionism still dominates natural systems modelling, there are some signs that attitudes may be changing. There is a growing realization that, despite their superficially rigorous scientific appearance, simulation models of the natural systems based on deterministic concepts are more extensions of our mental models and perceptions of the real world than necessarily accurate representations of the real world itself. The recent revived interest in the 'top-down' approach to modelling in the hydrological literature (e.g. Jothityangkoon *et al.*. 2001 and the references therein), for instance, is a response to the relative failure of the alternative reductionist ('bottom-up') philosophy in this area of study. Quite similar anti-reductionist views are also appearing in other areas of science: for instance, in a recent lecture (Lawton, 2001), the current Chief Executive of the U.K. *Natural Environment Research Council* (NERC) recounted the virtues of the top-down approach to modelling ecological systems.

But such scepticism is not new. It has its parallels in the environmental (e.g. Beck, 1983; Young, 1978,1983) and ecosystems (e.g. see prior references cited in Silvert, 1993) literature of the 1970s and early 1980s. Over this period, the present first author's contributions were set within the context of 'badly defined' environmental systems. This poor definition arises because their behavioral mechanisms of are often poorly understood and planned experiments, that might lead to improvements in such understanding, are difficult or even impossible to undertake. These early papers then went on to present initial thoughts on an objective, statistical approach to modelling poorly defined systems on the basis of time series data that tried to avoid the dangers of placing too much confidence in prior perceptions about the nature of the model. In the subsequent period since the earlier papers were published, however, he has sought to develop this statistical approach within a more rigorous systems setting termed *Data-Based Mechanistic* (DBM) modelling. This has led to the application of DBM modelling methods to time series data obtained from monitoring exercises in a number of different areas, from the environment, through ecology and engineering to economics. And latterly, the second author has successfully exploited the DBM modelling in the area of plant physiology (Jarvis *et al.*, 1999).

After outlining the main tenets of the DBM approach, the present Report discusses two interpretations of continuous-time stochastic state space models in order to set the scene for the modelling methods used in this Report. It then proceeds to outline the identification and estimation of a particular class of 'state dependent parameter' models for nonlinear, stochastic, dynamic systems that are playing an increasingly important

role in DBM modelling. Finally, an example based on the analysis of global climate data is presented that illustrates the utility of these data-based modelling methods when applied to real data.

2 Data-Based Mechanistic Modelling

The term 'data-based mechanistic modelling' was first used in Young and Lees (1992) but the basic concepts of this approach to modelling dynamic systems have developed over many years. Previous publications, ranging from Beck and Young (1975) to Young (1998a), as Reported in the latter paper, map the evolution of the DBM philosophy and its methodological underpinning in considerable detail, and so it will suffice here to merely outline the main aspects of the approach when sufficient time series data are available[2].

1. **Modelling Objectives** The important first step is to define the objectives of the modelling exercise and to consider the type of model that is most appropriate to meeting these objectives. Since DBM modelling requires adequate data if it is to be completely successful, this stage also includes considerations of scale and the data availability at this scale, particularly as they relate to the defined modelling objectives. However, the prior assumptions about the form and structure of this model are kept at a minimum in order to avoid the prejudicial imposition of untested perceptions about the nature and complexity of the model needed to meet the defined objectives.

2. **The Generic Model Form** Based on the considerations in 1., an appropriate model structure and order is identified by a process of statistical inference applied directly to the time-series data and based initially on a given generic class of linear, discrete or continuous-time, models whose parameters are allowed to vary over time, if this seems necessary to satisfactorily explain the data.

3. **Linear Model Identification** If the model is identified as predominantly linear or piece-wise linear, then the constant parameters that characterize the identified model structure in step 2. are estimated using advanced methods of statistical estimation for dynamic systems. The methods used in the present Report are based on optimal *Instrumental Variable* (IV) estimation algorithms (in particular, the *Refined Instrumental Variable* (RIV) algorithm[3]: see Young, 1984) that provide a robust approach to model identification and estimation and have been well tested in practical applications over many years.

4. **Nonstationary and Nonlinear Model Identification** The idea that model parameters may vary over the observation interval in order to reflect nonstationary aspects of the system under study is important to DBM modelling and has been a research topic for many years in the systems (e.g. Lee, 1964; Young, 1969) and statistical (e.g. Brown *et al.*, 1975) literatures. If significant model parameter variation is detected over the observation interval, using these or other methods then, in DBM modelling, the parameters are estimated by the application of an

[2] an alternative DBM approach is utilized when data are scarce and simulation models are the main medium of study (Young *et al.*, 1996).

[3] This is related to the IV algorithms used in Econometrics (e.g. Harvey, 1989) but is significantly different in some important respects.

approach to *time variable* or *state dependent* parameter estimation based on recursive fixed interval smoothing (see later). Such parameter variation will tend to reflect nonstationary and nonlinear aspects of the observed system behaviour. In effect, the fixed interval smoothing algorithm provides a method of non-parametric estimation, with the *Time Variable Parameter* (TVP) estimates defining the non-parametric relationship. And, as we shall see, this relationship can often be interpreted in nonlinear *State-Dependent Parameter* (SDP) terms (see Young, 1978, 1984[4], 1993; Priestley, 1988; Young and Beven, 1994; Young, 2000, 2001a,b,c; Lees, 2000).

5. **Final Model Estimation** If nonlinear phenomena have been detected and identified in stage 4, the non-parametric SDP relationships are normally parameterized in a finite form and the resulting (normally constant) nonlinear model parameters are estimated using some form of numerical optimization, such as nonlinear least squares, prediction error minimization or *Maximum Likelihood* (ML) optimization.

6. **Mechanistic Interpretation** Regardless of whether the model is identified and estimated in linear or nonlinear form, it is only accepted as a credible representation of the system if, *in addition to explaining the data well, it also provides a description that has direct relevance to the physical reality of the system under study, at the scale of interest.* This is a most important aspect of DBM modelling and differentiates it from more classical 'black-box' modelling methodologies, such as those associated with standard (Box-Jenkins) transfer functions, NARMAX[5] representations, most unobserved component models; neural network and neuro-fuzzy models.

7. **Predictive Validation** Finally, the estimated model is tested in various ways to ensure that it is conditionally valid. This can involve standard statistical diagnostic tests for stochastic, dynamic models, including analysis which ensures that the nonlinear effects have been modelled adequately (e.g. Billings and Voon, 1986). It also involves predictive validation, as well as exercises in stochastic uncertainty and sensitivity analysis using Monte Carlo simulation methods.

In philosophical terms, DBM modelling can be differentiated most clearly from alternative deterministic, top-down methods by its 'inductive' approach to model synthesis. Rather than basing the model development on an *a priori* assumed, conceptual model form (the 'hypothetico-deductive approach': e.g. Popper, 1959), the DBM model structure is inferred directly from the observational data in relation to a more general class of models (see Young, 2002a). Another important difference is its inherently stochastic nature. This means that the uncertainty in the estimated model is always quantified and this information can then be utilized in various ways. For instance, it allows for the application of Monte Carlo-based uncertainty and sensitivity analysis, as well as the use of the model in statistical forecasting and data assimilation algorithms, such as the Kalman filter (Kalman, 1960; Kalman and Bucy, 1961) and its nonlinear relatives.

Finally, a most important aspect of DBM modelling arises from considerations that derive from its origins in the development of models for use in control system design (e.g. Ljung and Söderstrom, 1983; Young, 1984). This requires the identification of parametrically efficient (parsimonious) models, as a way of avoiding the identifiability problems that are associated with the estimation of over-parameterized models from

[4] see pp 157-166, where the approach is first discussed within a hydrologic context.

[5] *Nonlinear AutoRegressive Moving Average eXogenous variables*: see e.g. Leontaritis and Billings, 1985.

limited time series data.[6]. It must be stressed, however, that such problems arise mainly from the specification of the dynamic model order (in the present Report, the order of the differential equations that are used to describe the system under study). So a parsimonious model, in this important dynamic sense, is one that has a lowest *dynamic* order that is consistent with the information content in the data and whose parameters are statistically significant. Typical model order identification statistics that are useful in this regard are the AIC and YIC criteria (see later).

Of course, the DBM model may well have *other* parameters that are not associated primarily with the dynamic order of the model: for instance, coefficients that parameterize any nonlinearity in the system. Here again, the presence of such parameters in the model should be justified by whether or not they are statistically significant. The statistical significance of parameter estimates can be evaluated by conventional statistical tests or, in these days of the fast digital computer, by *Monte Carlo Simulation* (MCS) analysis (see e.g. Report 6 in Saltelli *et al.*, 2000 and Report 7 in Beven, 2000b). Such MCS analysis is very useful for assessing the uncertainty associated with 'derived', physically interpretable parameters that are computed from the estimated model parameters, rather than being estimated directly (Young, 1999a). In the context of the later global climate example, for instance, these include parameters such as decay rates, steady state gains and time constants (residence times).

3 Continuous-Time State Dependent Parameter Models of Physical Systems

In this Report, continuous-time, stochastic, state space descriptions are considered from two standpoints. First, as we see below, *state equations* can provide a description of a dynamic system that has specified physical significance. This is the way Kalman (1960) and Kalman and Bucy (1961) viewed the stochastic state space in their seminal work on state estimation and filter theory. Second, the state space description can be exploited within *parameter estimation* context, to describe a certain class of 'unobserved components' model, where the unobserved components are not necessarily 'state variables', in the normal sense, but stochastic time variable or state-dependent parameters that characterize a nonstationary or nonlinear time series model. Here, the model normally appears not in the state equations themselves but in the associated *observation equation* (e.g. Mayne, 1963; West and Harrison, 1989; Harvey, 1989; Durbin and Koopman, 2001).

3.1 The Stochastic State Space Model I: State Estimation and the Transfer Function Model

Considering the first of the above formulations, a linear stochastic *State Space* (SS) model of a physical system can be written in the form of the following, first order, vector-matrix differential equation:

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t) + \boldsymbol{\eta}(t) \quad (1a)$$

$$\mathbf{y}(t) = \mathbf{C}\mathbf{x}(t) + \boldsymbol{\xi}(t) \quad (1b)$$

[6]Such identifiability problems can arise either because the inputs to the system are not 'persistently exciting' (see references above) or because the model is of too high a dynamic order. This leads to ambiguity, with numerous different plausible parameter sets providing an equally good explanation of the data (i.e latterly also termed 'equifinality' by Beven, 2000a,b).

where $\mathbf{x}(t) = [x_1(t)\ x_2(t) \dots\ x_n(t)]^T$ is an n dimensional state vector, whose elements usually have direct physical significance but are not often all measurable; $\mathbf{u}(t) = [u_1(t)\ u_2(t) \dots\ u_m(t)]^T$ is an m dimensional, deterministic (i.e. exactly known or measurable) input vector; $\mathbf{y}(t) = [y_1(t)\ y_2(t) \dots\ y_p(t)]^T$ is a p dimensional output vector representing the physical measurements that can be made on the system; $\boldsymbol{\eta}(t)$ is a n dimensional stochastic input disturbance vector; and $\boldsymbol{\xi}(t)$ is a p dimensional stochastic noise vector. These two stochastic inputs are assumed to be vectors, each composed of zero mean, white noise variables that may be instantaneously correlated with each other. However, normally (although this is not essential) $\boldsymbol{\eta}(t)$ and $\boldsymbol{\xi}(t)$ are assumed to be completely independent. In other words:

$$\boldsymbol{\eta}(t) = [\eta_1(t), \eta_2(t), \dots \eta_n(t)]^T; \quad \boldsymbol{\xi}(t) = [\xi_1(t), \xi_2(t), \dots \xi_p(t)]^T;$$

$$cov\{\boldsymbol{\eta}(t)\boldsymbol{\eta}(\tau))\} = E\{\boldsymbol{\eta}(t)\boldsymbol{\eta}^T(\tau))\} = \mathbf{Q}\,\delta(t-\tau);$$

$$cov\{\boldsymbol{\xi}(t)\boldsymbol{\xi}(\tau)\} = E\{\boldsymbol{\xi}(t)\boldsymbol{\xi}^T(\tau)\} = \mathbf{R}\delta(t-\tau)$$

$$cov\{\boldsymbol{\eta}(t)\boldsymbol{\xi}(\tau)\} = E\{\boldsymbol{\eta}(t)\boldsymbol{\xi}^T(\tau)\} = \mathbf{0}\ \ \forall\ t, \tau$$

where $\delta(t-\tau)$ is the Dirac delta function. Finally, the matrices $\mathbf{A}, \mathbf{B}$ and $\mathbf{C}$ are appropriately dimensioned matrices with real coefficients (see later).

One advantage of a continuous-time state space description, such as (1a,b), is that such a model often results naturally when modelling physical systems using physical concepts such as mass, energy or momentum conservation. In this situation, the nature of $\mathbf{A}$ and $\mathbf{B}$ in (1a), as well as the parameters that characterize them, will be specified by the nature of the physical system. In parametric terms, however, it is not a very efficient representation of a linear dynamical system. Moreover it is not a *unique representation*: there are an infinite number of state space realizations that can be associated with any specified input-output relationship (e.g. Isermann, 1989). A much more efficient and unique representation in this sense is the multi-order differential equation, or its equivalent the *Transfer Function* (TF) description in the *Observation Space* (OS): i.e. the space of the measured variables $\mathbf{y}(t)$ and $\mathbf{u}(t)$.

In order to derive this OS description from the SS description (1a,b), let us consider the scalar, *Single-Input, Single-Output* (SIS0) case where $\mathbf{u}(t) = u(t)$ and $\mathbf{y}(t) = y(t)$; and then define the model in the 'observable' or 'observer' canonical form (e.g. Iserman, 1989), where:

$$\mathbf{A} = \begin{bmatrix} -a_1 & 1 & 0 & \dots & 1 \\ -a_2 & 0 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \\ \dots & 0 & 0 & 0 & 1 \\ -a_n & 0 & 0 & 0 & 0 \end{bmatrix} \quad \mathbf{B} = \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ \dots \\ b_n \end{bmatrix} \tag{2}$$

$$\mathbf{C} = \mathbf{c}^T = [1\ 0\ \dots\ 0]$$

Note that, although there are $n^2 + 2n$ elements in this canonical form, only $2n$ are non trivial (i.e. neither zero or unity) and need to be estimated. These are, as we shall see, the parameters of the TF description.

Now, if we introduce the derivative operator $s = d/dt$, then the equations (1a,b) can be written in the form,

$$\mathbf{x}(t) = [s\mathbf{I} - \mathbf{A}]^{-1}\,\mathbf{b}\ u(t-\tau) + [s\mathbf{I} - \mathbf{A}]^{-1}\,\eta(t) \tag{3a}$$

$$y(t) = \mathbf{c}^T\mathbf{x}(t) + \xi(t) \tag{3b}$$

Here, τ has been introduced into the definition $u(t-\tau)$ to account for the kind of pure time delay that often occurs between the input $u(t)$ and the output $y(t)$ in real systems. With the definitions above, it is easy to compute the following input-output model from (3a,b):

$$y(t) = \frac{B(s)}{A(s)}u(t-\tau) + \zeta(t); \tag{4a}$$

$$\zeta(t) = \frac{C(s)}{A(s)}\eta(t) + \xi(t) \tag{4b}$$

where,

$$\begin{aligned} A(s) &= s^n + a_1 s^{n-1} + \ldots + a_n \\ B(s) &= b_1 s^{n-1} + \ldots + b_n \\ C(s) &= c_1 s^{n-1} + \ldots + c_n \end{aligned} \tag{5}$$

and the ratios of these polynomials appearing in (4a,b) are the 'transfer functions' in the derivative operator s. Multiplying throughout by $A(s)$ we obtain,

$$A(s)y(t) = B(s)u(t-\tau) + C(s)\eta(t) + A(s)\xi(t)$$

or, on substitution from (5) and expansion,

$$s^n y(t) + a_1 s^{n-1}y(t) + \ldots + a_n y(t) = b_1 s^{n-1}u(t-\tau) + \ldots + b_n u(t-\tau) + \mu(t) \tag{6}$$

where the stochastic variable $\mu(t)$ is defined as follows in terms of $\eta(t)$ and $\xi(t)$,

$$\mu(t) = c_1 s^{n-1}\eta(t) + \ldots + c_n \eta(t) + s^n\xi(t) + a_1 s^{n-1}\xi(t) + \ldots + a_n \xi(t) \tag{7}$$

And finally, converting back from this s operator form to the differential equation form, equation (6) becomes:

$$\frac{d^n y(t)}{dt^n} + a_1\frac{d^{n-1}y(t)}{dt^{n-1}} + \cdots + a_n y(t) = b_1\frac{d^{n-1}u(t-\tau)}{dt^{n-1}} + \cdots + b_n u(t-\tau) + \mu(t) \tag{8}$$

We see, therefore, that in the case of a SISO system, this familiar multi-order differential equation is a parametrically efficient representation of the state space system (1a,b) in the observation space; and that an alternative observation space representation of this model is the transfer function description (4a,b). A simple example of these model forms provides the starting point for the practical example considered later in section 4.

3.2 The Stochastic State Space Model II: Estimation of Nonstationary and Nonlinear Systems

The TF model (4a,b) represents a continuous-time, linear system with time-invariant parameters. The estimation of these parameters from sampled input-output data represents an 'error-in-variables' problem (e.g. Durbin, 1954) and it has has been the subject of much research over many years (see e.g. Young, 1981; Sinha and Rao, 1991 and references in the example below). In this Report, however, we consider the more difficult problem where the parameters may vary over time, either directly or because they are varying as a function of other variables or states. The second type of stochastic state space model considered here is formulated specifically to allow for the estimation of such time variable or state dependent parameter models. Here, the observation equation (equation (1b)

of the previous section) normally assumes the role of the system model; and the state equations are used to describe any stochastic time variable or state dependent parameters characterizing this model. Often, however, this state space formulation is carried out in continuous/discrete (continuous-time model, discrete-time observations) or purely discrete-time terms, since this is more straightforward in theoretical and practical terms.

The estimation of TVP models formulated in the above manner goes back a long way to research in the nineteen sixties (e.g. Mayne, 1963; Lee, 1964; Young, 1969a, 1970) based on the use of the Kalman filter or other recursive 'filtering' algorithms. The exploitation of recursive *Fixed Interval Smoothing* (FIS) for 'off-line' TVP estimation follows from the early development of FIS algorithms (see e.g Rauch *et al.*, 1965; Bryson and Ho, 1969). Since then, there has been a great deal of research and development on this off-line FIS approach, with contributions from Norton (1976); Harrison and his co-workers (e.g. West and Harrison, 1989 and the prior references therein), Harvey (e.g. 1984, 1989); Young (1984, 1988); Durbin and Koopman (2001); and many others.

A recent paper (Young, 1999b) has discussed in detail the recursive estimation of *slowly* time variable parameters in the *Dynamic AutoRegressive eXogenous variables* (DARX) transfer function model, the time invariant (ARX) version of which can be estimated using linear least squares methods (e.g. Ljung and Söderstrom, 1983). Here the variation is 'slow' in comparison with the variation of the system variables (input, output and states) in the model. TVP models of this type can describe a wide range of nonstationary dynamic behaviour but they are not able to characterize true nonlinear dynamics. For this reason, there has been much interest during the last few years in the development of statistically-based methods for modelling true nonlinear stochastic systems. Granger and Teräsvirta (1993), for instance, reviewed the state-of-the-art in this area of study at that time and described numerous non-parametric, semi-parametric and parametric approaches, including neural network models. And the recent book by Durbin and Koopman (2001) nicely presents the TVP estimation methodology in the context of later developments in nonlinear model estimation based on numerically intensive methods, formulated from either classical or Bayesian perspectives.

Currently, there is much interest in the exploitation of numerically intensive methods in the modelling of nonlinear stochastic systems, much of it deriving from Bayesian concepts. Contributions of this type are derived in relation to a particular area of application, although they nearly always have wider application potential. For instance, there is enormous current interest in financial modelling[7] that often relates to nonlinear models of stochastic volatility (e.g. Shephard, 1995); while engineers requiring true, on-line implementation have developed methods such as 'particle filtering' (e.g. Gordon *et al.*, 2000) that provide nonlinear extensions to Kalman filtering and prediction. Of course, such particle filters are not only used for on-line applications in engineering: for instance Rydberg and Shephard (2000) develop a particle filter for stock exchange behaviour. And they, or related approaches, have been developed and used in areas such as geophysics, where Kitagawa (e.g. 1996 and the references therein) has made numerous important contributions over many years, most of which are applicable to a wide variety of systems in other areas of study.

Most often, the numerically intensive approaches to nonlinear modelling assume that non-Gaussianity enters, at least in part, through non-Gaussian probability distributions that are assumed to characterize the stochastic inputs to the models. The present author and his colleagues (Young, 1993, 1998b, 2000, 2001a,b,c; Young *et al.*, 2002) have pursued a rather different strategy which assumes that these stochastic inputs are Gaussian in nature and that non-normality in the measured output variables derives from the

[7] of course not all of this research exploits numerically intensive methods

nonlinear mechanisms within the model itself. For this class of nonlinear system, the standard TVP estimation methods can be extended to handle stochastic models whose parameters are functions of the system variables, and so vary at a rate commensurate with these variables: normally the state variables. As a result, these *State Dependent Parameter* (SDP) models, which derive originally from earlier work by Young (1978) and Priestley (1988), can characterize dynamic systems that behave in a heavily nonlinear or even chaotic manner and yield output variables with probability distributions that are very far from normality.

Most of the examples discussed in the above references on SDP estimation have been concerned with discrete-time, sampled data systems. In this Report, however, we concentrate on the SDP version of the continuous-time model (4a), which takes the form:

$$y(t) = \frac{B(s, \mathbf{z}(t))}{A(s, \mathbf{z}(t))} u(t - \tau) + \zeta(t) \tag{9a}$$

where $\mathbf{z}(t) = [z_1(t) z_2(t) \dots z_{2n}(t)]$ is the vector of variables on which the parameters are dependent; while $A(s, \mathbf{z}(t))$ and $B(s, \mathbf{z}(t))$ are the following state dependent polynomials in the derivative operator s:

$$\begin{aligned} A(s, \mathbf{z}(t))) &= s^n + a_1\{z_1(t)\}s^{n-1} + a_2\{z_2(t)\}s^{n-2} + \dots + a_n\{z_n(t)\} \\ B(s, \mathbf{z}(t)) &= b_1\{z_{n+1}(t)\}s^{m-1} + b_2\{z_{n+2}(t)\}s^{m-2} + \dots + b_m\{z_{2n}(t)\}. \end{aligned} \tag{9b}$$

In general, $\zeta(t)$ will be a complex, nonlinear stochastic noise variable representing that part of the output $y(t)$ that cannot be explained by the input $u(t)$. However, consider initially the simpler situation where,

$$\zeta(t) = \frac{1}{A(s, \mathbf{z}(t))} e(t) \tag{9c}$$

and $e(t)$ is a zero mean, white noise process, with variance σ^2. This *State Dependent ARX* (SDARX) model is then the continuous-time SDP equivalent of the time variable parameter DARX model mentioned above.

From a parameter estimation standpoint, the TF model (9a), with $\zeta(t)$ defined by (9c), can be written in the sampled form:

$$(s^n y)_t = \mathbf{z}_t^T \mathbf{p}_t + e_t \qquad e_t = \mathrm{N}(0, \sigma^2); \quad t = 1, 2, \dots N \tag{10a}$$

where, N is the total sample size and,

$$\begin{aligned} \mathbf{z}_t^T &= \left[-(s^{n-1}y)_t \ -(s^{n-2}y)_t \ \cdots \ -y_t \ (s^{n-1}u)_{t-\delta} \ \cdots \ u_{t-\delta-m} \right] \\ \mathbf{p}_t &= \left[\, p_1(z_{1,t}) \, p_2(z_{2,t}) \cdots \, p_{2n}(z_{2n,t}) \, \right]^T \end{aligned} \tag{10b}$$

while δ is the pure time delay τ measured to the nearest integral number of sampling intervals. The elements of parameter vector $\mathbf{p}_t$ are defined as follows in relation to the TF model parameters in (9b):

$$p_1(z_{1,t}) = a_1(z_{1,t}); \ p_2(z_{2,t}) = a_2(z_{2,t}), \cdots, p_{2n}(z_{2n,t}) = b_{2n}(z_{2n,t})$$

Here, the nomenclature $(s^i y)_t$ and $(s^j u)_t$, $i, j = 1, 2, \dots n$, denotes the sampled values of the derivatives of y and u at the t^{th} sampling instant; and e_t is the assumed discrete-time white noise associated with the measurement of $(s_n y)_t$.

The main problem with this continuous-time model formulation from a parameter estimation standpoint is its requirement for sampled measurements of the input and output time derivatives,

$$(s^i y)_t = \left(\frac{d^i y(t)}{dt^i} \right)_t, i = 1, 2, ..., n; \quad \left(s^j u\right)_{t-\delta} = \left(\frac{d^j u(t-\delta)}{dt^j} \right)_t, j = 1, 2, ..., n$$

which are not usually available directly and cannot be computed easily because of the high frequency noise amplification associated with differentiation. This problem is not too severe in the case of linear, constant parameter TF models and was solved many years ago by the introduction of 'state variable filters' (see previous references and the later example), but it presents more difficulties in the present nonlinear context.

The recursive approach to the time derivative estimation problem used in the later example (Young, *et al.*, 1993; Young, 1993) is again based on FIS estimation. The variable in question is modelled as a multiple differentiation process in continuous-time and then converted to the discrete-time equivalent of this process. The time derivatives of the variable at the sampling instants are then recovered as the FIS estimated states of this model, with the smoothing operations solving the problem of derivative estimation, at least for reasonable noise levels. In the simplest, single derivative case used in the example discussed later, for instance, this takes the form of an integrated random walk process[8] with its parameter defined by the sampling interval, Δt. This process could be formulated more accurately in continuous-time terms but the discrete-time formulation works quite well, as we shall see in the later example. Note that this direct estimation of time derivatives is only used in the first, non-parametric identification stage of SDP estimation: it is not required in the final parametric estimation stage described below.

3.3 Final Parametric Estimation

Within DBM modelling, non-parametric SDP modelling normally provides a method for identifying the presence and location of nonlinearities in the SDARX model (or the more general transfer function model with coloured residuals: see Young, 2000, 2001a). In this manner, it serves as a prelude to the parameterization of the final nonlinear stochastic model and the more efficient estimation of the (normally constant) parameters that characterize this nonlinear model. Such estimation can be based on various approaches to model optimization, from nonlinear least squares, through maximum likelihood to the latest Monte Carlo-based methods of Bayesian estimation. But the methodology used in any particular application will normally depend on the nature of the system under study, the modelling objectives, and the scientific background of the model builder. In the example described in the next section, we exploit maximum likelihood based on prediction error minimization but, in other applications (e.g. Young, 2000), we have converted the SDP transfer function model into a canonical state space form and used the maximum likelihood method based on prediction error decomposition (Schweppe, 1965; Harvey, 1989).

4 A DBM Model of Global Carbon Cycle Dynamics

The DBM modelling philosophy and the associated SDP estimation methodology have been applied successfully to a number of simulated and real systems (e.g. Young, 1993,

[8] this is the *irwsm* algorithm in the CAPTAIN Toolbox: see Conclusions section.

1998b, 2000, 2001ab, 2002; Young and Beven, 1994; Young and Pedregal, 1999; Price *et al.*, 1999; Jarvis *et al.*, 1999). The present example is based on the analysis of global average climate data. One novelty of this example, in time series analysis terms, is that it concentrates on modelling in terms of continuous-time differential equations, as discussed above, rather than the discrete-time models preferred by most statisticians and time series analysts. As we shall see, this considerably aids the process of DBM modelling because it is much easier to interpret the estimated model in a physically meaningful manner.

4.1 Atmospheric CO_2 and Global Climate Change

This example provides the technical background to a short paper by Jarvis and Young (2002). It investigates the dynamic relationship, over the period 1856 to 2000, between globally averaged annual measures of CO_2 emissions (arising from both the use of carbon fuels and land-use changes); atmospheric CO_2; and the Northern Hemisphere temperature anomaly. In particular, it reveals the possible presence of a temperature-dependent nonlinearity in the dynamic relationship between CO_2 emissions and atmospheric CO_2 that has an interesting and potentially important physical interpretation.

Figure 1 presents the data used in the analysis and shows that there are clear increases in all three variables over the period from 1856 to the end of the last century. The normal statistical procedure would be either to reduce the series to stationarity in some manner (e.g. by differencing); or consider each series as the sum of unobserved components (e.g. as trends and the perturbations about these trends, perhaps with relationships between these trends, as in the 'cointegration' models used by econometricians: see e.g. Harvey, 1989; Stern and Kauffman, 2000). But the climate data have a clear physical meaning and we can be reasonably sure that the increase in the levels of atmospheric pCO_2 are the result of the increases in emissions. In other words, there is an obvious input-output relationship, with the nonstationarity in the input giving rise to nonstationarity in the output. What is much less certain, however, is that the rise in the level of the atmospheric pCO_2 is, in turn, leading to the observed increase in the temperature anomaly.

With these factors in mind, we will analyze the data directly in the form shown in Figure 1. For this analysis, the input CO_2 emissions, the output atmospheric pCO_2 perturbations about the assumed pre-industrial level (see caption to Figure 1), and the temperature anomaly will be denoted by $u(t)$, $y(t)$ and $T(t)$, respectively.

4.1.1 Linear model identification and estimation

The RIVC method for continuous-time transfer function identification[9] (see Young and Jakeman, 1980; Young, 2002b) identifies a number of linear, constant parameter, first order models that have good identification and estimation statistics; i.e. coefficients of determination based on the simulated output R_T^2 greater than 0.99 (i.e. the simulated output of the model explains $> 99\%$ of the pCO_2 variance), together with well defined, low standard error parameter estimates and, hence, a satisfactory YIC criterion (Young, 1989). However, all higher order models are rejected, either because the do not satisfy these statistical criteria or because they are not satisfactory in dynamic terms (e.g. they have unstable or imaginary eigenvalues).

However, two important factors emerge from this analysis: first, it is necessary to add a small additional constant input to obtain a good explanation of the $y(t)$ series (see

[9] the *rivcid* tool in the CAPTAIN Toolbox.

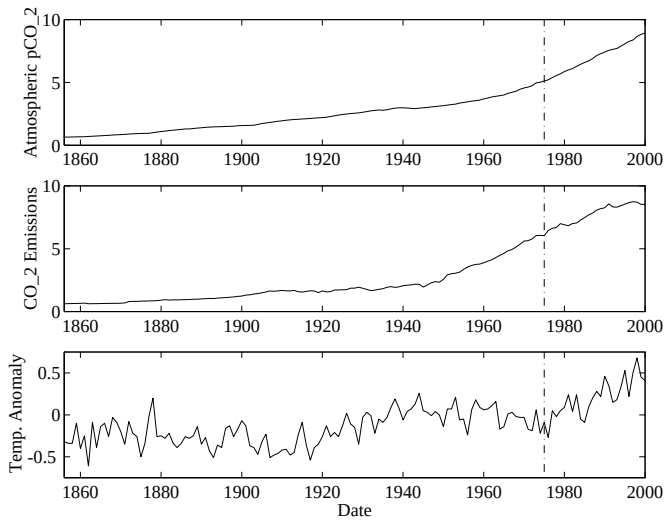

Figure 1. Annual carbon dioxide and temperature anomaly data 1856-2000. Upper panel, perturbations in atmospheric CO_2, (measured as partial pressure, pCO_2, relative to standard pressure, in pascals, pa) about an assumed pre-industrial level of 28 pa; middle panel, anthropogenic CO_2 emissions arising from fossil fuel usage and land use change ($Gt\ y^{-1}$); lower panel, Northern Hemisphere average temperature anomaly ($^{\circ}C$). The vertical dash-dot line marks the boundary between model estimation (1856-1975) and predictive validation (1976-2000) data (see text). All series are derived from data available at http://cdiac.esd.ornl.gov/.

below); second, there is a less well defined pure time delay of about 5 years. In other words, this initial analysis suggests a model of the form:

$$\frac{dx(t)}{dt} = a_1 x(t) + b_0 u(t-\tau) + c \tag{11a}$$

$$y(t) = x(t) + \xi(t) \tag{11b}$$

where $x(t)$ is the underlying, 'noise-free' pCO_2 perturbation; τ is the pure time delay; $\xi(t)$ is the residual coloured noise at the output of the model, with zero mean value and variance σ_ξ^2; and c is the additional constant input. The addition of c makes sense physically because it will correct for any small inaccuracy in the either assumed pre-industrial level of pCO_2 that has been removed from the pCO_2 data (see caption to Figure 1) or the CO_2 emissions.

In order to obtain an improved, possibly non-integral, estimate of the time delay, the model (11a) was estimated using the *leastsq* optimization tool in Matlab^{TM}, with the model simulated in Simulink^{TM}, using the *linsim* tool. All integrations of the model used in this optimization were initiated from the measured $y(0)$, since separate optimization of the initial condition had little effect on the estimates. Also, in order to allow for colour in the residuals $\xi(t)$, they were modelled as a *discrete-time* AutoRegressive (AR) process, i.e.,

$$\xi_t = \frac{1}{1 + d_1 L + ... + d_n L^n} e_t \tag{11c}$$

where $\xi_t = \xi(t_i)$ and $e_t = e(t_i)$ are, respectively, $\xi(t)$ and $e(t)$ sampled at the annual sample times $t_i, i = 1, 2, ..., N$, and N is the sample size. The sampled stochastic model residuals e_t are assumed to be a zero mean sequence of serially uncorrelated random variables with variance σ^2 (discrete white noise). This 'hybrid' approach to modelling was used because the discrete-time stochastic model (11c) is easier to handle within the optimization (and in theory). In any case, the noise model estimation makes only a small difference to the final estimated parameter values (although it does affect their estimated uncertainty) because the residual noise variance is so small.

Parameter estimation was based on optimization of the following least squares 'prediction error minimization' cost function (equivalent to maximum likelihood optimization under the assumption of normally distributed errors) with respect to the unknown parameters:

$$J\{\boldsymbol{\theta}\} = \sum_{t=1}^{t=N} \hat{e}_t^2 \qquad ; \qquad \boldsymbol{\theta} = [a_1 \ b_0 \ c \ d_1 \ d_2 \ ... \ d_n \ \tau]^T$$

where $\hat{e}_t$ are the stochastic model residuals (one-year-ahead prediction errors) at the annual sampling interval. The estimated parameters in the most important continuous-time part of the model, based initially on the whole data set ($N = 145$) are as follows:

$$\hat{a}_1 = -0.0167(0.0009); \quad \hat{b}_0 = 0.0371(0.0009); \quad \hat{c} = 0.0114(0.0006);$$

$$\hat{\tau} = 5.0(0.389); \quad \sigma_\xi^2 = 0.0041; \quad \sigma^2 = 0.0004$$

where the figures in parentheses here and elsewhere are the standard errors on the estimates. The noise model (11c) is identified as either an AR(8) or ARMA(2,2) process, with the final residuals e_t showing no significant auto-correlation and no cross-correlation with the input u_t (the annual samples of the input CO_2 emissions). However, the residuals $\hat{\xi}_t = y_t - \hat{x}_t$ are significantly correlated with the temperature T_t for all lags between 4 and 22 years and a maximum correlation coefficient of 0.4 (0.17) at a lag of 10 years. Moreover, recursive FIS estimation of the local cross correlation is much larger than this at high values of T_t. The model has a coefficient of determination based on the simulated deterministic model residuals $\hat{\xi}_t$ of $R_T^2 = 0.9991$; while the more conventional coefficient of determination based on $\hat{e}_t$ is $R^2 = 0.9999$. This is, of course, important in the present context since it means that the main differential equation which, as we shall see later has physical significance, is explaining the measured output of the dynamic system very well indeed.

4.1.2 Nonlinear model identification and estimation

Despite the apparently very good results obtained in linear modelling, the high correlation of the residuals $\hat{\xi}_t$ with the temperature anomaly T_t suggests that there may be a temperature dependent component in the model residuals that is capable of being absorbed within the model and so improving its descriptive ability still further. This is indeed the case: SDP non-parametric estimation suggests strongly that, while the input parameter b_0 is constant, the parameter estimate $\hat{a}_1$ appears to vary as a function of temperature anomaly T_t. This SDP estimate $\hat{a}_1$, plotted in the left hand panel of Figure 2, suggests that the parameter value is reducing as the temperature increases, although there is a tendency for the variations to 'flatten out' at the lower and upper extremes of the temperature anomaly range. But we must remember that these are non-parametric estimates and tend to be more poorly defined in these regions because of end effects and the paucity of data in these regions.

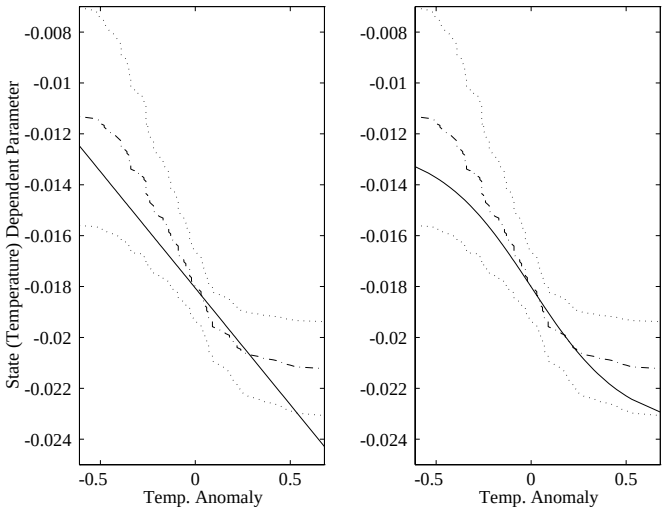

Figure 2. Initial, non-parametric SDP estimate (dash-dot line) and standard error bounds (dots) compared with the parametric model estimates: linear change with temperature (left panel); sigmoidal change with temperature (right panel). These temperature dependent variations can be compared with the linear model parameter value of $\hat{a}_1 = -0.0167$.

In order to investigate this problem in a statistically more efficient parametric manner, several different parameterizations of the temperature dependency suggested in Figure 2 were tried, including polynomial, radial basis function and an exponential decline. However, the best results were obtained with either simple linear (first order polynomial) or sigmoidal laws. In other words, the finally identified nonlinear model takes either of the following forms:

$$\frac{dx(t)}{dt} = \{\alpha + \beta T(t)\}x(t) + b_0 u(t-\tau) + c \tag{12a}$$

$$y(t) = x(t) + \xi(t) \tag{12b}$$

or,

$$\frac{dx(t)}{dt} = \{\alpha + \frac{1}{1+e^{-\beta T(t)}}(\gamma - \alpha)\}x(t) + b_0 u(t-\tau) + c \tag{12c}$$

$$y(t) = x(t) + \xi(t) \tag{12d}$$

In the case of (12a,b), which is the model we shall consider further below, the estimated parameters, again based initially on the whole data set ($N = 145$), are as follows[10]:

$$\hat{\alpha} = -0.0181(0.0016); \quad \hat{\beta} = -0.0092(0.0021); \quad \hat{b}_0 = 0.0402(0.0017);$$

$$c = 0.0069(0.0014); \quad \hat{\tau} = 5.0; \quad \sigma_\xi^2 = 0.0025; \quad \sigma^2 = 0.0006$$

[10]These results were obtained with a fixed $\tau = 5$: however, this was based on prior estimation with τ allowed to take on non integral values.

$$R_T^2 = 0.9995; \quad R^2 = 0.9999$$

where the AIC (Akaike, 1974) again identifies an AR(8) or ARMA(2,2) model for the noise ξ_t. As before, the final model residuals e_t show no significant auto-correlation and no cross-correlation with the input u_t; but now $\hat{\xi}_t$ also shows no significant correlation with T_t, as required. Bearing on our earlier discussion, note that the estimate of c is significant but very small, as anticipated

The linear-in-temperature law obtained in the above estimation is shown as the full line in the left hand panel of Figure 2 and we see that it coincides well with the non-parametric SDP estimate. The right hand panel in Figure 2 shows the results obtained with the best competing sigmoidal model (12c,d). This was investigated to allow for any possible flattening out of the relationship at higher levels of the temperature anomaly (see earlier discussion) which would have most effect on long-term model predictions. However, there is only a minor effect of this type. Also, despite its additional parameter, this model explains the data virtually the same as (12a,b) and two of its parameters are more poorly defined statistically (particularly β). So, it is sensible on parsimony grounds to proceed with the simpler model (12a,b).

4.1.3 Predictive validation

In order to investigate the predictive capacity of (12a,b), it is re-estimated on the basis of the estimation data set alone (i.e. only the first 120 annual samples up to 1975) and then its performance is evaluated by forecasting the perturbational pCO_2 variations over the last 25 years of the 20^{th} Century, without any re-estimation of the parameters over this period. To make this exercise more demanding, the model integrations are initiated in 1856, with the initial condition for the integrations set to the value of $y(0) = 0.6523$ *pa* on this date and *with no reference to the actual* $y(t)$ *measurements at all after this.* In other words, the forecast is based on a straightforward Monte Carlo simulation of the nonlinear model from this initial condition using only the measured CO_2 emissions and temperature anomaly as inputs to the model. This MCS analysis is based on the estimated covariance matrix of the model parameters and involves 1000 random realizations of the model. The results are shown in Figure 3, where we see that the $y(t)$ variations are predicted very well indeed ($R_T^2 = 0.9993$, only a little worse than obtained from model estimation based on all 145 samples) and the MCS estimated confidence region is small. For comparison, the sigmoidal model (12c,d) performed about the same in predictive validation terms; while the linear model (11a,b) was significantly worse, with $R_T^2 = 0.9985$.

It is possible to go further in evaluating the adequacy of the model by recognizing that equation (12a) represents a state dependent system with negative feedback of the temperature $T(t)$. Consequently, if the relationship between $y(t)$ and $T(t)$ is identified, then the model's predictive ability can be assessed using only the emissions input $u(t)$. As an initial illustration of this, a simple, linear, continuous-time transfer function model between $y(t)$ and $T(t)$ is estimated, again using the *rivcid* tool in the CAPTAIN Toolbox. The resulting model takes the form:

$$\frac{dz(t)}{dt} = a_1 z(t) + b_0\{y(t) - \bar{y}\} \tag{13a}$$

$$T_t = z(t) + \eta(t) \tag{13b}$$

where $\bar{y}$ is the mean value of $y(t)$ (subtracted from $y(t)$ so that the input is a perturbational series like the output temperature anomaly series, T(t)); $z(t)$ is the underlying 'noise-free' temperature anomaly; η_t is an AR(9) process and the estimates of the two

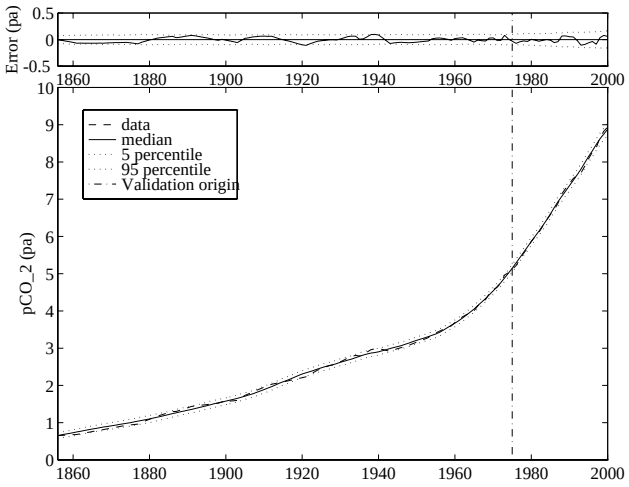

Figure 3. Monte Carlo Simulation and predictive validation results with all predictions based on simulation from initial conditions in 1856, using the model based on the first 120 samples to 1975: perturbations in atmospheric pCO_2 about the assumed pre-industrial level (dashed line); deterministic simulation and MCS median prediction (full line); 5%-95% percentile bounds (dotted lines). The error between the simulated and measured pCO_2 is shown in the top panel at a smaller scale, also with dotted 5%-95% percentile bounds.

parameters are:

$$\hat{a}_1 = 0.0514(0.009); \quad \hat{b}_0 = 0.0080(0.001)$$

It must be stressed that we are not claiming that this is necessarily a good model for the effects of the perturbations in $pCO2$ on global energy balance: its descriptive ability is too limited in this regard ($R_T^2 = 0.56$; $R^2 = 0.72$) and a more detailed analysis of this relationship is required[11]. Rather it is being used here merely for illustrative purposes and to ensure that the scaling between $y(t)$ and $T(t)$ is of the correct order to ensure that the simulation of the complete feedback system makes reasonable sense. Even with these limitations, however, the complete model (i.e. (12a,b) with $T(t)$ defined internally within the model by (13a,b)) is able to predict the pCO_2 very well over the historical period, as shown in Figure 4, with $R_T^2 = 0.9992$. The associated median estimate of $T(t)$, together with its $5\% - 95\%$ percentile bounds, is compared with the measured $T(t)$ in the lower panel of this figure.

4.1.4 Physical interpretation

Most conventional models of the *Global Carbon Cycle* (GCC) are based on a reductionist, 'bottom up' approach and take the form of high order deterministic differential equations (see e.g., Joos *et al.*, 1999). A typical example is the Enting-Lassey (EL) model of the GCC (Enting and Lassey, 1993), which consists of 23 coupled, nonlinear differential equations and represents a good example of the hypothetico-deductive approach to modelling.

[11] This is a current area of research for both authors.

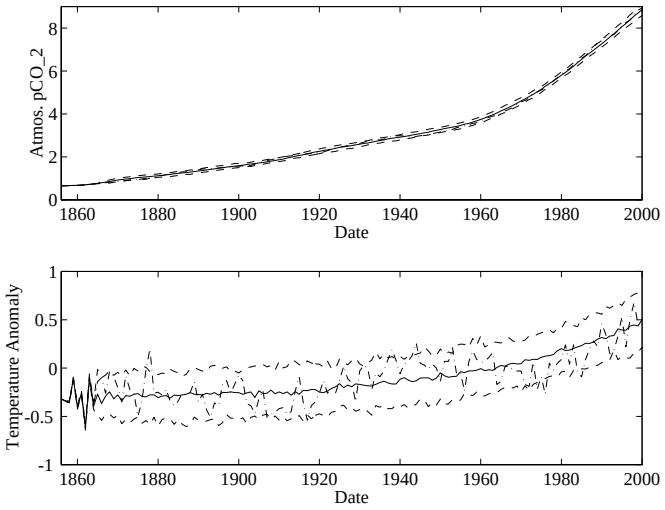

Figure 4. Monte Carlo Simulation (MCS) with internally generated, stochastic temperature feedback from 1864, using the complete nonlinear model based on the full 145 samples. Upper panel: perturbations in atmospheric pCO_2 (dashed line); MCS median prediction (full line). Lower Panel: temperature anomaly (dashed line); MCS median prediction (full line). The 5%-95% percentile bounds are shown as dotted lines in both panels.

At first sight, the contrast between this complex, high order model and the identified first order, stochastic models (12a,b) and (12c,d) is considerable. However, Young *et al.* (1996) have shown that the dynamic behaviour of the high order EL simulation model can be represented, almost completely, by a differential equation of only fourth order. The reason for this is that the observable dynamics of high order dynamic systems are almost always defined by the 'dominant modes' of the system, which are normally few in number. And it is, of course, only these observable dynamics that are identifiable from the measured data. As a result, we should not be too surprised that the models identified in this Report are so simple, particularly since they are based on globally averaged data. In effect, the global averaging ensures that the data represent the aggregative effects of all the relevant behaviour within the GCC and, as we can see from the data in Figure 1, the variations in the CO_2 emissions and the atmospheric pCO_2 are not particularly complicated as a result.

Given that the model (12a,b) has been estimated from global scale emissions and atmospheric pCO_2 perturbation data, it seems appropriate to interpret this model in terms of the mixing dynamics of anthropogenic CO_2 emissions within the active elements of the Global Carbon Cycle (GCC). We commence by assuming that variations in atmospheric pCO_2 are proportional to variations in the concentration of carbon in these active elements. Then, a perturbational representation of this single mixing unit may be given by the following mass balance (see Appendix),

$$\frac{wvdy\,(t)}{dt} = u\,(t-\tau) - w\,\{k_0 + mT\,(t)\}\,y\,(t) \tag{14}$$

Here, k_0 is the initial value of the first order loss constant k at $T(t) = 0$; m is the

sensitivity of this loss constant to $T(t)$; w is the proportionality between variations in the well mixed CO_2 concentration and the atmospheric pCO_2; and v is the effective volume actively involved in the mixing of anthropogenic CO_2 (the 'active mixing volume': see Young and Lees, 1992) such that $wvy(t)$ is the mass of anthropogenic CO_2 within this well mixed compartment.

The pure time delay τ signifies a five year delay before the emissions significantly impact on the state of anthropogenic CO_2 in the system. Given the relatively well mixed state of the atmosphere, and that emissions are into the atmosphere, it is hard to conceive how this delay could arise from pure advection prior to emergence within the atmospheric compartment of the GCC. Therefore, a more plausible explanation is obtained by considering the nature of the emissions exciting the observed perturbations in pCO_2. In particular, given the trend-like nature of these inputs, uncertainties over the time period between input and effect are likely to arise, especially since the 5 year pure time delay is small relative to the identified time constant of the system, which is given by $v/k_0 = 55.5\ (48.4, 64.9)$ years at $T = 0\ ^\circ C$, where the figures in parentheses are 5th and 95th percentiles for this non-Gaussian derived parameter. In addition, the identification of pure time delays within aggregated systems, such as the GCC, may be indicative of the presence of poorly defined higher order dynamic behaviour (see Young, 2001b)[12].

Having introduced the mechanistic counterpart to the identified data-based model, we are in a position to equate the remaining parameters between (12a) and (14) and evaluate some of the physical properties of the identified system. This yields the following estimates:

$$wv = 24.90\ (1.08)\ Gt\ pa^{-1}; \quad wk_0 = 0.45\ (0.022)\ Gt\ y^{-1}\ pa^{-1}$$

and

$$wm = 0.228\ (0.05)\ Gt\ y^{-1}\ pa^{-1}\ ^\circ C^{-1}$$

In order to compare these results with published work, we start by estimating the total mass of CO_2 in the identified mixing system in 1980, which is given by $33.85mv$ or $842.9(30.2)Gt$. This figure is close to, but significantly larger in statistical terms than, quoted figures for the mass of CO_2 in the atmosphere alone in 1980, which is given as 730 Gt (Farquhar *et al.*, 2001). This would indicate that, although the global scale mixing dynamics of anthropogenic CO_2, as observed in measurements of atmospheric pCO_2, are dominated by the effects of the atmospheric reservoir, approximately 15% of the mixing mass is contributed by some other components of the GCC. Likely candidates are the surface ocean and terrestrial carbon reservoirs (Harvey 2000). However, theoretical estimates of the mass of carbon in these two reservoirs, in 1980, are put at around $2500Gt$ (Farquhar *et al.*, 2001). This suggests that, contrary to current understanding, large fractions of the terrestrial and surface oceanic carbon reservoirs are effectively 'dead zones' that have played no significant role in the observed mixing process to date, and instead may have behaved as sinks for anthropogenic CO_2 over this period.

These conflicts are further illustrated by consideration of the non-conservative nature of (14), as revealed by the fact that there is no integrator in the model (the steady state gain is finite at $2.2\ (2.1, 2.4)\ pa\ (Gty^{-1})^{-1}$). By contrast, simulation models of the GCC invariably contain conservative elements (see e.g. Enting and Lassey 1993; Joos *et al.*,

[12] note that for completeness, any losses of CO_2 from the system during the pure time delay, as well as the effects of the offset c, should be taken into account (see Appendix). They are omitted here to make the analysis more transparent

1999). Again, this discrepancy may result from the limitations of the 145 year observation interval relative to the timescale for accumulation of anthropogenic carbon within the GCC as a whole. However, dominant mode analysis of these simulation models would suggest that, if such conservative behaviour were present in the form being specified, then it should be identifiable within the current time series data set (Young *et al.*, 1996).

The identified temperature dependency of the CO_2 loss rate constant k can be explained through the effects of temperature on the various processes associated with atmospheric CO_2 removal. Raising global temperature reduces the solubility of CO_2 in the oceans and promotes respiration, both of which should act to decrease k. Therefore, the temperature related increases in k we have estimated here could indicate temperature enhanced photosynthetic processes or surface water mixing over this time interval. Such effects are known as 'climatic stimulation of CO_2 removal processes' that act over and above the effects of the CO_2 fertilization implicit in (14) (Appendix). For the period 1950-1984 the cumulative losses attributable to this effect is 13.5 (1.8) Gt, which is comparable to the 20 (5) Gt estimated by Dai and Fung (1993) using a completely different approach. The estimated total climatic losses for the period 1856-2000 are 39.4 (6.2) Gt. This may provide a credible explanation for some of the so called 'missing sink' for CO_2 often cited in the literature (Farquhar et al 2001). If it is assumed that rising pCO_2 leads to rising global temperatures, then the identified effect of temperature on the CO_2 removal efficiency has acted as a stabilizing negative feedback as shown in Figures 5 and 6 of the next section. It has been proposed that temperature effects on respiration and CO_2 solubility in the oceans should dominate the climatic response of the GCC, leading eventually to a net positive climatic feedback (e.g. Cox *et al.*, 2001). This would suggest that the temperature dependency shown in Figure 2 is a transitory effect that may disappear either at higher temperatures or in time as the ocean temperature equilibrates with that of the surface. However, it is important to note that, to date, such effects are not observed in these global scale data. Finally, although these data provide no insight into the future persistence of the observed stabilization effect, the identification of the effects of global temperature rises within the relationship between emissions and pCO_2 perturbations provides an important independent validation of the significance of the observed increases in global temperature shown in Figure 1.

From this evaluation of the identified model (12a) in relation to its mechanistic counterpart (14), we have seen that certain inferences about the dynamics of the GCC can be made. As is sometimes the case, this diagnosis has highlighted both parallels and conflicts between the inferred and the identified dynamic behaviour, only some of which can be reconciled through careful consideration of the nature of the identified system in relation to the underlying behaviour being observed. In particular it must be stressed that the DBM model obtained here relates to the *global scale* observations from which it was derived, and that it does not attempt to describe the operation of the GCC at any smaller scale.

4.1.5 Hypothetical long-term forecasting

Let us now consider the model in a less serious, illustrative manner by investigating what implications it may have on the longer term behaviour of the global climate. In this regard, it must be emphasized that the results presented in this section are hypothetical and based not only on an assumption that the model parameters remain constant over the next two centuries, but also on an extrapolation of the nonlinearity in Figure 1a to higher

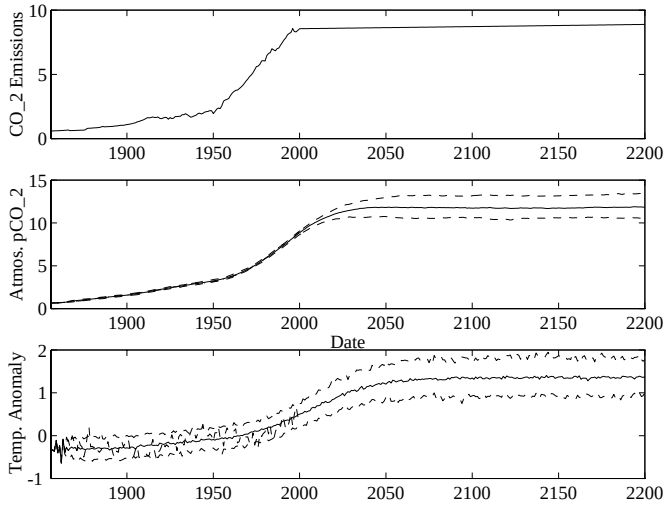

Figure 5. Hypothetical predictive Monte Carlo stochastic simulation of the complete nonlinear feedback model with internally generated temperature feedback from 1879 to 2200, based on the model estimated over the whole observational period to year 2000: CO_2 emissions (full line, upper panel); atmospheric pCO_2 perturbations (full line, middle panel); and Northern hemisphere temperature anomaly (full line, lower panel). Measured variations in the variables to 2000 are shown as dashed lines and the 5%-95% percentile bounds are denoted by dotted lines.

levels of the temperature anomaly, up to about 1.5°C.[13] The forecasts are also dependent on a forecast of the CO_2 emissions, $u(t)$, over the next two centuries, as shown in the top panel of Figure 5. This was obtained using an SDP estimate of the emissions growth rate and averaging this over the years 1995-2000 to generate future predictions of $u(t)$. This additional averaging was introduced because the rate is changing quite rapidly over this last portion of the historical data due to recent reductions in the emissions, leading to a predicted decline, which seem rather doubtful. Naturally, these future emissions will be based on many factors and a purely historical extrapolation such as this is unlikely to be accurate. Again, however, it suffices for these illustrative purposes.

Under these assumptions, the full nonlinear feedback model produces the MCS-based forecasts shown in the bottom two panels of Figure 5. Both the pCO_2 and the temperature continue to increase for some time, but with a very much reduced rate of increase caused by the levelling-off of the CO_2 emissions and the temperature feedback effect. The latter effect becomes clear if these results are compared with the forecasts generated in the same manner by the linear model (11a,b), as shown in Figure 6, where we see that pCO_2 in the year 2200 is some 8 *pa* higher than that forecast by the nonlinear model; and this leads to a 1.3°C higher temperature anomaly.

As we point out in the next section 4.1.6, these forecasts of ours differ markedly from

[13] At first, it would seem to be more cautious, if this was intended as an entirely serious exercise, to utilize the model (12c,d), with its apparently more conservative sigmoidal nonlinearity. However, this nonlinearity is a quite sensitive to the β parameter in (12c), which has a high variance estimate, so its is not a very satisfactory long term forecasting model.

those obtained using complex simulation models of the GCC, (see also our comments on this in Young and Jarvis, 2002). There are two main reasons for these differences. First, the non-conservative behaviour within the complex, reductionist models means that there is no stabilization of the atmospheric $pCO2$ for *any* positive emissions level. Secondly, the effects of temperature on reductions in the solubility of CO_2 in the oceans is thought to dominate the climatic effects on the GCC, such that losses of CO_2 from the atmosphere reduce rather than increase with elevating temperatures.

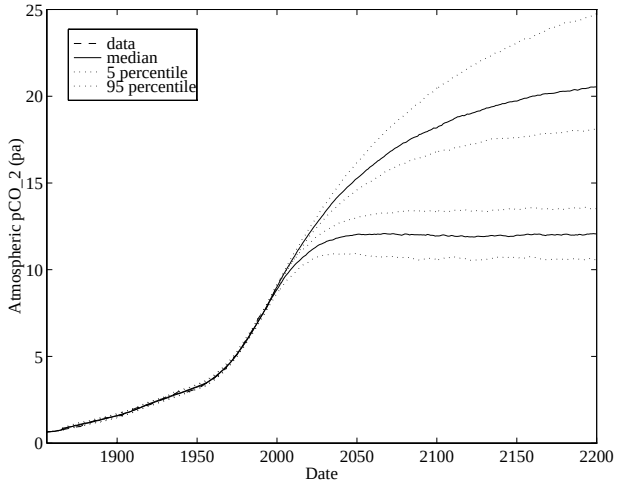

Figure 6. Hypothetical long term Monte Carlo predictions of the nonlinear SDP (obtained as for Figure 5) and the constant parameter linear model. Also shown are the 5%-95% percentile bounds (dotted lines) and the atmospheric pCO_2 data to year 2000 (dashed line).

4.1.6 Some additional observations on prediction

Considering the use of the nonlinear models in hypothetical long term forecasting raises a number of questions about the nature of the nonlinearities and the definition of the emissions scenario into the future. The three models we have considered so far are the linear model (11a,b); and the two nonlinear SDP models with feedback nonlinearities that are either linear (12a,b) or sigmoidal (12c,d) in the temperature anomaly. The linear model has a temperature-invariant coefficient of -0.0167; while the latter two have the temperature dependent coefficients plotted again[14] in figure 7.

So which of these models should we choose for our hypothetical predictive exercises? The most obvious approach is to first consider the range of predictions that they produce for any specified emissions scenario. For instance, figure 8 compares the predictions of all three models for the emissions scenario in the upper panel of figure 5, with the percentile bounds only shown for the model with the sigmoidal nonlinearity to avoid confusion on the plot. Of these three, we see that this sigmoidal-in-temperature model represents a

[14]this figure is added for completeness: the only difference between this and Figure 2 is that, here, the percentile bounds are those that relate to the parametric estimates.

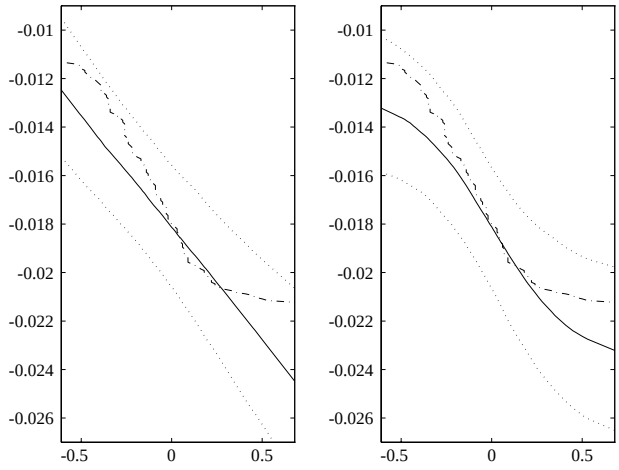

Figure 7. The estimated parametric nonlinearities in the models (12a,b) and (12c,d): linear change with temperature (left panel); sigmoidal change with temperature (right panel). The $5\% - 95\%$ percentile bounds are shown dotted and the non-parametric estimate is shown as a dash-dot line for comparison

reasonable compromise between the pessimism of the linear model and the optimism of the linear-in-temperature model.

Of course, the predictions in figure 8 are constrained by the assumption of the rather optimistic future emissions scenario. Also, such analyses should take into consideration the uncertainty associated with the emissions measurements themselves which, up to now, have been assumed error free (except for the inclusion of the offset parameter c in all the models). This latter concern apart, one approach to the wider and more discerning definition of such emission scenarios is to consider the 'inverse problem' (e.g. Wigley, 2000): i.e. compute the emission scenarios that are able to achieve a range of 'stabilization concentration profiles' for atmospheric CO_2, such as those utilized in the studies carried out by the IPCC (Schimel,*et al.*, 1996). An alternative and more flexible approach is to exploit automatic control theory and so generate an emissions scenario (control input) that achieves some required objective, as defined by a defined 'optimal' criterion function.

However, if we consider the results obtained using approaches such as these, based on the models obtained in the present report, they are significantly different from those obtained heretofore by climate scientists. For example, Wigley (2000), using his 1993 carbon balance model (Wigley, 1993), generates a range of emissions scenarios that achieve a whole range of stabilization concentration profiles, with steady CO_2 levels ranging from 350 to 750 *ppmv* (i.e. perturbations in pCO_2 from 7 to 47 *pa*). If we consider the 450 *ppmv* (17 *pa*) case, for instance, his required future emission scenario reduces to a steady level of *circa* 2.3 $Gt\ y^{-1}$ by the year 2200. By contrast, Figures 9 and 10 illustrate the results of an automatic control exercise based on our linear model (11a,b).

Figure 9 is the block diagram of the Simulink system used to generate the MCS realizations in this exercise (calling this simulation repeatedly from the Matlab workspace). From 1856 to 2000, the emissions input to the model is based on the measured emissions. After this, however, the switch shown towards the centre of the block diagram introduces

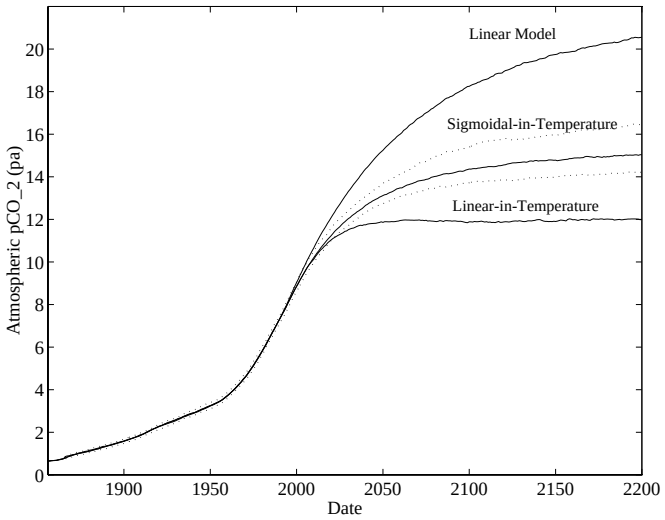

Figure 8. Comparison of the hypothetical long term Monte Carlo predictions of the two nonlinear SDP models and the constant parameter linear model (percentile bounds only shown for the sigmoidal-in-temperature nonlinear model to avoid confusion; the percentile bounds for the other two models are shown in Figure 7).

the computed emissions input based on a *Proportional-Integral-Plus* (PIP) feedback controller (Young *et al.*, 1987, 2002; Taylor *et al.*, 2001) designed to follow a defined future CO_2 profile (in this case similar to the Wigley example mentioned above, although other profiles could be used equally easily using this approach). This is designed to stabilize the atmospheric pCO_2 perturbation at a level of $17.6pa$ ($456ppmv$) and the temperature anomaly at a mean level of *circa* 2.6°C. Figure 10 shows the results of this exercise and we see that the objectives have been realized by 2200, with an emissions scenario stabilizing at a level of 7.4 $Gt\ y^{-1}$, with a $5\% - 95\%$ percentile range between 6.1 and 8.5 $Gt\ y^{-1}$; i.e. between 3.6 to 6 $Gt\ y^{-1}$ higher than that computed by Wigley (2000) for a similar profile (i.e. the same result achieved with a much smaller reduction in the CO_2 emissions).

Note that one advantage of this automatic control approach is that we can choose any desired criterion for the future emissions control, since this only entails modifying our criterion function. For example, the criterion function used in achieving the results shown in Figure 10 is based on generating a future emissions strategy (control input) that minimizes the error between the desired future profile and the future pCO_2 variations. However, this could be modified to include other factors, such as economic costs and benefits.

Of course, it must be emphasized that both Wigley's results and ours are speculative 'what-if' studies, characterized by considerable uncertainty, even if it is assumed that the generated emissions scenario is achievable. They can also be considered as providing a range of extreme speculations, with the Wigley results representing a pessimistic future requiring major reductions in emissions; while ours are much more optimistic in this regard[15]. The credibility attached to these speculations will, of course, depend largely

[15] although, ironically, they are based here on our most *pessimistic* model: the nonlinear models

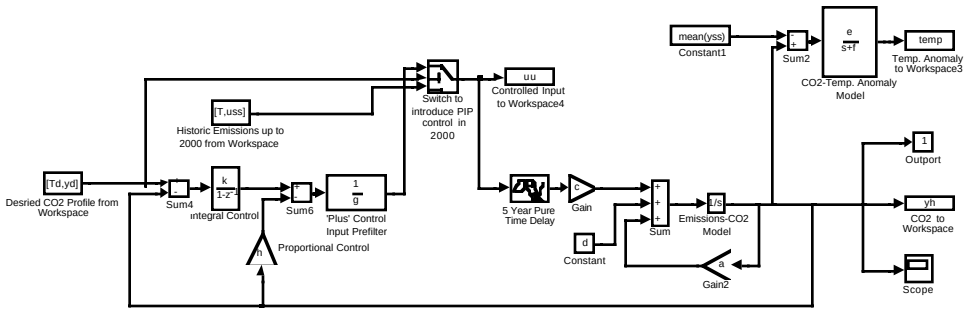

Figure 9. Simulink block diagram of the PIP automatic control system (at the left) controlling the CO_2 emissions to the DBM linear model of atmospheric CO_2 (at the right), in order achieve a desired atmospheric CO_2 stabilization profile.

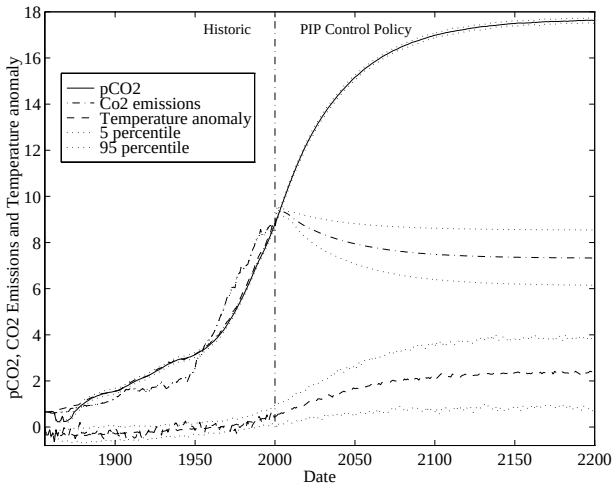

Figure 10. MCS simulation of the DBM linear model, showing how a PIP designed automatic control system is able to produce a reasonable CO_2 emissions policy (dash-dot line) that stabilizes 200 year-ahead levels of the simulated atmospheric CO_2 (full line) at a level of $17.6pa$ ($456ppmv$) and the simulated temperature anomaly (dashed line) at a mean level of *circa* 2.6°C.

on one's scientific background. If we exaggerate the situation somewhat, in order to clarify the nature of the dilemma, then two extreme viewpoints can be discerned:

1. Scientists educated within a deterministic, hypothetico-deductive tradition, will argue correctly that a simulation model, such as Wigley's, reflects the current state-of-the-art understanding of the mechanisms operative in those multiple com-

(12a,b) and (12c,d) would provide still more optimistic predictions because of the temperature feedback effects.

partments of the GCC system that are thought necessary to characterize its the dynamic behaviour. They will point out that it is a representation that utilizes all of the information available in this regard, assembled in a model form that reflects the scientist's well-supported perception of how the different physical and biological processes interact with each other in dynamic terms. And they will emphasize that the level of detail in the model reflects a widely held view that the environment, particularly at the global scale, is a very complex system that can only be represented by a similarly complex model.

2. On the other hand, scientists who follow a statistically-based, inductive approach, of the kind employed in the present report, will argue that data-based, mechanistic models, identified and estimated in stochastic terms, better reflect the information content of the available, uncertain data; and that such models are less prone to the prior prejudice that can sometimes result from over-confidence in current paradigmatic judgement. They will also point out that large and complex models cannot be estimated properly in rigorous statistical terms, since they are over-parameterized and so not uniquely identifiable from the available data. As a result, they will argue that such a model has not been adequately validated against the available data and so is a questionable vehicle for making predictions into the distant future. And, finally, they will be able to show that, despite their complexity, large mathematical models behave in a quite simple dynamic manner and can be mimicked in this regard by much simpler 'dominant mode' mathematical models of the DBM kind (e.g. Young *et al.*, 1996; Shackley *et al.*, 1996).

Both of these extreme viewpoints can be defended, of course, and the reader will not be surprised that we subscribe rather strongly to the latter. But they are, nonetheless, rather dogmatic: the most reasonable approach, in any given practical situation, probably lies somewhere between them. After all, *there is never only one model of a real system* and the choice between them will depend largely on the objectives of the modelling exercise. Certainly, although we exploit data-based mechanistic modelling whenever the availability of data allow for this, we also make good use of large simulation models (although normally considered within a stochastic setting and utilizing stochastic simulation: see Parkinson and Young, 1998; Beven *et al.*, 2000; Young and Parkinson, 2002).

Finally, there is one paradox raised by the comparison of our results with those of Wigley (2000) that we will leave the reader to contemplate. Figure 11 is a reproduction of Figure 21.1 in Wigley (2000) which compares the simulated atmospheric CO_2, as generated by his rather heavily parameterized simulation model, with the measured data (see 'FULL OPT' and 'OBSERVED' lines). If these results are compared with those obtained above (figure 8), then it is clear that despite the complexity of the Wigley model, the simple DBM models (12a,b) or (12c,d) explain the observational data rather better. Moreover this DBM model, although simple, cannot be dismissed as an exercise in curve fitting. It is *not* a 'black-box' representation: as we have shown above, its parameters, as estimated or derived, are physically meaningful; and the physical deductions drawn from these parameters, as well as the model predictions, are all reasonable (albeit controversial) from a scientific standpoint.

This situation cannot arise because the more complex model, with its larger number of parameters, is unable to explain the data better: with so many parameters it would be straightforwrad to achieve a better explanation of the data. So it would seem to us that two major (but not mutually exclusive) possibilities exist. First, it could be because constraints that may have been applied to the values of the model's 'physically meaningful' parameters during the model building process are too severe and this limits

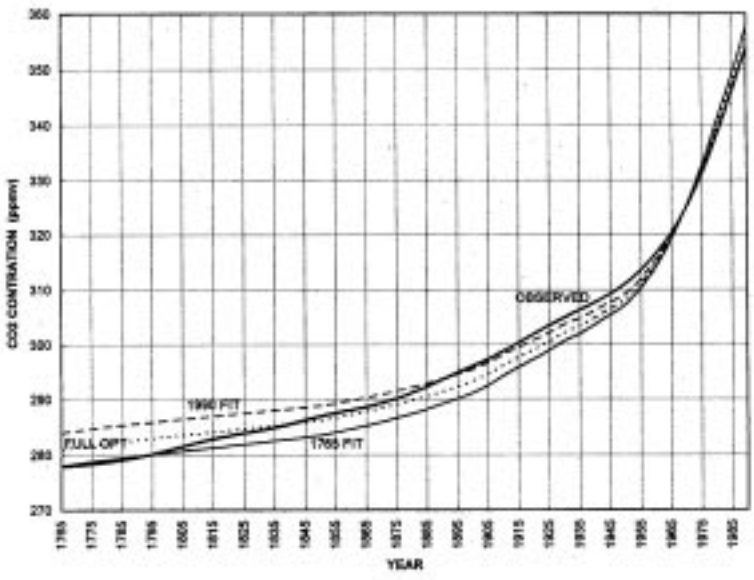

Figure 21.1: Optimized forward fits to observed concentration changes based on different fitting constraints. The bold solid curve gives the observations; the thin solid curve denotes modeled concentration fixed at the observed value in 1765 (27820ppmv), the long-dashed curve (C(1765) = 284 ppmv) denotes modeled concentration fixed to match the observed value in 1990; and the short-dashed curve (C(1765) = 281 ppmv) is fully optimized with no constraints.

Figure 11. (Reproduced from Wigley, 2000)

the further reduction of the simulation response errors. Second, it could be a result of the difficulties in model optimization caused by the obvious over-parameterization of the Wigley model and associated lack of identifiability. Often, for instance, some of the model parameters are fixed[16] at 'well known' values and only a subset of lesser known parameters are optimized against the data in an attempt to avoid these problems.

4.1.7 Relationship to the results of Jarvis and Young (2002)

Finally, it is important to comment on the relationship of the results presented here and those reported in Jarvis and Young (2002). In order to communicate with climate change scientists who are more familiar with nonlinear least squares optimization based on the response error, Jarvis and Young used this simpler optimization approach rather than the prediction error optimization used in the present report (see section 5.1.1). It is well known in time series analysis that if the model residuals (here $\hat{\xi}_t$) are serially correlated (coloured noise), then this response error approach can produce biased and statistically inefficient model parameter estimates, where these effects are dependent on the variance of the model residuals and level of their serial correlation. In the present case, the variance of residuals is very small but the serial correlation is quite high. The practical consequences of this situation are that the bias on the estimates is insignificant but the estimated uncertainty in the parameter estimates is too low. For instance, the response error optimization results in the case of the model (12a,b) are as follows (see

[16] An alternative Bayesian approach to this problem would not set parameters to fixed values but it would need to severely constrain the range of their estimated values by the specification of very tight prior distribution functions about the assumed initial estimates.

Jarvis and Young, 2002):

$$\hat{\alpha} = -0.0181(0.0007); \quad \hat{\beta} = -0.0100(0.0010); \quad \hat{b}_0 = 0.0402(0.0007);$$

$$c = 0.0065(0.0014); \quad \hat{\tau} = 5.0; \quad \sigma_\xi^2 = 0.0025; \quad \sigma^2 = 0.0006$$

$$R_T^2 = 0.9995; \quad R^2 = 0.9999$$

so that the parameter estimates are almost the same as those obtained by prediction error optimization in section 5.1.2, but the estimated level of uncertainty associated with three of these estimates is about half as large, so that they are too optimistic.

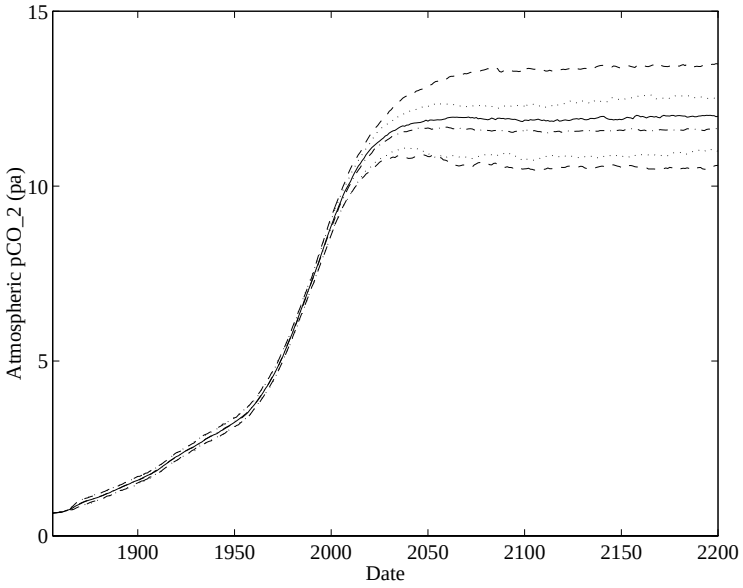

Figure 12. Comparison of the hypothetical long term Monte Carlo predictions of the nonlinear SDP optimized using prediction error (full line: percentile bounds shown dashed) and response error (dash-dot line: percentile bounds shown dotted) cost functions.

There are two main consequences of these lower estimation error variances. First, the confidence in the derived, physically meaningful parameters cited in Jarvis and Young is somewhat too high, although this does not affect at all their conclusions about the temperature dependent feedback effect, which are the same as those reported above in section 5.1.4 (i.e. only the confidence bounds on the estimates are changed to any significant degree). Second, as shown in figure 12, while there is not very much difference in the median of the predictive distribution, the confidence bounds are too narrow and engender more confidence in the prediction than is warranted. Again, however, the difference is not too large and it does not affect the main conclusions of the exercise very much at all.

5 Conclusions

Models of non-Gaussian and nonlinear processes do not necessarily require the assumption of non-Gaussian inputs. As we have seen in this Report, a fairly wide class of non-Gaussian and nonlinear time series can be represented by state dependent (SDP) parameter, nonlinear, stochastic models with Gaussian inputs. When it is possible (and the methods do seem quite widely applicable), this is clearly advantageous, since it allows for the use of well tried and robust algorithms that are computationally much less demanding than even the 'classical' non-Gaussian methods (see Durbin and Koopman, 1999, 2001). It is also clearly possible to develop state estimation and control system design methods based on SDP models. Research on such developments is continuing (e.g. Young *et al.*, 2002; Young and Jarvis, 2002) and has so far led to encouraging initial results.

In contrast to many other methods of nonlinear modelling, the methods of SDP estimation discussed in this Report involve the data-based identification of the nonlinear model form and structure, *prior* to the estimation of the parameters in the finally identified model. This helps to ensure that this final nonlinear model is efficiently parameterized (parsimonious) and it should avoid the over-parameterization that often accompanies 'black-box' nonlinear time series models, such as neural network, neuro-fuzzy and, to a lesser extent, NARMAX models . A practical example of this is given in Young (2001c).

We have also shown that the SDP approach is a primary tool in 'top-down' *Data-Based Mechanistic* (DBM) modelling, where its ability to obtain parametrically efficient and physically meaningful models from time series data is essential. This approach can be contrasted with the more conventional 'bottom-up' *hypothetico-deductive* method of modelling where the often overly complex and unidentifiable model structure is based on prior, physically-based (and possibly subjective) assumptions. The global climate example demonstrates how this novel top down approach can extract information from the globally averaged data in a manner which contrasts quite markedly to the 'bottom-up', reductionist approach used by most climate scientists (e.g. Enting and Lassey, 1993; Wigley, 1993). In this way, it addresses the important question of how the climate behaves at this global scale and whether the alternative, reductionist approach is entirely appropriate to explaining the dominant modes of dynamic behaviour at this global scale. Whilst not rejecting the reductionist philosophy, nor the very large models that are often developed using this philosophy, we feel that simpler, data-based models should be playing a more important role in research on global climate change (see Young *et al.*, 1996; Shackley *et al.*, 1998).

Finally, it should be noted that most of the time series analysis and modelling methods used or mentioned in this Report are available in the CAPTAIN Toolbox that has been developed at Lancaster over the last 15 years for use in the Matlab/Simulink^{TM}software environment. The latest version of this Toolbox is currently in the final stages of β-testing and will be generally available towards the end of 2002. Further information on the Toolbox can be obtained via: http://www.es.lancs.ac.uk/cres/captain/.

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Appendix: Derivation of an Aggregated, Perturbational, Single Mixing Unit Model for Anthropogenic Carbon.

The apparent suitability of the first order dynamic model (11a,b) and its nonlinear counterparts (12a,b) and (12c,d), for describing the relationship between anthropogenic carbon emissions and variations of the perturbations in pCO_2 points to a single mixing process that aggregates the 'active' contributions of the atmospheric, terrestrial and oceanic carbon reservoirs in a global scale mixing process. A mass balance for this 'well mixed' mass of carbon may be given by,

$$\frac{vdC(t)}{dt} = U(t-\tau) - k\left\{T(t)\right\}C(t) \tag{A1}$$

where $C(t)$ is the effective well-mixed concentration of carbon; $U(t-\tau)$ is the net input of carbon into this system delayed τ years; $k\{T(t)\}$ is the first order loss constant of the system (which has earlier been identified as being temperature dependent); and v is the effective volume actively involved in the mixing process (see Young and Lees 1992), such that $vC(t)$ is the mass of carbon within this well mixed compartment.

As a result of the mixing process, the measured variations in atmospheric pCO_2 should be good surrogates for variations in $C(t)$. Therefore, assuming that $C(t) = w\{pCO_2(t)\}$ where w is the proportionality constant, and $pCO_2(t) = 28 + y(t)$, as before, then on substitution (A1) becomes:

$$\frac{wvdy(t)}{dt} = U(t-\tau) - wk\left\{T(t)\right\}y(t) - 28\left\{T(t)\right\} \tag{A2}$$

Now the input of carbon into the system is comprised of two fluxes. Firstly, there is the net natural input, uN, which not only comprises additions of carbon to the system from, for example, upwelling of carbon rich deep oceanic waters, but also losses of carbon from the system that arise from CO_2 independent processes (i.e. processes not affected by CO_2 fertilisation). This term is assumed to be unaffected by any anthropogenic disturbance, reflecting the pre–industrial base level inputs and outputs of carbon.

Secondly, there is the anthropogenic input from fossil fuel burning, cement manufacturing and land use change, $u(t)$. Considering these two inputs separately within (A2) gives,

$$\frac{wvdy(t)}{dt} = u(t-\tau) - wk\left\{T(t)\right\}y(t) + \left[u_N - 28\left\{T(t)\right\}\right] \tag{A3}$$

The form of (A3) is now comparable to that of (11a,b) and its nonlinear counterparts (12a,b) and (12c,d) so that,

$$a_1 = \frac{k\left\{T(t)\right\}}{v}; \quad b_0 = \frac{1}{wv}; \quad c = \frac{u_N - 28\left\{T(t)\right\}}{wv}$$

From this equivalence we note that, as discussed, the offset term c arises from potential inaccuracies in specifying either the pre–industrial pCO_2 level required to exactly balance the natural net steady state inputs of carbon to the system, uN, or the base level of $u(t)$ that would otherwise added to uN. Further analysis has revealed that the predominant source of error contributing to small but significant values of c appears to arise from the latter source, which is not surprising given the uncertainties associated with the emissions inventory. The fact that the SDP analysis was unable to detect any temperature dependency in the c parameter, as inferred in (A3), is consistent with the fact that c is so small, hence having only a minor effect on the overall model behaviour.

One notable difference between (A3) and, say, (11a,b) is the absence of any pure time delay between the input, and its effect on the output. The DBM modelling procedure objectively identified this as being around five years. As a result, the effects of any decay in the input over this time should really be accommodated into the model (A3). This requires making some assumption about the nature of any such decay process. Previously, for example, Young and Beck (1974), applying a similar DBM methodology to mixing within river systems, assumed that the same decay process that is operative within the mixing process is also operative over the pure time delay. Then, simply integrating these losses over the pure time delay gives $u^*(t-\tau) = e^{-k\tau}u(t-\tau)$, where $u^*(t-\tau)$ is the decayed input. However, since the inclusion of the pure time delay here may act to accommodate poorly defined dynamic behaviour rather than pure advection, as discussed in section 4.1.4, such assumptions may not be valid. For simplicity, therefore, we have assumed that no losses of CO_2 occur during this five year interval[17].

References

Akaike, H. (1974) A new look at statistical model identification, *I.E.E.E. Trans. Auto. Control*, **ACl9**, 716-722.

Beck, M. B. (1983) Uncertainty, system identification and the prediction of water quality. Report 2 in *Uncertainty and Forecasting of Water Quality*, M.B. Beck and G. Van Straten (Eds.), Springer-Verlag: Berlin, 3-68.

Beck, M. B. and Young, P. C. (1975) A dynamic model for BOD-DO relationships in a non-tidal stream, *Water Research*, **9**, 769-776.

Beven, K. J. (2000a) Uniqueness of place and process representations in hydrological modelling, *Hydrology and Earth System Sciences*, **4**, 203-213.

Beven, K. J. (2000b) *Rainfall-Runoff Modelling: the Primer*, J. Wiley: Chichester.

Billings, S.A. and Voon, W.S.F. (1986) Correlation based model validity tests for nonlinear models, *International Journal of Control*, **44**, 235-244.

Brown, R.L., Durbin, J. and Evans, J.M. (1975) Techniques for testing the constancy of regression relationships over time, *Jnl. Royal Stat. Soc., Series B*, **37**, 141-192.

Bryson, A.E. and Ho, Y.C. (1969) *Applied Optimal Control*, Blaisdel: Waltham Mass.

Cox, (2001) ?????????

Dai, A. and Fung, I.Y. (1993) Can climate variability contribute to the missing CO2 sink? *Global Biogeochem. Cycles*, **7**, 599-609.

Durbin, J. (1954) Errors in variables, *Review Int. Stat. Inst.*, **22**, 23-32.

Durbin, J. and Koopman, S.J. (2000) Time series analysis of non-Gaussian observations based on state space models from both classical and Bayesian perspectives, *Jnl. Royal Stat. Soc., Series B*, **62**, 3-56.

Durbin, J. and Koopman, S.J. (2001) *Time Series Analysis by State Space Methods*, Oxford University Press: Oxford.

Enting, I. G. and Lassey, K. R. (1993) *Projections of Future Atmospheric CO_2*, Technical Paper No. 27, Division of Atmospheric Research, Commonwealth Scientific and Industrial Research organisation, Melbourne, CSIRO: Melbourne.

Farquhar, G. D, Fasham, M. J. R., Goulden, M. L., Heimann, M., Jaramillo, V. J., Khesgi, H. S., Le Quere, C., Scholes R. J. and Wallace D. W. R. (2000) The carbon cycle and atmospheric carbon dioxide, in: *Climate Change 2001: The Scientific Basis*, contribution of working group I to the third assessment Report of the *Intergovernmental Panel on Climate Change*, J. T. Houghton *et al.* (Eds.), Cambridge University Press: Cambridge (U.K.) and New York (U.S.A).

[17] Again, this is a matter of further research for both authors, especially since it is unclear whether the nonlinear temperature effects of any decay process also needs to be considered here.

Gordon, N., Marrs, A. and Salmond, D. (2000) Sequential analysis of nonlinear dynamic systems using particles and mixtures, in *Nonlinear and Nonstationary Signal Processing*, W.J. Fitzgerald, A. Walden, R. Smith and P.C. Young (Eds.), Cambridge University Press: Cambridge, 42-73.

Granger, C. W. J. and Teräsvirta, T (1993) *Modelling Nonlinear Economic Relationships*, Oxford University Press: Oxford.

Harvey, A.C. (1984) A unified view of statistical forecasting procedures (with comments), *Jnl. of Forecasting*, **3**, 245-283.

Harvey, A.C. (1989) *Forecasting Structural Time Series Models and the Kalman Filter*, Cambridge University Press: Cambridge.

Harvey L. D. D. (2000) *Global Warming: The Hard Science*, Prentice Hall: New Jersey.

Isermann, R. (1989) *Digital Control Systems: Vols. 1 and 2*, Springer-Verlag: Berlin.

Jarvis, A. J, Young, P. C, Taylor, C. J and Davies, W. J, (1999) An analysis of the dynamic response of stomatal conductance to a reduction in humidity over leaves of *Cedrella odorata*, *Plant Cell and Environment*, **22**, 913-924.

Jarvis, A. J, Young, P. C. (2002) Identification of temperature dependency in the relationship between global anthropogenic CO_2 emissions and atmospheric CO_2, 1856-2000, letter submitted to *Nature*.

Joos, F., Plattner G. K., Stocker,T.F., Marchal, O. and Schmittner, A. (1999) Global warming and carbon cycle feedbacks on future atmospheric CO_2, *Science*, **284**, 464-467.

Jothityangkoon, C., Sivapalan, M. and Farmer, D. L. (2001) Process controls of water balance variability in a large semi-arid catchment: downward approach to hydrological model development, *Journal of Hydrology*, **254**, 174-198.

Kalman, R.E. (1960) A new approach to linear filtering and prediction problems, *ASME Transactions Journal Basic Engineering*, **82D**, 35-45.

Kalman, R. E. and Bucy, R. S. (1961) New results in Linear filtering and prediction theory, *ASME Trans., Journal Basic Eng.* **83-D**, 95-108.

Kitagawa, G. (1996) Monte Carlo filter and smoother for non-Gaussian nonlinear state space models, *Journal of Computational and Graphical Statistics*, **5**, 1-25.

Lawton, J. (2001) Understanding and prediction in ecology. *Institute of Environmental and Natural Sciences, Lancaster University*, Distinguished Scientist Lecture.

Lee, R. C. K. (1964) *Optimal Identification, Estimation and Control*, MIT Press: Mass.

Lees, M. J. (2000) Data-based mechanistic modelling and forecasting of hydrological systems, *Journal of Hydroinformatics*, **2**, 15-34.

Leontaritis, I. J. and Billings, S. A. (1985) Input-output parametric models for nonlinear systems. Part I: deterministic nonlinear systems, *International Journal of Control*, **41**, 303-328.

Ljung, L. and Söderstrom, T. (1983) *Theory and Practice of Recursive Identification*, M.I.T. Press: Cambridge, Mass.

Mayne, D. Q. (1963) Optimal nonstationary estimation of parameters of a linear system with Gaussian inputs, *Journal of Electronics and Control*, **14**, 101-112.

Norton, J. P. (1976) Identification by optimal smoothing using integrated random walks, *Proceedings Institute Electrical Engineers*, **123**, 451-452.

Popper, K. (1959) *The Logic of Scientific Discovery*, London: Hutchinson.

Price, L. E., Young, P. C., Berckmans, D. Janssens, K. and Taylor, J. (1999). Data-based mechanistic modelling and control of mass and energy transfer in agricultural buildings, *Annual Reviews in Control*, **23**, 71-82.

Priestley, M. B. (1988) *Nonlinear and Nonstationary Time Series Analysis*, Academic Press: London.

Rauch, H. E., Tung, F. and Streibel, C. T. (1965) Maximum likelihood estimates of linear dynamic systems, American Institute of Aeronautics and Astronautics Journal. **3**, 1445-1450.

Rydberg, T. H. and Shephard, N. (2000) A modelling framework for the prices and times of trade made on the New York Stock Exchange, in *Nonlinear and Nonstationary Signal Processing*, W.J. Fitzgerald, A. Walden, R. Smith and P.C. Young (Eds.), Cambridge University Press: Cambridge, 217-246.

Saltelli, A., Chan, K and Scott, E. M. (2000) *Sensitivity Analysis*, J. Wiley: Chichester.

Schimel, D., Alves, D., Enting, I., Heimann, M., Joos, F., Raynaud, D. and Wigley, T. M. L. (1996) CO_2 and the carbon cycle, in *Climate Change 1995: The Science of Climate Change, Contribution of Working Group I to the Second Assessment Report of the Intergovernmental Panel on Climate Change*, J. T. Houghton *et al.*, (Eds.), Cambridge University Press: Cambridge, 65-86.

Schweppe, F. (1965) Evaluation of likelihood function for Gaussian signals, *IEEE Transactions on Information Theory*, **11**, 61-70.

Shackley, S., Young, P. C., Parkinson, S., and Wynne, B. (1998). Uncertainty, complexity and concepts of good science in climate change modelling: Are GCMs the best tools? *Climate Change*, **38**, 159-205.

Shephard, N. (1995) Statistical aspects of ARCH and stochastic volatility, in D.R. Cox, O.E. Barndorff-Nielsen and D. V. Hinkley (Eds.), *Time Series models in Econometrics, Finance and Other Fields*, Chapman and hall: London, 1-63.

Silvert, W. (1993) Top-down modelling in ecology, in *Concise Encyclopedia of Environmental Systems*, P. C. Young (Ed.), Pergamon Press: Oxford, 605.

Sinha, N. K. and Rao, G. P. (Eds.) (1991) *Identification of Continuous-Time Systems*, Kluwer Academic Publishers: Dordrecht.

West, M. and Harrison, J. (1989) *Bayesian Forecasting and Dynamic Models*, Springer-Verlag: Berlin.

Wigley, T. (1993) Balancing the carbon budget: implications for projections of future carbon dioxide concentration changes, *Tellus*, **45B**, 409-425.

Wigley, T. (2000) Stabilization of CO_2 concentration levels, in T. Wigley and D, Schimel (Eds.), *The Carbon Cycle*, Cambridge University Press: Cambridge, 259-276.

Young, P.C. (1969) Applying parameter estimation to dynamic systems: Part l, Theory, Control Engineering, **16**, 10, 119-125; 'Part lI Applications', **16**, 11, 118-124.

Young, P.C. (1970) An instrumental variable method for real-time identification of a noisy process, *Automatica*, **6**, 271-287.

Young, P.C. (1978) A general theory of modeling for badly defined dynamic systems, in *Modeling, Identification and Control in Environmental Systems*, G.C. Vansteenkiste (Ed.), North Holland: Amsterdam, 103-135.

Young, P. C., 1981, Parameter estimation for continuous-time models - a survey, *Automatica*, **17**, 23-39.

Young, P.C. (1983) The validity and credibility of models for badly defined systems, Report 2 in *Uncertainty and Forecasting of Water Quality*, M.B. Beck and G. Van Straten (Eds.), Springer-Verlag: Berlin, 69-100.

Young, P.C. (1984) *Recursive Estimation and Time-Series Analysis*, Springer-Verlag: Berlin.

Young, P.C. (1988) Recursive extrapolation, interpolation and smoothing of non-stationary time-series, in H.F.Chen (Ed.) *Identification and System Parameter Estimation 1988*, Pergamon Press: Oxford, 33-44

Young, P. C. (1989) Recursive estimation, forecasting and adaptive control, Report in C.T. Leondes (Ed.) *Control and Dynamic Systems: Advances in Theory and Applications*, **30**, Academic Press: San Diego, 119-166.

Young, P.C. (1993) Time variable and state dependent modelling of nonstationary and nonlinear time series, in *Developments in Time Series Analysis*, T. Subba Rao (Ed.), Chapman and Hall: London, 374-413.

Young, P.C. (1998a) Data-based mechanistic modelling of environmental, ecological, economic and engineering systems, *Environmental Modelling and Software*, **13**, 105-122.

Young, P.C. (1998b) 'Data-based mechanistic modelling of engineering systems', *Journal of Vibration and Control*, **4**, 5-28.

Young, P.C. (1999a) Data-based mechanistic modelling, generalised sensitivity and dominant mode analysis, *Computer Physics Communications*, **117**, 113-129.

Young, P.C. (1999b) Nonstationary time series analysis and forecasting, *Progress in Environmental Science*, **1**, 3-48.

Young, P.C. (2000) Stochastic, dynamic modelling and signal processing: time variable and state dependent parameter estimation, in *Nonlinear and Nonstationary Signal Processing*, W.J. Fitzgerald, A. Walden, R. Smith and P.C. Young (Eds.), Cambridge University Press: Cambridge, 74-114.

Young, P.C. (2001a) The identification and estimation of nonlinear stochastic systems, in *Nonlinear Dynamics and Statistics*, A.I. Mees (Ed.), Birkhauser: Boston, 127-166.

Young, P. C. (2001b) Data-based mechanistic modelling and validation of rainfall-flow processes, in *Model Validation: Perspectives in Hydrological Science*, M. G. Anderson and P. D. Bates (Eds.), J. Wiley: Chichester, 117-161.

Young, P.C. (2001c) Comment on 'A quasi-ARMAX approach to the modelling of nonlinear systems' by J. Hu *et al*, *International Journal of Control*, **74**, 1767-1771.

Young, P.C. (2002a) Advances in real-time flood forecasting, *Philosophical Transactions of the Royal Society: Mathematical, Physical and Engineering Sciences*, **360**, 1433-1450.

Young, P.C. (2002b) Comments on the estimation of continuous-time transfer functions, *Int. Journal of Control*, **75**, 693-697.

Young, P.C. and Beck M. B. (1974) The modelling and control of water quality in a river system, *Automatica*, **16**, 281-294.

Young, P.C. and Beven, K.J. (1994) Data-based mechanistic modelling and the rainfall-flow nonlinearity, *Environmetrics*, **5**, 335-363.

Young, P. C. and A. J. Jakeman (1980) Refined instrumental variable methods of recursive time-series analysis: part III, extensions, *International Journal of Control*, **31**, 741-764.

Young, P. C. and Jarvis, A. J. (2002) *Data-Based Mechanistic Modelling, the Global Carbon Cycle and Global Warming*, CRES Report No. TR/177, Department of Environmental Science, Lancaster University.

Young P.C. and Lees, M.J. (1992) The active mixing volume: a new concept in modelling environmental systems, in *Statistics and the Environment*, Barnett and R. Turkman (Eds.), J. Wiley: Chichester, 2-43.

Young, P. C. and D. J. Pedregal (1999). Macro-economic relativity: government spending, private investment and unemployment in the USA 1948-1998. *Jnl. Structural Change and Economic Dynamics*, **10**, 359-380.

Young, P. C., Foster, M, and Lees, M. J. (1993) A direct approach to the identification and estimation of continuous-time systems from discrete data based on fixed interval smoothing, *Proc. 12th IFAC World Congress, Vol. 10*, G. Goodwin (Ed.), Pergamon Press: Oxford, 27-30.

Young, P. C., Parkinson, S. and Lees, M. J. (1996). Simplicity out of complexity: Occams razor revisited, *Journal of Applied Statistics*, **23**, 165-210.

Young, P.C., McKenna, P. and Bruun, J. (2001) Identification of nonlinear stochastic systems by state dependent parameter estimation, *International Journal of Control*, **74**, 1837-1857.

Young, P. C., McCabe, A. P. and Chotai, A. (2002) State dependent parameter nonlinear systems: identification, estimation and control. *Proceedings IFAC World Congress, Barcelona, July 2002*, Pergamon: Oxford, in press.