Jul 1st, 12:00 AM

Data-Based Mechanistic and Top-Down Modelling

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Abstract: The paper discusses the problems associated with environmental modelling and the need to develop simple, 'top-down', stochastic models that match the information content of the data. It introduces the concept of Data-Based Mechanistic (DBM) modelling and contrasts its inductive approach with the hypothetico-deductive approaches that dominate most environmental modelling research at the present time. The major methodological procedures utilized in DBM modelling are outlined and two practical examples illustrate how it has been applied in a hydrological and water quality context. The use of this same methodology as a basis for the evaluation and simplification of large deterministic simulation models is also discussed briefly.

Keywords: Top-down; Data-Based Mechanistic (DBM); inductive; stochastic; transfer function.

1 INTRODUCTION

The environment is 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 environmental science research. 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. Such deterministic reductionism appears to be guided by a belief that physical 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 deterministic reductionism still dominates environmental 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 environment 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. [12] 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.

But such scepticism is not new. It has its parallels in the environmental (e.g. [25][26][2]) and ecosystems (e.g. see prior references cited in [19]) literature of the 1970s and early 1980s . Over this period, the present author's contributions were set within the context of 'badly defined' environmental systems. These early papers ([25][26]) then went on to present initial thoughts on an objective, statistical approach to modelling poorly defined systems that tried to avoid the dangers of placing too much confidence in prior perceptions about the nature of the model. They also adumbrate very similar anti-reductionist arguments that have appeared recently in the hydrological literature and express some of these same views within a hydrological context ([10][5]). In the subsequent period since the earlier papers were published, however, the author has sought to develop this statistical approach

*The author is grateful to the U.K. Engineering and Physical Sciences (EPSRC) , Biotechnology and Biological Sciences (BBSRC), and Natural Environment Research (NERC) Councils, all of whom supported various aspects of the research discussed in this paper.

within a more rigorous systems setting that he has termed *Data-Based Mechanistic* (DBM) modelling. Prior to discussing the DBM approach, the present paper will first discuss briefly the philosophical basis for modelling natural systems and outline the major concepts of statistical modelling that are important in any modelling process. Subsequently, two examples will be presented that illustrate the utility of DBM modelling in practical environmental science and systems analysis.

2 PHILOSOPHIES OF MODELLING

Within the history of science, two main approaches to mathematical modelling can be discerned; approaches which, not surprisingly, can be related to the more general deductive and inductive approaches to scientific inference that have been identified by philosophers of science from Francis Bacon to Karl Popper and Thomas Kuhn.

- The *hypothetico-deductive* approach. Here, the *a priori* conceptual model structure is effectively a theory of behaviour based on the perception of the scientist/modeller and is strongly conditioned by assumptions that derive from current scientific paradigms.

- The *inductive* approach. Here, theoretical preconceptions are avoided as much as possible in the initial stages of the analysis. In particular, the model structure is not prespecified by the modeller but, wherever possible, it is inferred directly from the observational data in relation to a more general class of models. Only then is the model interpreted in a physically meaningful manner, most often (but not always) within the context of the current scientific paradigms.

In common with much of the scientific investigation that occurred *prior* to the 20^{th} Century, The DBM approach to modelling is of this latter inductive type and it forms the basis for the research described in the rest of this paper. Previous publications ([30] and the prior references therein) map the evolution of this DBM philosophy and its methodological underpinning in considerable detail. As these references demonstrate, DBM models can be of various kinds depending upon the nature of the system under study. In the context of the present paper, however, they take the form of linear and nonlinear, stochastic *Transfer Function* (TF) models.

3 STATISTICAL IDENTIFICATION, ESTIMATION AND VALIDATION

Inductive modelling is concerned with the analysis of data from planned experiments or monitoring exercises. As a result, the methodology required for inductive modelling is strongly statistical in its motivation. This statistical approach to modelling assumes that the model is stochastic: in other words, no matter how good the model and how low the noise on the observational data happens to be, a certain level of uncertainty will remain after modelling has been completed. Consequently, full stochastic modelling requires that this uncertainty, which is associated with both the model parameters and the stochastic inputs, should be quantified in some manner as an inherent part of the modelling analysis.

In the statistical time series literature, stochastic modelling is normally considered in two main stages: *identification* of an appropriate, identifiable model structure; and *estimation* (optimization, calibration) of the parameters that characterize this structure, using some form of estimation or optimization. Normally, a further stage of *validation* (or *conditional validation*: see later) is defined, in which the ability of the model to explain the observed data is evaluated on data sets different to those used in the model identification and estimation stages.

In the DBM approach to modelling, the identification stage is considered as a most important and essential prelude to the later stages of model building. It usually involves the identification of the most appropriate model order, as defined in dynamic system terms. However, the model structure itself can be the subject of the analysis if this is also considered to be ill-defined. In the inductive DBM approach, for instance, the nature of linearity and nonlinearity in the model is not assumed *a priori* (unless there are good reasons for such assumptions based on previous data-based modelling studies). Rather it is identified from the data using non-parametric and parametric statistical estimation methods based on a suitable generic model class. Once a suitable model structure has been defined within this class, there are a variety of statistical methods for identifying model order, some of which are mentioned later. In general, however, they exploit some order identification statistics, such as the correlation-based statistics popularized by Box and Jenkins [7], the well known Akaike Information Criterion (AIC: [1]), and the more heuristic YIC statistic (see e.g. [35][37][42]) which provides an alternative to the AIC in the case of transfer functions (where the AIC

tends to identify over-parameterized models).

Once the model structure and order have been identified, the parameters that characterize this structure need to be estimated in some manner. There are many automatic methods of estimation or optimization available in this age of the digital computer. These range from the simplest, deterministic procedures, usually based on the minimization of least squares cost functions, to more complex numerical optimization methods based on statistical concepts, such as Maximum Likelihood (ML). In general, the latter are more restricted, because of their underlying statistical assumptions, but they provide a more thoughtful and reliable approach to statistical inference. It is an approach which, when used correctly, includes the associated statistical diagnostic tests that are considered so important in statistical inference. In the present DBM modelling context, the estimation methods are based on optimal, linear *Instrumental Variable* (IV) methods for transfer function models (e.g. [27] and the prior references therein) and nonlinear modifications of these methods [33][34].

Validation is a complex process and even its definition is controversial. Some academics (e.g. [13], within a ground-water context; [15], in relation to the whole of the earth sciences) question even the possibility of validating models. Nevertheless, one specific, quantitative aspect of validation is widely accepted; namely 'predictive validation' (often referred to as just 'validation'), in which the predictive potential of the model is evaluated on data other than that used in the identification and estimation stages of the analysis. While the authors of [15] dismiss this approach, which they term 'calibration and verification', their criticisms are rather weak and appear to be based on a perception that "models almost invariably need additional tuning during the verification stage". While some modellers may be unable to resist the temptation to carry out such additional tuning, so negating the objectivity of the validation exercise, it is a rather odd reason for calling the whole methodology into question.

On the contrary, provided it is practically feasible, there seems no doubt that conditional validation, in the predictive sense used here, is an essential prerequisite for any definition of model efficacy, if not validity in a wider sense. In the rainfall-flow context considered later, for example, it implies that, on the basis of the new measurements of the model input (rainfall) from the validation data set, the model produces flow predictions that are acceptable within the predicted uncertainty bounds.

4 DATA-BASED MECHANISTIC (DBM) MODELLING

The term 'data-based mechanistic modelling' was first used in [38] but the basic concepts of this approach to modelling dynamic systems have developed over many years. It was first applied within a hydrological context in the early 1970s, with application to modelling water quality in rivers ([3]) and rainfall-flow processes ([22][24]). Indeed, the DBM water quality and rainfall-flow models discussed later in the present paper are a direct development of these early models.

In DBM modelling, the most parametrically efficient (parsimonious) model structure is first inferred statistically from the available time series data in an *inductive* manner, based on a generic class of black-box models (normally linear or nonlinear differential equations or their difference equation equivalents). *After this initial black-box modelling stage is complete*, the model is interpreted in a physically meaningful, mechanistic manner based on the nature of the system under study and the physical, chemical, biological or socio-economic laws that are most likely to control its behaviour. By delaying the mechanistic interpretation of the model in this manner, the DBM modeller avoids the temptation to attach too much importance to prior, subjective judgement when formulating the model equations. This inductive approach can be contrasted with the alternative *hypothetico-deductive* 'Grey-Box' modelling, approach. Here, the physically meaningful but simple model structure is based on prior, physically-based and possibly subjective assumptions; and the parameters that characterize this simplified structure are estimated from data only *after* this structure has been specified by the modeller.

Other previous publications, as cited in [30], 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:

1. 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. Appropriate model structures are identified by a process of objective statistical inference applied directly to the time-series data and based initially on a given generic class of linear Transfer Function (TF) models whose parameters are allowed to vary over time, if this seems necessary to satisfactorily explain the data.

3. If the model is identified as predominantly linear, linear with slowly varying parameters or piece-wise linear, then the 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 paper are based on optimal, recursive Instrumental Variable (IV) estimation algorithms (see [27]) that provide a robust approach to model identification and estimation and have been well tested in practical applications over many years. Here the important identification stage means the application of objective statistical methods to determine the dynamic model order and structure. Full details of these time series methods are provided in the above references and they are outlined more briefly in [35], [37] and [42].

4. If *significant* parameter variation is detected over the observation interval, then the model parameters are estimated by the application of an approach to time dependent parameter estimation based on the application of recursive Fixed Interval Smoothing (FIS) algorithms (e.g. [8][14][27]). Such parameter variation will tend to reflect statistically significant nonstationary and nonlinear aspects of the observed system behaviour. In effect, the FIS algorithm provides a method of non-parametric estimation, with the *Time Variable Parameter* (TVP) estimates (e.g. [32]) defining the non-parametric relationship, which can often be interpreted in *State-Dependent Parameter* (SDP) terms (see later).

5. If nonlinear phenomena have been detected and identified in stage 4, the non-parametric state dependent relationships are normally parameterized in a finite form and the resulting nonlinear model is estimated using some form of numerical optimization, such as nonlinear least squares or Maximum Likelihood (ML) optimization.

6. 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*. This is a most important aspect of DBM modelling and differentiates it from more classical 'black-box' and 'grey-box' modelling methodologies, such as those associated with standard TF, nonlinear autoregressive-moving average-exogenous variables (NARMAX), neural network and neuro-fuzzy models (see discussion in [36]).

7. Finally, the estimated model is tested in various ways to ensure that it is conditionally valid (see above discussion and [34][35]). 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. [6]). It also involves validation exercises, as well as exercises in stochastic uncertainty and sensitivity analysis.

Of course, while step 6 should ensure that the model equations have an acceptable physical interpretation, it does not guarantee that this interpretation will necessarily conform exactly with the current scientific paradigms. Indeed, one of the most exciting, albeit controversial, aspects of DBM models is that they can tend to question such paradigms. For example, DBM methods have been applied very successfully to the characterization of imperfect mixing in fluid flow processes and, in the case of pollutant transport in rivers, have led to the development of the *Aggregated Dead Zone* (ADZ) model ([4][20][31]). Despite its initially unusual physical interpretation, the acceptance of this ADZ model (e.g. [9] and the prior references therein) and its formulation in terms of physically meaningful parameters, seriously questions certain aspects of the ubiquitous Advection-Dispersion Model (ADE) which preceded it as the most credible theory of pollutant transport in stream channels (see the comparative discussion in [40]).

One aspect of the above DBM approach which differentiates it from alternative deterministic 'top-down' approaches is its inherently stochastic na-

ture. 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. The uncertainty analysis is particularly useful because it is able to evaluate how the covariance properties of the parameter estimates affect the probability distributions of physically meaningful, derived parameters, such as residence times and partition percentages in parallel hydrological pathways (see e.g. [28] [31] and the examples below).

Finally, it should be emphasized that the DBM approach to modelling is widely applicable: it has been applied successfully to the characterization of numerous environmental and other systems (see e.g. [30] and the prior references therein), including the macro-economy of the USA [39].

5 PRACTICAL EXAMPLES

Two practical examples will be considered here, both concerned with hydrological systems. The first will show how even purely linear DBM modelling can provide a powerful approach to analyzing experimental data. However, many environmental systems are nonlinear and so the second example will show how *State Dependent Parameter* (SDP) modelling procedures can be exploited to handle such nonlinearity.

5.1 A Linear Example: Modelling Solute Transport

The first model to be considered seriously in DBM terms was the ADZ model for the transport and dispersion of solutes in river systems, as mentioned earlier. This model has also led to related models that describe the imperfect mixing processes that characterize mass and energy flow processes in the wider environment (see e.g. [17][38])

This example is concerned with the DBM/ADZ modelling of input-output data obtained from a 'gulp' (impulsive input) bromide tracer experiment carried out in a Florida wetland area receiving treated domestic wastewater for further nutrient removal. The experiment was part of a study carried out by Chris Martinez and Dr. William R. Wise of the Environmental Engineering Sciences Department, University of Florida for the City of Orlando. The study objective was to determine residence times for each wetland cell in the system and to assess whether the same degree of treatment could be maintained should the wastewater loading be raised from 16 to 20 million gallons per day. The bromide tracer was injected 765 metres upstream of a weir, at which samples were taken with a sampling interval Δt of 2 hours.

The first step in DBM modelling is to identify a suitable model from a generic model class that is both capable of explaining the data in a parametrically efficient manner and producing a model that can be interpreted in physical terms. Based on the previous research described in the above references, a reasonable model class is the linear TF model in continuous or discrete time form. As we shall see, such TF models are not only able to explain the tracer data well, they can also be interpreted in multi-reach ADZ model terms that have physical meaning. Here, we will consider the discrete-time TF model and utilize the SRIV algorithm (a simplified version of the optimal IV algorithm mentioned earlier) to identify the model order and estimate the parameters[2].

The impulsive input is not persistently exciting but the SRIV algorithm has no difficulty identifying and estimating a low order model. The best identified TF, based on the YIC criterion, is either 3^{rd} or 4^{th} order but subsequent analysis, described below, suggests that the latter is superior from a physical standpoint. The estimated [4, 2, 22] (4^{th} order denominator, 2^{nd} order numerator and a 22 sampling interval pure time delay) TF model takes the form:

$$y_t = \frac{\hat{B}(z^{-1})}{\hat{A}(z^{-1})} u_{t-22} + \xi_t \qquad (1)$$

where,

$$\hat{A}(z^{-1}) = 1 - 3.67z^{-1} + 5.06z^{-2} - 3.11z^{-3} + 0.72z^{-4}$$

$$\hat{B}(z^{-1}) = 0.00103 - 0.00101z^{-1}$$

Here the 'hat' denotes the estimated value; z^{-i} is the backward shift operator (i.e. $z^{-i}y_t = y_{t-i}$); y_t is the observed tracer concentration at the weir and u_t is the impulsive input of tracer (186.33 mg/l), both measured at the t^{th} sampling instant. Note that the large 'advective' time delay of 22 sampling intervals (44 hrs.) is the time taken for the solute to first reach the weir. The noise ξ_t, which represents the quantification of all stochastic influences, including unmeasured inputs and measurement noise,

[2] Continuous time TF estimation using the continuous-time SRIV algorithm yields very similar results but the discrete-time analysis is more convenient in this paper.

is small and the model explains the data very well with a *Coefficient of Determination* (or *Nash Efficiency* in the hydrological literature) based on the simulation or 'response error' of $R_T^2 = 0.997$ (i.e. 99.7% of the output variance is explained by the model).

Unfortunately, despite its ability to describe the data very well, the model (1) is not immediately acceptable from a DBM standpoint, primarily because the eigenvalues are $\{0.988, 0.964, 0.860 \pm 0.132j\}$ and the pair of complex roots is difficult to justify in ADZ modelling terms. In particular, the elemental, single reach, ADZ model [4][20][31] is a first order, mass conservation, differential equation and so, other than in exceptional circumstances, multiple reach ADZ models must be characterized by real eigenvalues when considered in TF terms.

In the present circumstances, the most obvious approach is to re-estimate the model in a form where the eigenvalues are constrained to be real. This was carried out by means of constrained nonlinear least squares optimization using the *leastsq* optimization procedure in Matlab™. To ensure that the most parametrically efficient model was obtained, both [3, 2, 22] and [4, 2, 22] models were considered in this analysis but the latter yielded much the best constrained model, which has the following form:

$$y_t = \frac{\hat{B}(z^{-1})}{\hat{A}(z^{-1})} u_{t-22} + \xi_t \qquad (2)$$

where,

$$\hat{A}(z^{-1}) = (1 - 0.980z^{-1})(1 - 0.855z^{-1})^3$$

$$\hat{B}(z^{-1}) = 0.00127 - 0.00121z^{-1}$$

This model is well defined statistically and it explains 99.7% of the output data variance ($R_T^2 = 0.997$), the same as the unconstrained model (1). Figure 1 compares the model output (full line) with the measured tracer output y_t (circular points).

Unlike the TF model (1), the model (2) not only has four real eigenvalues, as required, but three of these are repeated, so defining three identical ADZ reaches. These eigenvalues define ADZ residence times (time constants) of 99 hours and 12.8 hours (x3), giving a total estimated residence time for the wetland cell of 137.4 hours (99+3x12.8). One particular physically meaningful decomposition and interpretation of the model defined in this manner is obtained by partial fraction expansion of the TF in (2). This consists of two parallel pathways, each consisting of three ADZ reaches, as shown in the top block diagram of Figure 2.

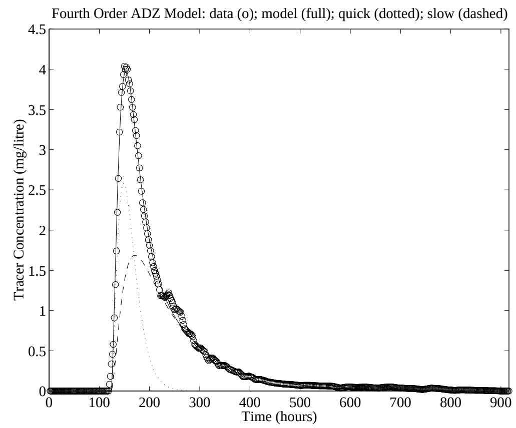

Figure 1: Comparison of the DBM model output (full line) and tracer experiment data (circular points). Also shown are the inferred slow flow (dashed line) and quick flow (dotted line) components.

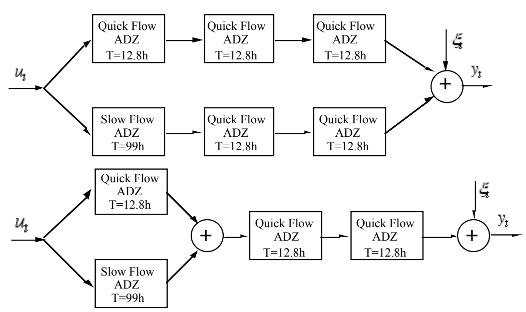

Figure 2: Block diagram of transfer function decompositions that can be interpreted in physical terms: fully parallel decomposition (upper plot); equivalent parallel-serial decomposition (lower plot).

The 'quick-flow' pathway has three identical ADZ reaches connected in series, each with a residence time of 12.8 hours; while the 'slow-flow' pathway is similar but with one of the reaches replaced by the longer ADZ residence time of 99 hours associated with the other identified eigenvalue (0.98). The total *travel time* for this complete system is 181.4 hours (the sum of the 44 hour advective time delay and the cumulative overall time constant of 137.4 hours). This means that the '*dispersive fraction*' (see [20][31][40]) is 0.76 (i.e. $137.4 \div 181.5$): in other words, 76% of the water appears to be effective in dispersing the solute. This is a very high proportion, reflecting the nature of the system in this case, with a much higher potential for dispersion of tracer than in normal, faster moving streams, where the dispersive fraction is normally

in the range 0.3-0.4 (see e.g. [4][20]). The inferred responses of the two parallel pathways are plotted in Figure 1: the dotted line shows the estimated concentration changes in the quick pathway, which accounts mainly for the initial response measured at the weir; the dashed line are the estimated changes in the slow pathway, and these are responsible for the raised tail of the measured response.

It is possible to compute estimates of other physical attributes associated with the model. First, the steady state gains associated with the two parallel pathways define the partitioning of the flow, with 33% of flow associated with the quick pathway and 67% with the slow pathway. And since the flow rate is known in this example, the *Active Mixing Volumes* (AMVs: [38]), based on the estimated partitioned flow, are 361 m^3 in the quick pathway and $5,656$ m^3 in the slow pathway. As a result, the total estimated AMV is $5,656 + 3\text{x}361 = 6739$ m^3, which seems reasonable when compared with the $9,749$ m^3 for the total volume of the wetland, estimated by physical measurement. This suggests that about 70% of the wetland is important in dispersing the tracer (and, therefore, the waste water) and compares reasonably with the dispersive fraction derived percentage of 76%.

Of course, all of the results above are statistical estimates and so they are inherently uncertain. The advantage of the DBM approach is that we can quantify and consider the consequences of this uncertainty. For instance, based on the covariance matrix of the parameters produced by the SRIV estimation analysis, empirical probability distributions, in the form of histograms, can be computed for the 'derived' physical parameters, such as the residence times, partition percentages, AMVs, total AMV and steady state gains, using *Monte Carlo Simulation* (MCS) analysis. Figure 3 is a typical example of such analysis: it shows the normalized empirical distributions for the two residence times obtained by MCS using 10,000 random realizations (the procedure used here is discussed in [31]).

Of course, it should be noted that the parallel decomposition of the estimated TF used above is not unique: there are other decompositions that are just as valid and give precisely the same y_t response. For example, two other examples are: (i) a parallel decomposition of the two ADZs with residence times 99 and 12.8 hours, in series with two other identical ADZs, both with residence times 12.8 hours (see lower block diagram of Figure 2); (ii) various decompositions including feedback processes. However the latter seem less supportable in physical terms and are rejected according to the DBM ethos.

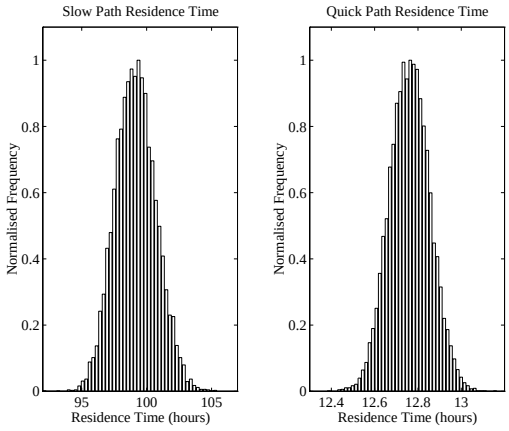

Figure 3: MCS analysis results: empirical probability distributions of the slow (left panel) and quick (right panel) residence times.

Finally, how can decompositions of ADZ reaches, such as those shown in Figure 2 be interpreted in terms of the wetland system? The most plausible mechanism is that the quick parallel pathway represents the 'main stream-flow' that is relatively unhindered by the vegetation; while the slow pathway represents the solute that is captured by the heavy vegetation and so dispersed more widely and slowly before reaching the weir. It is this latter pathway, which we have shown above accounts for some 67% of the flow, together with the large associated dispersive fraction of 76%, that is most useful in terms of nutrient removal, since it allows more time for the biological activity to take place.

5.2 A Nonlinear Example: Rainfall-Flow Modelling

This example is concerned with the analysis of daily rainfall, flow and temperature data from the 'ephemeral' Canning River in Western Australia which stops flowing over Summer, as shown in Figure 4. These data have been analyzed before and reported fully in [41]. The results of this previous analysis are outlined briefly below but most attention is focussed on more recent analysis that shows how the inductive DBM modelling can help to enhance alternative hypothetico-deductive, conceptual models that have been developed previously ([22][10][11]; see later). In particular, the nonlinearity inferred in the DBM modelling suggests significant modifications to the conceptual model.

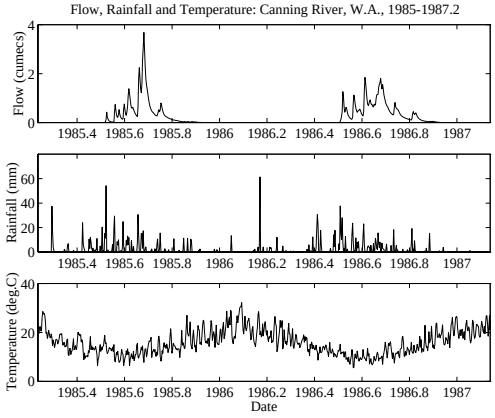

Figure 4: Daily rainfall-flow and temperature data for the ephemeral Canning River in Western Australia for the period 23^{rd} March 1985 to 26^{th} February, 1987.

Young *et al*. [41] show that, in this example, the most appropriate generic model form is the nonlinear *State-Dependent Parameter* (SDP) model class (see above, section 4). Analysis of the rainfall-flow data in Figure 4, based on this type of model, is accomplished in two stages. First, non-parametric estimates of the SDPs are obtained using the specific *State Dependent parameter Auto-Regressive eXogenous Variables* (SDARX) model form (see [33][34] and [35] where it is discussed at some length within a rainfall-flow context). This SDARX model can be written in the vector form:

$$y_t = \mathbf{z}_t^T \mathbf{p}_t + e_t \qquad e_t = N(0, \sigma^2) \qquad (3)$$

where,

$$\mathbf{z}_t^T = [y_{t-1} \quad \dots \quad y_{t-n} \quad r_{t-\delta} \dots \quad r_{t-\delta-m}]$$

$$\mathbf{p}_t = [a_1(z_t) \dots a_n(z_t) \quad b_0(z_t) \dots b_m(z_t)]^T$$

Here, y_t and r_t are, respectively, the measured flow and rainfall; δ is a pure advective time delay; and $n = 2$, $m = 3$, $\delta = 0$. All the model parameters are assumed initially to be dependent on a state variable z_t. In this case, the SDP analysis then shows that the state dependency is apparently in terms of the measured flow variable (i.e. $z_t = y_t$: see later explanation) and *is limited to those parameters associated with the rainfall* r_t.

In the second stage of the analysis, the non-parametric estimate of the nonlinearity is parameterized in the simplest manner possible; in this case as a power law in y_t. The constant parameters of this parameterized nonlinear model are then estimated using a nonlinear optimization procedure (see [35]). The resulting model is the following simplified version of the nonlinear *SDP Transfer Function* (SDTF) model [33][34]:

$$y_t = \frac{\hat{B}(z^{-1})}{\hat{A}(z^{-1})} u_t + \xi_t; \quad u_t = c.y_t^{\hat{\beta}}.r_t \qquad (4)$$

where,

$$\hat{A}(z^{-1}) = 1 - 1.646z^{-1} + 0.658z^{-2}$$

$$\hat{B}(z^{-1}) = 0.058 + 0.092z^{-1} - 0.138z^{-2}$$

with $\hat{\beta} = 0.85$. This shows that the input variable u_t is a nonlinear function in which the measured rainfall r_t is multiplied by the flow raised to a power $\hat{\beta}$, with the normalization parameter c simply chosen so that the steady state gain of the linear TF between u_t and y_t is unity[3]. In other words, the SDP analysis shows, in a relatively objective manner, that the underlying *dynamics* are predominantly linear but the overall response is made nonlinear because of a very significant input nonlinearity.

This model not only explains the data well ($R_T^2 = 0.96$) it is also consistent with hydrological theory, as required by the tenets of DBM modelling. This suggests that the changing soil-water storage conditions in the catchment reduce the rainfall to an '*effective*' level and that the relationship between the measured rainfall and this effective rainfall (sometimes referred to as 'rainfall excess') u_t is quite nonlinear. For example, if the catchment is very dry because little rain has fallen for some time, then most new rainfall will be absorbed by the dry soil and little, if any, will be effective in promoting increases in river flow. Subsequently, however, if the soil-water storage increases because of further rainfall, so the '*run-off*' of excess water from the catchment rises and the flow increases because of this. In this manner, the effect of rainfall on flow depends upon the antecedent conditions in the catchment and a similar rainfall event occurring at different times and under different soil-water storage conditions can yield markedly different changes in river flow.

The linear TF part of the model conforms also with the classical 'unit hydrograph' theory of rainfall-flow dynamics: indeed, its unit impulse response at any time is, by definition, the unit hydrograph. And the TF model itself can be seen as a parametrically efficient method of quantifying this unit hydrograph. Additionally, as in the solute transport example, the TF model can be decomposed by partial fraction expansion into a parallel pathway form

[3]This is an arbitrary decision in this case. However, if the rainfall and flow are in the same units, then this ensures that the total volume of effective rainfall is the same as the total flow volume.

which has a clear hydrological interpretation. In particular, it suggests that the effective rainfall is partitioned into three pathways: the instantaneous effect which, as might be expected, accounts for only a small 5.8% of the flow; a fast flow pathway with a residence time of 2.63 days which accounts for the largest 54.4% of the flow; and a slow flow pathway of 25.9 days residence time accounting for the remaining 39.8% of the flow. It is this latter pathway that leads to an extended tail on the associated hydrograph and can be associated with the slowly changing baseflow in the river. (for a more detailed explanation and other examples, see [28][29] [30][35][37][41]).

The most paradoxical and, at first sight, least interpretable model characteristic is that the effective rainfall nonlinearity is a function flow. Although this is physically impossible, the analysis produces such a clearly defined relationship of this sort that it must have some physical connotations. The most hydrologically reasonable explanation is that the flow is acting as a surrogate for soil water storage. Of course, it would be better to investigate this relationship directly by measuring the soil-water storage in some manner and incorporating these measurements into the SDP analysis. Unfortunately, it is much more difficult to obtain such 'soil moisture' measures and these were not available in the present example.

The temperature measurements are available, however, and this suggests that we should explore the model (4) further, with the object of enhancing its physical interpretation using these additional data. Two interesting conceptual ('grey-box') models of rainfall-flow dynamics are the Bedford-Ouse River model (e.g. [22]); and a development of this, the IHACRES model ([11]). Both of these '*Hybrid-Metric-Conceptual*' (HCM) models ([21]) have the same basic form as (4), except that the nature of the effective rainfall nonlinearity is somewhat different. In the case of the IHACRES model ([10][11]), for instance, this nonlinearity is modelled by the following equations:

$$\tau_s(T_t) = \tau_s e^{\frac{\bar{T}_t - T_t}{f}} \quad (5a)$$

$$s_t = s_{t-1} + \frac{1}{\tau_s(T_t)}(r_t - s_{t-1}) \quad (5b)$$

$$u_t = c.s_t^{\beta}.r_t \quad (5c)$$

where T_t is the temperature; $\bar{T}_t$ is the mean temperature; s_t represents a conceptual soil-water storage variable; and c, τ_s, f and β are *a priori* unknown parameters. Comparing (5c) with (4), we see that the main difference between the two models is that the measured y_t in (4), acting as a surrogate for soil-water storage, has been replaced by a modelled (or latent) soil-water storage variable s_t. The model (5b) that generates this variable is a first order discrete-time storage equation with a residence time $\tau_s(T_t)$ defined as τ_s multiplied by an exponential function of the difference between the temperature T_t and its mean value $\bar{T}_t$, as defined in (5a).

In the original IHACRES model (e.g. [10][11]), $\bar{T}_t$ is normally set at $20°$C, but the estimation results are not sensitive to this value. Also, s_t is not raised to a power, as in (5c). Some later versions of IHACRES have incorporated this parameter, but it has been added here so that the two nonlinearities in (4) and (5c) can be compared. More importantly, its introduction is practically important in this particular example since, without modification, the standard IHACRES model is not able to model the ephemeral Canning flow very well.

Using a constrained nonlinear optimization procedure procedure similar to that in the previous example, the parameters in this modified IHACRES model are estimated as follows:

$$A(z^{-1}) = 1 - 1.748z^{-1} + 0.755z^{-2}$$

$$\hat{B}(z^{-1}) = 0.029 + 0.141z^{-1} - 0.163z^{-2}$$

$$\hat{\tau}_s = 65.8, \hat{f} = 32.6; \hat{\beta} = 6.0; T_t = 15.9$$

These parameters are all statistically well defined and the model explains 97% of the flow y_t ($R_T^2 = 0.97$), marginally better than the DBM model. Moreover, as shown in Figure 5, it performs well in validation terms when applied, without re-estimation, to the data for the years 1977-78. In this case, $R_T^2 = 0.92$ which is again better than the $R_T^2 = 0.88$ achieved by the DBM model. However, when validated against the 1978-79 data, the positions are reversed, with only $R_T^2 = 0.81$ for the modified IHACRES model compared with $R_T^2 = 0.93$ for the DBM model. Overall, therefore, the two models are comparable in their ability to explain and predict the Canning River data.

Not surprisingly with its inclusion such a high value power law ($\hat{\beta} = 6.0$), the nonlinear transformation produced by equations (5a)-(5c) has a marked effect: in particular, it considerably modifies the soil-water storage s_t, effectively reducing it to zero, in relative terms, over the Summer period, as required. The reason why the modified IHACRES and DBM models perform similarly becomes clear when we compare the normalized (since they differ by a scale factor) effective rainfall variables for both models. The two variables are very similar indeed: in other

words, the optimized nonlinear transformation has forced the hypothetico-deductive IHACRES model dynamics to closely resemble those of the inductive DBM model.

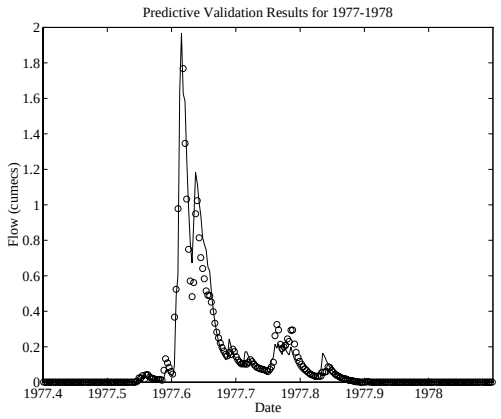

Figure 5: DBM rainfall-flow modelling of the Canning River: validation results on 1977-78 data.

It must be emphasized that this example is purely illustrative and it is not suggested that the modified IHACRES model identified here cannot be improved upon by the introduction of some alternative nonlinear mechanism. For instance, the estimation of a power law nonlinearity with such a large power of 6.1 seems a rather odd way to handle this type of nonlinearity, although the reader will see that it is very effective. Nevertheless, the example illustrates well how DBM modelling can, in a reasonably objective manner, reveal the *nature* of the nonlinearity required to model the data well and then seek out a parameterization that achieves this. In this example, it clearly demonstrates that the standard IHACRES model nonlinearity cannot do this unless it is modified in some manner. Of course, the power law nonlinearity is not the only, and definitely not the best, way of achieving this. For example, [23] introduces a threshold-type nonlinearity on s_t and obtain reasonable results but with R_T^2 values significantly less than those obtained with the above model (around 0.88-0.89 for estimation and 0.82-0.88 for validation). Clearly more research is required on the characterization of the effective rainfall-flow nonlinearity in models such as these.

6 THE EVALUATION OF LARGE DETERMINISTIC SIMULATION MODELS

This paper has concentrated on data-based modelling and analysis. However, as we have pointed out, many environmental scientists and engineers, including the present author, use more speculative simulation models of the deterministic-reductionist kind. Although we would not advocate the use of such models if adequate experimental or monitored data are available, they can provide a very good method of extending our 'mental models' of environmental systems, often as a valuable prelude to the design of experimental and monitoring exercises or, more questionably, as an aid in operational control, management and planning exercises.

If speculative simulation models are exploited in these latter ways, however, it is important that their construction and use is preceded by considerable critical evaluation. For instance, in a series of papers ([16][31][42]), the author and his colleagues have shown how *Monte Carlo Simulation* (MCS) and the related technique of *Generalized Sensitivity Analysis* (GSA) can be used to assess the sensitivity of a deterministic, 23rd order, nonlinear, global carbon cycle simulation model to input and parametric uncertainties, as defined by climate scientists.

Also in these papers, a technique known as *Dominant Mode Analysis* (DMA), based on the same SRIV methods of TF model estimation employed in the above DBM modelling, is used to obtain much simpler, reduced (e.g. 4th) order representations of the high order simulation model that are able to reproduce its dynamic behaviour to a remarkable degree.

All of these simulation model evaluation procedures are generally applicable and have been in continual use over the past few years, particularly in relation to the modelling and automatic control of the microclimate in large horticultural glasshouses and other agricultural buildings (e.g. [17][42]). They can also act as a prelude to the use of similar procedures in data assimilation and forecasting, as described elsewhere in this Conference [18].

7 CONCLUSIONS

For too long in the environmental sciences, deterministic reductionism has reigned supreme and has had a dominating influence on mathematical modelling in almost all areas of the discipline. In general, such 'bottom-up', reductionist models are over-parameterized in relation to the information content of the experimental data, and their determinism sits uncomfortably with the acknowledged uncertainty that characterizes most environmental systems. This paper has argued that parsimonious,

'top-down' models provide a more appropriate parameterization in most situations and that the uncertainty which pervades most environmental systems demands an alternative stochastic approach. Most often, however, the conventional statistical approach to stochastic model building is posed in a 'black-box' manner that fails to produce models that can be interpreted in physically meaningful terms. The *Data-Based Mechanistic* (DBM) approach to modelling discussed in the present paper tries to correct these deficiencies. It provides a parsimonious modelling strategy that not only exploits powerful statistical techniques but also produces models that can be interpreted in physically meaningful terms and are normally more acceptable to environmental scientists and engineers.

Finally, it should be noted that most of the analysis and modelling described in this paper was carried out using the Lancaster CAPTAIN Toolbox in Matlab (see http://www.es.lancs.ac.uk/cres/captain/).

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