DATA-BASED MECHANISTIC MODELLING AND VALIDATION OF RAINFALL-FLOW PROCESSES

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

Peter Young[1]

Centre for Research on Environmental Systems and Statistics,

Institute of Environmental and Natural Sciences,

Lancaster University, Lancaster LA1 4YQ

1. INTRODUCTION

One of the most interesting modelling problems in hydrology is the characterisation of the nonlinear dynamic relationship between rainfall and runoff. This has received considerable attention over the past thirty years, with mathematical and computer-based models ranging from simple ‘black-box’ representations to complex, physically-based catchment models. Wheater *et al.* (1993) have categorised such models into the following four, broad types.

- *Metric Models*, which are based primarily on observational data and seek to characterise the flow response largely on the basis of these data, using some form of statistical estimation or optimisation (e.g. Young, 1986). These include purely black-box, time-series models, such as the discrete-time transfer function or the neural network representations. Often, such models derive from, or can be related to, the earlier unit hydrograph theory but this is not always recognised overtly.

- *Conceptual Models*, which vary considerably in complexity but are normally based on the representation of internal storages, as in the original Stanford Watershed Model of the nineteen sixties (Crawford and Linsley, 1966), although the hypothesis of catchment-scale response is sometimes included, as in TOPMODEL (Beven and Kirkby, 1979). The essential feature of all these models, however, is that the model structure is specified *a priori*, based on the hydrologist/modeller’s perception of the relative importance of the component processes at work in the catchment; and then an attempt is made to ‘optimise’ the model parameters in some manner by ‘calibration’ against the available rainfall and flow data.

- *Physics-Based Models*, in which the component processes within the models are represented in a more classical, mathematical-physics form, based on continuum mechanics solved in an approximate manner via finite difference or finite element spatio-temporal discretisation methods. A well known example is the Système Hydrologique Européen

[1] Also, Adjoint Professor, Centre for Resource and Environmental Studies, Australian National University, Canberra, Australia.

(SHE) model (e.g. Abbot *et al*, 1986). The main problems with such models, which they share to some degree with the larger conceptual models, are two-fold: first, the inability to measure soil physical properties at the scale of the discretisation unit, particularly in relation to sub-surface processes; and second, their complexity and consequent high dimensional parameterisation. This latter problem makes objective optimisation and calibration virtually impossible, since the model is normally so over-parameterised that the parameter values cannot be uniquely identified and estimated against the available data.

- *Hybrid Metric-Conceptual* (HMC) Models, in which (normally quite simple) conceptual models are identified and estimated against the available data to test hypotheses about the structure of *catchment scale* hydrological storages and processes. In a very real sense, these models are an attempt to combine the ability of *Metric Models* to efficiently characterise the observational data in a statistical terms (the principle of *parsimony*: Box and Jenkins, 1970), with the advantages of *Conceptual Models* that have a prescribed physical interpretation within the current scientific paradigm.

The models in the two middle categories, above, are often characterised by a large number of unknown parameters that need to be estimated ('optimised' or 'calibrated') in some manner against the observational rainfall-flow time series. Because the number of parameters is normally very large in relation to the information content of the data, however, such models are often *over-parameterised* and not normally *identifiable*, in the sense that it is impossible to estimate their parameters uniquely without imposing prior restrictions on a large subset of the parameter values prior to estimation (see e.g. Young *et al*, 1996). The author and his co-workers have addressed these problems of over-parameterisation and poor identifiability associated with large environmental models many times over the past quarter century (e.g. Young, 1978, 1983, 1992, 1993, 1998a,b, 1999; Young and Minchin, 1991; Young and Lees, 1993; Young and Beven, 1994; Young *et al*, 1996; Shackley *et al*, 1998). And recently, Keith Beven and his co-workers (e.g. Franks *et al*, 1997; Beven Chapter ? of this Volume) have used the term *equifinality* to describe the consequences of such over-parameterisation and non-identifiability: namely the existence of many different parameterisations and model structures that are all able to explain the observed data equally well, so that no unique representation of the data can be obtained within the prescribed model set.

There appear to be two main reasons for these identifiability problems. First, any limitations of the observational data can be important, since the available time series may not be sufficiently informative to allow for the estimation of a uniquely identifiable model form. In particular, the inputs to a system may not be *sufficiently exciting* (see e.g. Young, 1984), in the sense that they do not perturb the system sufficiently to allow for unambiguous estimation of all the model parameters within an otherwise identifiable model structure. Secondly, even if the input does sufficiently excite the system, there are usually only a limited number of dynamic modes - the *dominant modes* of the system - that are excited to any significant extent; and the observed output of the system is dominated by their cumulative effect. The importance of this dominant mode concept in model identification and estimation is illustrated by the example in Appendix 1, which shows how the response of a 26th order simulation model can be duplicated with exceptional accuracy (0.001% error by variance) by a much simpler 7th order dominant mode model. This is typical of most high order linear systems and appears to carry over to nonlinear systems. For example, Young *et al* (1996) and Young (1998b) have used similar analysis to show how the response of high dimensional, nonlinear global carbon cycle simulation models are accurately reproduced by differential equation models of much reduced order. This is also reflected in other recent work on the simplification of global climate models (Hasselman *et al*, 1997; Hasselman, 1998).

In the above references, the author has stressed that dominant modal behaviour is a generic property of dynamic systems (see Young *et al*, 1996 and the prior references therein) and that it is probably the main reason for the limitation on the number of clearly identifiable parameters that can be estimated from observational data. The largest order identifiable system that the author has encountered from the analysis of real time series data, over the past forty years, is a 10th order differential equation model for the vibrations in a cantilever beam (Young, 1998a), where the very low damping of the system results in four dominant complex modes and the resulting model explains 99.74% of the experimental data. However, the identifiable order is normally much lower than this and many previous rainfall-runoff modelling studies (e.g. Kirkby, 1976; Hornberger *et al*, 1985; Jakeman and Hornberger, 1993; Young, 1993, 1998b; Young and Beven, 1994; Young *et al*, 1997, 1998; Ye *et al*, 1998) suggest that a typical set of rainfall-runoff observations contain only sufficient information to estimate up to a maximum of less than ten parameters within simple, nonlinear dynamic models of *dynamic order* three or less. In the rainfall-runoff example discussed later, for instance, there is clear evidence in the data of only three dominant modes between the effective rainfall input and the flow response (as described by a second order transfer function model with only five parameters): an instantaneous component, in which rainfall affects flow within the daily sampling interval; a ‘quick’ mode with a time constant of 1.02 days; and a ‘slow’ mode, with a time constant of 12.2 days. Other, less significant aspects of the flow response are a seasonal evapo-transpiration component, modelled as the response of a first order transfer function to temperature variations; and a constant component. As a result, the total number of parameters, including those associated with the nonlinear effective rainfall generation, is only nine.

Given the above considerations, one has to seriously question whether it is possible to validate the large Conceptual and Physics-Based models in any rigorous statistical sense, since non-uniqueness is endemic in such models and their over-parameterisation presents formidable obstacles to the application of the available statistical modelling and numerical optimisation procedures. Of course, this does not mean that model optimisation and limited forms of validation are impossible: there are many examples where large models have been successfully constructed and used to good effect in a variety of applications, from research studies to environmental management and planning. But it does mean that unconstrained, holistic optimisation of the model parameters in such large models is virtually impossible. It also limits the more rigorous application of statistical diagnostic and testing procedures, of the kind discussed in this Chapter.

Both the Metric and HMC approaches avoid these 'large model' problems to some extent but the practical utility of the basic Metric model is limited by its lack of any clearly defined physical interpretation. In this Chapter, therefore, attention is limited to the identification, estimation and validation of HMC-type models, where the problems of identifiability and optimisation are minimised (although, as we shall see, not eliminated) and the questions of validity can at least be approached in a statistically meaningful manner. Within the category of HMC models, however, two main approaches to modelling can be discerned; approaches which, not surprisingly, can be related to the more general *deductive* and *inductive*[2] approaches to scientific inference that have been identified by philosophers of science from Francis Bacon (1620), to Karl Popper (1959) and Thomas Kuhn (1962).

In the first hypothetico-deductive approach, the *a priori* conceptual model structure is effectively a theory of hydrological behaviour based on the perception of the hydrologist/modeller and is strongly conditioned by assumptions that derive from current hydrological paradigms (e.g. the IHACRES model of Jakeman *et al* 1990). The alternative *Data-Based Mechanistic* (DBM) approach is basically inductive, in the sense that it tries to avoid theoretical preconceptions as much as possible in the initial stages of the analysis. In particular, the model structure is not pre-specified by the modeller but, wherever possible, 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 hydrological paradigm: e.g. the models of rainfall-flow data in Young (1993, 1998b), Young and Beven (1994) and Young *et al* (1997, 1998).

This physical interpretation is an essential element in all DBM modelling: no matter how well the DBM model explains the data, it is only considered truly credible if it can be interpreted in physically meaningful (albeit not always conventional - see below) terms. In this, the DBM

[2] The term 'induction' is open to different interpretations and inductive methods have, for example, tended to dominate many areas of social science. Here, we utilise the term more narrowly, within the context of statistical inference, in order to differentiate the DBM approach from the related but more conventional hypothetico-deductive approaches to HMC modelling.

approach harks back to the father of modern statistical inference, Karl Friedrich Gauss, who held that no hypothesis was satisfactory which rested on a formula and was not also a consequence of physical conjecture. For this reason, Gauss abandoned his work on the attraction between charged particles because he was unable to find a plausible physical interpretation of the formula he had obtained for the relationship between the relative motion and position of two particles. Of course, this lack of credibility does not preclude the purely data-based model from being used for certain applications, such as forecasting and control, where the physical interpretation may be relatively unimportant and where the success of 'black-box' models is well documented.

Since the DBM approach is inductive, it is not wedded as strongly to the current paradigms as the hypothetico-deductive approach: indeed, its intention is always to respect these paradigms but not allow them to dictate the structure of models (here rainfall-flow) if the data suggest otherwise. In other words and to use a Kuhnian (Kuhn, 1962) interpretation of science, the DBM approach encourages the continual questioning of current paradigms and rejoices in its ability to promote paradigm change *if this is supported by observational data*. Examples of this ability to promote paradigm change in an evolutionary manner, based primarily on the statistical analysis of data, are the development of the *Aggregated Dead Zone* (ADZ) model for solute transport in rivers (e.g. Beer and Young, 1983; Wallis *et al*, 1989; Young and Wallis, 1994); and recent research on modelling the relationship between government spending, private capital investment and unemployment in the USA during the last half century (Young and Pedregal, 1998, 1999).

Another important aspect of the IHACRES and DBM approaches to rainfall-flow modelling relates to the *objectives* of the modelling exercise in each case. In the author's opinion, the search for a single, all encompassing model of any dynamic system is futile. Rather, the model builder should be seeking *a model that suits the nature of the study objectives*. Of course, this objective orientation does not have to be precisely defined, since a model can simultaneously serve more than one purpose. But even more loosely defined objectives need to be considered carefully before the modelling exercise begins. In this sense, we will see that the IHACRES and DBM models of rainfall-flow processes appear to have overlapping but not identical objectives. And these objectives affect, and have to be taken into account when evaluating, the overall 'validity' of the models.

On the basis of the above observations, the present chapter discusses the IHACRES and DBM approaches to rainfall-flow modelling within the context of daily rainfall, flow and temperature time series from the well known archive of data from the Coweeta Catchment (as collected over many years by scientists at the U.S. Forest Service). Prior to this, however, some background to the statistical methods utilised in the Chapter is presented. In particular, the basic aspects of statistical identification, estimation and validation are outlined and the DBM approach is described briefly. The historical development of the IHACRES and DBM rainfall-flow models and their inter-relationships are then discussed briefly, preparatory to the presentation of the Coweeta example. Four HMC models are considered in this example: the standard DBM model; a modified version of the IHACRES model which is appropriate to the Coweeta data; the Bedford-Ouse model, the progenitor of the IHACRES model; and a 'simulation' version of the DBM model. All of these models are optimised using a similar numerical optimisation scheme based on a 2000 sample set of daily data (see Appendix 2). Following optimisation, the models are subjected to standard statistical diagnostic tests, prior to predictive validation on separate sets of data.

This detailed modelling analysis of the Coweeta data helps to highlight certain important questions about the wider definition of model validation within the HMC context; questions that relate back to the different approaches and objectives of modelling discussed above, and are considered briefly at the end of the Chapter. It is concluded that none of the HMC models can be considered well validated at this time, although they can be deemed valid in the 'conditional' sense defined in this Chapter (i.e. they have not been falsified by the analysis here: which is arguably all that can be achieved by models anyway). In particular, the nature of the nonlinearity in the models is not sufficiently well defined and requires more detailed scientific study. Despite this, all the models appear to have advantages over alternative rainfall-flow models and are undoubtedly useful in both scientific and predictive terms.

2. STATISTICAL IDENTIFICATION, ESTIMATION AND VALIDATION

The 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. This statistical approach involves three main stages, as shown in fig.1: *identification* of an appropriate, identifiable model structure; *estimation* (optimisation, calibration) of the parameters that characterise this structure, using some form of estimation or optimisation; and predictive validation of the model on data sets different to those used in the model identification and estimation. In this section, we consider these three stages in order to set the scene for the later analysis. This discussion is intentionally brief, however, since the topic is so large that a comprehensive review is not possible in the present context.

INSERT Fig.1

2.1 Structure and Order Identification

In the hypothetico-deductive approach to model building, the model constitutes a hypothesis or 'theory of behaviour' and it is normally selected beforehand, based on the current scientific paradigm. However, the subsequent processes of model estimation and validation are often considered as exercises in Popperian 'falsification' (Popper, 1959) and so the initial perceived model structure may well be modified in the light of these. In the DBM approach, this questioning of the hypothetical model is more overt and the identification stage is considered as a most important and essential prelude to the later stages of model building. Nevertheless, in the case of HMC models, both approaches make use of statistical identification procedures to some extent. These usually involve the identification of the most appropriate *model order,* as defined in dynamic system terms, although the *model structure* itself can be the subject of the analysis if this is also considered to be ill-defined. In the 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) but is identified from the data using non-parametric and parametric statistical estimation methods. Once a suitable model structure has been defined, there are a variety of statistical methods for identifying model order, some of which are discussed later in connection with the Coweeta example (see Appendix 3). In general, however, they exploit some *order identification statistics*, such as the correlation-based statistics popularised by Box and Jenkins (1970) and the well known Akaike Information Criterion (AIC: Akaike, 1974).

2.2 Estimation (Optimisation)

Once the model structure and order have been identified, the parameters that characterise this structure need to be estimated in some manner. There are many automatic methods of estimation or optimisation available in this age of the digital computer, from the simplest, deterministic procedures, usually based on the minimisation of least squares cost functions; to more complex numerical optimisation 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; an approach which, when used correctly, includes the associated statistical diagnostic tests that are considered so important in statistical inference. Moreover, the power of the modern computer is such that some of these restrictions are gradually being lifted, with the advent of stochastic approaches, such as Markov Chain Monte Carlo (MCMC) procedures. In the present context, however, the estimation methods are based on nonlinear modifications of linear *Instrumental Variable* (IV) methods (e.g. Young, 1984 and the references therein).

2.3 Conditional Validation

As the concluding section of this paper will stress, validation is a complex process and even its definition is controversial. Some academics (e.g. Konikow and Brederhoeft, 1992, within a ground-water context; Oreskes *et al.*, 1994, in relation to the whole of the earth sciences) question even the possibility of validating models. To some degree, however, these latter arguments are rather philosophical and linked, in part, to questions of semantics: what is the 'truth'; what is meant by terms such as validation, verification and confirmation? etc. Nevertheless, one specific, quantitative aspect of validation is widely accepted; namely predictive 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 Oreskes *et al.* (1994) 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 proves practically feasible, there seems no doubt that predictive validation is an essential pre-requisite for any definition of model efficacy, if not validity.

It appears normal these days to follow the Popperian view of validation (Popper, 1959) and consider it as a continuing process of 'falsification'. Here, it is assumed that scientific theories (models in the present context) can never be proven universally 'true'; rather, they are 'not yet proven to be false'. In fig.1, it is suggested that this yields a model that is considered 'conditionally valid', in the sense that it can be assumed to represent the best theory of behaviour currently available that has not yet been falsified. Thus, conditional predictive validation means that the model has proven valid in this more narrow predictive sense. In the rainfall-flow context, for example, it implies that, on the basis of the 'new' measurements of the model inputs (e.g. rainfall, temperature or evaporation) from the validation data set, the model produces flow predictions that are acceptable *within the uncertainty bounds associated with the model.* Note this stress on the question of the inherent uncertainty in the estimated model: one advantage of statistical estimation, of the kind considered in this chapter, is that the level of uncertainty associated with the model parameters and the stochastic inputs is quantified in the time series analysis. Consequently, the modeller should not be looking for perfect predictability (which no-one expects anyway) but *predictability which is consistent with the quantified uncertainty associated with the model.*

It must be emphasised, of course, that conditional predictive validation is simply a useful statistical diagnostic which ensures that the model has certain desirable properties. It is not a panacea and it certainly does not prove the complete validity of the model if, by this term, we mean the 'establishment of the truth' (Oreskes *et al.*, 1994). Models are, at best, approximations of reality designed for some specific objective; and conditional predictive validation merely shows that this approximation is satisfactory in this limited predictive sense. As we point out in the concluding section of this chapter, this may well not satisfy all of our requirements and the efficacy of the model will often need to be evaluated in much wider and practical terms.

3. Data-Based Mechanistic (DBM) Modelling

Previous publications (Beck and Young, 1975; Whitehead and Young, 1975; Young, 1978, 1983, 1992, 1993, 1998a,b,c; Young and Minchin, 1991; Young and Lees, 1993; Young and Beven, 1994; Young *et al*, 1996; Young and Pedregal, 1998, 1999) 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.

The main stages in DBM model building are as follows:

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. 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. An appropriate model *structure* is identified by a process of objective statistical inference applied directly to the time-series data and based on a given *general 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 or piece-wise linear, then the *constant parameters* that characterise the identified model structure in step 2. are estimated using advanced methods of statistical estimation for dynamic systems. The methods used in the present chapter are the Refined Instrumental Variable (RIV) and Simplified RIV (SRIV) algorithms, which provide a robust approach to model identification and estimation that has been well tested in practical applications over many years. Full details of these methods are provided in Young and Jakeman (1979, 1980); Young, (1984, 1985). They are also outlined in Young and Beven (1994) and Young et al. (1996).
4. If significant parameter variation is detected then the model parameters are estimated by the application of an approach to time (or state) dependent parameter estimation based on recursive Fixed Interval Smoothing (FIS): e.g. Young (1984, 1988, 1993, 1998a,b,c, 1999b); Young and Beven (1994). Such parameter variation will tend to reflect *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 defining the non-parametric relationship, which then can often be interpreted in State-Dependent Parameter (SDP) terms (see Young, 1993; Young and Beven, 1994; Young, 1998a,b,c). These methods are outlined in Appendix 2.

5. If nonlinear phenomena have been detected and identified in stage 4, the non-parametric state dependent relationships are normally parameterised in a finite form and the resulting nonlinear model is estimated using some form of numerical optimisation, such as nonlinear least squares or ML based on prediction error decomposition (Schweppe, 1965). In the present paper, this approach to nonlinear identification and estimation is required only to define the nature of the effective rainfall nonlinearity, which appears only at the input to the model, as described in subsequent sections. This approach is also outlined in Appendix 2.
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 statistical modelling methodology.
7. Finally, the estimated model is tested in various ways to ensure that it is conditionally valid in the sense discussed above. This involves 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), as well as exercises in predictive validation and stochastic sensitivity analysis (see the later example).

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 characterisation 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 (Beer and Young, 1983; Wallis *et al.*, 1989). Despite its initially unusual physical interpretation, the practical success of this ADZ model 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 (Young and Wallis, 1994).

4. THE BEDFORD-OUSE, IHACRES AND DBM MODELS

The IHACRES and DBM models have a common origin in the discrete-time rainfall-flow model developed by the author and his colleagues for the Bedford-Ouse Study in the early 1970's (Young, 1974; Whitehead and Young, 1975). This section introduces first this seminal model; and then discusses briefly the later development of the IHACRES and DBM models.

4.1 The Bedford-Ouse Model (BM)

This was probably the first HMC model to be suggested and it takes the following form:

$$y_t = \frac{B(z^{-1})}{A(z^{-1})} u_t + \xi_t \qquad ; \qquad t = 1,2,\ldots,N \tag{1}$$

$$\begin{aligned} r_t &= r_t \frac{T_r - T_m}{c} && \text{(i)} \\ s_t &= s_{t-1} + \frac{1}{\tau_s}\left\{ r_t - s_{t-1} \right\} && \text{(ii)} \\ u_t &= s_t . r_t && \text{(iii)} \end{aligned} \tag{2}$$

where,

$$A(z^{-1}) = 1 + a_1 z^{-1} + \ldots + a_n z^{-n} \qquad ; \qquad B(z^{-1}) = b_0 + b_1 z^{-1} + \ldots + b_m z^{-m}$$

and z^{-i} is the backward shift operator: i.e. $z^{-i} y_t = y_{t-i}$ Equation (1) is a linear *Transfer Function* (TF) relationship between the effective rainfall (rainfall excess) input u_t and the measured flow y_t. This can be written in the following alternative equation form,

$$y_t = -a_1 y_{t-1} - \ldots - a_n y_{t-n} + b_0 u_t + b_1 u_{t-1} + \ldots + b_m u_{t-1} + \eta_t \tag{3}$$

where δ represents the potential presence of any pure advective time delay in the system; $\eta_t = \xi_t + a_1 \xi_{t-1} + \ldots + a_n \xi_{t-n}$; and ξ_t represents uncertainty in the relationship arising from a combination of measurement noise, the effects of other unmeasured inputs and modelling error. Normally, ξ_t is modelled as an AutoRegressive (AR) or AutoRegressive-Moving Average (ARMA) stochastic process (see e.g. Box and Jenkins, 1970; Young, 1984).

The equations 2(i) to 2(iii) describe the assumed nonlinear relationship between the measured rainfall r_t and u_t, which takes the form of a multiplicative nonlinearity between r_t and a measure of soil moisture s_t. This soil moisture variable can be considered as an unobserved state of the system that has to be estimated from the data (see later discussion). The modified rainfall input r_t is a nonlinear function of the measured rainfall r_t and the mean monthly temperature T_m, as defined in equation 2(i). Like the linear TF parameters $a_i, i = 1,2,\ldots,n$, and

$b_j, j = 0,1,2,...,m$, the nonlinear model parameters τ_s, T_r and c, are all unknown *a priori* and need to be estimated from the rainfall, flow and temperature measurements. In addition the TF polynomial orders n and m (which are normally $\leq$ 3), and any associated time delay δ, need to be identified as part of the identification and estimation procedure, which is discussed in the next section of the Chapter.

The conceptual justification for the model defined by equations (1) and (2) is straightforward. First, the linear part of the model, as represented by the TF model in equation (1), can be considered in its alternative *infinite dimensional*, discrete-time 'convolution equation' form,

$$y_t = \sum_{i=1}^{\infty} g_i . u_{t-i} + \xi_t \tag{4}$$

which is obtained by simply dividing the numerator polynomial $B(z^{-1})$ by the denominator polynomial $A(z^{-1})$. This form of the model is interesting because the coefficients $g_i, i = 1,2,...,\infty$ are the ordinates of the impulse response function; or, in hydrological terms, the associated infinite dimensional unit hydrograph (IUH). The more conventional finite dimensional approximation of the IUH (the *Finite Impulse Response* (FIR) in systems terms) is obtained from the g_i by curtailing the number of these coefficients to only those that are numerically significant. This interpretation demonstrates that the TF model is a parametrically efficient ('parsimonious') representation of the unit hydrograph model which, given our comments in the previous section, has important implications on the statistical identification and estimation of the model.

Second, the nonlinear equations in (2) are an attempt to represent, in a simple manner, the soil-moisture, groundwater and seasonal evapo-transpiration mechanisms in the system and modify the rainfall to account for these effects. In this regard, equation 2(i) multiplies the 'raw' rainfall measurements by a factor which is a function of the difference between a reference temperature T_r and the current monthly mean temperature T_m, thereby adjusting the rainfall to allow for seasonal factors. This initially modified rainfall r_t is then passed through the first order filter in equation 2(ii), which has a time constant or residence time τ_s. This can be conceptualised as a catchment storage equation which yields a constantly changing index of catchment storage s_t reflecting antecedent rainfall that has fallen on the catchment. In times of no rainfall, this index will reduce in a manner defined by τ_s; while during high rainfall episodes it will increase sharply in value. The final effective rainfall measure u_t is obtained as the product of s_t and r_t, so modifying the measured rainfall to reflect the temperature and antecedent rainfall effects. Interpreted in these terms, the input nonlinearity can be considered as a refinement of the conventional 'antecedent precipitation index' approach (e.g. Weyman, 1975) used in previous rainfall-runoff models (since the dynamic equation 2(ii) yields s_t as an exponentially-weighted measure of the input r_t into the past, with the exponential decay defined by τ_s). The main difference lies in the overall framework of the model and the fact that the model in (1) and (2) is couched within a stochastic framework and so is identified and estimated using statistical methods.

4.2 The IHACRES Model

The IHACRES model (Jakeman *et al*, 1990; Jakeman and Hornberger, 1993) is quite similar to the Bedford-Ouse model, from which it was derived, but its conceptual basis is perceived to be somewhat more acceptable in hydrological terms. The only differences lie in the nonlinear part of the model, where the equations in (2) are replaced by the following:

$$\begin{aligned} &\tau_s(T_t) = \tau_s.\exp\left[20 - T_t / f\right] && \text{(i)} \\ &s_t = c.s_{t-1} + \frac{1}{\tau_s(T_t)}\left\{r_t - s_{t-1}\right\} && \text{(ii)} \\ &u_t = s_t.r_t && \text{(iii)} \end{aligned} \qquad \text{(2a)}$$

Here, the main change relates to the time constant $\tau_s(T_t)$ in the storage equation 2a(ii) which, in the BM model, is a time-invariant parameter estimated from the data. In 2a(ii), it is now a nonlinear function of the temperature T_t, as defined by equation 2a(i). This temperature dependent time constant $\tau_s(T_t)$, which now applies differential exponential weighting to the antecedent rainfall r_t, is inversely related to the rate at which catchment wetness declines (or potential evapo-transpiration): this is arbitrarily defined as a constant τ_s at $20^\circ C$. The parameter f is a temperature modulation factor which accounts for the fluctuations in potential evapo-traspiration and determines how $\tau_s(T_t)$ changes with temperature. Both parameters τ_s and f are estimated from the data, while the parameter c is set so that the volume of the effective rainfall (rainfall excess) is equal to the total stream flow volume over the estimation period of N samples[3].

4.3 The DBM Model

The nonlinear part of the DBM model is much simpler than in either of the two previous models. Following the DBM approach discussed in the last section and the procedures outlined in Appendix 2, it is based on non-parametric estimation from the data and takes the form,

$$u_t = c.y_t^{\beta}\, r_t \qquad \text{(2b)}$$

---

[3] In the published IHACRES model, this parameter c is selected by the modeller and appears in equation 2a(ii), but it performs the same function as here.

In other words, the catchment storage term s_t in the IHACRES model equation 2a(iii) is replaced by the term y_t^{β}. As pointed out in the above references, this relationship should *not* be interpreted as saying that effective rainfall is physically a function of flow, which is obviously impossible. Rather, the measured flow y_t is effectively acting here as an objectively identified *surrogate* for the catchment storage s_t. This seems sensible from a hydrological standpoint, since flow is clearly a function of the catchment storage and its pattern of temporal change is likely to be similar. The power law appears in (2b) because it is identified objectively from the data during the non-parametric estimation phase of the analysis. In fact, this has been substantiated by subsequent research on the IHACRES model (e.g. Ye *et al*, 1998), which has shown the advantage of incorporating such a power law. Consequently, later versions of the IHACRES model replace 2a(iii) by $u_t = c.s_t^{\beta}\, r_t$, thus making the similarity between the two models even more transparent.

It will be noted that the DBM model (equations (1) and (2b)) does not include any temperature dependent terms and so, in this basic form, it cannot account for seasonal, transpiration effects. Following the DBM approach, these should be identified and estimated from the data, rather than included *a priori*, as in the Bedford-Ouse and IHACRES models. As we shall see later, such analysis applied to the Coweeta data suggests strongly that the temperature dependency enters through a separate TF relationship, so that the more general DBM model takes the form:

$$y_t = b + \frac{B_1(z^{-1})}{A_1(z^{-1})} u_{t-\delta_1} + \frac{B_2(z^{-1})}{A_2(z^{-1})} T_{t-\delta_2} + \xi_t \qquad \text{(i)}$$

(2c)

$$u_t = c.y_t^{\beta}\,.r_t \qquad \text{(ii)}$$

where,

$$A_1(z^{-1}) = 1 + a_{11}z^{-1} + ... + a_{1n1}z^{-n1} \quad ; \quad B_1(z^{-1}) = b_{10} + b_{11}z^{-1} + ... + b_{1m1}z^{-m1}$$
$$A_2(z^{-1}) = 1 + a_{21}z^{-1} + ... + a_{2n2}z^{-n2} \quad ; \quad B_2(z^{-1}) = b_{20} + b_{21}z^{-1} + ... + b_{2m2}z^{-m2}$$

and b is a constant or very slowly varying flow component, which seems to be present in the Coweeta flow data and is probably due to deep aquifer effects of some kind.

4.4 The DBMS Model

Unfortunately, the simplification of the nonlinear relationships in the above DBM models is obtained at a cost. Although the models so defined can function very well indeed in a forecasting context, they cannot be used directly for *simulation* purposes, where only the rainfall and temperature measurements are used to generate purely simulated flow outputs (e.g.

in applications such as off-line management, planning and 'what-if' studies). This arises because the flow variable y_t, which is not available in such studies, is required to generate the effective rainfall via equations (2b) and 2c(ii). Related DBM simulation models can be constructed, however, by introducing a catchment storage equation into the model that mirrors the identified DBM model rainfall-flow dynamics but does not utilise the flow measurement directly. The exact form of this storage equation cannot mimic the DBM model rainfall-flow dynamics exactly, of course, and so it has to be identified from the data by comparing the estimation results obtained with various possible approximations. In the case of the Coweeta catchment data discussed in the next section, for example, this has yielded the following DBM Simulation (DBMS) model:

$$y_t = b + \frac{B_1(z^{-1})}{A_1(z^{-1})} u_{t-\delta_1} + \frac{B_2(z^{-1})}{A_2(z^{-1})} T_{t-\delta_2} \qquad \text{(i)}$$

$$s_t = b + \frac{g}{1+\alpha z^{-1}} r_t + \frac{B_2(z^{-1})}{A_2(z^{-1})} T_{t-\delta_2} \qquad \text{(ii)} \qquad \text{(2d)}$$

$$u_t = c.s_t^{\beta} r_t \qquad \text{(iii)}$$

In equation 2d(ii),$\alpha = 1-(1/\tau_s)$, g and β are parameters optimised within the nonlinear storage part of the model; while b, $A_2(z^{-1})$ and $B_2(z^{-1})$ are assumed to be the same as those estimated in the linear TF part of the model 2d(i). In other words, since the effective rainfall (a direct function of flow in the standard DBM model) is not available in this simulation mode of solution, the storage equation 2d(ii) is an approximation of the rainfall flow equation in 2d(i) but with the measured rainfall entering linearly through the first order TF $g/(1+\alpha z^{-1})$. Here, the simple first order TF form, with only two unknown parameters to be estimated (g and α), is necessary because the assumption of a higher order TF, such as $B_1(z^{-1})/A_1(z^{-1})$ in 2d(i), leads to over-parameterisation and associated identifiability problems during optimisation.

In relation to the nonlinear storage equation in the IHACRES model, note that the two input model in 2d(ii) effectively replaces equations (i) and (ii) of (2a) and the overall DBMS model, excluding the model for the noise term ξ_t, has 11 parameters to be estimated, compared with 9 for the IHACRES model and 9 for the standard DBM. This suggests that either the IHACRES is under-parameterised or the DBMS has too many parameters: this is discussed in the next section.

5. A PRACTICAL EXAMPLE: HMC MODELS OF RAINFALL-FLOW PROCESSES IN THE COWEETA CATCHMENT

Fig.2 is a plot of the rainfall, flow and temperature time series from the Coweeta catchment that are used for model identification and estimation in this example: these are 2000 daily measurements of each variable, from sample number 8310-10309 out of a full data set of 17532 daily samples. Independent one year long subsets, from sample 10310-10674 and 14310-14674, respectively, are used for the predictive validation tests reported here, although these are representative of the validation results obtained over all sections of the complete data set.

INSERT Fig.2

5.1 DBM Model Identification and Estimation

The first stage in DBM model identification confirms that the relationship between rainfall and flow is nonlinear and the non-parametric State Dependent Parameter (SDP) analysis, as outlined in Appendix 2, yields the results shown in fig.3. This is a plot of the estimated SDP against the flow y_t (where the star superscript indicates that the flow has been sorted in ascending magnitude) and the FIS non-parametric estimate $\hat{b}_{0,t|N}$ is shown as dots, with the standard errors shown dashed (see Appendix 2 for further explanation) . The full line curve is the weighted least squares estimate of a power law relationship, which does not fit the data too badly and confirms, to some extent, the results of previous analysis of data from other catchments in the UK, Australia and the tropics (Young, 1993; Young and Beven, 1994; Young *et al.*, 1997, 1998; Ye *et al.*, 1998; Young, 1998b; Chappell *et al.*, 1999). It might be better, in this case, to consider a two segment linear relationship, as used by Young (1993), rather than the power law. However, selection of the latter has the advantage of maintaining continuity with earlier work on both DBM and IHACRES models which have utilised such a relationship. Nevertheless, it must be emphasised that further research on the nature of the nonlinearity is required and it is clear that the power law relationship may not always be optimum.

INSERT Fig.3

Based on this power law parameterisation of the nonlinearity, the identification and estimation analysis outlined in Appendix 2 yields the following DBM model, which is simply a special example of equations (2c):

$$y_t = 2.05 + \frac{0.170 - 0.118z^{-1} - 0.022z^{-2}}{1 + 1.298z^{-1} - 0.347z^{-2}} u_t + \frac{-0.0042z^{-6}}{1 - 0.97z^{-1}} T_t + \xi_t \qquad \text{(5a)}$$

$$u_t = c.y_t^{0.711}.r_t \quad ; \quad c = \left\{ \sum_{t=1}^{t=N} y_t \Big/ \sum_{t=1}^{t=N} y_t^{0.711}.r_t \right\}$$

where the noise term ξ_t is modelled as an AR(5) process,

$$\xi_t = \frac{1}{1 - 0.269z^{-1} - 0.192z^{-2} - 0.062z^{-3} - 0.040z^{-4} - 0.056z^{-5}} e_t \quad ; \quad \text{var}(e_t) = 1.46 \qquad \text{(5b)}$$

the parameter c is selected so that total effective rainfall u_t over the observation interval is equal to the total flow $\sum y_t$; and T_t is the temperature minus its mean value. The estimated covariance matrices associated with the 3 component model parameters and the noise model are given below:

<u>Effective Rainfall - Flow TF</u>

$$P(A_1,B_1) = 10^{-3} \begin{bmatrix} 0.9901 & -0.8596 & -0.0013 & 0.1983 & -0.1173 \\ -0.8596 & 0.7499 & 0.0016 & -0.1735 & 0.1046 \\ -0.0013 & 0.0016 & 0.0044 & -0.0067 & 0.0026 \\ 0.1983 & -0.1735 & -0.0067 & 0.0527 & -0.0308 \\ -0.1173 & 0.1046 & 0.0026 & -0.0308 & 0.0203 \end{bmatrix} \qquad \text{(5c)}$$

<u>Temperature - Flow TF</u>

$$P(A_2,B_2) = 10^{-5} \begin{bmatrix} 0.6353 & -0.0665 \\ -0.0665 & 0.0093 \end{bmatrix} \qquad \text{(5d)}$$

<u>Nonlinear Catchment Storage parameters</u>

$$P(\beta, b) = 10^{-4} \begin{bmatrix} 1.8795 & 4.3312 \\ 4.3312 & 5.3894 \end{bmatrix} \qquad \text{(5e)}$$

<u>Noise Process</u>

$$P(AR) = 10^{-3} \begin{bmatrix} 0.5025 & -0.1375 & -0.0983 & -0.0366 & -0.0278 \\ -0.1375 & 0.5393 & -0.1128 & -0.0940 & -0.0366 \\ -0.0983 & -0.1128 & 0.5559 & -0.1128 & -0.0985 \\ -0.0366 & -0.0940 & -0.1128 & 0.5394 & -0.1377 \\ -0.0278 & -0.0366 & -0.0985 & -0.1377 & 0.5032 \end{bmatrix}$$

Fig. 4 compares the output of the deterministic part of the model (5a), $\hat{y}_t$, where,

$$\hat{y}_t = 2.05 + \frac{0.170 - 0.118z^{-1} - 0.022z^{-2}}{1 + 1.298z^{-1} - 0.347z^{-2}} u_t + \frac{-0.0042z^{-6}}{1 - 0.97z^{-1}} T_t$$

with the observed flow y_t: clearly the data are fitted well with the coefficient of determination $R_t^2 = 0.91$ (i.e. 91% of the flow data are explained by $\hat{y}_t$: see Appendix 3). After incorporating the AR(5) noise model, the coefficient of determination based on the one-step-ahead prediction errors $R^2 = 0.93$. Fig.5 is a plot of the deterministic output from the temperature - flow model, $\hat{y}_{2,t}$ (see below and Appendix 2) compared with the residual $y_t - b - \hat{y}_{1,t}$ (dotted), where $\hat{y}_{1,t}$ is the deterministic output of the effective rainfall - flow model. This shows how well the temperature - flow model explains the seasonal variations in flow due, presumably, to long term evapo-transpiration effects. Note also the 'spikes' in the residual $y_t - b - \hat{y}_{1,t}$, which suggests that there are outliers in the data during high flow events (see later).

INSERT Figs.4 and 5

Figs.6 to 9 present the results of correlation analysis applied to the model residuals. Fig.6 is the auto-correlation function (acf) of the deterministic model residuals $y_t - \hat{y}_t$: it is clear that there is considerable correlation in these residuals but, as shown in fig.7, the final stochastic residuals $\hat{e}_t$ (the one-step-ahead prediction errors) are not correlated and subscribe to the assumption of white noise[4]. However, the 'spikes' mentioned above are clear also on the plot of $\hat{e}_t$ in the top panel of the figure and a histogram of the $\hat{e}_t$, coupled with tests for normality and a normal probability plot, confirm that the amplitude distribution is far from Gaussian normality. Given this observation, it is necessary to be careful about the interpretation of the covariance matrices in (5c) to (5e), which are computed on the assumption of normally distributed residuals. However, the matrices still provide an indication of the uncertainty on the estimates and are useful in this regard for subsequent stochastic analysis, provided we bear in mind the distortions that will arise from the non-normality .

Fig.8 shows the cross-correlation function (ccf) between $\hat{e}_t$ and the temperature input T_t: although there is a larger correlation at lag zero, it falls only on the boundary of the significance bands (dotted) and so we can assume that $\hat{e}_t$ and u_t are reasonably uncorrelated, as required. Finally, fig.9 is the ccf between $\hat{e}_t$ and the effective rainfall input u_t: here, there is evidence of just significant correlation at some lags, although the magnitude is always quite small. Apart from the clear deviation from normality, this is the only way in which the model (5a) fails its

[4] More precisely, the residual series constitutes 'weak white noise', in the sense that there is some autocorrelation when the squared or absolute values of the residuals are considered.

statistical diagnostic tests and these failures appear common in all rainfall-flow models that we have investigated using these statistical diagnostic methods.

INSERT Figs 6 to 9

One of the main reasons for the correlation between the stochastic residuals $\hat{e}_t$ and u_t, as well as the non-normality of $\hat{e}_t$, is the presence of the 'spikes' mentioned above. Fig.10 is a plot of $\hat{e}_t$ with the outliers (defined as values lying outside the ±3 standard deviations bound) marked as circles . It is clear that there are numerous samples within the series $\hat{e}_t$ that appear to be outliers in this sense, and these most often occur at times of high rainfall and flow when one might expect measurement errors and extremes of behaviour to be present. One straightforward approach, in this situation, would be to repeat the identification and estimation analysis under the assumption that the outliers represent errors in the data and either should be given less weight in the estimation or considered as missing samples. A related approach would be to consider that the $\hat{e}_t$ are heteroscedastic (i.e. their variance is not the same at all samples) and utilise some method of estimation which allows for this (e.g. Johnston and DiNardo, 1997). These approaches have not been attempted in the present illustrative analysis, but it seems unlikely that it would make a great difference to the final estimated model's predictive performance (although it would affect the parameter estimates). Unfortunately, other approaches to the problem of non-normality, such as the use of Markov Chain Monte-Carlo (MCMC) methods (e.g. Gamerman, 1997), involve new, relatively untried methodology and can be computationally very intensive. However, the non-normality of the residuals in rainfall-flow models is clearly significant and constitutes a suitable topic for future research.

INSERT Fig.10

5.2 Mechanistic Interpretation of the DBM Model

As discussed in Young (1992, 1998b) and following the procedure used in the previous publications mentioned above, the TF part of the model (5a) can be written in the following alternative form:

$$y_t = 2.05 + \left[0.17 + \frac{0.077}{1 - 0.38z^{-1}} + \frac{0.026}{1 - 0.92z^{-1}} \right] u_t + \frac{-0.0042z^{-6}}{1 - 0.97z^{-1}} T_t + \xi_t \quad (5f)$$

Considering only the deterministic parts of this model, the deterministic output $\hat{y}_t$ is given by,

$$\hat{y}_t = 2.05 + \hat{y}_{1,t} + \hat{y}_{2,t} \quad (5g)$$

where:

$$\hat{y}_{1,t} = \left[0.17 + \frac{0.077}{1-0.38z^{-1}} + \frac{0.026}{1-0.92z^{-1}} \right] u_t \quad ; \quad \hat{y}_{2,t} = \frac{-0.0042z^{-6}}{1-0.97z^{-1}} T_t$$

Here, the variables $\hat{y}_{1,t}$ and $\hat{y}_{2,t}$ are, respectively, the modelled flow due to the effective rain and the temperature effects, with the former TF decomposed into a three pathway, parallel flow form. A systems diagram of the model in this decomposed parallel form is shown in fig. 11 and the details of the decomposition are given below in Table 1.

Table 1

Instantaneous TF (A)			
Eig	SSG	TC	% of $\hat{y}_{1,t}$ flow
0	0.17	0.00	27.3
Fast Flow TF (B)			
Eig	SSG	TC	% of $\hat{y}_{1,t}$ flow
0.38	0.12	1.02	19.9
Slow Flow TF (C)			
Eig	SSG	TC	% of $\hat{y}_{1,t}$ flow
0.92	0.33	12.21	52.8
Slow Temperature (Seasonal) Effect (D)			
Eig	SSG	TC	TD
0.97	- 0.14	32.9	6
Constant Base flow			
2.05 (t)			

Table 1. Eig denotes the eigenvalue associated with the component; SSG denotes steady state gain; TC denotes time constant (residence time); TD denotes pure time delay.

We now see that *one interpretation* of the model (5a)[5] is that the effective rainfall u_t reaches the river and affects the flow via three pathways; and that the flow is also affected by the prevailing temperature variations. This interpretation has the advantage that it makes reasonable physical sense. In particular, it suggests that the river flow is composed of 5 components: a very rapid instantaneous (i.e. within one day) effect; a 'fast flow' component with residence time 1.02 days, probably associated with surface processes; a 'slow flow' component with residence time 12.21 days, probably associated with sub-surface and groundwater processes; and a very slow, 'base flow' component in the form of a 'constant flow' of 2.05 mm, probably due to deep aquifer effects and apparently constant over the 2000 days of data (but varying very slowly over the whole 17532 data set). Note that the TF's associated with 'fast' and 'slow' flow parallel pathways can be interpreted directly as dynamic mass balance or storage equations (see Young and Beven, 1994). The 5th, temperature dependent component (the temperature variations about the mean passed through a TF with time constant 32.9 days) clearly accounts

[5] This decomposition is not unique: serial and feedback decompositions are equally feasible in mathematical system terms but the parallel decomposition seems most logical on physical grounds.

for long term temperature dependent effects, such as those arising from evapo-transpiration processes.

Fig.12 is a plot of the flow estimates associated with each of the parallel pathways. The instantaneous effect is shown in the upper panel; the fast and slow flows below this; and the temperature dependent effect in the lower panel. Fig.13 lumps these effects together: in the upper panel is the sum of the instantaneous and fast flow components; while the cumulative slow flows are plotted in the lower panel. The dashed line in this lower plot is the temperature dependent component, showing how it dominates the slower flow components in the longer term.

INSERT Figs.11, 12 and 13

5.3 Predictive Validation of the DBM Model

The model (5a) has been validated in a predictive sense, as discussed in earlier sections, by applying it to two other, one year long, segments of the data: from samples 10310-10674 and 14310-14674, respectively. Over the first segment, the coefficients of determination are $R_T^2 = 0.90$ and $R^2 = 0.91$, respectively; while over the second segment, they are $R_T^2 = 0.92$ and $R^2 = 0.95$. Since both of these results show that the model, without any re-estimation, continues to explain the data to a level commensurate with that obtained over the original estimation period between samples 8310 to 10309, we can conclude that the model is 'conditionally valid' and can be used for forecasting applications. In such applications, the model would be best transformed into discrete-time, stochastic state space form embedded within a Kalman filter mechanism (see e.g. Young, 1984; Young *et al*, 1997; Young and Tomlin, 2000). However, while the predictive validation results obtained above engender confidence in the model for such forecasting applications, it cannot be considered fully validated in a wider sense, as discussed later in section 6.

5.4 The Effects of Uncertainty in the DBM Model

One final evaluation of the DBM model (5a) concerns the effects of the parametric uncertainty on the mechanistic interpretation of the model. The easiest approach to such analysis is to utilise Monte-Carlo Simulation (MCS) methods (see Young *et al*, 1996; Parkinson and Young, 1998; Young, 1999a). Here, the model is simulated many times (here between 1000 and 5000 times) with the model parameters for each 'random realisation' of this kind generated by randomly sampling the parameters from their parent probability distribution functions (pdf's). In the present context, these pdf's, are assumed to be multivariate Gaussian, with the mean values and covariance matrices shown in equations (5a) to (5e)[6]. Two types of output are obtained from this analysis: first, a response analysis, where the model is perturbed by the actual measured inputs used during the estimation (i.e. y_t , r_t and T_t), with the stochastic noise ξ_t generated, for each realisation, from independent samples of white noise, via equation (5b); and second, a parametric analysis, where each realisation is used to calculate only the 'derived', mechanistically meaningful parameters associated with the parallel flow decomposition. Typical MCS results in the present example are presented in figs.14 to 16. These are not meant to be comprehensive in any way: they are simply illustrative of the kind of uncertainty analysis that is possible using stochastic simulation methods.

INSERT Figs.14 to 16

Fig.14 compares the mean of an ensemble of 1000 stochastic realisations (full line) with the actual data (circles) over the shorter period between samples 8550 and 8660, which is selected to avoid congestion in the graph. This mean response is virtually identical to the deterministic model output $\hat{y}_t$, as would be expected in this case. The dashed lines mark the envelope of the ensemble and thus show the limits of the uncertainty propagation arising from the various uncertain elements in the model. The measured response falls mainly within these bounds, showing that the stochastic model provides a reasonable description of the data. Figs. 15 and 16 are typical of the results obtained from the parametric MCS analysis based on 5000 random realisations: fig.15 shows the histograms of the residence time parameters for the slow and fast parallel TF's (see Table 1); while fig.16 displays the histograms of the partition percentages associated with the parallel pathways, including the instantaneous flow effect. The ensemble mean values agree almost exactly with the values of these parameters derived from the estimated TF parameters, as listed in Table 1.

The sample distributions in figs. 15 show that the estimated slow pathway residence time is much more uncertain than that of the fast pathway; and, while both show signs of minor skewness towards larger values, that of the slow pathway is more pronounced. These results make physical sense, since there is less information in the data on the dynamics of the slow pathway over the sampling interval and it is also describing subsurface processes which are likely to be less well defined. In the case of fig.16, there are some minor signs of skewness in the fast and slow pathway partition percentages, with the former skewed towards higher and the latter towards lower values. The instantaneous distribution seems quite symmetric.

[6] Note the earlier comment on the non-normality of the model residuals. In this case, it means that the covariance matrices will tend to underestimate the parametric uncertainty and this will naturally affect the propagation of this uncertainty in the MCS analysis.

5.5 Comparison of HMC Models

Similar analysis to that described in sections 5.1 to 5.4 has been carried out on the other HMC models discussed in section 4 and some of the estimation results are reported in Appendix 4. There are many ways in which the models can be compared and any one set of comparisons can be misleading. However, the results shown in Table 2, which compares the coefficients of determination R_T^2 and R^2 obtained for each model over the estimation and predictive validation periods, provide a reasonable impression of the comparative performance in this example.

Table 2

	Estimation (8310-10309)		Validation 1 (10310-10674)		Validation 2 (14310-14674)		Validation 3: all 17532 samples	
Model	R_T^2	R^2	R_T^2	R^2	R_T^2	R^2	R_T^2	R^2
DBM	0.91	0.93	0.90	0.91	0.92	0.95	0.85	0.90
DBMS	0.86	0.88	0.87	0.90	0.90	0.92	0.82	0.87
IHACRES	0.82	0.86	0.89	0.91	0.87	0.90	0.82	0.87
BM	0.84	0.87	0.88	0.91	0.91	0.92	0.82	0.86
Best	DBM	DBM	DBM	DBM=	DBM	DBM	DBM	DBM
2nd Best	DBMS	DBMS	IHACRES	IHACRES =	BM	DBMS =	DBM=	DBM=

Table 2 Comparison of coefficients of determination of the HMC models: the equals (=) sign shows that one or more model performed virtually the same

These results are also reflected in the statistical diagnostics. The DBM and DBMS models are clearly superior in this regard: both satisfy most of the statistical requirements on the final stochastic residuals $\hat{e}_t$, failing only marginally in relation to the ccf between these residuals and the effective rainfall input, but with clearly non-normal $\hat{e}_t$. On the other hand, the IHACRES and BM models only satisfy the acf requirement on their $\hat{e}_t$ series: they fail both of the ccf requirements, with many significant violations of confidence bounds at a range of lags. As expected, the distribution of the residuals is clearly non-normal with many outliers.

An indication of how well or badly the model parameters are defined in any nonlinear least squares optimisation exercise is provided by how well the optimisation procedure converges, combined with the resulting covariance properties of the estimates. Here again, there are indications of some problems with the IHACRES and BM models. Whereas convergence is rapid and well defined in the case of the DBM and DBMS models, neither of the other two models converge under the same convergence criteria; and the Matlab algorithm *leastsq*, as used for optimisation in these studies, reports difficulties during convergence for both models. The covariance properties of the optimised estimates are also worse, with some 't' values (the estimated parameter divided by its standard error) noticeably lower in the case of the IHACRES and BM models (although it is well known that the covariance properties obtained during nonlinear numerical optimisation can be misleading).

One common aspect of all four models is the use of a TF model to describe the predominantly linear relationship between the effective rainfall and flow. But, as pointed out previously, the TF model is basically a parametrically efficient way of characterising the largely invariant, unit hydrograph characteristics of the catchment, which is quantified in the present context by the impulse response of the TF model. These TF derived unit hydrographs for all four models are compared in fig.17 and it is clear that they are all very similar: the initial responses, which are dominated by the 'quick flow' component, are virtually identical; while the somewhat longer tails of the IHACRES and BM hydrographs reflect the rather longer residence times of the 'slow flow' components in these cases (see Appendix 4). This is also confirmed by the TF-based flow decomposition results shown in Table 3, where the partition percentages for all the models are reasonably similar.

Table 3

Component	Instantaneous (%)	Fast (%)	Slow (%)
DBM	27.3	19.9	52.8
DBMS	26.1	25.6	48.3
IHACRES	21.0	29.7	49.3
BM	18.4	25.0	56.6
Average	23.2±4.2	25.0±4.0	51.8±3.8

Table 3 Comparison of TF-based flow decomposition partition percentages for the HMC models

These results are comforting in practical terms: they show that, although the four models are rather different in the manner that they characterise the nonlinear catchment storage characteristics, they are quite similar in their quantification of the underlying unit hydrograph aspects of the catchment dynamics which are, of course, such an important icon in both the theory and practice of hydrology.

INSERT Fig.17

Since the catchment storage part of all the four HMC models provides a nonlinear mechanism for generating the effective rainfall series, it is interesting to compare the relationship between the rainfall and effective rainfall series in each case. However, since this relationship is quite complex, a simple graph of effective rainfall against measured rainfall takes the form of a 'scatter plot' and it is difficult to compare these plots in any meaningful manner. One approach to this problem is to exploit the FIS approach to non-parametric estimation outlined in Appendix 2 and estimate a smooth relationship between effective rainfall and measured rainfall for each of the models. The results of this analysis, as shown in fig.18, reveal that there are quite significant differences in the pattern of the transformation in each case: in particular, the DBM model nonlinear transform (full line) lies a little below the others (DBMS, dash-dot; IHACRES, dotted; BM, dashed) for rainfall less than 45 mm; and above them for rainfall greater than this. Moreover, this difference is very significant for rainfall greater than 70 mm, as we see in fig.19: this shows plots of the difference between the effective and measured rainfall for all four models and the increased magnitude of the high rainfall events in the case of the DBM model (upper plot) is obvious. It seems, therefore, that since the linear parts of the models are reasonably well defined and quite similar, the superiority of the DBM model derives from its superior definition of effective rainfall during the higher rainfall episodes.

INSERT Figs.18 and 19

Finally, it is necessary to ask why the DBM model performs significantly better than the other three models. The answer is fairly obvious: the DBM modelling strategy has uncovered the fact that the flow series itself provides a *surrogate measure* of catchment storage and so the model is able to exploit this in the definition of the effective rainfall nonlinearity. In the other models, on the other hand, the catchment storage is an entirely unobserved, latent variable, an *estimate* of which is computed from the rainfall input using the conceptualised storage equations. The differences between these other models lies mainly, therefore, in the nature of these storage equations. The message from this result is also clear: a model should extract all of the useful information in the observational data. If measured variables are available which provide either direct (e.g. soil moisture or evapo-transpiration measurements) or indirect (e.g. the flow measurement as a surrogate for catchment storage) quantification of important variables within the model, they should be incorporated into the model wherever this is possible.

This does not mean, however, that the concept of unobserved (sometimes termed ‘latent’) variables should be dismissed. On the contrary, it is essential in the present context for the construction of models that are useful in a simulation context. Moreover, systems research has shown how the definition and estimation of such latent state variables (state variable estimation and reconstruction, as the in Kalman filter) provides a very powerful, general approach to modelling stochastic dynamic systems. Indeed, one obvious development of the HMC models discussed in this paper is to incorporate them into such a state estimation framework for both optimisation and on-line purposes. This is discussed later in the Conclusions section 6.

5.6 Discussion

The results presented in previous sub-sections show that all of the HMC models considered here perform reasonably well on the Coweeta catchment data. The DBM model (5a) is best in statistical diagnostic and predictive validation terms, with its simulation version, DBMS, having very similar diagnostics but not performing quite as well in the predictive validation tests.

However, these DBMS validation results are not bad (see Table 2) and the model seems marginally superior to the IHACRES and BM models in this regard. Although the latter two models perform poorly in the diagnostic tests, their predictive validation results are quite acceptable. Indeed, they could be used with some confidence in forecasting applications, although they would probably be out-performed by the DBM model in most cases.

The only disadvantage of the DBM model is its inability to function directly in simulation terms. In such applications, its simulation version, DBMS, would have to be used and, as shown above, the differences between this version and both the IHACRES and BM models is not nearly as significant: all three would provide reasonable models in simulation terms, with little to choose between them; and their predictive performance is quite similar, with only a marginal advantage to the DBMS model. Perhaps surprisingly, given its age, the BM model is still very competitive with both the IHACRES and DBMS models in all simulation and predictive respects. If we are to choose between the models, therefore, it is necessary to look further than these quantitative performance measures and consider other, more qualitative, properties of the models, such as their conceptual interpretations. This must be carried out very carefully, however, because it means moving away from objective measures of performance into much less trustworthy subjective areas, where the prior perceptions of the modeller can tend to bias rational judgement.

6. CONCLUSIONS

This chapter has been concerned with the process of constructing models for stochastic, dynamic systems. It has argued that there is no unique mathematical model of any real system; that, in consequence of this, the model has to be chosen on the basis of carefully defined objectives; and that the Data-Based Mechanistic (DBM) approach to modelling stochastic, dynamic systems provides a suitably rigorous statistical framework for such objective-oriented modelling exercises. In more specific terms, the chapter has been concerned with a detailed exploration of the Hybrid Metric-Conceptual (HMC) class of rainfall-flow models; and it has shown how such models may be statistically identified, estimated and validated using DBM methods, as demonstrated by the modelling of rainfall-flow processes in the Coweeta catchment. In relation to the topic of this book, the chapter has also raised questions about the meaning of the term ‘validation’ and to what extent quantitative procedures of predictive validation can engender confidence in a model. The Popperian concept of model falsification, combined with the idea of ‘conditional validation’, has been promoted as a reasonable approach to verifying the practical utility of DBM models, but the possible limitations of such quantitative methods have been mentioned.

Clearly, predictive validation of a data-based rainfall-flow model, as defined in this chapter, is a *necessary* condition for its acceptance, regardless of the study objectives. If the model fails to perform adequately in this predictive sense, then it is hard to see how it can be considered acceptable in any meaningful role, except as a vehicle for scientific debate. But, just as obviously, predictive validation is not a *sufficient* condition for the model's acceptance within the wider hydrological community. The hydrologist is rightly suspicious of the 'black-box' model which performs well in forecasting terms but whose abstract form makes its contact with hydrological reality very tenuous. In this sense, it has been argued that a model needs to have a physically interpretable conceptual basis which is reasonably acceptable within current hydrological paradigms. On the other hand, the model should not be overly constrained by these existing paradigms and the modeller should be willing, even anxious, to attack them if the DBM modelling procedure secures evidence from the experimental data that they may have serious limitations.

In relation to the specific rainfall-flow modelling exercise considered in this chapter, we have seen that a number of HMC models are competitive in their explanation and prediction of the time series data from the Coweeta catchment. If the modelling objective is *forecasting*, then the standard DBM model, particularly if it is made adaptive, has definite theoretical and practical advantages. However, if the model is required for *simulation* purposes, in applications such as management, planning and certain aspects of scientific investigation, then the DBM model is not so useful and the alternative DBMS, IHACRES and BM models come into their own.

In regard to these latter three models, it would appear that the IHACRES and BM models are less satisfactory in statistical terms and the estimated parameters of the nonlinear parts of the models, in particular, are not very well defined. Equifinality plots (Franks *et al*, 1997; Young, 1999a) tend to confirm this and suggest that there are some identifiability problems for these models, deriving mainly from the effective rainfall nonlinearity. Although the DBMS is marginally superior in statistical terms, its nonlinear catchment storage model is also rather ill-defined. Overall, then, it would appear that there is little to choose between the different catchment storage equations used in the three simulation models and, indeed, that any reasonable conceptual storage model would yield similar predictive performance. This is a classic case of equifinality and it means that the models cannot be judged or 'validated' on the basis of their conceptual structure, even though hydrologists may hold great store by this aspect of the model. On the other hand, although all three simulation-type models are statistically inferior to the DBM model, they perform sufficiently well in a predictive sense to make them conditionally valid under our definition of this term. Moreover, they all have a conceptual basis which seems reasonably acceptable within current hydrological paradigms; and they can be employed easily within a simulation context, whether deterministic or stochastic.

It is their ability to function in this stochastic simulation sense that sets these latest HMC models apart from the deterministic simulation models that have so dominated rainfall-flow modelling in the past. The advent of very fast, desktop (and portable[7]) computers, as well as developments in Monte-Carlo simulation methods, mean that deterministic simulation should no longer be the norm: all systems are uncertain to some degree and even models constructed on a largely deterministic basis can now be subjected quite easily to powerful stochastic uncertainty and sensitivity analysis (see e.g. Young *et al*, 1996; Parkinson and Young, 1998; Young 1999a).

Another advantage of the HMC models is that they can be incorporated easily into a stochastic state-space setting. This is useful for two main reasons. First, it can provide a framework for final *stochastic* optimisation, in which the associated Kalman filter is exploited to obtain maximum likelihood estimates of the model parameters (see Appendix 2). Second, the stochastic state space formulation is inherently recursive so that, when combined with the recursive estimation of the model parameters, which is straightforward in the case of the TF models considered here (Young, 1984), it provides a vehicle for on-line adaptive modelling, forecasting and data assimilation. The DBM model appears to be particularly attractive in this context.

So what can we conclude at the end of this investigation of HMC rainfall-flow modelling? Unambiguously, there are good reasons for preferring the DBM model in forecasting applications. But which of the other three HMC models (DBMS, IHACRES or BM) is preferable within the alternative simulation environment? This is almost an impossible question to answer since it requires us to reflect on what is meant by the term 'validation' in wider, semi-quantitative or qualitative terms, where personal subjective judgement becomes a factor. In particular, because all three models perform equally well, with only marginal statistical advantages to the DBMS model, it is necessary to decide which of them has the most attractive conceptual base. Whilst the author has some preferences in this regard, only time will tell which of the models, or any future developments of them, will perform better in practical terms. And it is surely on such practical grounds that any preference should be given.

As regards future developments of the HMC models considered in this chapter, there remain two major problems which need attention. First, the poor identifiability and consequent equifinality of the nonlinear effective rainfall equations in the BM, IHACRES and DBMS models suggest strongly that more research is required on the nature and modelling of the rainfall-flow nonlinearity in such 'simulation' models. The DBM approach may help in such research, since the nonlinearity in the DBM model is much better defined and demonstrates the value of using measured rather than 'latent' variables in defining the nonlinear mechanisms.

---

[7] All of the analysis described in this chapter was carried out on a Macintosh Powerbook 3400c, within a Matlab™ software environment.

Second, in these models and most other rainfall-flow models the author has investigated, the model residuals are clearly non-normal and dominated by large outliers. The statistical analysis in this chapter has largely ignored this problem, but it is clear that superior estimation results and better quantification of the uncertainty in the stochastic models would be obtained if this aspect of rainfall-flow data was taken fully into account.

ACKNOWLEDGEMENTS

The author is grateful for the support of the U.K. Engineering and Physical Sciences Research Council under grant GR/G53866; and to Professor A.J. Jakeman of CRES, Australian National University, for his support during visits to CRES which have strongly influenced the research reported in this Chapter. He is also grateful to his colleagues Dr. Laura Price, Dr. Paul McKenna, Dr. Nick Chappell and Prof. Keith Beven for checking the chapter. Of course, the author remains responsible for any errors or omissions.

APPENDIX 1 DOMINANT MODE BEHAVIOUR

This Appendix presents a simulation example which demonstrates the importance of dominant modal behaviour in model identification and estimation. The simulated model is of 26th order with one sample pure (advective) time delay and consists of 26 first order processes in series, each with unity gain and lag coefficient ranging from 0.1 in steps of 0.02 to 0.6 (e.g. time constant (residence times) from 0.43 to 1.96 days). In this sense, it could represent a ‘lag and route’ model of flow in a long river; or an ADZ model of solute transport, also in a long river. Since the model is an ‘all pole’ TF (i.e. the numerator TF is a scalar), the SRIV identification stage in the analysis is constrained to such models and a selection of the results are presented in Table A1 (even better fitting models can be identified if this restriction is removed). These were obtained from the analysis of the noise-free impulse response data (unit hydrograph in hydrological terms) generated by the 26th order simulation model. Although the best identified model is only 7th order with a pure time delay of 3 sampling intervals, it is extremely well identified, with a very negative YIC value and a coefficient of determination R_T^2 of nearly unity. Neither the SRIV algorithm nor the PEM algorithm in Matlab converged at all for model orders greater than 10, indicating severe identifiability problems in these higher order cases. In other words, it is impossible to identify the true model from the simulation data, despite the fact that the data are noise-free.

Table A1 SRIV Identification Results

Model Structure	YIC	R_T^2	σ_ξ^2	% error by variance	% error by stand.dev.
7 1 3	-26.0291	0.999990	0.000139	0.0010	0.3131
6 1 4	-22.8568	0.999936	0.000907	0.0064	0.7999
7 1 2	-22.3942	0.999833	0.00235	0.0166	1.2876
6 1 3	-22.5934	0.999819	0.00256	0.0181	1.3439
5 1 5	-20.9560	0.999740	0.00367	0.0259	1.6091

The best identified 7th order model takes the following form:

$$y_t = \frac{0.0001169}{1 - 5.65z^{-1} + 13.93z^{-2} - 19.39z^{-3} + 16.47z^{-4} - 8.54z^{-5} + 2.50z^{-6} - 0.32z^{-7}} u_{t-3}$$

where the denominator polynomial coefficients have been rounded to 2 decimal places. The standard errors on the estimated parameters are very small and so these are not reported. The steady state gain of this reduced order model is insignificantly different from the unity value of the 26th order model. If the 26th order model is now perturbed by a *different* input, in the form of the Coweeta rainfall data from sample 8310 to 8810, then the above model performs in a very similar manner, with a percentage error by variance of 0.001 and by standard deviation of 0.3205, despite the fact that the input data is so different in this 'validation' test.

These results are confirmed by the power decomposition analysis of Liaw (1986), which shows that the percentage power contributed to the response of the 26th order model by the first seven modes is 99.6% of the total power in the model response, and this power is distributed as follows:

Table A2 Liaw Analysis Results

dynamic mode	1	2	3	4	5	6	7
% power	48.30	28.47	11.67	6.37	2.60	1.69	0.49

In other words, practically all of the model response is explained by the effect of these dominant modes and, in fact, the first five modes explain approximately 97.5% of the response.

The message provided by this example is clear: a high order linear system can be approximated almost exactly by a much lower order linear system (often including an additional pure time delay) which reflects the dominant modes of the system's dynamic behaviour. Since this result is generic and certainly applies to most linear dynamic systems of the kind encountered in environmental and hydrological science, the consequences on model identification and parameter estimation are profound. In particular, the identifiable order of a dynamic system is clearly limited by its dominant mode characteristics; and it is impossible, in almost all practical situations, to unambiguously estimate the parameters from experimental data, even when the level of noise of the data is very low.

APPENDIX 2 NON-STATIONARY AND NONLINEAR MODEL ESTIMATION

This Appendix outlines the approach to time variable and state dependent parameter estimation employed in the DBM modelling of non-stationary and nonlinear systems. In the main text, this is used to identify the nature of the effective rainfall nonlinearity shown in fig.3.

The TVP/SDP Model

In discrete-time, sampled data terms, the behaviour of a typical measured variable y_t can be described by a general stochastic, dynamic equation of the form,

$$y_t = \quad \{\chi_t, \mu_t\} \qquad \text{(A2.1)}$$

where $\{\,\}$ is a reasonably behaved, nonlinear function of the variables in an extended or *Non-Minimum State Space* (NMSS; see Young *et al*, 1987) defined by the following NMSS state vector,

$$\chi_t = [y_{t-1} \cdots y_{t-n}\ \mathbf{u}_t^T \cdots \mathbf{u}_{t-m}^T\ \mathbf{U}_t^T \cdots \mathbf{U}_{t-q}^T]^T$$

We see that χ_t is composed of the past values of y_t, as well as present and past values of a deterministic input (or exogenous) variable vector $\mathbf{u}_t$ with elements $u_{i,t}, i = 1,2,...,r$; and the present and past values of a vector $\mathbf{U}_t$ of other exogenous variables $U_{j,t}, j = 1,2,..., p$. Finally, μ_t is an unobserved, zero mean, stochastic process with fairly general properties, which is the source of all stochasticity in the system and is assumed to be independent of the input variables $u_{i,t}$ and $U_{j,t}$.

This model assumes that y_t is causally related to the *primary* input variables $u_{i,t}$; while the vector $\mathbf{U}_t$ represents any other associated variables which *may* affect the system nonlinearly but whose relevance in this regard may not be clear prior to time-series analysis. For example, in the rainfall-flow case, y_t is the flow measurement, $u_{1,t} = r_t$ is the rainfall; and $U_{1,t} = T_t$ is the temperature.

If, for simplicity, we consider the case of a single, primary, input variable, so that $r = 1$ then, following arguments similar to those presented in Young (1993) and Young and Beven (1994), the nonlinear model (A2.1) can be approximated by the following general TF model with time or state dependent parameters,

$$y_t = \frac{B(t,z^{-1})}{A(t,z^{-1})} u_{t-\delta} = \frac{b_{0,t} + b_{1,t}z^{-1} + \cdots + b_{m,t}z^{-m}}{1 + a_{1,t}z^{-1} + \cdots + a_{n,t}z^{-n}} u_{t-\delta} + \xi_t \qquad \text{(A2.2a)}$$

or,

$$y_t = x_t + \xi_t \tag{A2.2b}$$

where x_t, which can be considered as the noise free output of the model, is defined as,

$$x_t = \frac{B(t,z^{-1})}{A(t,z^{-1})} u_{t-\delta} \tag{A2.2c}$$

ξ_t is a stochastic noise term arising from the stochastic disturbance μ_t in (A2.1) which, like μ_t, is assumed to be statistically independent of the input variable u_t; and δ is any pure time delay affecting the relationship between u_t and y_t.

The model (A2.2) is a time/state dependent parameter version of a standard TF model, such as equation (1) in the main text, where the polynomial parameters are assumed to be possible functions of the time index t. In the present context, these Time Variable (TVP) or State Dependent (SDP) parameters will reflect the nature of any nonstationary or nonlinear aspects of the system behaviour; and their statistical estimates, based on the data $\{y_t, u_t\}$, should provide a potential source of information on the nature of the nonstationarity and/or nonlinearity in the system. The approximation of the nonlinear system by a TVP/SDP model such as (A2.2) is the key assumption in the first stage of DBM modelling. As shown in Young (1984, 1988, 1993, 1998a,b,c, 1999b) and Young and Beven (1994), TVP/SDP estimation is based on a powerful *Fixed Interval Smoothing* (FIS) method of recursive estimation. The details of FIS estimation are given in these prior publications and so it will suffice here to present only the latest improvements to the procedures described in these earlier publications.

FIS Estimation of TVP's

The FIS algorithm is applied to the following alternative vector form of the TF model (A2.2), where the pure time delay δ has been omitted to simplify the presentation:

$$y_t = \mathbf{z}_t^T \mathbf{a}_t + \eta_t; \qquad t = 1,2,\cdots,N \tag{A2.3}$$

where,

$$\mathbf{z}_t^T = [-y_{t-1} \; -y_{t-2} \; \cdots -y_{t-n} \; u_t \; \cdots \; u_{t-m}];$$
$$\mathbf{a}_t = [a_{1,t} \; a_{2,t} \; \cdots \; a_{n,t} \; b_{0,t} \; \cdots \; b_{m,t}]^T$$

and η_t is a stochastic noise term arising from the presence of ξ_t in (A2.2). We can say little about the statistical properties of η_t because of the general TVP nature of the model. Consequently, it will be assumed that, once again, it is statistically independent of the input variable u_t.

Based on this model form, the FIS algorithm provides an estimate $\hat{\mathbf{a}}_{t|N}$ of the model parameter vector $\mathbf{a}_t$ at every sampling instant, conditional on the time-series data $\{y_t,\ u_t\}$ over the whole observation interval $t = 1,2,\cdots,N$. In addition, if the noise η_t is assumed to be a zero mean sequence of serially uncorrelated random variables (discrete white noise), it also yields an estimate, at each sampling instant, of the covariance matrix $\mathbf{P}_t = E\{\tilde{\mathbf{a}}_{t|N}\tilde{\mathbf{a}}_{t|N}^T\}$, where $\tilde{\mathbf{a}}_{t|N} = \hat{\mathbf{a}}_{t|N} - \mathbf{a}_t$ is the estimation error. If η_t is not white noise, then the matrix $\mathbf{P}_t$, as derived from the FIS algorithm in the same manner, will not provide an accurate estimate of the covariance properties of the FIS estimates. Nevertheless, it still provides information on the *relative* accuracy of the parameter estimates which can, as we shall see, prove useful in evaluating the detailed nature of the estimated parameter variations.

FIS Estimation of SDP's by Sorting and Backfitting

FIS estimation of the TVP vector $\mathbf{a}_t$ in (A2.3) is limited to slowly varying parameters: i.e. parameters that vary slowly in relation to the variations in the input and output variables y_t and u_t. In the case where $\mathbf{a}_t$ is a SDP vector, on the other hand, the estimation procedure normally needs to be modified. In particular, it becomes necessary to sort the data in a non-temporal order, so that the SDP variations are smoother and less rapid. In this manner, the FIS algorithm is able to estimate the parametric variations more easily and so obtain more accurate, lower variance estimates. For example, if the time series are sorted in some common 'ascending order' manner (the *sort* operation in Matlab), then the rapid natural variations in y_t and u_t are effectively eliminated from the data and replaced, in the sorted data space, by much smoother and less rapid variations. And if the SDP's are, indeed, related to these variables, then they will be similarly affected by the sorting. Following FIS estimation, however, these SDP estimates can be 'unsorted' (a trivial *unsort* operation to reverse Matlab's *sort*) and their true, rapid variation becomes apparent.

One obvious requirement with this new approach to SDP estimation is that the sorting of data, prior to FIS estimation, must be *common to all of the variables in the relationship* (A2.3). If an 'ascending order' strategy is selected, therefore, it is necessary to decide upon which variable in the model the sorting should be based. The simplest strategy is to sort according to the ascending order of the 'dependent' variable y_t (here flow). Depending upon the nature of each SDP in the vector $\mathbf{a}_t$, however, a single variable sorting strategy, such of this, may not produce entirely satisfactory results. If this is the case, then a more complicated, but still straightforward, 'backfitting' procedure is exploited. Here, each parameter is estimated *in turn*, based on the 'partial residual' series obtained by subtracting all the other terms on the right hand side of

(A2.3) from y_t. In this situation, the sorting at each such backfitting iteration can be based on the single variable associated with the current SDP being estimated.

To clarify this backfitting procedure, let us consider the DBM rainfall-flow model discussed in the main text. The analysis starts by considering the simplest TVP/SDP relationship that might explain the dynamic relationship between the rainfall r_t, temperature T_t and flow y_t. Initial SRIV identification suggests that, in the case of the Coweeta data, this is the following first order model:

$$y_t = b + \frac{b_{0,t}}{1 + a_{1,t} z^{-1}} r_t + \frac{f z^{-6}}{1 + g z^{-1}} T_t + \xi_t \qquad \text{(A2.4)}$$

where it will be noted that the second TF between T_t and flow is identified as being linear with *constant* parameters. If all terms except the noise ξ_t and TF between r_t and y_t are taken to the left hand side of the equation (since they involve only parameters that have been identified as constant over time), then equation (A2.4) can be written in the form,

$$y_t = \frac{b_{0,t}}{1 + a_{1,t} z^{-1}} r_t + \xi_t \qquad \text{(A2.5a)}$$

where,

$$y_t = y_t - b - \frac{f z^{-6}}{1 + g z^{-1}} T_t \qquad \text{(A2.5b)}$$

or, considering (A2.5a) in equation form,

$$y_t = -a_{1,t} y_{t-1} + b_{0,t} r_t + \eta_t \qquad \text{(A2.5c)}$$

which is a first order example of the general model (A2.3) with y_t replaced by y_t.

In this case, sorting according to the ascending order of y_t yields sensible FIS estimation results (see fig.3), in the sense that the smoothed SDP estimates are relatively smooth and the SDP model explains the data well with $R_T^2 = 0.9$. However, if this were not the case, backfitting would need to be invoked. A typical algorithmic approach would then be as follows:-

- Assume that, without any sorting (i.e. as in the previous studies of Young, 1993, Young and Beven, 1994), FIS estimation has yielded prior TVP estimates $\hat{a}^1_{1,t|N}$ and $\hat{b}^1_{0,t|N}$ of $a_{1,t}$ and $b_{0,t}$, respectively[8]. An SDP estimation equation for $a_{1,t}$ can then be formulated as,

[8] These could be simply the SRIV *constant* parameter estimates, since the convergence of the backfitting procedure is not too sensitive to the prior estimates, provided they are reasonable. Here, for example, the SRIV constant parameter estimates yield an $R_T^2 = 0.74$ and SDP estimation raises this to $R_T^2 = 0.9$.

$$[y_t - \hat{b}^1_{0,t|N} r_t]^{sy} = a^{sy}_{1,t} (y_{t-1})^{sy} \tag{A2.6}$$

where the superscript sy denotes that all the variables are sorted in the ascending order of the right hand side variable y_{t-1} in (A2.5c), which is associated with the SDP $a_{1,t}$. This yields the FIS estimate $a^{sy}_{1,t|N}$ of $a^{sy}_{1,t}$.

- $a^{sy}_{1,t|N}$ is then 'unsorted' so that the SDP estimation equation for $b_{0,t}$ can be formulated as,

$$[y_t + \hat{a}_{1,t|N} y_{t-1}]^{su} = b^{su}_{0,t} r^{su}_t \tag{A2.7}$$

with the variables now sorted according to the ascending order of the rainfall variable r_t associated with $b_{0,t}$. This yields the FIS estimate $\hat{b}^{su}_{0,t|N}$ and the first iteration of the 'backfitting' algorithm is complete.

- This process is continued in an iterative manner (each time unsorting, forming the partial residual, and sorting according to the current right hand side variable, prior to FIS estimation), until the FIS estimates of the SDP's $\hat{a}_{1,t|N}$ and $\hat{b}_{0,t|N}$ (which are each time-series of length N) do not change significantly between iterations. The smoothing 'hyper-parameter' required for FIS estimation at each iteration is optimised by Maximum Likelihood (ML), based on prediction error decomposition (see Young, 1999b).

Since the SDP estimates resulting from this backfitting algorithm are themselves time series, the algorithm constitutes a special form of non-parametric estimation and, as such, can be compared with the Generalised Additive Modelling (GAM) approach of Hastie and Tibshirani (1996). However, in both conceptual and algorithmic terms, the algorithm is significantly different from this earlier approach. Indeed, in the current dynamic modelling context, the GAM backfitting algorithm will only produce unbiased estimates of the SDP's in (A2.5c) if the noise η_t is zero mean, serially uncorrelated and independent of any noise on the model variables y_t and u_t (i.e. the SDP version of the AutoRegressive eXogenous variable (ARX) model, rather than the more general TF model considered here). However, by exploiting a new instrumental variable form of the FIS algorithm (Young and McKenna, 1999), the proposed backfitting algorithm is not limited in this manner and is able to produce unbiased non-parametric estimates of the TF model parameters.

Final Nonlinear Model Estimation.

The primary aim of the non-parametric FIS analysis in previous sections of this Appendix is to identify a sensible functional form for any nonlinearities in the model; *in other words, the* *analysis is aimed at nonlinear model structure identification.* In general, this identification phase is completed by fitting a *finite dimensional* parametric function to the non-parametric estimate of the nonlinearity using Weighted Least Squares (WLS) estimation, as discussed in Young (1993) and Young and Beven (1994), where the weighting is a function of the error covariance matrix $\mathbf{P}_t$ generated by the FIS algorithm. Fig.3 illustrates this procedure within the present rainfall-flow modelling context: the dots show the estimate $\hat{b}_{0,t|N}$ plotted against the modified flow variable y_t and the full line is the WLS estimate of a power law relationship of the form $\hat{b}_{0,t|N} = \alpha(y_t)^{\beta}$ (see the comments about this in the main text). The backfitting procedure suggest that the lag parameter $a_{1,t}$ does not change too significantly over the observation interval and so it is assumed time-invariant in this case. As a result, the identified model, incorporating the power law, takes the form,

$$y_t = \frac{b_0}{1 - a_1 z^{-1}} u_t + \xi_t \quad ; \quad u_t = c(y_t)^{\beta} \qquad \text{(A2.8)}$$

where $b_0.c = \alpha$. This constitutes the end of the first stage of nonlinear DBM model identification.

The model (A2.8) explains the Coweeta data reasonably well but further SRIV identification and estimation with u_t defined as in (A2.8) suggests that the dynamics are a little more complicated than this, with a second order relationship indicated between the modified (effective) rainfall u_t and y_t. As a result the finally identified model structure takes the form shown in equation (5a) of the main text. Once a plausible structural form for the nonlinear model, such as this has been identified, however, it is then necessary to finally re-estimate the model against the time-series data by some form of numerical optimisation (e.g. deterministic minimisation of the model residual variance; maximum likelihood estimation; prediction error minimisation etc.), the exact nature of which will tend to depend on the identified form of the model.

In the present rainfall-flow example, the nonlinearity resides only in the effective rainfall input, so that the linear and nonlinear parts of the model are relatively separable. As a result, the optimisation method used to obtain the model (5a) involves optimising the nonlinear component parameters with, at each step in the optimisation, the linear TF model parameters estimated by SRIV estimation. As pointed out in the Conclusions section of the paper, this can be considered as an approximation to a more elegant (but computationally more demanding) Maximum Likelihood (ML) procedure based on prediction error decomposition (see Schweppe, 1965; Harvey, 1989). Recent research (Young, 1999c, which considers the modelling of blowfly population dynamics) has suggested, however, that the recursive ML methodology is feasible for highly nonlinear stochastic systems and its application to rainfall-flow modelling is now being considered.

A SUMMARY OF THE COMPLETE DBM PROCEDURE FOR A SISO SYSTEM

In the case of a single input-single output system, the analysis discussed in the previous sub-sections can be summarised as follows:

(1) Examine the available time-series data $\{y_t, u_t\}$ and use these to estimate the parameters in the best identified, constant parameter TF model using a reliable method of TF model identification and estimation (here the SRIV method). Apply standard statistical tests to the model residuals, including tests for nonlinearity (e.g. Billings and Voon, 1986): if the results indicate linearity then the linear model can be accepted and the analysis is complete. Alternatively, proceed to step (2)

(2) Based on the analysis in (1) and any knowledge about the physical nature of the system, select: (a) the variables that could characterise the NMSS vector; and (b), the simplest TF model that appears capable of characterising the behaviour of the output variable y_t in relation to the observed input u_t (this will often be a first or second order model).

(3) Use FIS estimation to obtain initial non-parametric TVP estimates of the parameters in the initial, simple TF model and define those parameters in $\hat{\mathbf{a}}_t$ which show significant variation over the observation interval. If any TVP/SDP parameters are identified, then obtain the FIS estimate of the TF model parameter vector $\hat{\mathbf{a}}_{t|N}$, if necessary (in the SDP case) using the backfitting algorithm. Note the relative accuracy of these estimates over time by reference to the appropriate diagonal elements of the covariance matrix $\mathbf{P}_{t|N}$.

(4) Examine the nature of the FIS estimated time variation in the parameters in relation to all the variables in the defined NMSS vector, using devices such as scatter plots, correlation analysis etc., in all cases taking into account the relative accuracy of the FIS estimates identified in (3). On the basis of these results and a physically meaningful interpretation of the model, define nonlinear, parametric relationships that are able to approximate the FIS estimated non-parametric relationships.

(5) On the basis of the results in (4), use WLS estimation to estimate the constant parameters which characterise these nonlinear laws, with the weighting defined by the diagonal elements of the covariance matrix $\mathbf{P}_{t|N}$.

(6) Use the estimates of the parameters in (5) as starting values in a final model estimation stage where the (hopefully constant) parameters in the identified nonlinear, stochastic model are estimated by some form of numerical optimisation based on the identified nonlinear model form and all the relevant data in the NMSS vector.

(7) Analyse the residuals from the nonlinear estimation to ensure that there is no evidence of any residual nonlinearity not identified in steps (1)-(6). This should include standard statistical tests, such as correlation analysis and normality statistics, as used in the main text, as well as nonlinearity tests on the residuals (e.g. Billings and Voon, 1986).

APPENDIX 3 MODEL ORDER IDENTIFICATION

In DBM modelling, model order identification is based around the R_T^2, YIC and AIC criteria, which are defined as follows, where y_t is the measured output of the system:-

(i) $R_T^2 = 1 - \frac{\hat{\sigma}^2}{\sigma_y^2}$; $\sigma_y^2 = \frac{1}{N}\sum_{t=1}^{t=N}[y_t - \bar{y}]^2$; $\bar{y} = \frac{1}{N}\sum_{k=1}^{k=N} y_t$

(ii) $\text{YIC} = \log_e \frac{\hat{\sigma}^2}{\sigma_y^2} + \log_e\{\text{NEVN}\}$; $\text{NEVN} = \frac{1}{np}\sum_{i=1}^{i=np}\frac{\hat{\sigma}^2.\hat{p}_{ii}}{\hat{a}_i^2}$

(iii) $\text{AIC}(np) = N\log_e \hat{\sigma}^2 + 2.np$

Here $\hat{\sigma}^2$ is the variance of the model residuals; σ_y^2 is the variance of $y_t - \bar{y}$; $np=n+m+1$ is the number of estimated parameters in the $\hat{\mathbf{a}}_N$ vector; $\hat{p}_{ii}$ is the *ith* diagonal element of the $\hat{\mathbf{P}}_t$ covariance matrix obtained from the estimation analysis (so that $\hat{\sigma}^2.\hat{p}_{ii}$ can be considered as an approximate estimate of the variance of the estimated uncertainty on the *ith* parameter estimate); and $\hat{a}_i^2$ is the square of the *ith* parameter estimate in the $\hat{\mathbf{a}}_N$ vector.

We see that the coefficient of determination R_T^2 is a statistical measure of how well the model explains the data: if the variance of the model residuals $\hat{\sigma}^2$ is low compared with the variance of the data σ_y^2, then R_T^2 tends towards unity; while if $\hat{\sigma}^2$ is of similar magnitude to σ_y^2 then it tends towards zero (and can become negative). Note, however, that R_T^2 is based on the variance of the model errors $\hat{e}(k)$ and it is *not* the more conventional coefficient of determination R^2 based on the variance of the *one step ahead prediction errors*: this is because R_T^2 is a more discerning measure than R^2 for TF model identification.

The YIC is more a more complex, heuristic criterion. From the definition of R_T^2, we see that the first term is simply a relative measure of how well the model explains the data: the smaller the model residuals the more negative the term becomes. The second term, on the other hand, provides a measure of the conditioning of the Instrumental Product Matrix (IPM), which needs to be inverted when the IV normal equations are solved (see Young, 1984): if the model is over-parameterised, then it can be shown that the IPM will tend to singularity and, because of its ill-conditioning, the elements of its inverse $\hat{\mathbf{P}}_t$ will increase in value, often by several orders of magnitude. When this happens, the second term in the YIC tends to dominate the criterion function, indicating over-parameterisation. An alternative, justification of the YIC can be obtained from statistical considerations (see e.g. Young, 1989). Although heuristic, the YIC has proven very useful in practical identification terms over the past ten years: it should not, however, be used as a sole arbiter of model order and improvements in its definition are being researched.

Finally, the Akaike Information Criterion AIC is a well known identification criterion for AR processes (Akaike, 1974) and is used here to identify the order of AR models for the noise process ξ_t, based on the analysis of the model residuals $\hat{e}_t$. Here, the first term is a measure of how well the model explains the data; while the second term is simply a penalty on the number of parameters in the model. Thus, as in the YIC, the AIC seeks a compromise between the degree of model fit and the complexity of the model.

APPENDIX 4 BM, IHACRES AND DBMS ESTIMATION RESULTS

This Appendix reports the most significant of the estimation results for the BM, IHACRES and DBMS models. The complete results are not reported to conserve space.

BM Model

Instantaneous TF (A)			
Eig	SSG	TC	% of $\hat{y}_{1,t}$ flow
0	0.17	0.00	18.4
Fast Flow TF (B)			
Eig	SSG	TC	% of $\hat{y}_{1,t}$ flow
0.52	0.22	1.49	25.0
Slow Flow TF (C)			
Eig	SSG	TC	% of $\hat{y}_{1,t}$ flow
0.98	0.51	43.0	56.6
Constant Base flow			
0.50 (t)			

$\hat{\beta}$ = 0.95(0.02); $\hat{T}_r$ = 31.32(0.52); τ_s = 7.16(0.48)

(Note: to allow for comparison with the IHACRES model, T_m in equation 2(i) was replaced by the daily temperature T_t)

IHACRES Model

Instantaneous TF (A)			
Eig	SSG	TC	% of $\hat{y}_{1,t}$ flow
0	0.17	0.00	21.0
Fast Flow TF (B)			
Eig	SSG	TC	% of $\hat{y}_{1,t}$ flow
0.52	0.24	1.53	29.7
Slow Flow TF (C)			
Eig	SSG	TC	% of $\hat{y}_{1,t}$ flow
0.97	0.40	33.9	49.3
Constant Base flow			
0.88 (*t*)			

DBMS Model

Instantaneous TF (A)			
Eig	SSG	TC	% of $\hat{y}_{1,t}$ flow
0	0.17	0.00	26.1
Fast Flow TF (B)			
Eig	SSG	TC	% of $\hat{y}_{1,t}$ flow
0.38	0.17	1.03	25.6
Slow Flow TF (C)			
Eig	SSG	TC	% of $\hat{y}_{1,t}$ flow
0.92	0.32	12.66	48.3
Slow Temperature (Seasonal) Effect (D)			
Eig	SSG	TC	TD
0.97	- 0.23	9.63	6
Constant Base flow			
1.82 (*t*)			

$\hat{\beta} = 1.49(0.07)$; $\hat{c} = 0.87(0.007)$; 0.036(0.001)

REFERENCES

Abbott, M.B., Bathurst, J.C., Cunge, J.A., O'Connell, P.E. and Rasmussen, J.L. (1986) An introduction to the European Hydrology System (SHE). 2: Structure of a physically based distributed modelling system. *Journal of Hydrology,* **87**, 61-77.

Akaike, H. (1974) A new look at statistical model identification, *IEEE Trans. Auto. Control*, **AC-19**, 716-723.

Bacon, F. (1620) *Novum Organum.*

Beck, M.B. and Young, P.C. (1975) A Dynamic Model for DO-BOD Relationships in a Non-Tidal Stream, *Water Research,* **9**, 769-776

Beer, T. and Young, P.C. (1983) Longitudinal Dispersion in Natural Streams, *Am. Soc. of Civil Eng., Jnl. Env. Eng.,* **109**, 1049-1067.

Beven, K.J. (1999) Chapter ?, in this book.

Beven, K.J. and Kirkby, M.J. (1979) A physically-based variable contributing area model of basin hydrology, *Hydrological Sciences Journal*, **24**, 43-69.

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

Box, G.E.P. and Jenkins, G.M. (1970) *Time Series analysis Forecasting and Control*, Holden-Day: San Francisco.

Chappell, N.A., McKenna, P., Bidin, K., Douglas, I. and Walsh, R.P.D. (1999) Parsimonious modelling of water and suspended-sediment flux from nested-catchments affected by selective tropical forestry, *Philosophical Transactions: Biological Sciences*, in press.

Crawford, N.H. and Linsley, R.K. (1966) Digital simulation in hydrology: the Stanford Watershed Model IV, *Tech. Report 39, Stanford University, California.*

Franks, S., Beven, K.J., Quinn, P.F. and Wright, I (1997) On the sensitivity of soil-vegetation-atmosphere transfer (SVAT) schemes: equifinality and the problem of robust calibration, *Agric. Forest Meteorol.*, **86**, 63-75.

Gamerman, D. (1997). *Markov Chain Monte Carlo*, Chapman and Hall: London.

Goodwin, G.C. and Payne, R.L. (1977) *Dynamic System Identification: Experiment Design and Data Analysis.* Academic Press, New York.

Hasselmann, K. (1998) Climate-change research after Kyoto, *Nature,* **390**, 225-226.

Hasselmann, K., Hasselmann, S., Giering, R., Ocana, V. and Storch, H. von (1997) Sensitivity study of optimal CO_2 emission paths using a simplified structural integrated assessment (SIAM), *Climate Change,* **37**, 345-386.

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

Hastie, T.J. and Tibshirani, R.J. (1996) *Generalized Additive Models,* Chapman and Hall: London.

Hornberger, G.M., Beven, K.J., Cosby, B.J. and Sappington, D.E. (1985) Shenandoah watershed study: calibration of a topography-based variable contributing area hydrological model for a small forested catchment, *Water Resources Research*, **21** 1841-1850.

Jakeman, A.J. and Hornberger, G.M. (1993) How much complexity is warranted in a rainfall-runoff model? *Water Resources Research*, **29**, 2637-2649.

Jakeman, A.J. and Young, P.C. (1981) Recursive filtering and the inversion of ill-posed causal problems, *Utilitas Math.*, **25**, 351-376

Jakeman, A.J., Littlewood, I.G and Whitehead, P.G. (1990) Computation of the instantaneous unit hydrograph and identifiable component flows with application to two small upland catchments, *Journal of Hydrology*, **117**, 275-300.

Johnston, J. and DiNardo, J. (1997) *Econometric Methods (4th edition)*, McGraw-Hill: New York.

Kirkby, M.J. (1976) Hydrograph modelling strategies, in R.J. Peel, M. Chisholm and P. Haggett (eds.), *Processes in Physical and Human Geography*, Academic Press: London, 69-90.

Konikow, L.F. and Bredehoeft, J.D. (1992) Ground water models cannot be validated, *Advances in Water Resources*, **15**, 75-83.

Kuhn, T. (1962: 2nd edition 1980) *The Structure of Scientific Revolutions*, University of Chicago: Chicago.

Lees, M., Young, P.C., Beven, K. J., Ferguson, S. and Burns, J. (1994) An adaptive flood warning system for the River Nith at Dumfries, in W. R. White and J. Watts (eds.) *River Flood Hydraulics*, Institute of Hydrology: Wallingford.

Liaw, C.M. (1986) Model reduction of discrete systems using the power decomposition method, *IEE Proc*., **133**, Pt.D, 30-34.

Oreskes, N., Shrader-Frechette, K. and Belitz, K. (1994) Verification, validation, and confirmation of numerical models in the earth sciences, *Science*, **263**, 641-646.

Parkinson, S.D. and Young, P.C. (1998) Uncertainty and sensitivity in global carbon cycle modelling, *Climate Research*, in press.

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

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

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

Wallis, S.G., Young, P.C. and Beven, K.J. (1989) Experimental investigation of the aggregated dead zone model for longitudinal solute transport in stream channels, *Proc. Inst. of Civil Engrs, Part 2*, **87**, 1-22.

Weyman, D.R. (1975) *Runoff Processes and Streamflow Modelling*, Oxford Univ. Press: Oxford.

Wheater, H.S., Jakeman, A.J. and Beven. K.J. (1993) Progress and directions in rainfall-run-off modelling. Chapter 5 in A.J. Jakeman, M.B. Beck and M.J. McAleer (eds.), *Modelling Change in Environmental Systems*, Wiley: Chichester.

Whitehead, P.G. and Young, P.C. (1975) A recursive approach to time series analysis for multivariable systems, in G.C. Vansteenkiste (ed.), *Modeling and Simulation of Water Resource Systems*, 39-58, North Holland: Amsterdam.

Ye, S., Jakeman, A.J. and Young, P.C. (1998) Identification of improved rainfall-runoff models for an ephemeral low yielding Australian catchment, *Environmental Modelling and Software*, **13**, 59-74.

Young, P.C. (1974) Recursive approaches to time series analysis, *Bull. of Inst. Maths and its Applications*, **10**, 209-224.

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

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

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

Young, P.C. (1985) The instrumental variable method: a practical approach to identification and system parameter estimation, in H.A.Barker and P.C.Young (eds.), *Identification and System Parameter Estimation*, Pergamon Press: Oxford, 1-16

Young, P.C. (1986) Time-series methods and recursive estimation in hydrological systems analysis, Chapter 6 in D.A. Kraijenhoff and J.R. Moll (eds.), *River Flow Modelling and Forecasting*, D. Reidel: Dordrecht, 129-180.

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*, 33-44, Pergamon Press: Oxford.

Young, P.C. (1992) Parallel processes in hydrology and water quality: a unified time series approach, *Jnl. Inst. of Water and Env. Man.*, **6**, 598-612,.

Young, P.C. (1993) Time variable and state dependent parameter modelling of nonstationary and nonlinear time series, Chapter 26 in T. Subba Rao (ed.), *Developments in Time Series*, 374-413, Chapman and Hall: London.

Young, P.C. (1994) Time variable parameter and trend estimation in nonstationary economic time series, *Journal of Forecasting, special issue on Time Series Advances in Economic Forecasting*, **13**, 179-210.

Young, P.C. (1996) Identification, estimation and control of continuous-time and delta operator systems, in M.I. Friswell and J.E. Mottershead (eds.), *Identification in Engineering Systems*, , University of Wales: Swansea, 1-17.

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

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

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

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

Young, P.C. (1999c) Data-based mechanistic modelling and the Nicholson blowfly experiments, in preparation.

Young, P.C. and Jakeman, A.J. (1979) Refined instrumental variable methods of recursive time-series analysis: part I, single input, single output systems. *Int. Jnl. of Control*, **29**, 1-30.

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

Young, P.C. and Lees, M.J. (1993) The Active Mixing Volume (AMV): a new concept in modelling environmental systems, Chapter 1 in V. Barnett and K.F. Turkman (eds.), *Statistics for the Environment*, , 3-44, J. Wiley: Chichester.

Young, P.C. and Minchin, P. (1991) Environmetric time-series analysis: modelling natural systems from experimental time-series data, *Int. Jnl. Biol. Macromol.*, **13**, 190-201.

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

Young, P.C. and Chotai, A. (1997) Data-based mechanistic modelling of natural systems, in *Proc. IFAC Conference on Biomedical Systems, Warwick*, Pergamon Press: Oxford.

Young, P.C. and McKenna, P. (1999) An instrumental variable method of fixed interval smoothing for time variable and state dependent parameter estimation, in preparation.

Young, P.C and Pedregal, D.(1998) Data-based Mechanistic Modelling, Chapter 6 in C. Heij and H. Schumacher (eds.), *System Dynamics in Economic and Financial Models*, , J. Wiley: Chichester, 169-213.

Young, P.C and Pedregal, D.(1999) Macro-economic relativity: Government spending, private investment and unemployment in the USA 1948-1998, *Structural Change and Economic Dynamics*, in press.

Young, P. C. and Tomlin, C. M. (2000) Data-based mechanistic modelling and adaptive flow forecasting, in P. Walshe and M. Lees (eds.) *Flood forecasting: what does current research offer the practitioner?* British Hydrological Society Occasional Paper, in press.

Young, P.C. and Wallis, S.G. (1994) Solute transport and dispersion in channels, appears as Chapter 6 in K.J. Beven and M.J. Kirkby (eds.) *Channel Networks*. Wiley: Chichester, 129-173.

Young, P.C., Jakeman, A.J. and Post, D. (1998) Recent advances in the data-based modelling and analysis of hydrological systems, *Water Science and Technology*, **36**, 99-116.

Young, P.C., Parkinson, S.D., and Lees, M. (1996) Simplicity out of complexity in environmental systems: Occam's Razor revisited. *J. Appl. Stat.*, **23**, 2&3, 165-210.

Young, P.C., Behzhadi, M.A., Wang, C.L. and Chotai, A. (1987) Direct digital and adaptive control by input-output, state variable feedback, *Int. Jnl. of Cont.*, **46**, 1861-1881.

Young, P.C., Schreider, S. Yu., and Jakeman, A.J. (1997) A streamflow forecasting algorithm and results for the Upper Murray Basin, *Proc. MODSIM 97 Congress on Modelling and Simulation, Hobart, Tasmania*.

FIGURE CAPTIONS

Fig.1 Stochastic dynamic modelling: A general statistical procedure for identification, estimation and conditional validation.

Fig.2 Daily rainfall, flow and temperature data from the Coweeta catchment used for model identification and estimation: samples 8310 to 10309.

Fig.3 FIS non-parametric estimate of the rainfall-flow nonlinearity as a function of flow.

Fig.4 DBM modelling results: comparison of the deterministic model output $\hat{y}_t$ and the flow measurements y_t between samples 8310 and 8675.

Fig.5 DBM modelling results: comparison of the deterministic output $\hat{y}_{2,t}$ of the temperature-flow model and the residual series $y_t - b - \hat{y}_{1,t}$.

Fig.6 DBM modelling results: auto (ACF) and partial autocorrelation (PACF) functions of the deterministic model residuals $\hat{\xi}_t = y_t - \hat{y}_t$.

Fig.7 DBM modelling results: auto (ACF) and partial autocorrelation (PACF) functions of the stochastic model residuals $\hat{e}_t$ (one-step-ahead prediction errors).

Fig.8 DBM modelling results: cross correlation function (CCF) between the stochastic residuals $\hat{e}_t$ and the temperature input T_t.

Fig.9 DBM modelling results: cross correlation function (CCF) between the stochastic residuals $\hat{e}_t$ and the effective rainfall input u_t.

Fig.10 DBM modelling results: the stochastic residuals $\hat{e}_t$, with the outliers marked as circled points.

Fig.11 Systems block diagram of the DBM rainfall-flow model, showing the parallel flow decomposition inferred from the TF model.

Fig.12 DBM modelling results: TF derived decomposition of flow showing the extracted instantaneous (within one day), fast flow, slow flow and seasonal (temperature dependent) components.

Fig.13 DBM modelling results: TF derived decomposition of flow showing the combined instantaneous and fast flow effects (upper); and the combined slow flow and temperature dependent components (lower) Also, temperature dependent component shown separately (dashed) in lower plot.

Fig.14 DBM modelling results. MCS flow response: mean (full line) and ensemble envelope (dashed), compared with the measured flow (circles).

Fig.15 DBM modelling results. MCS generated histograms for the TF derived slow (left) and quick (right) residence time (time constant) parameters.

Fig.16 DBM modelling results. MCS generated histograms for the TF derived slow (left), quick (middle) and instantaneous (right) partition percentage parameters.

Fig.17 Comparison of the TF derived instantaneous unit hydrographs for the four HMC models: DBM (full line); DBMS (dashed); IHACRES (dashed); and BM (dash-dot).

Fig.18 Comparison of the FIS estimated effective rainfall nonlinearities for the four HMC models: DBM (full line); DBMS (dash-dot); IHACRES (dotted); and BM (dashed).

Fig.19 Comparison of the differences between the effective and measured rainfall for the four HMC models: DBM (top); DBMS (second); IHACRES (third); BM (lower).

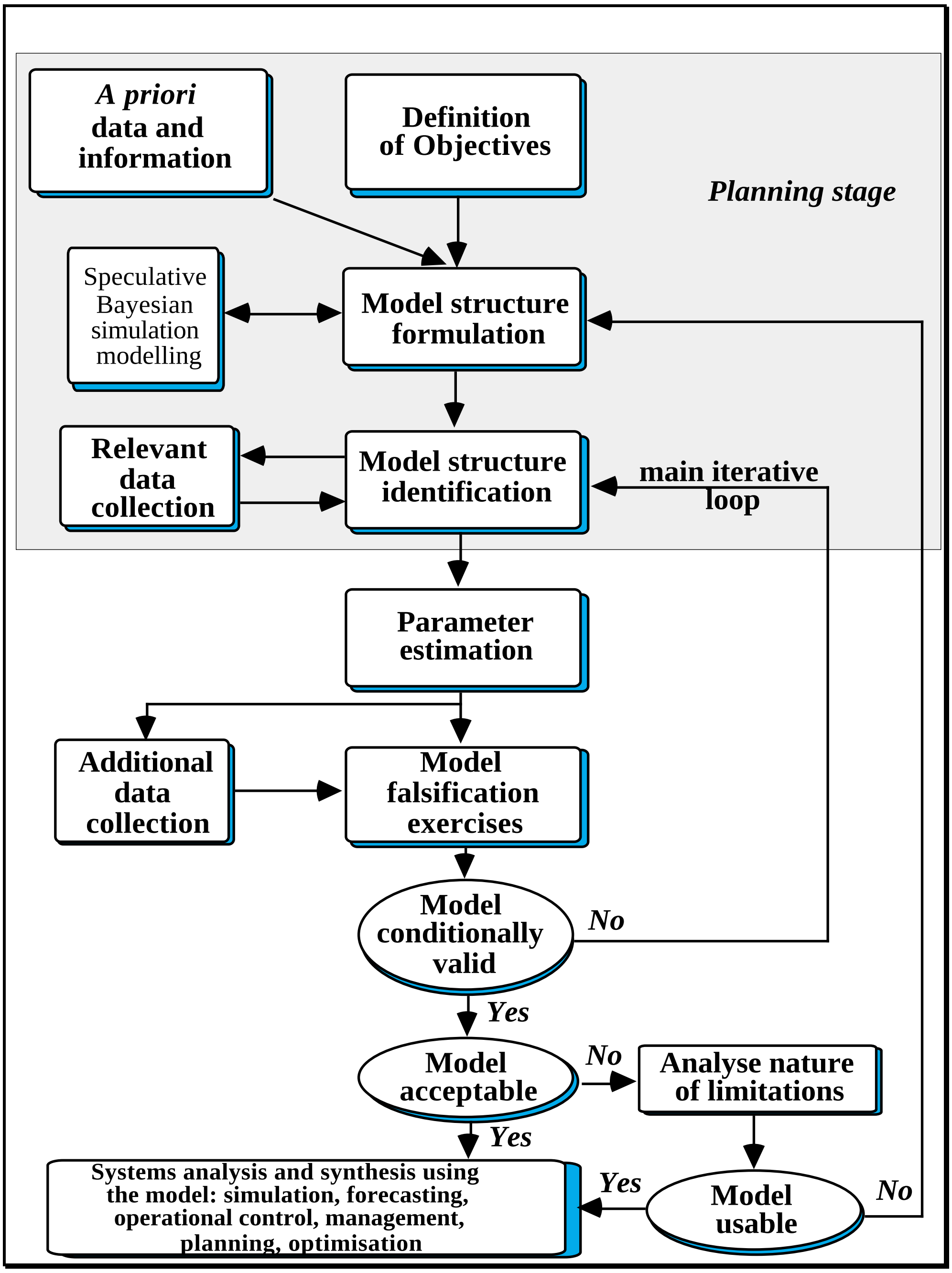


Fig.1 Stochastic dynamic modelling: A general statistical procedure

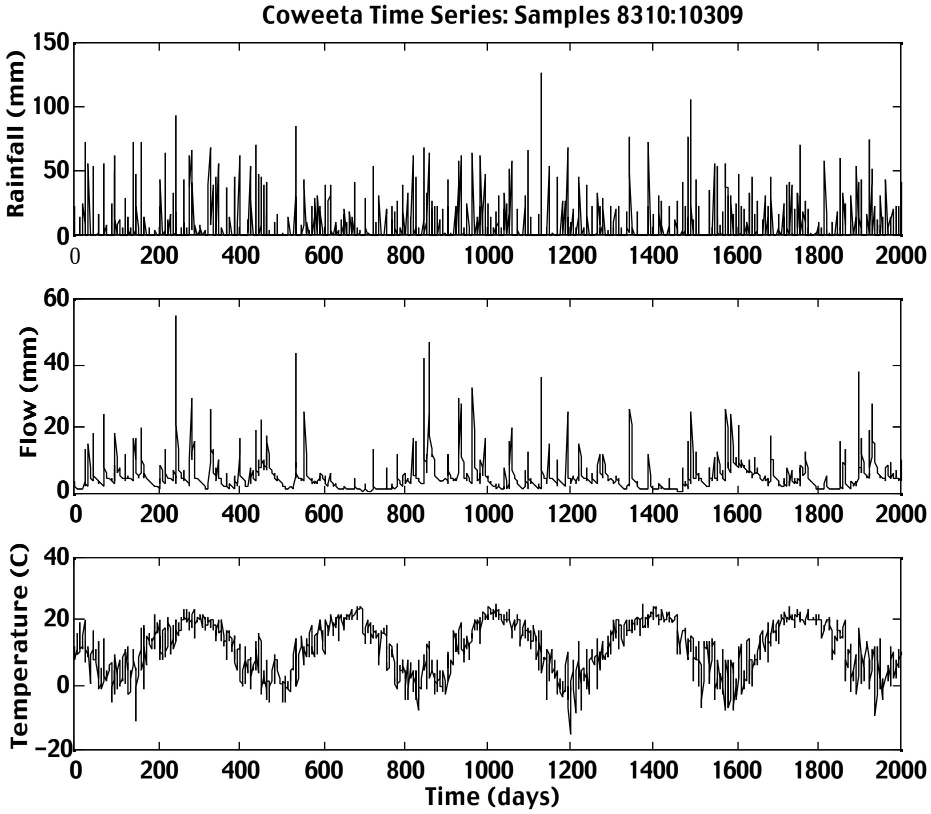

Coweeta Time Series: Samples 8310:10309
Rainfall (mm)
Flow (mm)
Temperature (C)
Time (days)

Fig.2

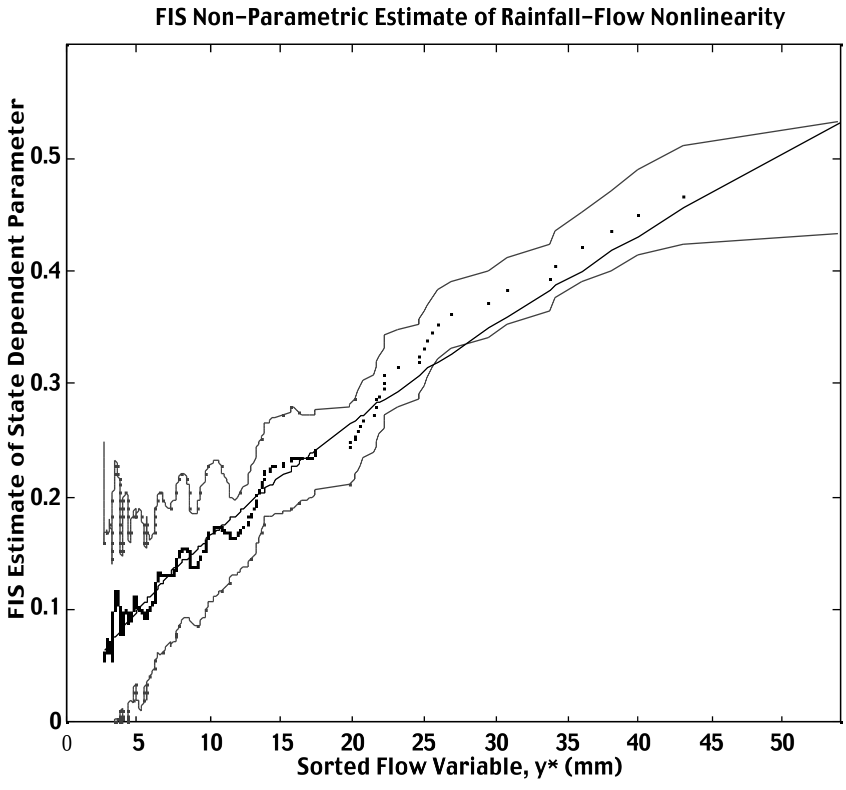

FIS Non-Parametric Estimate of Rainfall-Flow Nonlinearity
FIS Estimate of State Dependent Parameter
Sorted Flow Variable, y* (mm)

Fig. 3

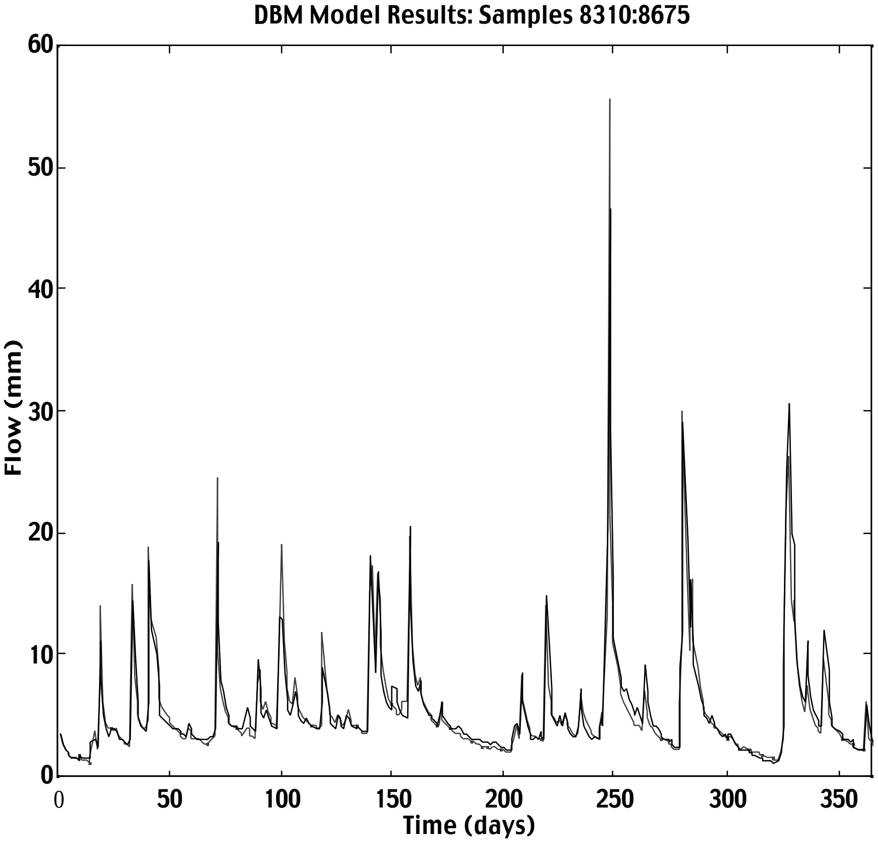

DBM Model Results: Samples 8310:8675
Flow (mm)
Time (days)
0
10
20
30
40
50
60
0
50
100
150
200
250
300
350

Fig. 4

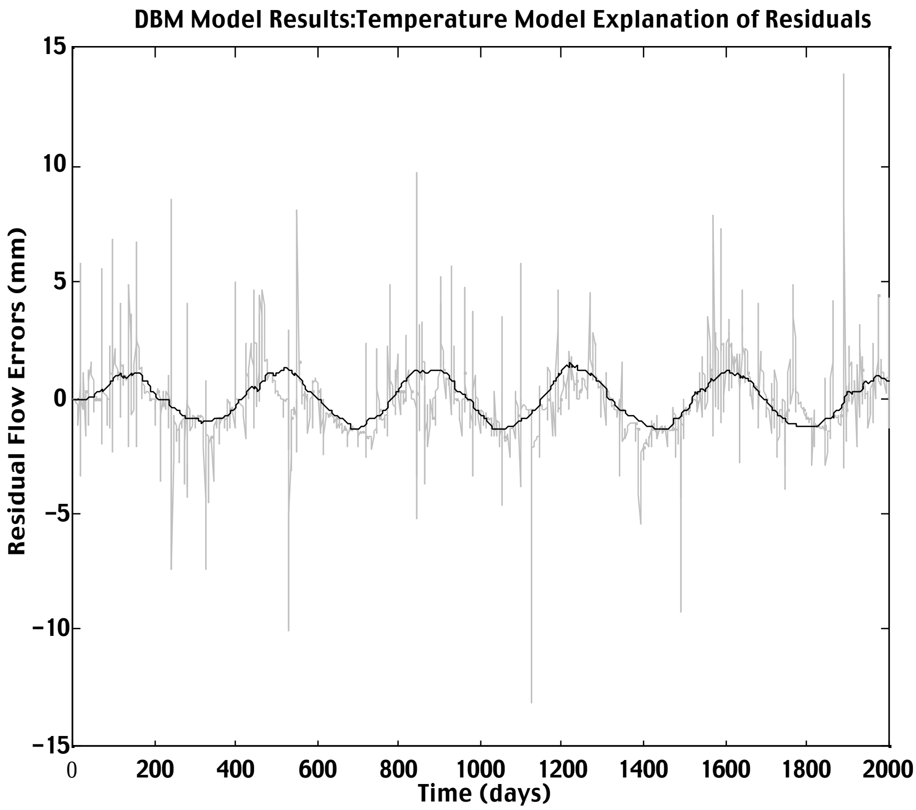

DBM Model Results:Temperature Model Explanation of Residuals
Residual Flow Errors (mm)
Time (days)
15
10
5
0
−5
−10
−15
0
200
400
600
800
1000
1200
1400
1600
1800
2000

Fig. 5

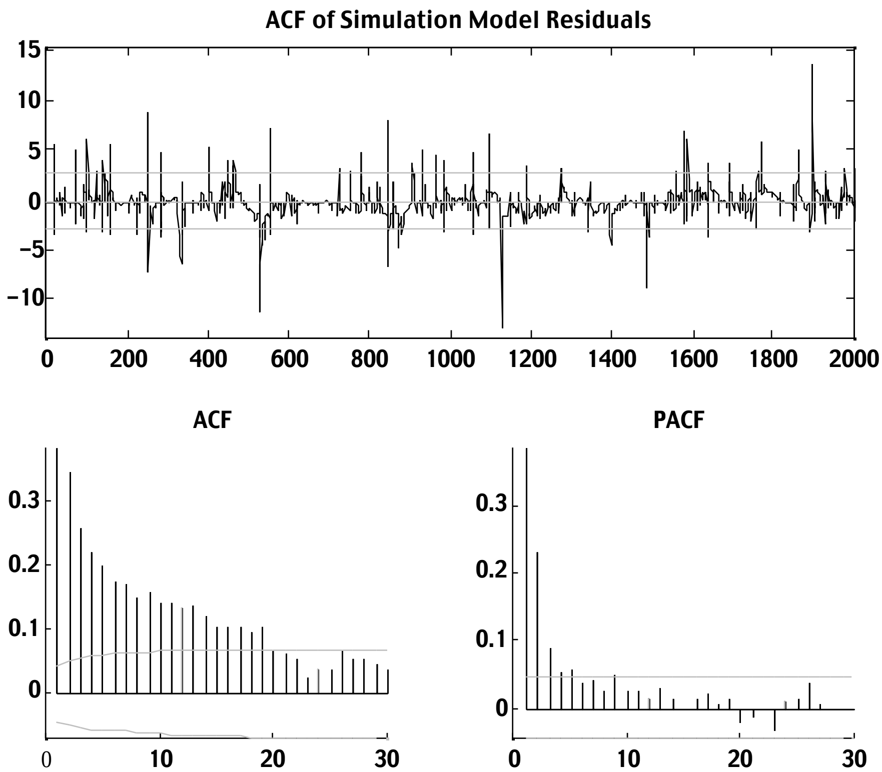

ACF of Simulation Model Residuals
15
10
5
0
−5
−10
0 200 400 600 800 1000 1200 1400 1600 1800 2000
ACF
0.3
0.2
0.1
0
0 10 20 30
PACF
0.3
0.2
0.1
0
0 10 20 30

Fig. 6

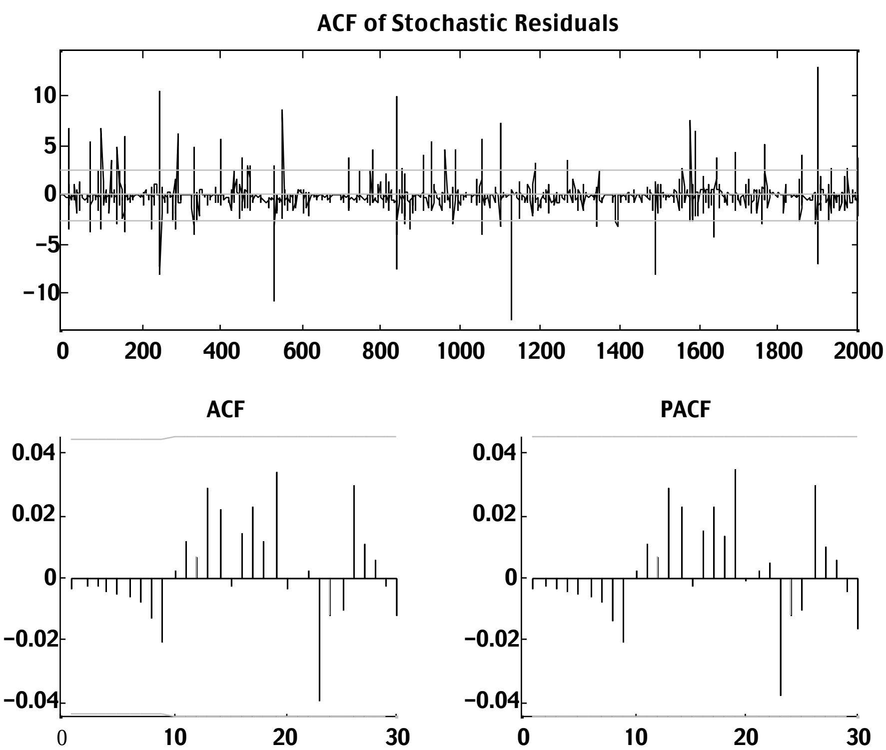

ACF of Stochastic Residuals
10
5
0
−5
−10
0 200 400 600 800 1000 1200 1400 1600 1800 2000
ACF
0.04
0.02
0
−0.02
−0.04
0 10 20 30
PACF
0.04
0.02
0
−0.02
−0.04
0 10 20 30

Fig. 7

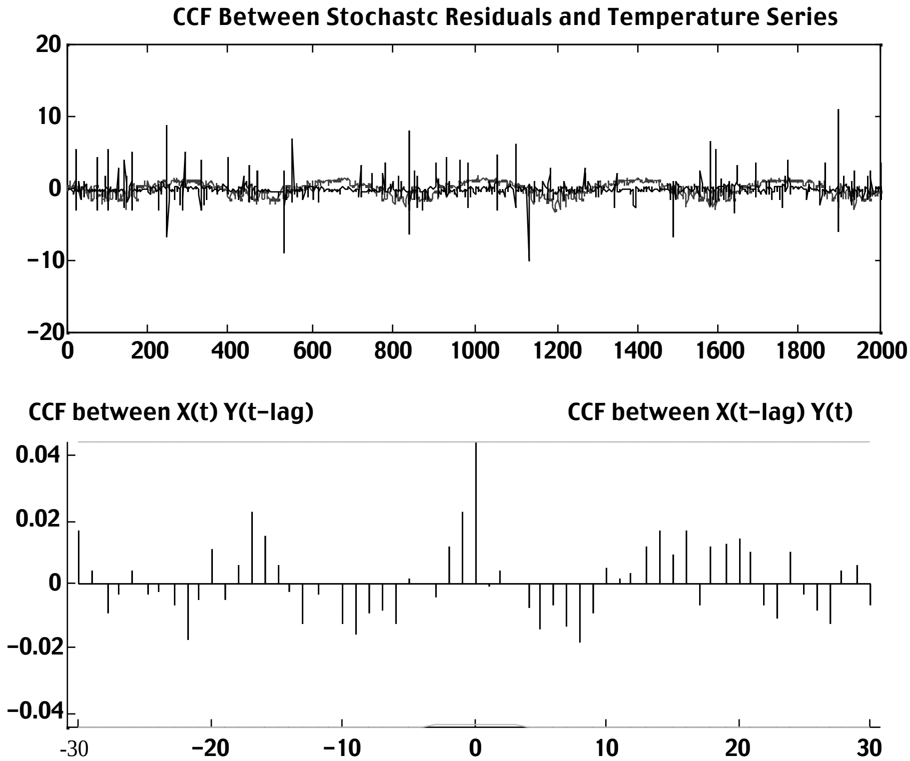

CCF Between Stochastc Residuals and Temperature Series
20
10
0
−10
−20
0
200
400
600
800
1000
1200
1400
1600
1800
2000
CCF between X(t) Y(t−lag)
CCF between X(t−lag) Y(t)
0.04
0.02
0
−0.02
−0.04
-30
−20
−10
0
10
20
30

Fig. 8

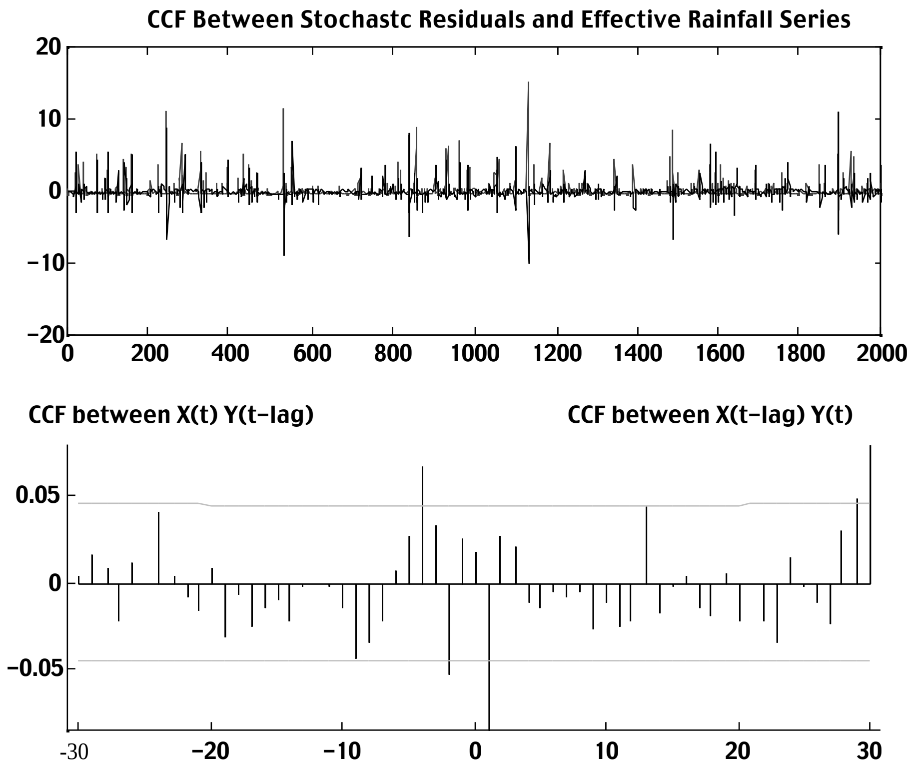

CCF Between Stochastc Residuals and Effective Rainfall Series
20
10
0
−10
−20
0
200
400
600
800
1000
1200
1400
1600
1800
2000
CCF between X(t) Y(t−lag)
CCF between X(t−lag) Y(t)
0.05
0
−0.05
-30
−20
−10
0
10
20
30

Fig. 9

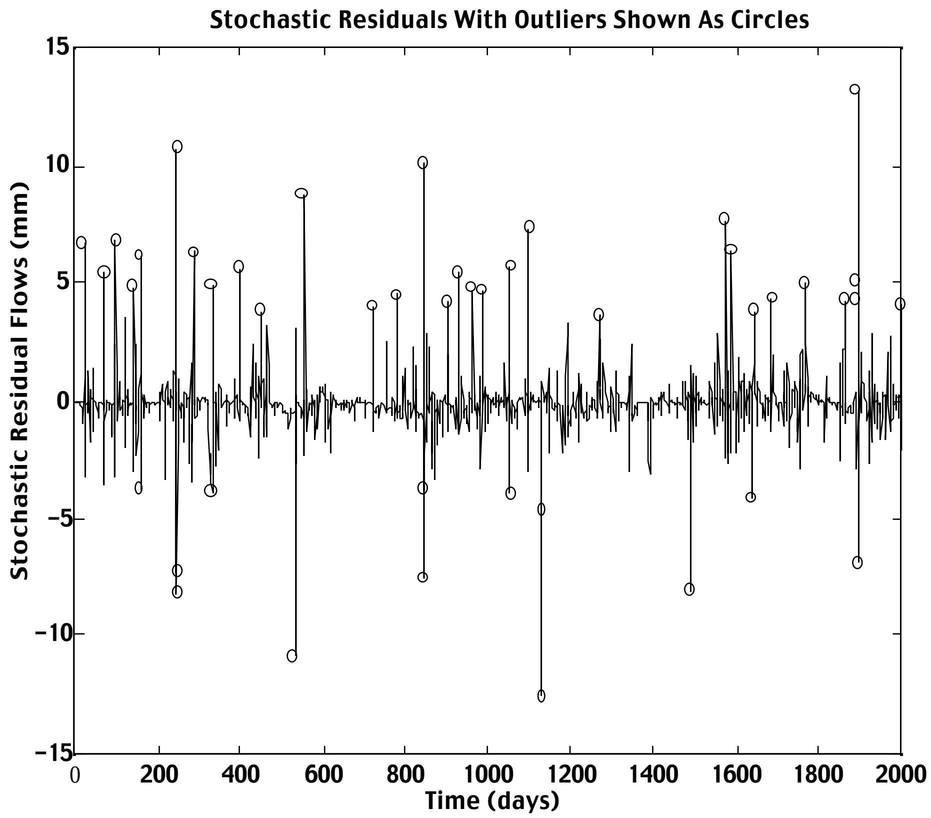

Stochastic Residuals With Outliers Shown As Circles
Stochastic Residual Flows (mm)
15
10
5
0
−5
−10
−15
0
200
400
600
800
1000
1200
1400
1600
1800
2000
Time (days)

Fig. 10

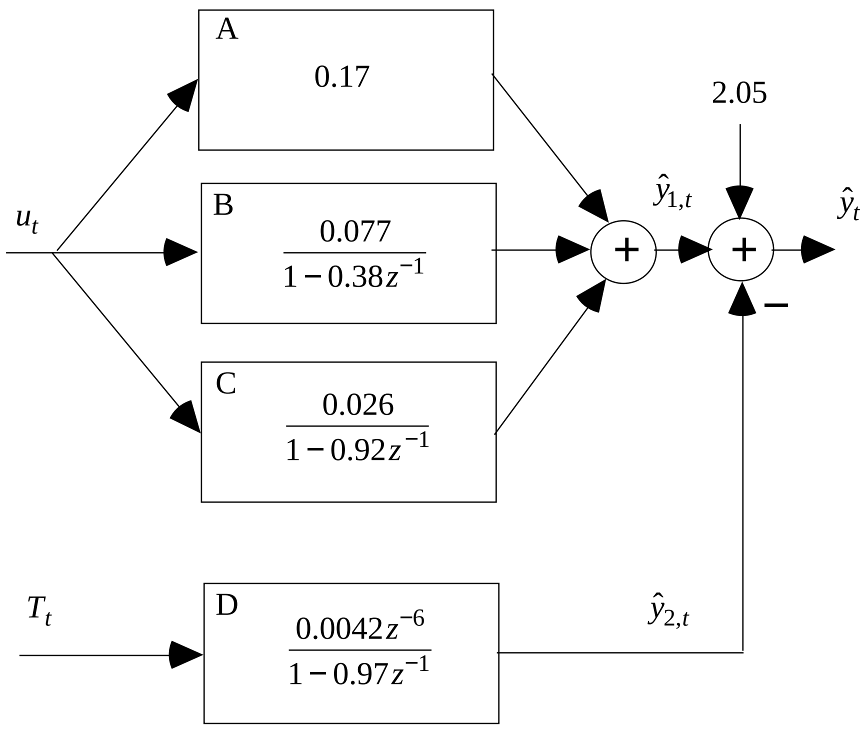
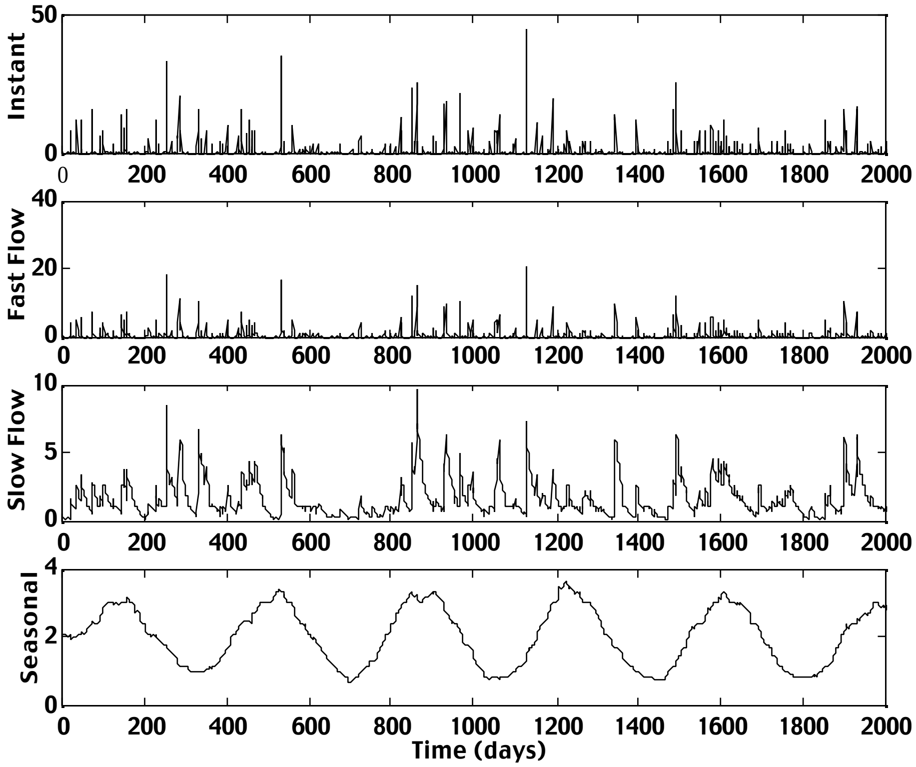
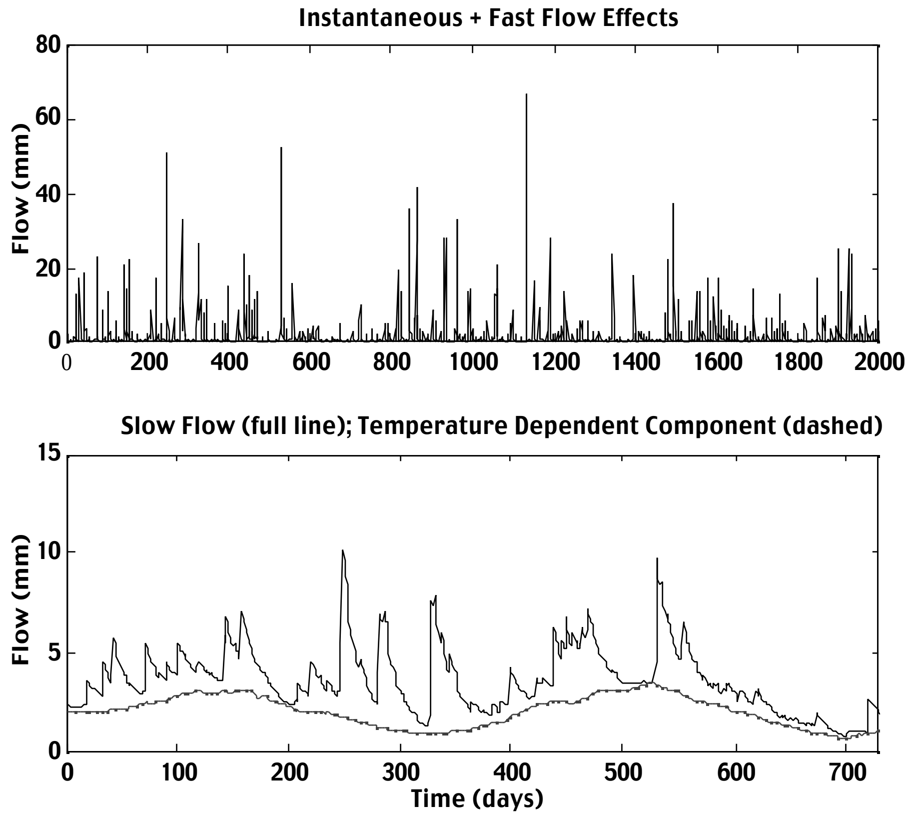

A
0.17
B
$\frac{0.077}{1-0.38z^{-1}}$
C
$\frac{0.026}{1-0.92z^{-1}}$
D
$\frac{0.0042z^{-6}}{1-0.97z^{-1}}$
u_t
T_t
2.05
$\hat{y}_{1,t}$
$\hat{y}_{2,t}$
$\hat{y}_t$
+
+
−

Fig.11



Instant
Fast Flow
Slow Flow
Seasonal
Time (days)

Fig. 12



Instantaneous + Fast Flow Effects
Flow (mm)
Slow Flow (full line); Temperature Dependent Component (dashed)
Flow (mm)
Time (days)

Fig. 13

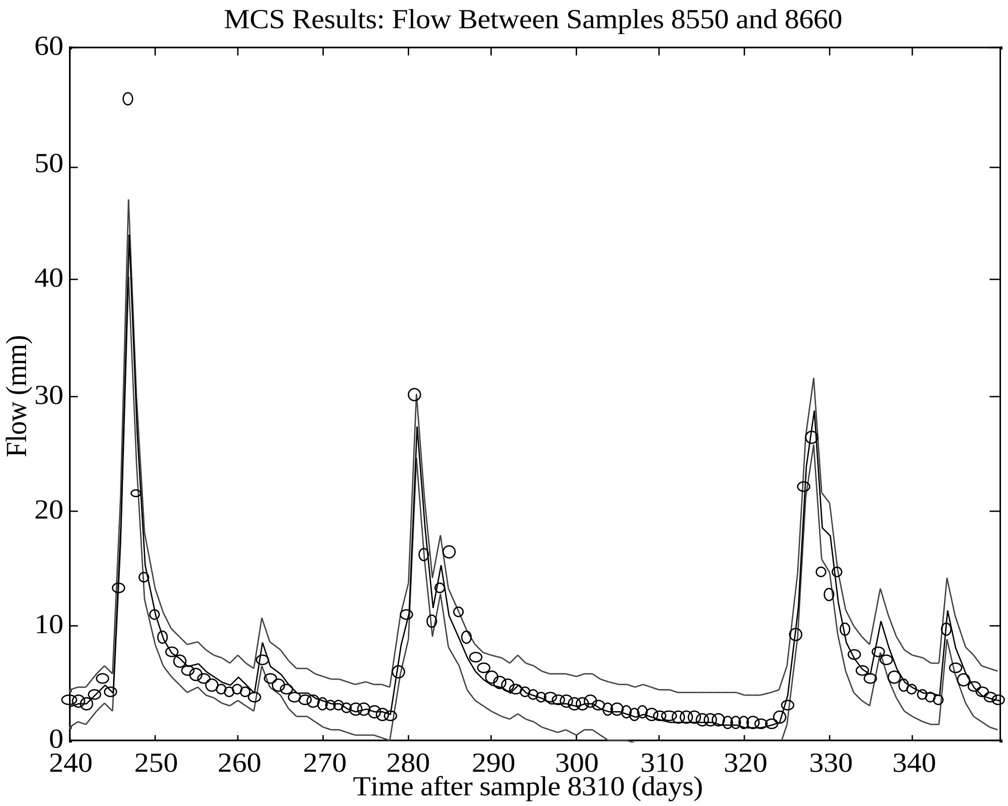

MCS Results: Flow Between Samples 8550 and 8660
Flow (mm)
Time after sample 8310 (days)
0
10
20
30
40
50
60
240
250
260
270
280
290
300
310
320
330
340

Fig. 14

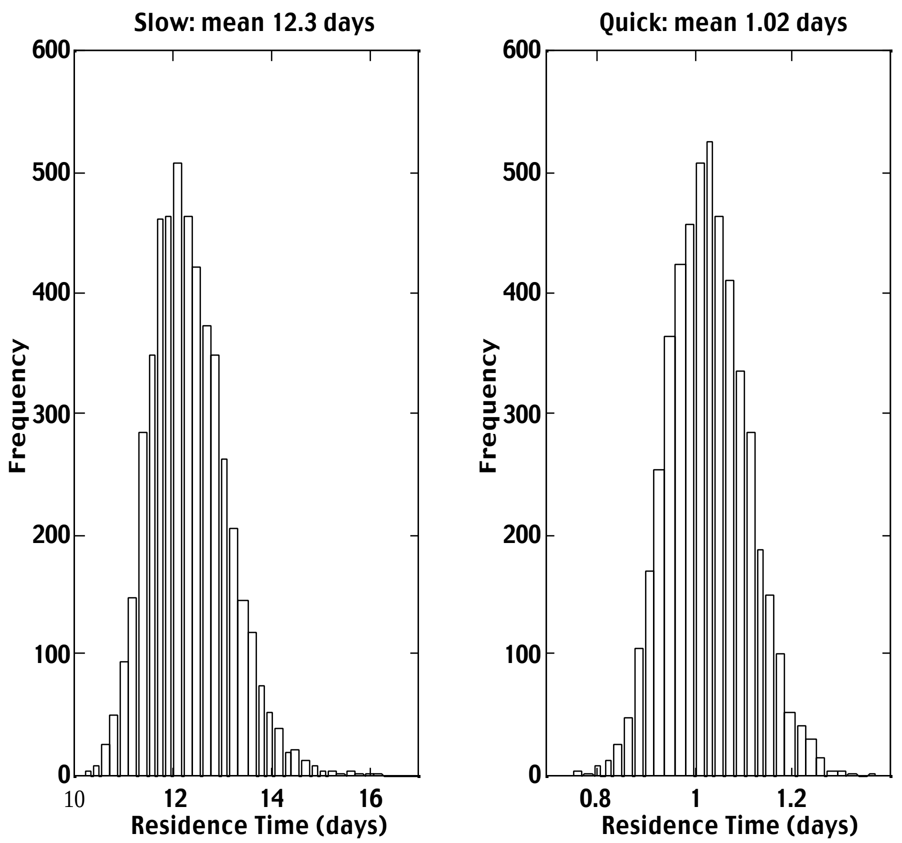

Slow: mean 12.3 days
Quick: mean 1.02 days
Frequency
Residence Time (days)
0
100
200
300
400
500
600
10
12
14
16
0.8
1
1.2

Fig. 15

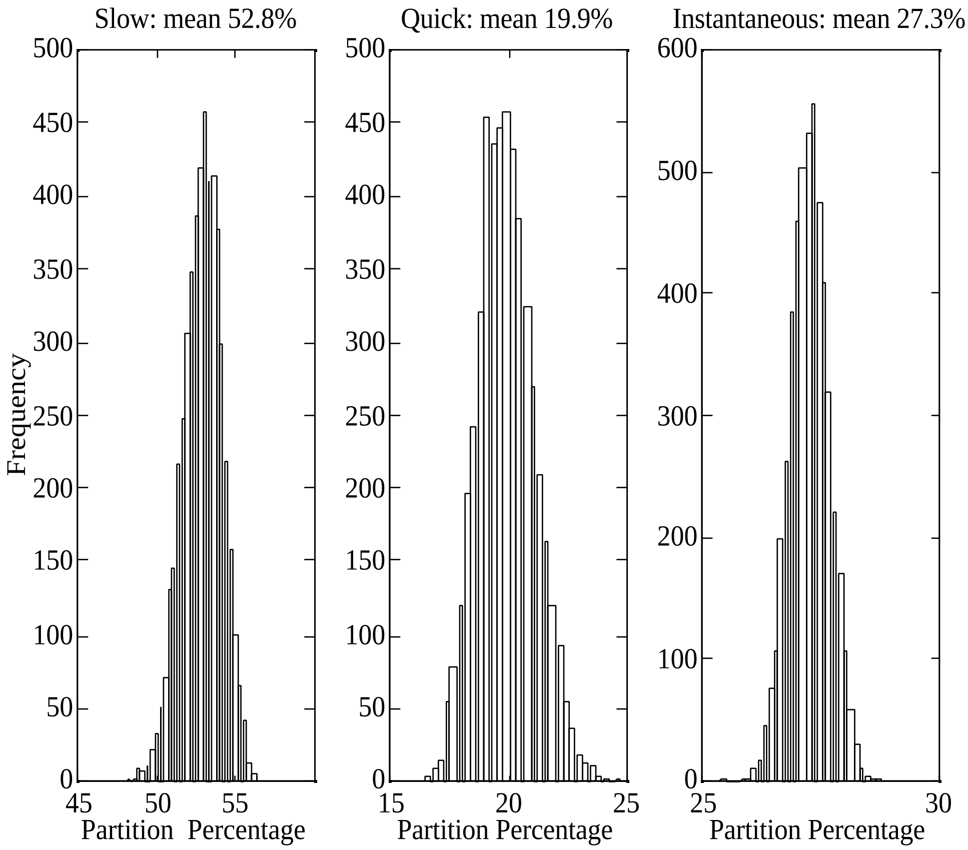

Slow: mean 52.8%
Quick: mean 19.9%
Instantaneous: mean 27.3%
Frequency
Partition Percentage
Partition Percentage
Partition Percentage

Fig. 16

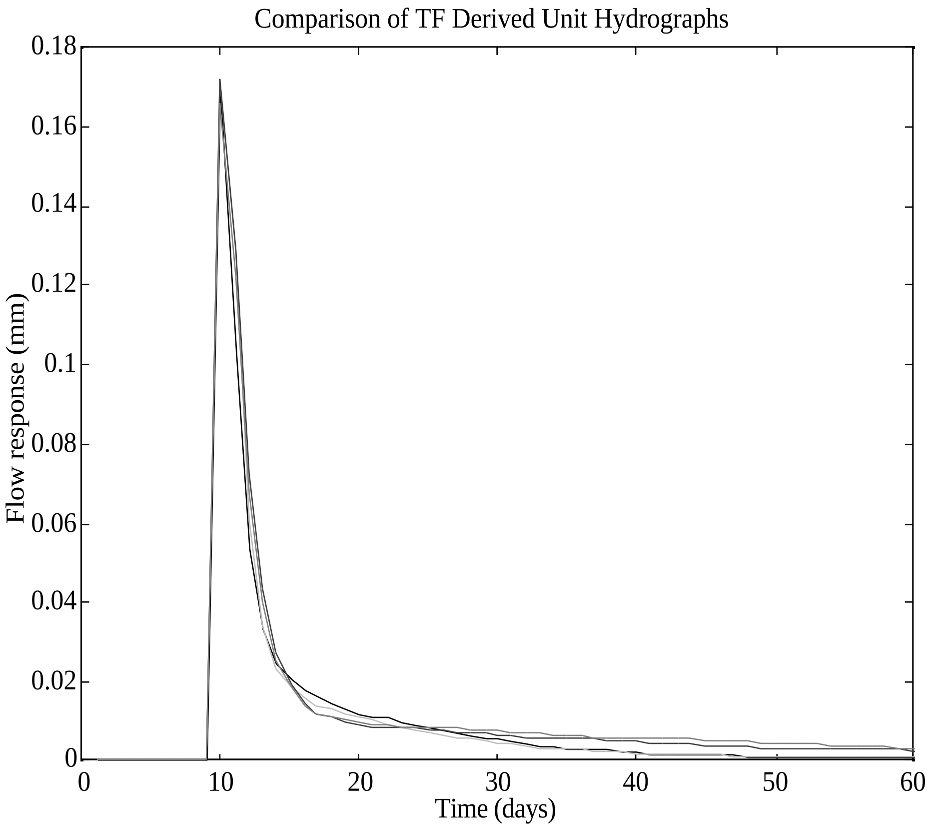
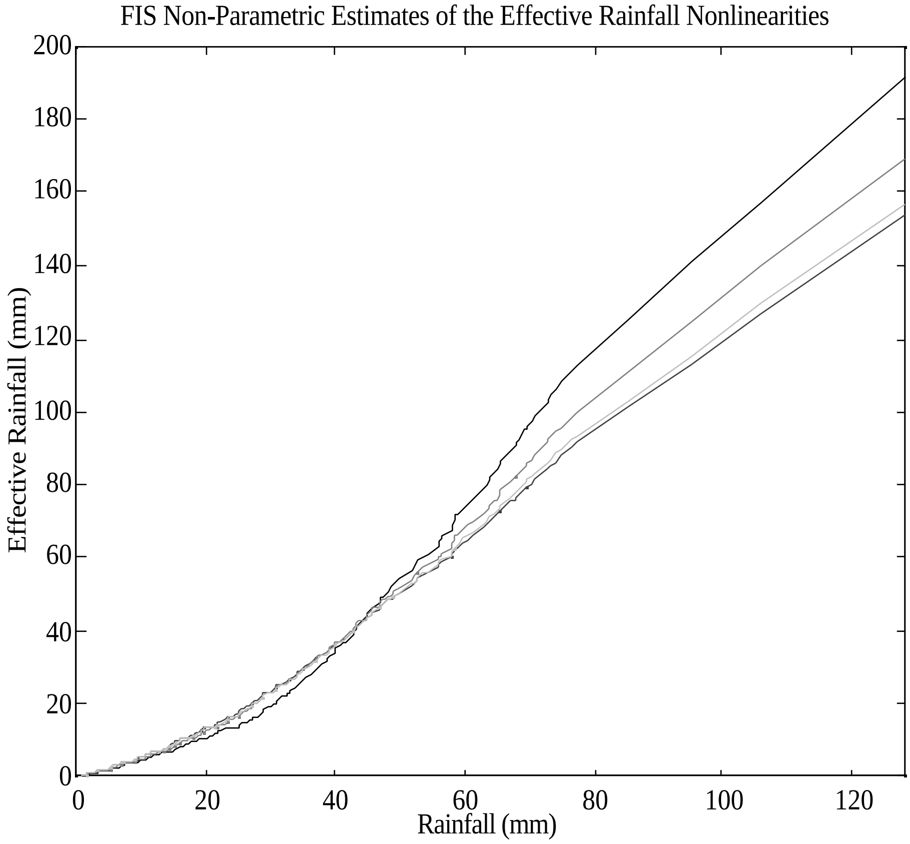
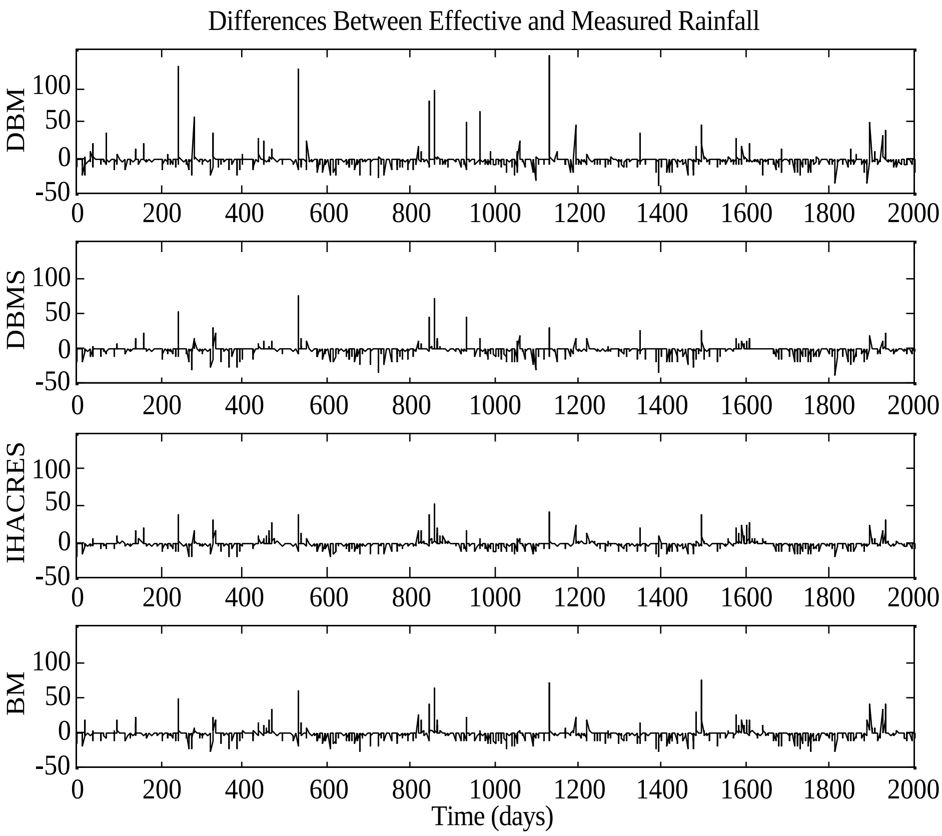

Comparison of TF Derived Unit Hydrographs
Flow response (mm)
Time (days)

Fig. 17



FIS Non-Parametric Estimates of the Effective Rainfall Nonlinearities
Effective Rainfall (mm)
Rainfall (mm)

Fig. 18



Differences Between Effective and Measured Rainfall
DBM
DBMS
IHACRES
BM
Time (days)

Fig. 19