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Summary

This report constitutes a User Focussed Measurable Outcome (UFMO) of work carried out under Work Package 3 of the FRMRC and describes methods for real-time flood forecasting that involve the real-time updating of states (river levels or flows) and parameters in flood forecasting models. The Work Package 3 has involved a number of contributions. However, this UFMO Report is based only on the research and development carried out under WP 3.4 at Lancaster University. The other contributors to WP 3 will be reporting on their work at a later date.

The Lancaster contribution to WP 3 is based around a Case Study that involves a Data-Based Mechanistic (DBM) model of the River Severn from its upper reaches down to Bewdley. However, the same basic approach can be applied to any model of this general, ‘quasi-distributed’ type: i.e. lumped parameter models for rainfall-level and level routing (or the flow equivalents), connected in a manner that represents the geographical nature of the catchment and the location of rainfall and flow gauges within the catchment.

The Lancaster Real-Time Flood Forecasting System utilises a state-space form of the complete DBM catchment model, which provides the basis for data assimilation and forecasting of water levels or flows at specified geographical locations, using a modified Kalman Filter (KF) forecasting engine. Here, the predicted model states (here water levels for reasons discussed in the Report), as well as important adaptive gain parameters, are updated recursively in response to input data received in real-time from remote sensors in the catchment. In this way, the extraction of information content in the data is maximised, leading to improved stochastic forecasts of water level or flow.

The work discussed in this UFMO is entirely compatible with the developments underway in the National Flood Forecasting System (NFFS), a dedicated user interface being developed for the Environment Agency that provides for the incorporation of user-specified hydrological and hydraulic models; as well as the efficient import and processing of numerical weather predictions, radar data and on-line meteorological and hydrological data. Therefore, the tools and routines that are described in the present Report, must fulfil the requirements of the NFFS. In this regard, the Lancaster team have cooperated with the developers of the NFFS, Delft Hydraulics, in the initial incorporation of the Lancaster River Severn forecasting system into the NFFS, thus demonstrating that these modern forecasting tools, with updating, can be used within the NFFS for other catchment areas.

The main part of this Report describes all aspects of the real-time flood forecasting system. Following an introduction in Section 4, Section 5 outlines the methodological basis for its design; and Section 6 illustrates its practical utility when applied to the case study on the River Severn. Section 7 discusses briefly the initial incorporation of the system into the NFFS and Section 8 considers associated research being carried on the River Dee. Finally, in this main part of the report, Sections 9 and 10 present comments and conclusions on the system and the case study.

The methodology exploited in the development of the Lancaster real-time flood forecasting system involves quite advanced mathematics and statistics. For this reason, we have included three, semi-tutorial, Appendices that we hope will assist the reader in understanding the topics introduced and discussed in the main part of the Report.

Appendix 1 discusses the Choice of Models in Flood Forecasting by considering different types of models and their suitability in real-time flood forecasting applications.

Appendix 2 provides a long tutorial on Transfer Function Models, which includes some background into the use of transfer function models in hydrology, as well sections on the formulation of such stochastic models in continuous time (differential equations) and discrete-time (difference equations: the discrete-time equivalent of differential equations). It also discusses how such models can be estimated statistically from real data and how they can be extended to allow for nonstationarity (the

model parameters change over time) or nonlinearity, in the form of State-Dependent Parameter (SDP) models. A practical example of a DBM model is included to illustrate how the nonlinear SDP transfer function models can be interpreted in physically meaningful terms and used in flow forecasting. This also provides the background to the development of the River Severn DBM model in the main part of the Report.

Appendix 3, Recursive Estimation and the Kalman Filter, deals with other topics that are of importance in the main part of the Report, this time relating to the development of the modified Kalman Filter forecasting engine and its associated recursive (adaptive) parameter updating algorithms. Again, the Appendix is intended as a tutorial introduction to these important topics.

Finally, the development of real-time updating methods for on-line flood forecasting requires the development of generic tools, together with guidelines for using them in various hydrological conditions. Generic software modules have been developed for the DBM/KF-based forecasting system described in this Report and will be part of the FRMRC Uncertainty Estimation Methods Catalogue. Guidelines for users will be prepared to help them in the choice of the appropriate structure of the on-line flood forecasting system and, subsequently, for developing the on-line updating aspects of the flood forecasting modules. In addition, the CAPTAIN Toolbox, designed for use in the MATLAB numeric computation software environment, contains all the routines used in the development of the forecasting system and a fully functional, 3 month demonstration version of this Toolbox is available for download at <http://www.es.lancs.ac.uk/cres/captain/>.

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1. Preface

The work programme on real-time flood forecasting in the FRMRC Work Package 3 has involved a number of contributions. However, this UFMO Report is based only on the research and development carried out under WP 3.4 at Lancaster University. The other contributors to WP 3 will be reporting on their work at a later date.

A number of people have helped in the Lancaster Study, especially in the provision of information and hydrological data for the River Severn Catchment. Particular thanks are due to Jo Cullen of the Welsh Environment Agency and Dr. Micha Werner of Delft Hydraulics, who have both assisted the work described in this Report. In her Ph.D research at Lancaster, Dr. Cullen is developing a *Data-Based Mechanistic* (DBM) model and associated real-time forecasting system for the River Dee, of a similar type to that developed in the Lancaster Study and described in the present Report. She has kindly allowed us to incorporate a plot of her initial forecasting results in the present Report.

Dr. Werner's assistance was essential for the initial incorporation of the Lancaster flood forecasting system into the *National Flood Forecasting System* (NFFS) software. This has demonstrated that the Lancaster system is compatible with the NFFS and has provided initial promising results. It is hoped that this work will be continued in the future, if possible based on Jo Cullen's system for the River Dee. However, this work is not funded by the FRMRC and, although additional funding is being sought, this has not been successful so far.

2. Introduction

Recent extensive flood events in Britain have focussed the interest of the hydrological community on improved methods of flood forecasting that could help to decrease flood losses under the increasing probability of flood occurrence. Disasters such as floods, which might arise from human-induced environmental changes, are not only dangerous for the natural environment but also for human beings. Consequently, new methodologies are required to mitigate the effects of such flooding both before and during events. In this Report, we consider various aspects of model-based, real-time flood forecasting, concentrating on the research being carried out at Lancaster under the aegis of the FRMRC. In particular, we discuss the development of models and methods that allow for the real-time updating of forecasts and model parameters in flood forecasting models.

Refsgaard (1997) gives a review of different updating techniques used in real time flood forecasting systems, as well as the comparison of two different updating procedures applied to a conceptual hydrological model of a catchment, including rainfall-flow and the flow routing models. In relation to his classification, the methods developed in the present Report utilize both parameter and state updating. However, unlike approaches such as the EKF algorithm used by Refsgaard, where the updating is carried out within a single, nonlinear, state space setting, with the parameters considered as adjoined state variables, our state and parameter estimation procedures are carried out separately but concurrently, employing coordinated recursive estimation algorithms, as in Young (2001c, 2002a). This avoids the well known deficiencies of the EKF (such as problems with covariance estimation and convergence for multi-dimensional, non-linear models) and yields more statistically

efficient estimates of the model parameters. (i.e. it reduces the uncertainty on these estimates). Based on the results of previous research (Romanowicz et al. [2004b]), the present study also considers an implementation based on the modelling and forecasting of water level (stage) rather than flow. This approach avoids the errors introduced by the conversion of levels to flow; it can be applied in the situation where flow observations are not available; and it yields directly the forecasts of water levels that are normally required for flood forecasting and warning.

The real-time adaptive updating procedures applied in this project follow the methodology for the on-line forecasting of rainfall-flow processes described originally by Young (2001c, 2002a). This exploits the top-down, objective orientated, *Data-Based Mechanistic* (DBM) approach to the modelling of environmental processes (e.g. Young 2001b, 2003 and the prior references therein), concentrating on the identification and estimation of those ‘dominant modes’ of dynamic behaviour (Young, 1999a) that are most important for the objective of high quality flood prediction. This DBM approach involves inductive modelling, where the dominant mode model structure is identified from the available data; the parameters that characterize this model structure are estimated from the same data; and the model is validated against other, separate data sets. In the resulting model, which can be interpreted directly in hydrological terms, the most important hydrological processes active in the catchment are modelled using the *State Dependent Parameter* (SDP) method of estimating the effective rainfall nonlinearity, together with a *Stochastic Transfer Function* (STF) method for characterising both the linear effective rainfall-water level behaviour and the water level routing processes (see e.g. Young, 2000, 2001a; Young *et al.*, 2001; and Appendix 2).

The complete model consists of these linear and nonlinear stochastic, dynamic, hydrological elements connected in a manner that represents the physical structure of the catchment, accounting for both surface and groundwater effects on river water level or flow. Bearing in mind that the objective of flood forecasting is to predict the water level of the river at future times, the Lancaster system has been developed specifically for water level (stage) forecasting, thus avoiding the uncertainties associated with the stage-discharge calibration relationship. It is important to note, however, that there have been numerous previous studies where DBM models have been concerned with flow modelling and forecasting and that the procedures developed here for water level forecasting could be used equally well for flow forecasting, if this is required.

The adaptive forecasting system utilises a state-space form of the complete catchment model, which provides the basis for data assimilation and forecasting of water levels at specified geographical locations using a modified *Kalman Filter* (KF: see Kalman, 1960) forecasting engine. Here, the predicted model states (water levels) and important adaptive gain parameters are updated recursively, in real-time, in response to input data received in real-time from remote sensors in the catchment. In this way, the extraction of information content in the data is maximised, leading to improved stochastic forecasts of water level or flow.

3. Research Background

The main objective of work package 3.4 is the development of a methodology for operational real-time flood forecasting systems at extended lead times and a strat-

egy for updating both the states (here river water levels or flows) and associated model parameters in real time. The research reflects the developments underway in the *National Flood Forecasting System* (NFFS), a dedicated user interface that provides for the incorporation of user-specified hydrological and hydraulic models; as well as the efficient import and processing of numerical weather predictions, radar data and on-line meteorological and hydrological data. Therefore, the tools and routines that are described in this UFM0, must fulfil the requirements of the NFFS. In this regard, the team at Lancaster have cooperated with the developers of the NFFS, Delft Hydraulics, in the initial incorporation of the Lancaster River Severn forecasting system, as described later in the Report, into the NFFS, thus demonstrating that the system is compatible with the NFFS.

The Lancaster contribution to WP 3 is primarily focused on the development of a formal but practical framework for on-line, real-time updating of parameters and states in either DBM or the related *Hybrid-Metric-Conceptual* (HMC: see Wheater *et al.*, 1993) forecasting models. The same basic approach can be applied to any model of this general, quasi-distributed type: i.e. lumped parameter models for rainfall-level and level routing (or flow equivalents), connected in a manner that represents the geographical nature of the catchment and the location of rainfall and flow gauges within the catchment. However, some difficulties in parameter updating may be experienced in large models whose parameters are not identifiable from the data because the model is over-parameterized (see Appendix 1). Although the basic tools are also appropriate for fully distributed (partial differential equation) hydrological and hydraulic models, they have not been developed nor tested in this framework and further research would be necessary in this connection.

We have also considered the use of other procedures, such as the topical numerical Bayesian approach to forecasting, as in the *Ensemble Kalman Filter* (EnKF) and other more complex methods that exploit *Monte Carlo Simulation* (MCS) analysis. However, since these methods are computationally expensive and complicated to implement because of the need for multi-realization MCS, they should only be used if the nonlinear stochastic structure is such that much simpler, and computationally inexpensive, analytic Bayesian procedures, such as the KF are inappropriate. In the present context, this does not seem to be the case.

In particular, DBM model identification, echoing many previous conceptual catchment modelling studies, shows that rainfall-flow (or water level) processes can be represented by the serial connection of an ‘effective rainfall’ nonlinearity, that represents the nonlinear catchment storage (soil moisture) dynamics, and a linear process, here in the form of a STF, which is simply the discrete-time equivalent of a differential equation model (see Appendix 2). The impulse response function of this STF module nicely reflects the underlying unit hydrograph properties of the catchment and it can be decomposed into a parallel pathway form that represent fast (surface and near-surface) processes, as well as slow, groundwater processes that affect the base-flow of the river. Stochastic forecasting using such a ‘Hammerstein’ model can be carried out by a simple modification of the KF that allows for the nonlinear input and the heteroscedasticity (changing variance) of the prediction errors.

It could be argued that the simple distributional assumptions that are required for the Bayesian interpretation of the KF are not entirely valid. However, it should be realized that the KF does not require such assumptions (Kalman developed the

algorithm using orthogonal projection theory) and it is robust to their violation. Moreover, from a practical standpoint, recent comparison of the results obtained from the EnKF (Moradkhani, 2005b) and analytical KF results using a DBM model (Young, 2006a) for the Leaf River in the USA show that the simpler KF-based approach produces results that are as good, if not better, than the much more computational expensive and complicated EnKF approach (see Appendix 2).

An on-line flood forecasting system should be capable of producing forecasts over a whole range of lead-times. Long lead-time forecasts may be important in flood warning, because of the need to make decisions about demountable defences. Although the accuracy of such long lead-time forecasts is naturally compromised by the inevitable uncertainty propagation that affects the forecasts, reasonable results have been obtained so far (Romanowicz *et al.*, 2006a; Young *et al.*, 2006). On the other hand, the short-to-medium (4 to 10-hour-ahead) forecasts in NFFS are critical in decisions about public flood warnings and it is here where a stochastic system, inherently optimized for the minimization of forecasting errors and uncertainty at specified lead-times, has particular advantages over more conventional deterministic alternatives.

The development of real-time updating methods for on-line flood forecasting requires the development of generic tools, together with guidelines for using them in various hydrological conditions. Generic software modules have been developed for the DBM/KF-based forecasting system described in this Report and these will be contributed to the Uncertainty Toolbox. Guidelines for users will be prepared to help them in the choice of the appropriate structure of the on-line flood forecasting system and, subsequently, for developing the on-line updating aspects of the flood forecasting modules. In addition, the CAPTAIN Toolbox for MatlabTM (e.g. Taylor *et al.*, 2006) contains all the routines used in the development of the forecasting system and a fully functional 3 month demonstration version of this Toolbox is available for download at <http://www.es.lancs.ac.uk/cres/captain/>. Finally, the efficacy of the methodology is illustrated using the River Severn data set that has provided the basis for the design of the Lancaster Real-Time Flood Forecasting system, as described in the next Section 4.

4. The Lancaster Real-Time Flood Forecasting System

In this Report, flood forecasting is understood in a specific sense: namely the derivation of real-time updated, on-line forecasts of the flood level at certain strategic locations along the river, over a specified time horizon into the future, based on the information about the rainfall and the behavior of the flood wave upstream. Depending on the length of the river reach and the slope of the river bed, a realistic forecast lead time, obtained in this manner, may range from hours to days. The information upstream can include the observations of river water levels and/or rainfall measurements. In the situation where meteorological ensemble forecasts are available, they can be used to further extend the forecast lead times (e.g. Cluckie *et al.*, 2006), as in the approach presented by Krzysztofowicz (1999, 2002a,b) and Pappenberger *et al.*, (2005), but we have not utilized such information in the present Study.

The flow forecasting procedures described here are incorporated within a two-step Data Assimilation (DA) procedure based on DBM models, formulated within

a stochastic state space setting for the purposes of recursive state estimation and forecasting. In the first step, available observations of rainfall and river water levels at different locations along the river are sequentially assimilated into the forecasting algorithm, based on the statistically identified and estimated stochastic, dynamic DBM models, in order to derive the multi-step-ahead forecasts. These forecasts are then updated in real-time, using a Kalman Filter-based approach (Kalman, 1960), when new data become available. The incorporation of new observations into the dynamic model via DA is performed on-line for every time step (here every hour) of the forecasting procedure.

DA techniques have found wide application in the fields of meteorology and oceanography and an extensive review of sequential DA techniques, together with examples of their application in oceanography is presented in Bertino et al. (2003). The problems described there involve the integration of multi-dimensional, spatio-temporal observations into fully distributed numerical ocean models and thus differ from the flood forecasting systems, which have much smaller spatial dimensionality (these are usually interconnected quasi-distributed systems of lumped rainfall-flow and flow routing models), but require longer lead times for the forecasts. However, certain aspects of the problem remain the same and this has led to recent applications of the EnKF (see earlier) in a flow forecasting context.

The EnKF was developed by Evensen (1994) as an alternative to the *Extended Kalman Filter* (EKF) approach. The EnKF is an adaptation of the standard, analytic KF algorithm to non-linear systems using Monte Carlo sampling in the prediction (or propagation) step and linear updating in the correction (or analysis) step. It has been applied to rainfall-flow modelling by Vrugt et al. (2005) and Moradkhani et al. (2005b). In these latter papers, the authors exploit sequential, EnKF-based estimation of both the hydrological model parameters and the associated state variables for a single rainfall-flow model (in contrast to the present paper which considers a much more complicated, quasi-distributed catchment model, involving a number of inter-connected rainfall-water level and routing models). Moradkhani et al., (2005a) also apply a *Particle Filter* (PF) algorithm to implement sequential hydrologic data assimilation. Yet another approach to data assimilation is presented by Madsen et al. (2003) and Madsen and Skotner (2005), who apply updating to the modelling error of the distributed Mike-11 flow forecasts, at the observation sites, using a constant-in-time, proportional gain depending on the river chainage. Essentially, this gain is included to adjust for a hydrological model bias.

One problem with both PF and EnKF is that they are computationally intensive approaches to DA and forecasting, requiring many Monte Carlo realizations at each propagation step. Moreover, due to the high complexity of these approaches, there may be questions about the identifiability of parameters involved in the different aspects of the applied routines (e.g. the estimation of the variance hyper-parameters associated with stochastic inputs: see later, Section 5(c) and Appendix 3). In order to reduce the computational burden of EnKF and other MCS-based schemes, regularization may be introduced, as discussed by Sørensen et al. (2004). However, as we shall see in this paper, the relatively simple nonlinear nature of the rainfall-flow and flow routing processes means that there are simpler and computationally much less intensive alternatives to DA that are able to provide comparable forecasting performance.

There are a number of simplified, conventional approaches to flow routing that

have been applied to flow forecasting. Amongst others, for example, these include the Muskingham model with multiple inputs (Khan, 1993) and multiple regression (MR) models (Holder, 1985). The Muskingum model is deterministic and does not give the required uncertainty bounds for the forecasts. Moreover, these more conventional models tend to have a completely linear structure and so, naturally, they do not perform as well as nonlinear alternatives within the nonlinear rainfall-flow context.

In contrast, a considerable amount of research has been published recently on the application of nonlinear methods in flood forecasting. Amongst others, Porporato and Ridolfi (2001) present the application of a nonlinear prediction approach to multivariate flow routing and compare it successfully with ARMAX model forecasts. However, this approach does not have a recursive form and requires on-line automatic optimization when applied to on-line forecasting. Another nonlinear approach is the application of neural networks (NN) for flood forecasting (e.g. Thirumalaiyah and Deo, 2000; Park *et al.*, 2005). As discussed in these papers, NN models can yield better forecasts than conventional linear models and, if designed appropriately, they also allow on-line data assimilation. However, the NN based models normally have an overly complex nonlinear structure and so can provide over-parameterized representations of the fairly simple nonlinearity that characterizes the rainfall-flow process (see later). They are also the epitome of the black-box model and provide very little information on the underlying physical nature of the rainfall-flow process: information that can instill confidence in the model and allows for better implementation of the forecasting algorithm within a recursive estimation context.

In this Report, we consider another, newer approach to simplified modelling that utilizes statistical estimation to identify the special, serially connected nature of the rainfall input nonlinearity in the rainfall-water level process and then exploits this in order to develop a computationally efficient forecasting algorithm. This is based on statistically estimated, stochastic-dynamic DBM models of the rainfall-water level and level routing components of the system, which are then integrated into an adaptive, modified version of the standard recursive Kalman Filter (KF) state estimation algorithm that generates both the state variable forecasts and their 95% confidence bounds. Here, the state variables are defined as the ‘fast-flow’ and ‘slow-flow’ water levels, that together characterize the main inferred variables in the identified DBM rainfall-water level models. The serial input nonlinearity in the rainfall-flow model represents an effective rainfall transformation of the measured rainfall, the nature of which is estimated directly from the data using a method of *State Dependent Parameter* (SDP) estimation for nonlinear stochastic systems (e.g. Young, 2000, 2001a, Young *et al.*, 2001).

In contrast to the model predictions produced by a fully distributed parameter model, the water level forecasts in this case are made only at the location of measurements, in accordance with the goal of the flood forecasting system under consideration. Of course, the resulting water level forecasts could be used to update the predictions of inundation risk along a river by conditioning the risk predictions of a fully distributed flood forecasting model in real time (see Romanowicz and Beven, 1998; Romanowicz *et al.*, 2004a).

The methodology used in this study is presented in the next Section. It exploits the top-down, DBM approach to the stochastic-dynamic modelling of environmental processes, concentrating on the identification and estimation of those physically

interpretable, ‘dominant modes’ of dynamic behavior that are most important for flood prediction (e.g. Young, 2001c, 2002a). In particular, hydrological processes active in the catchment are modeled using the SDP method for estimating the location and nature of significant nonlinearities in the system (here the effective rainfall input nonlinearity), together with a *Stochastic Transfer Function* (STF) method for characterizing both the linear effective rainfall-water level behavior and the water level routing processes. The complete model consists of these linear and nonlinear, stochastic-dynamic elements connected in a manner that represents the physical structure of the Severn River catchment.

The adaptive forecasting system utilizes a state-space form of the complete catchment model, including allowance for heteroscedastic errors, as the basis for data assimilation and forecasting using a modified KF forecasting engine. Here, the updating is applied to three features of the forecasting system: the predicted model states (water levels including the inferred fast and slow components: see later, Section 5(b) and Appendix 2); adaptive gain parameters that allow for unpredictable changes in the catchment behavior; and the state-dependent heteroscedasticity (changing variance) that is associated with the model residuals. These are all updated recursively in response to input data received in real-time from remote sensors in the catchment. It is worth noting that this same methodology may be used when backwater effects are not negligible (e.g. from tidal effects). Such effects can be considered as a second (downstream) input to the STF elements in the DBM model, so that a *Multi-Input, Single-Output* (MISO) model can be incorporated within the same methodological framework. This latter approach was not necessary in the present case study but it would be necessary if the current forecasting system, which currently forecasts down to Bewdley, were to be extended further downstream to where tidal effects are encountered.

5. Methodology

In this paper, we develop further an earlier approach to forecasting system design for a single component rainfall-flow model (Young, 2001c, 2002a) so that it can be used with a complete, multi-component, quasi-distributed model covering a large part of the River Severn Catchment in the U.K. An early version of this system has been outlined in Romanowicz *et al.* (2004b). Later, in the Section 6, we describe, in some detail, a considerably enhanced version, where water levels are forecast instead of flows and there is a modified approach to the on-line adaption of the variance ‘hyper-parameters’. These enhancements were introduced to facilitate the incorporation of the forecasting system into the *National Flood Forecasting System* (NFFS) developed for the *UK Environment Agency* (EA) by Delft Hydraulics (Beven *et al.*, 2005). The extension also includes the application of a larger number of rainfall gauging stations; the development of an enhanced method of dealing with the rainfall-water level nonlinearity; and a simpler, more robust method of accounting for the heteroscedastic variance. As a result of these changes, the forecasts have smaller bias, lower uncertainty levels and longer lead times.

The use of water levels, instead of flows, enables much better utilization of existing water level observations, including those stations for which rating curves do not exist or are not reliable. All of the river gauging stations provide water level measurements which, as usual, could be transformed into flow using the rating

curve specific to each station. However, variations in flow velocity and the way that losses of energy due to friction change with water level and gradient, mean that this transformation is not very well defined, particularly for high flows. Moreover, it is normally based on historic calibration that may well have become out-of-date or could have been changed during an extreme flood event. Hence, by using water level measurements instead of the flows, we by-pass these uncertainties related to water level-flow conversion. Additionally and conveniently, we also tend to decrease the heteroscedasticity of the prediction errors, as explained later. Since water levels are usually measured relative to a base level (i.e. the historically justified minimum water level at a given gauging station) a correction for this reference datum is introduced for each gauging station.

(a) *The Nonlinear Rainfall-Water Level Model*

It is assumed that the rainfall and water level measurements, $r(t)$ and $y(t)$ are sampled uniformly in time at a sampling interval of Δt time units (here hours) and that these discrete-time, sampled measurements are denoted by r_k and y_k , respectively. It has been shown (Young, 1993; Young and Beven, 1994; Young and Tomlin, 2000; Young, 2002a, 2003, 2004a, 2006a; Romanowicz *et al.*, 2004a,b) that the nonlinearities arising from the relationship between measured rainfall r_k and effective rainfall, denoted here by u_k , can be approximated using gauged flow or water level as a surrogate measure of the antecedent wetness or soil-water storage in the catchment. In particular, the scalar function describing the nonlinearity between the rainfall r_k and the soil moisture surrogate y_k is initially identified non-parametrically using SDP estimation (see Appendix 2 and the cited references).

As in the case of the flow modelling and forecasting studies considered previously and cited above, this shows that the SDP nonlinearity can often be parameterized to reasonable accuracy by a power-law relationship. However, in the present application, this relation has been modified to take into account the nature of the non-parametric SDP estimation results, where there is a flattening of the flood wave due to the over-bank flooding. It should be mentioned that this flattening effect is visible both for the flows and water levels. The modified relation, which allows the gain associated with the power law to change for higher water levels, takes the form†:

$$u_k = c_0 \cdot c(y_k) \cdot y_k^\gamma \cdot r_k; \quad c(y_k) = \begin{cases} 1 & \text{for } y_k < y_0 \\ c_p & \text{for } y_k \geq y_0 \end{cases} \quad (1.1)$$

where u_k denotes the effective rainfall; r_k denotes measured rainfall; c_0 is a scaling constant; $c_p (0 < c_p \leq 1.0)$ is a constant describing the degree of flattening of the flood wave; and y_0 is related to the bank-full water level. The power-law exponent γ and constants $\{c_p\}$ and $\{y_0\}$ are estimated by a special optimization procedure that includes the concurrent estimation of the following linear STF model (see Appendix

† The non-parametric estimation results suggest a more complicated function: this minor modification to the standard power law was selected for simplicity at this phase of the Study and a superior function, that better matches the non-parametrically estimated shape of the nonlinearity, is being investigated.

2) between the delayed effective rainfall $u_{k-\delta}$ and water level, denoted here by y_k :

$$y_k = \frac{B(z^{-1})}{A(z^{-1})} u_{k-\delta} + \xi_k \quad (1.2)$$

where δ is a pure, advective time delay of $\delta\Delta t$ time units, while $A(z^{-1})$ and $B(z^{-1})$ are polynomials in the backward shift operator of the following form:

$$\begin{aligned} A(z^{-1}) &= 1 + a_1 z^{-1} + a_2 z^{-2} + \cdots + a_n z^{-n} \\ B(z^{-1}) &= b_0 + b_1 z^{-1} + b_2 z^{-2} + \cdots + b_m z^{-m} \end{aligned}$$

Here, ξ_k is usually a heteroscedastic (changing variance) noise term that is assumed to account for all the uncertainty associated with the inputs affecting the model, including measurement noise, un-measured inputs, and uncertainty in the model. The orders of the polynomials n and m are identified from the data during the estimation process and are usually in the range 1-3. The triad $[n \ m \ \delta]$ is normally used to describe this model structure. Finally, combining equations (1.1) and (1.2), the complete rainfall-flow model can be written as:

$$y_k = \frac{B(z^{-1})}{A(z^{-1})} u_{k-\delta} + \xi_k \quad u_k = \{c(y_k) y_k^\gamma\} r_k \quad (1.3)$$

where the scaling constant c_p is incorporated into $c(y_k)$.

Note that, the STF model (1.2) can be written in the discrete-time equation form,

$$y_k = -a_1 y_{k-1} - \cdots - a_n y_{k-n} + b_0 u_{k-\delta} + b_1 u_{k-\delta-1} + \cdots + b_m u_{k-\delta-m} + \eta_k \quad (1.4)$$

where $\eta_k = A(z^{-1})\xi_k$ is the transformed noise input. This shows that the river water level at the k^{th} hour is dependent on water level and effective rainfall measurements made over previous hours, as well as the uncertainty η_k arising from all sources. Note also that, while the STF relationship between effective rainfall and water level is linear, the noise η_k is dependent on the model parameters, thus precluding linear least squares estimation and requiring more advanced STF model estimation procedures (see Appendix 2). And, of course, the complete model between measured rainfall and water level is quite heavily nonlinear because of the effective rainfall nonlinearity in (1.3).

(b) State Space Formulation of the Rainfall-Water Level Model

In a typical STF model describing the hourly changes of water levels in response to rainfall inputs, $n = m = 2$, so that the general model (1.3) reduces to:

$$y_k = \frac{b_0 + b_1 z^{-1}}{1 + a_1 z^{-1} + a_2 z^{-2}} u_{k-\delta} + \xi_k \quad \{c(y_k) y_k^\gamma\} r_k \quad (1.5)$$

The decomposition of the STF component of this DBM model into the fast and slow water level components $y_{1,k}$ and $y_{2,k}$ then has the form:

$$\text{Fast Component: } y_{1,k} = \frac{\beta_1}{1 + \alpha_1 z^{-1}} u_{k-\delta} \quad (1.6)$$

$$\text{Slow Component: } y_{2,k} = \frac{\beta_2}{1 + \alpha_2 z^{-1}} u_{k-\delta} \quad (1.7)$$

where $\alpha_1, \alpha_2, \beta_1$ and β_2 are parameters derived from the model parameters in (1.2) and the total gauged flow is the sum of these two components and the noise ξ_k , i.e.,

$$y_k = y_{1,k} + y_{2,k} + \xi_k \quad (1.8)$$

The associated residence times (time constants) $\{T_1, T_2\}$, steady state gains $\{G_1, G_2\}$ and partition percentages $\{P_1, P_2\}$, are given by the following expressions, as discussed in Appendix 2:

$$T_i = \frac{\Delta t}{\log_e(\alpha_i)}; G_i = \frac{\beta_i}{1 + \alpha_i}; P_i = \frac{100G_i}{G_1 + G_2} \quad i = 1, 2$$

The parameters of this DBM model are derived from statistical model identification and estimation analysis based on the observed rainfall-water level data. The value of the DBM method depends on the amount of information available in these data to statistically estimate the model parameters. Here, the SRIIV (Simplified Refined Instrumental Variable) algorithm from the CAPTAIN Toolbox for MatlabTM, as well as associated DBM statistical modelling concepts, are used to identify the order of the STF model (the values of n, m and δ) and to estimate the associated parameters (see Appendix 2 and the cited references).

For forecasting purposes, the DBM model (1.5), considered in its decomposed form (1.6) to (1.8), is converted to a stochastic state space form. This then allows for the solution of the resulting state equations within a Kalman filter framework. It also facilitates the on-line, real time estimation of both water level components, as well as the optimization of the hyper-parameters (parameters associated with the stochastic inputs: see next sub-Section (c)) of the state space model, based on a multi-step-ahead forecast error criterion. The state space form of the decomposed DBM model has the form:

$$\begin{aligned} \mathbf{x}_k &= \mathbf{F}\mathbf{x}_{k-1} + \mathbf{G}u_{k-\delta} + \boldsymbol{\zeta}_k \\ y_k &= \mathbf{h}^T \mathbf{x}_k + \xi_k \end{aligned} \quad (1.9)$$

where

$$\mathbf{F} = \begin{bmatrix} -\alpha_1 & 0 \\ 0 & -\alpha_2 \end{bmatrix} \quad \mathbf{G} = \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} \quad \boldsymbol{\zeta}_k = \begin{bmatrix} \zeta_{1,k} \\ \zeta_{2,k} \end{bmatrix} \quad \mathbf{h}^T = [1 \quad 1]$$

Here, the elements of the state vector $\mathbf{x}_k = [x_{1,k} \ x_{2,k}]^T$ are, respectively, the fast and slow components of the rainfall-water level process; while the system noise variables in $\boldsymbol{\zeta}_k$ are introduced to allow for un-measurable stochastic inputs to the system. For simplicity, it is assumed that these are zero mean, serially uncorrelated and statistically independent random variables, with a purely diagonal covariance matrix.

In hydrological applications, the observation noise ξ_k is often complex in form, being correlated in time (coloured noise), heteroscedastic (changing variance: see later, sub-Sections (c) and (e)(ii) and it does not necessarily have rational spectral density. However, as pointed out in Appendix 2, in the circumstances where it can be assumed to have rational spectral density, it can be modelled using an AutoRegressive, Moving Average (ARMA) process of an order that is identified from the data. This can then be incorporated into the Kalman filter DA and forecasting procedure by extending the state vector. This is an alternative to the ‘error correction’

or ‘error updating’ procedures that have been suggested over a number of years (e.g. Goswami *et al.*, 2005)†

(c) *The Modified Kalman Filter Forecasting Engine*

For water level forecasting purposes, the state space model discussed in the previous Section is used as the basis for the implementation of the following, special KF state estimation and forecasting algorithm, which is a modified version of the standard KF algorithm developed in Appendix 3:

A priori prediction:

$$\hat{\mathbf{x}}_{k|k-1} = \mathbf{F}\hat{\mathbf{x}}_{k-1} + \mathbf{G}\{c(y_{k-\delta})y_{k-\delta}^\gamma\}r_k \quad (1.10a)$$

$$\mathbf{P}_{k|k-1} = \mathbf{FP}_{k-1}\mathbf{F}^T + \sigma_k^2\mathbf{Q}_r \quad (1.10b)$$

A posteriori correction:

$$\hat{\mathbf{x}}_k = \hat{\mathbf{x}}_{k|k-1} + \mathbf{P}_{k|k-1}\mathbf{h}[\sigma_k^2 + \mathbf{h}^T\mathbf{P}_{k|k-1}\mathbf{h}]^{-1}\{(y_k - \mathbf{h}^T\hat{\mathbf{x}}_{k|k-1}\}\} \quad (1.10c)$$

$$\mathbf{P}_k = \mathbf{P}_{k|k-1} - \mathbf{P}_{k|k-1}\mathbf{h}[\sigma_k^2 + \mathbf{h}^T\mathbf{P}_{k|k-1}\mathbf{h}]^{-1}\mathbf{h}^T\mathbf{P}_{k|k-1} \quad (1.10d)$$

$$\sigma_k^2 = \sigma_0^2 + \sigma^2(y_k^2) \quad (1.10e)$$

In these equations, \mathbf{P}_k is the error covariance matrix associated with the state estimates; \mathbf{Q}_r is the 2×2 *Noise Variance Ratio* (NVR) matrix, as discussed in the next sub-Section (d); and the subscript notation $k|k-1$ denotes the estimate at the k^{th} sampling instant (here hour), based on the estimate at the previous $(k-1)^{th}$ sampling instant. The differences between this version of the KF and the standard version in Appendix 2 are: the nonlinear input entering in equation (1.10a); the state-dependent NVR matrix term $\sigma_k^2\mathbf{Q}_r$, replacing the constant covariance matrix \mathbf{Q} in equation (1.10b); and the state-dependent variance defined in equation (1.10e) and appearing in equations (1.10b), (1.10c) and (1.10d).

The f -step-ahead forecasts are obtained by simply repeating the prediction f times, without correction (since no new data over this interval are available). The f -step ahead forecast variance is then given by:

$$\text{var}(\hat{y}_{k+f|k}) = \hat{\sigma}_k^2 + \mathbf{h}^T\mathbf{P}_{k+f|k}\mathbf{h} \quad (1.10f)$$

where $\mathbf{P}_{k+f|k}$ is the error covariance matrix estimate associated with the f -step ahead prediction of the state estimates. This estimate of the f -step ahead prediction variance is used to derive approximate 95% confidence bounds for the forecasts, under the approximating assumption that the prediction error can be characterized as a nonstationary Gaussian process (i.e. twice the square root of the variance at each time step is used to define the 95% confidence region).

† It should be noted that the present paper utilizes TF models for rainfall-water level and flood routing forecasts, taking account of system nonlinearities, but the models used by Goswami *et al.* are linear TF models that are not appropriate to the modelling of nonlinear hydrological processes, except perhaps for single events, because they do not account for catchment storage effects.

(d) *State Adaption*

In the above KF equations (1.10a) and (1.10b), the model parameters $\alpha_i, i = 1, 2$ and $\beta_j, j = 1, 2$, that define the state space matrices \mathbf{F} and \mathbf{G} in (1.9), are known initially from the model identification and estimation analysis based on the estimation data set. However, by embedding the model equations within the KF algorithm, we have introduced additional, unknown parameters, normally termed ‘hyper-parameters’ to differentiate them from the model parameters†. In this example, these hyper-parameters are the elements of the NVR matrix \mathbf{Q}_r and, in practical terms, it is normally sufficient to assume that this is purely diagonal in form. These two diagonal elements, in this example, are defined as $NVR_i = \sigma_{\zeta_i}^2 / \sigma^2, i = 1, 2$. These specify the nature of the stochastic inputs to the state equations and so define the level of uncertainty in the evolution of each state (the quick and slow water level states respectively) relative to the variance of the measurement uncertainty σ^2 . The inherent state adaption of the KF arises from the presence of the NVR parameters, since these allow the estimates of the state variables to be adjusted to allow for presence and effect of the unmeasured stochastic disturbances that naturally affect any real system.

Clearly, the NVR hyper-parameters have to be estimated in some manner on the basis of the data. One well known approach is to exploit *Maximum Likelihood* (ML) estimation based on *Prediction Error Decomposition* (see Schweppe, 1964, 1973; Young, 1999b). Another, used in the River Severn forecasting system described later, is to optimize the hyper-parameters by minimizing the variance of the multi-step-ahead forecasting errors. In effect, this optimizes the memory of the recursive estimation and forecasting algorithm (see e.g. Young and Pedregal, 1999) in relation to the rainfall-water level data. In this numerical optimization, the multi-step-ahead forecasts $\hat{y}_{k+f|k}$, where f is the forecasting horizon. The main advantage of this latter approach is, of course, that the integrated model-forecasting algorithm is optimized directly in relation to the main objective of the forecasting system design; namely the minimization of the multi-step prediction errors.

(e) *Parameter Adaption*

Although the parameters and hyperparameters of the KF-based forecasting system can be optimized in the above manner, we cannot be sure that the system behaviour may not change sufficiently over time to require their adjustment. In addition, it is well known that the measurement noise ξ_k is quite highly heteroscedastic: i.e. its variance can change quite radically over time, with much higher variance occurring during storm events. For these reasons, it is wise to build some form of parameter adaption into the forecasting algorithm.

(i) *Gain Adaption*

It is straightforward to update *all* of the parameters in the rainfall-flow model since the RIV/SRIV estimation algorithms can be implemented in a recursive form that allows for sequential updating and the estimation of time-variable parameters (See

† Of course this differentiation is rather arbitrary since the model is inherently stochastic and so these parameters are simply additional parameters introduced to define the stochastic inputs to the model when it is formulated in this state space form

Appendix 3 and Young, 1984). However, this adds complexity to the final forecasting system and previous experience suggests that a simpler solution, involving a simpler scalar gain adaption is often sufficient. This is the approach that was used successfully for some years in the Dumfries flood warning system (Lees *et al.*, 1993, 1994) and it involves the recursive estimation of the gain g_k in the following relationship:

$$y_k = g_k \cdot \hat{y}_k + \epsilon_k \quad (1.11)$$

where ϵ_k is a noise term representing the lack of fit and, in the case of the second order model (1.5),

$$\hat{y}_k = \hat{y}_{1,k} + \hat{y}_{2,k} = \frac{\hat{b}_0 + \hat{b}_1 z^{-1}}{1 + \hat{a}_1 z^{-1} + \hat{a}_2 z^{-2}} u_{k-\delta} \quad (1.12)$$

In other words, the time variable scalar gain parameter g_k is introduced so that the model gain can be continually adjusted to reflect any changes in the steady state (equilibrium) response of the catchment to the effective rainfall inputs.

The associated recursive estimation algorithm for g_k is one of the simplest examples of the KF, in which the single state variable is the unknown gain g_k , which is assumed to evolve stochastically as a *Random Walk* (RW) process (e.g. Young, 1984)†:

$$p_{k|k-1} = p_{k-1} + q_g \quad (1.13a)$$

$$p_k = p_{k|k-1} - \frac{p_{k|k-1}^2 \hat{y}_k^2}{1 + p_{k|k-1} \hat{y}_k^2} \quad (1.13b)$$

$$\hat{g}_k = \hat{g}_{k-1} + p_k \hat{y}_k \{y_k - \hat{g}_{k-1} \hat{y}_k\} \quad (1.13c)$$

Here, \hat{g}_k is the estimate of g_k ; while q_g is the NVR defining the stochastic input to the RW process, the magnitude of which needs to be specified. The adapted forecast is obtained by simply multiplying the initially computed forecast by \hat{g}_k . Note that gain adaption of this kind is quite generic and can be applied to *any* model, not just the DBM model discussed here. If sufficiently motivated, the interested reader can derive the estimation equations (1.13a) to (1.13c) from the general KF equations in Appendix 3.

(ii) Variance Adaption

The heteroscedasticity of the observational noise suggests that the noise variance should be updated in some manner. Sorooshian and Dracup (1980) present an approach to deal with correlated and heteroscedastic errors of flow measurements, based on a maximum likelihood approach and an alternative procedure of either transforming the observation errors using an AR(1) model to obtain uncorrelated error, or introducing a Box-Cox transformation (Box and Cox, 1964) to deal with heteroscedasticity. Their methodology follows an *en-bloc* estimation procedure with hydrological model and error transformation parameters treated as deterministic variables. Vrugt *et al.* (2005), on the other hand, apply a nonparametric, local

† It is also a scalar example of *Dynamic Linear Regression* (DLR) algorithm (see Young, 1999b) available as a routine in the CAPTAIN Toolbox.

difference-based estimator of the observation error variance, based on Hall *et al.* (1990), to model the error heteroscedasticity in their EnKF solution of the rainfall-flow model.

In order to account for the heteroscedasticity in the present study, a new approach is used, where the variance σ_k^2 of ξ_k is identified from the data as a state-dependent function of a simulated output, taking the following form:

$$\sigma_k^2 = \lambda_0 + \lambda_1 \hat{y}_k^2 \quad (1.14)$$

where λ_0 and λ_1 are new hyper-parameters that are optimized together with the NVR hyper-parameter that controls the gain updating procedure discussed in (i). The estimate $\hat{\sigma}_k^2$ of σ_k^2 is fed back to the recursive Kalman filter engine (see previously, sub-Section (c)) as an estimate of the observational variance.

It is interesting to note at this point, that an analysis of the heteroscedastic characteristics of the noise, in the above manner manner, has revealed the advantage of modelling in terms of the water level variable instead of the flow. In particular, the transformation of the water level y_k into the flow variable, Q_k through the rating curve, may be written in the form $Q_k = f(y_k)$. According to delta-method calculations (Box and Cox, 1964), for a smooth function $f(\cdot)$, the asymptotic variance $AV(Q_k)$ of the flow Q_k as $y \rightarrow y_k$ will have the form

$$AV(Q_k) = \dot{f}(y_k)^2 \text{var}(y_k); \quad \dot{f}(y_k) = \left[\frac{df}{dy} \right]_{y=y_k} \quad (1.15)$$

Here, the function denotes the rating curve relationship, which often can be approximated by a power function of water levels, with the power greater than 1. Hence the variance of the flow is increased in comparison with the water level variance, in particular for larger flows. In this regard, it is interesting to note that Sorooshian and Dracup (1980) regarded error in the rating curve transformation of the water level observations as a main source of heteroscedasticity of the flow data.

(f) Single Module Summary

The combination of a Kalman filter incorporation of the state space model with the gain and variance updating described above in Sections e(i) and e(ii), provides a tool for on-line data assimilation. The NVR hyper-parameters associated with the stochastic inputs to the state space equation (1.9) are estimated in the first place by maximum likelihood based on ‘prediction error decomposition’ (Schweppe, 1964, 1973). Subsequently, in line with the current forecasting objectives, the hyper-parameters minimizing the variance of the N-step ahead prediction errors for the maximum water levels are estimated using an optimization routine from the MatlabTM computational software environment (based on the simplex direct search method of Nelder and Mead (1965)). The optimization is performed only during the calibration stage, the optimal values obtained in this manner are then used during the application of the real-time forecasting scheme.

In summary, the procedure for developing a single module of the forecasting system can be summarized as follows:

1. Estimate the complete nonlinear DBM model, including the effective rainfall nonlinearity, using the RIV and SDP estimation algorithms in the CAPTAIN

Toolbox, based on the available input-output data and ensuring that the chosen model is physically meaningful, in accordance with DBM modelling requirements.

2. Formulate the state space model and optimize the hyper-parameters, without on-line updating, using maximum likelihood estimation based on prediction error decomposition.
3. Optimize the updating and heteroscedastic variance parameters using a set of optimization criteria based on the N-step ahead forecast error.

Three criteria are used during the identification of the model structure and estimation of its parameters. The first is a coefficient of determination associated with the water level predictions $R_p^2 = (1 - \sigma_{inn}^2/\sigma_y^2)$, presented as a percentage, with σ_{inn}^2 and σ_y^2 denoting the variances of N-step prediction error and observations, respectively. This is a multi-step-ahead forecasting efficiency measure, similar in motivation to the Nash-Sutcliffe efficiency measure used for model calibration (Nash and Sutcliffe, 1970). The others are the YIC and AIC (Akaike, 1974) criteria, which are model order identification (identifiability) statistics: a low relative measure of these criteria ensures that the chosen model has a dynamic structure that reflects the information content of the data, so ensuring well identified parameters and no over-parameterization (see Appendix 2 and Young (1989)).

(g) River Water Level Routing

To begin with, following previous practice with flow routing, the water level routing down the river utilized linear dynamic models in a transfer function form. For instance, a first order example of such a model takes the form:

$$y_{i,k} = \frac{b_0}{1 + a_1 z^{-1}} y_{i-1,k-\delta} + \xi_k \quad (1.16)$$

where $y_{i-1,k}$ and $y_{i,k}$ are, respectively, the upstream and downstream water level measurements from the gauges and δ is the advective delay. If the noise ξ_k can be modelled well by an AR or ARMA process, then this can further enhance the model in forecasting terms. Model identification and estimation of this model is based on the same statistical procedures used in the rainfall-water level modelling, except that the added complexity of the SDP nonlinearity is now removed.

Once again, if the TF model is of this first order form, it represents a single linear store, whilst if it is higher order, it can be decomposed into a number of linear stores arranged in series or parallel, depending on the identification and estimation results (see Appendix 2). The incorporation of this model into the KF forecasting engine also involves the same procedure as in the rainfall-water level case, except that now the component of the KF devoted to this sub-model will be in its standard linear form, if necessary incorporating an SDP model for heteroscedastic noise. As we shall see in the Section 6, this approach to flow-routing is applied to the River Severn reach between Abermule and Welsh Bridge, where the model is first order with a pure advective time delay of $\delta = 23$ hours.

Further research has shown that this linear approach to flow routing can be improved by following the same SDP approach used in the case of rainfall-water

level modelling. This leads again to a ‘Hammerstein’ model form with an input nonlinearity that transforms the upstream water level before it enters the linear store. In the first order case, this SDP model takes the form:

$$y_{i,k} = \frac{b_0}{1 + a_1 z^{-1}} f(y_{i-1,k-\delta}) + \xi_k \quad (1.17)$$

where $f(y_{i-1,k-\delta})$ represents the nonlinearly transformed, advectively delayed upstream water level. Once again, if the noise ξ_k can be modelled well by an AR or ARMA process then this can be introduced to good effect. For forecasting, this model is introduced into the KF forecasting engine but now with the input nonlinearity present, as in the rainfall-water level case. In Section 6, this nonlinear approach to flow-routing is applied to the River Severn reaches between Buildwas and Bewdley.

(h) The Complete Catchment Forecasting System

Each rainfall-water level forecasting sub-system, together with the other sub-systems associated with the linear and nonlinear routing models, constitute modules in the complete forecasting system for the entire catchment. These are connected in a manner defined by the geographical location of the rainfall and flow sensors. The forecasts at each of the gauging stations are then based only on the upstream gauging station. The forecast lead times may be extended following the approach of cascading the predictions from upstream reaches as inputs to downstream reaches (see Romanowicz *et al.*, 2006b) but the forecasting accuracy is affected as a result. Of course, the use of this kind of routing model relies on data acquisition along the river at as many points as is economically justified in order to obtain the required accuracy of the distributed forecasts along the river.

The complete model synthesised in this manner could be incorporated as a single large state space model within the modified KF forecasting engine. While this approach was evaluated and found to function satisfactorily, it was naturally simpler to disaggregate the system into a combination of suitably interconnected KF algorithms, each defined on the basis of the appropriate rainfall-water level or water level-water level model at the specified location. For the lead times not exceeding the natural sub-reach delay, these modules are effectively independent from each other. However, for larger lead times, when the forecasts of the rainfall-flow and routing modules are introduced instead of observed input, the modules become coupled. The influence of the uncompensated correlation between the modules on the forecasting performance does not seem to be large but it is a subject for future research.

In line with our decomposition of the KF, the optimization of the hyper-parameters for the whole forecasting system is based on the separate optimization of the hyper-parameters in each module. Overall optimization was attempted but this failed because the optimization hyper-surfaces were too flat to allow for satisfactory convergence. Of course, this optimization can be based on a number of different criteria. For example, it could seek to:

1. maximize a statistical Likelihood function (ML optimization);
2. minimize overall forecasting errors, or at specific forecasting horizons;

3. minimize forecasting errors at flood peaks;
4. satisfy multi-objectives (multi-objective optimization), etc.

However, for simple illustrative purposes, in the present Case Study, optimization was based on 2., namely, minimizing the sum of the squares of the forecasting errors at specific forecasting horizons.

6. Case Study: The River Severn

The methodology outlined in the previous Sections has been used to derive a real-time, adaptive forecasting system for the River Severn in the U.K, as far downstream as the gauge at Bewdley. A map of the River Severn catchment is shown in Figure 1, where the locations considered are shown as black dots, with associated place names. The River Severn above Buildwas has one major tributary, the River Vyrnwy, which enters the main river upstream of the Montford gauging station. The data used in this study consist of hourly measurements of rainfall at the Dollyd, Cefn Coch, Vyrnwy Llanfyllin and Pen y Coed, in the Upper Severn and Vyrnwy catchments; and hourly water level measurements at Meifod, on the Vyrnwy, and Abermule, Welsh Bridge (Shrewsbury) and Buildwas, on the River Severn. The Severn catchment area at Abermule is 580 km^2 , at Welsh Bridge 2325 km^2 and at Buildwas 3717 km^2 . The Vyrnwy catchment area at Meifod is 675 km^2 . The length of the River Severn between Abermule and Welsh Bridge is about 80 km ; the distance between Welsh Bridge and Buildwas is about 37 km and the distance between Buildwas down to Bewdley is 40 km . There are 12 bridges on the 18 km long reach between Buildwas and Bridgnorth Bridge and a similar number on the 22 km long reach between Bridgnorth Bridge and Bewdley. There are also a number of rapids and weirs. It is worth noting that releases from the Llyn Clywedog reservoir, on Severn above Abermule, and Lake Vyrnwy, on the Vyrnwy tributary of Severn, are used to enhance low flows. Also, the water releases for water level maintenance may have an effect on low water level behaviour at Abermule and Meifod. As regards the data used for DBM modelling, model structure identification and estimation is based the October 1998 year flood event data; and the validation data starts at 9am on the 24th of October 2000. In addition, the flood event in February 2002 is used for the validation of the sub-reaches between Buildwas and Bewdley.

The aim of the forecasting system design is the development of a relatively simple, robust, on-line forecasting system, with acceptable accuracy and the longest possible lead-time. In order to maximize the lead-times, rainfall measurements are used as an input to the rainfall-water level forecasts in the upper part of the Severn catchment. The sequential structure of the DBM forecasting model is shown as a block diagram in Figure 2, which also defines the nomenclature for the rainfall and water level variables down the system. So far, the forecasting system has only been developed as far as Bewdley because, further downstream, there are numerous weirs controlling water levels locally along the river and the flow is no longer at all natural. We will only be able to extend the system to the lower part of the Severn when the additional information about the man-induced changes on the river are available.

In the following sub-Sections 6.1(a) to 6.3(g), we present the rainfall-water level and water level routing models for the River Severn from Abermule down to Be-

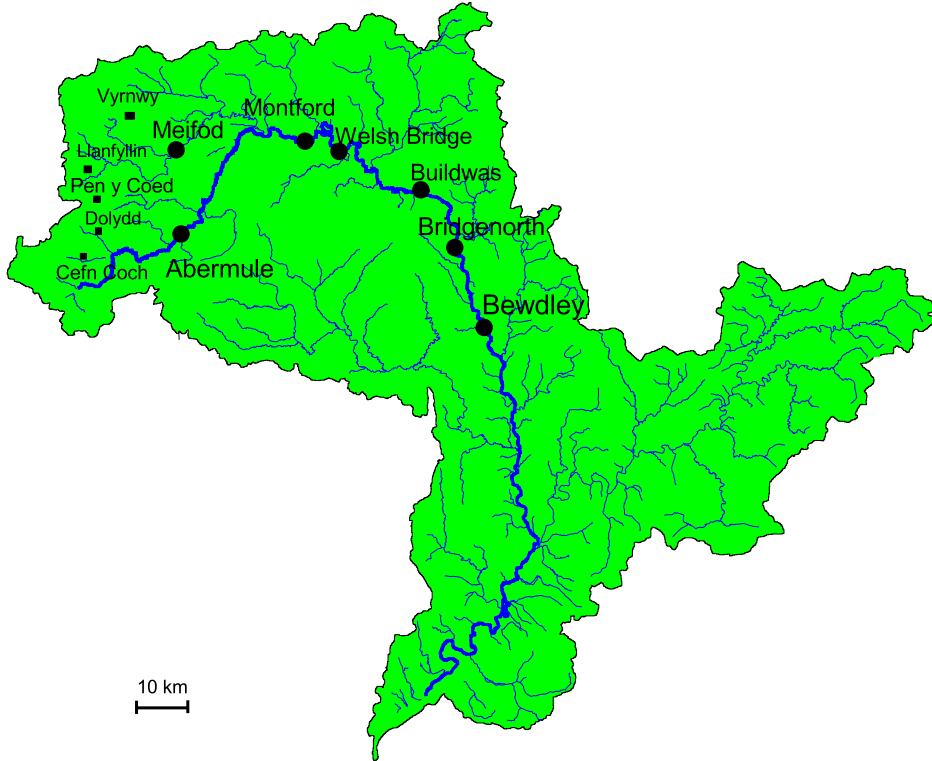


Figure 1. The River Severn catchment showing the water level/flow (black circles) and rainfall (small black squares) measurement sites used in the Study.

Table 1. Model Structure Identification Results

Model Type	Location	Model Structure	Forecast Lead [h]	R^2_T Calibration	R^2_T Validation
nonlinear	Abermule	[2 2 5]	5	0.954	0.945
nonlinear	Meifod	[2 2 5]	5	0.970	0.953
linear	Welsh Bridge	[1 1 23]	28	0.947	0.948
linear	Buildwas	[2 2 7]	35	0.970	0.961

wdley. The water level routing model for Welsh Bridge uses the averaged water levels from Abermule (Severn) and Meifod (Vyrnwy) as a single input variable: the use of these observations as two separate input variables was not possible due to their high cross-correlation and the associated poor identifiability of the model parameters (multi-collinearity). All the DBM sub-models in this network are estimated using the statistical identification and estimation procedures discussed in the previous Section 5. The results from the RIV/SDP analysis of the DBM models for Abermule, Meifod, Welsh Bridge and Buildwas, as well as their diagnostic performance measures are summarized in Table 1.

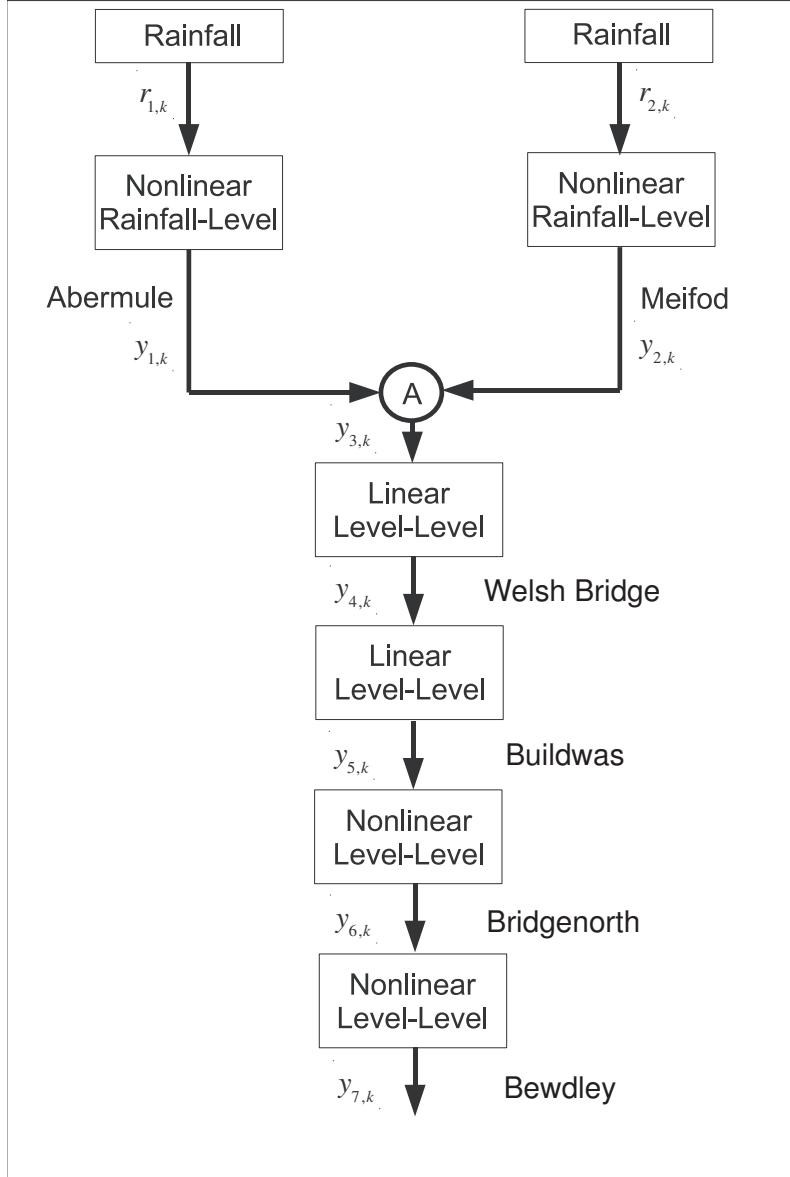


Figure 2. Block diagram of the River Severn Forecasting System DBM model.

6.1 Rainfall-Water Level Modelling

The two nonlinear models described in this first sub-Section relate composite rainfall measures, obtained as a linear combination of rainfall gauge measurements with optimized weights, to the water levels measured at each location.

(a) *Rainfall-Water Level Model for Abermule*

The rainfall-water level model for Abermule uses rainfall measurements from three gauging stations in the Upper Severn catchment, Cefn Coch, Pen-y-Coed and Dolydd, as inputs. The weights for the rainfall measurements are derived through the least squares optimization of the difference between the observed and modelled water levels at Abermule. The nonlinearity between the rainfall and water levels is identified initially using the non-parametric SDP estimation tool from the CAPTAIN toolbox. This non-parametric (graphical) relation is then parameterized using a step-wise power law parameterization of the form given in (1.1) and the coefficients c_p, y_0 and γ are optimized simultaneously with the estimation of the other model parameters. The model, after the decomposition into slow and fast components, has the form:

$$y_{1,k} = \frac{0.0038}{1 - 0.9955z^{-1}} u_{1,k-5} + \frac{0.134}{1 - 0.9304z^{-1}} u_{1,k-5} + \xi_k \quad (1.18a)$$

$$u_{1,k} = \begin{cases} 1 & y_{1,k} < 3.36 \\ 0.68 & y_{1,k} \geq 3.36 \end{cases} y_{1,k}^{0.7} \cdot r_{1,k} \quad (1.18b)$$

The identified residence times for the fast and slow flow components of this model are 13 hours and 9 days, respectively. This model explains 93% of the variance of the observations, with the variance of the simulation modelling errors equal to 0.037 m^2 .

The prediction error series shows both autocorrelation and heteroscedasticity, even though the latter is noticeably smaller than in the case of the model based on flow rather than water level measurements. In the case of the autocorrelation, an AR(3) model for the noise is identified based on the AIC criterion. The noise model could be incorporated into the forecasting model, as mentioned previously. However, in order to make the whole catchment model as simple as possible, and in compliance with the design objectives, it was decided not to do this in the upper reaches, down to Buildwas, but to retain the adaptive estimation of heteroscedastic variance of the predictions, with the option of introducing a noise model if the performance needed improvement and the added complexity could be justified at a later stage. As we shall see later in sub-Section 6.2, however, AR noise models are incorporated in the nonlinear routing models from Buildwas to Bewdley. Note that, although the standard errors on the parameters of the TF model are generated during the RIV/SDP estimation, the standard error estimates on the decomposed model parameters, shown here in (1.18a)–(1.18b), would need to be obtained by Monte Carlo simulation (e.g. Young, 1999a, 2001b, 2003) and this was not thought necessary in this illustrative example.

Based on these initial results, the gain and heteroscedastic variance updating procedures described earlier were applied to the rainfall-water level model (1.18a)–(1.18b). At the calibration stage, the resulting 5-step-ahead forecasts of water levels explained 95.4% of the observational variance. The subsequent validation stage was carried out for the year 2000 floods and the results are shown in Figure 3, where the 5-hour-ahead forecast explains 94.5% of the variance of observations, only a little less than that obtained during calibration. The bank-full level at this site is at about 3.7 meters.

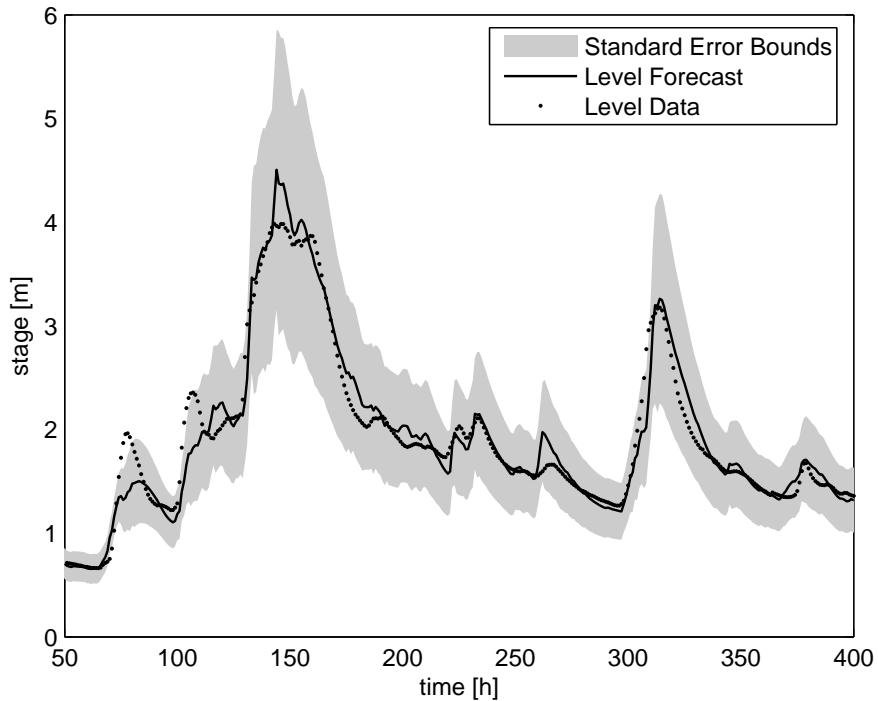


Figure 3. Abermule: 5-hour-ahead validation forecast, 24th October 2000

The results obtained so far, of which those shown in Figure 3 are typical, suggest that the adaptive forecasting system predicts the high water levels well, which is the principal objective of the forecasting system design. The magnitude and timing of the lower peaks is not captured quite so well. This may be due to a number of factors, such as the changes in the catchment response times arising from a dependence on the catchment wetness. These possibilities have not been investigated so far, however, because the forecasting performance is considered satisfactory in relation to the current objectives.

(b) Rainfall-Water Level Model for Meifod

The same procedure used in the last sub-Section was applied to derive the DBM model for the Meifod gauging station on the River Vyrnwy. Amongst the rainfall measurement stations on the Vyrnwy catchment, three were chosen: Pen-y-Coed, Llanfyllin and Vyrnwy. The weights for the rainfall measurements were optimized, together with the parameters of the DBM model. The best rainfall-water level model, without any adaptive updating, has the same form as for Abermule, that is [2 2 5], and explains 92% of the variance of the observations. The full model equation, with the TF decomposition and the modified power-law transformation

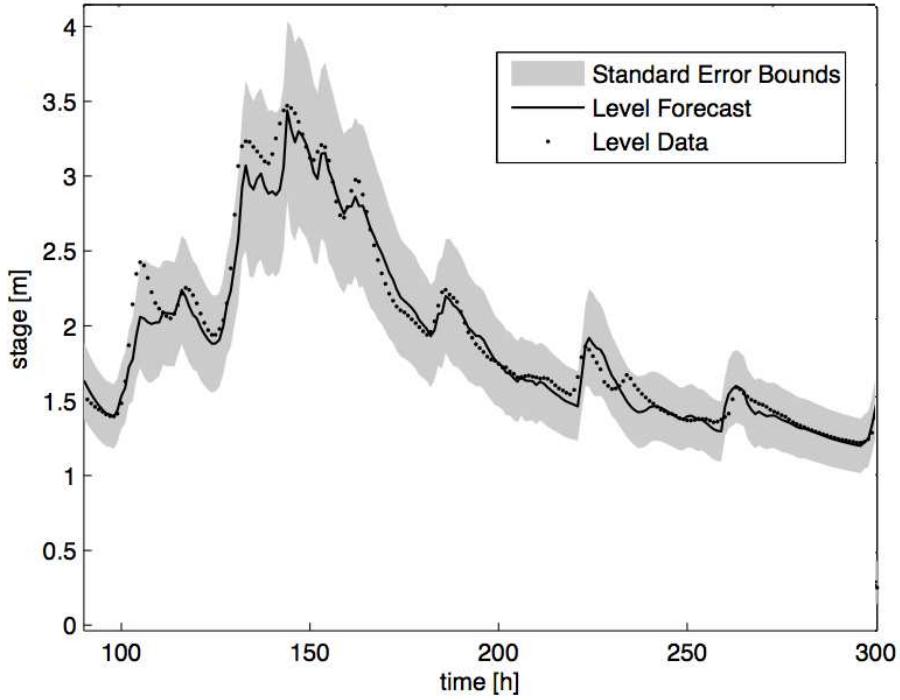


Figure 4. Meifod: 5-hour-ahead validation forecast based on upstream water level and rainfall inputs.

of the rainfall is given below:

$$y_{2,k} = \frac{0.0247}{1 - 0.9711z^{-1}} u_{2,k-5} + \frac{0.0424}{1 - 0.8491z^{-1}} u_{2,k-5} + \xi_k \quad (1.19a)$$

$$u_{2,k} = \begin{cases} 1 & y_{2,k} < 2.1 \\ 0.72 & y_{2,k} \geq 2.1 \end{cases} \quad (1.19b)$$

The identified residence times for the fast and slow flow components of this model are 6 hours and 34 hours, respectively.

The on-line updated 5-hour-ahead forecast for Meifod, over the calibration period in October 1998, explains 97% of the variance of observations. The validation was performed on the same time period in the year 2000 as the Abermule model and the results are shown in Figure 4. Here, the model explains 95.3% of the variance of observations. As in the case of Abermule, the results show some nonlinearity in timing. However, we do not have any information about the bank-full level for this site.

6.2 Linear Water Level Routing

The part of the River Severn down from Meifod and Abermule to Bewdley is modelled using two linear routing models, each of the form outlined in Section 5(g). At

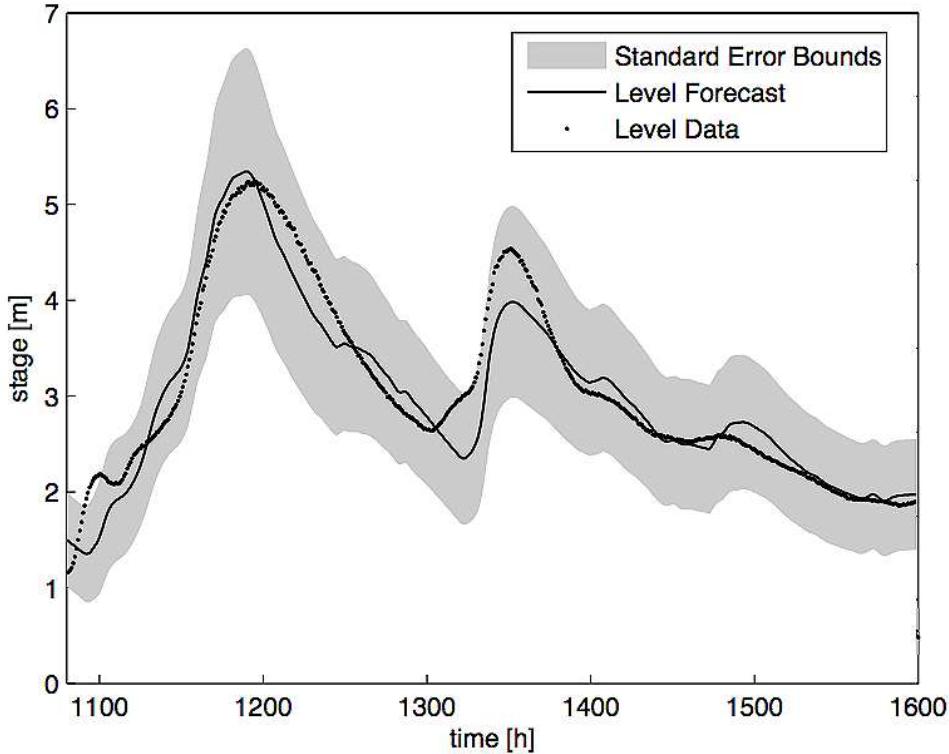


Figure 5. Welsh Bridge: 28-hour-ahead validation forecast based on upstream water level and rainfall inputs.

each gauging station, the linear STF model is identified and estimated based on the water level measurements at each gauge and the nearest downstream gauging station. The first order form of equation (1.16) is identified for the two models using the RIV algorithm for linear TF model estimation (see Appendix 2).

(c) Water Level-Routing Model for Welsh Bridge

The best results for the water level data between Abermule, Meifod and Welsh Bridge were obtained when the TF model was calibrated on the water level data with the minimum water level at Welsh Bridge removed for identification and estimation purposes. It was then re-introduced for implementation of the model in the forecasting engine. The first order model estimated in this manner is given below: it has a time delay of 23 hours and a residence time of about 28 hours.

$$y_{4,k} = \frac{0.0692}{1 - 0.9650z^{-1}} y_{3,k-23} + \xi_k \quad (1.20)$$

where $y_{3,k-23}$ denotes the average (circled A in Figure 2) of the water level measurements $y_{1,k}$ and $y_{2,k}$ at Meifod and Abermule, respectively, delayed by 23 hours; and $y_{4,k}$ denotes water level at Welsh Bridge. The 5 hour-ahead forecasts of water levels for Abermule and Meifod enable the Welsh Bridge water level forecasts

to be extended to 28 hours, which should be more than adequate for flood warning purposes at Shrewsbury. The resulting, adaptively updated, water level forecast at Welsh Bridge explains 94.7% of the output variation.

Validation of the model at Welsh Bridge was performed using all of the upstream models: i.e., rainfall-water level models for Meifod and Abermule and water level routing model for Welsh Bridge, with summed water level observations/forecasts for Abermule and Meifod. The resulting on-line updated 28-hour-ahead forecasts are shown in Figure 5, validated on year 2000 floods. These forecasts explain 94.8% of the observed water level variance at Welsh Bridge, a little better than the calibration performance.

(d) Water Level Routing Model for Welsh Bridge-Buildwas

Identification and estimation of the water level routing model for Welsh Bridge-Buildwas resulted in a [2 2 7] model, which explains 98% of the variance of the observations. This model has the following decomposed TF form:

$$y_{5,k} = \frac{0.0034}{1 - 0.9866z^{-1}} y_{4,k-7} + \frac{0.6456}{1 - 0.4669z^{-1}} y_{4,k-7} + \xi_k \quad (1.21)$$

where $y_{4,k-7}$ denotes the water level measurement at Welsh Bridge, delayed by 7 hours and $y_{5,k}$ denotes water level at Buildwas. Here, the residence times are about 1 hour for the fast component and about 3 days for the slow component. The bank-full level at this site is at about 6 meters. It is not clear what physical interpretation can be given to this identified parallel pathway model but it is probably a reflection of some complexity of the flow process in the river between Welsh Bridge and Buildwas and it would be interesting to investigate this further.

Finally, when the adaptive updating procedures were applied to the model and the 28 hour-ahead forecasts were used to extend the total forecast lead time of the final model to 35 hours, the forecast explains nearly 97% of the variance of observed water levels at Buildwas. The validation of the model was performed on the November floods from the year 2000 and the results are shown in Figure 6. The model explains 96% of the variance of the water level observations at Buildwas. The high peak values are predicted with reasonable accuracy, while the lower water level changes are over-predicted and there is a visible time difference between the simulated and observed water levels for the smaller peaks.

6.3 Nonlinear Water Level Routing

The three, nonlinear routing models described in this sub-Section relate the upstream water levels to the downstream water levels measured at each location. The part of the River Severn down from Welsh Bridge to Bewdley is modelled using three nonlinear routing models, each of the form outlined in Section 5(g). The Welsh Bridge-Buildwas reach was incorporated again in order to extend the forecast downstream using the same nonlinear modelling approach. At each gauging station, the nonlinear STF model is identified and estimated based on the water level measurements between this gauge and the nearest downstream gauging station. The first order form of equation (1.17) is identified for all three of these models using the same statistical approach to that described for the rainfall-water level models discussed in previous Sections. In each case, the identified non-parametric SDP

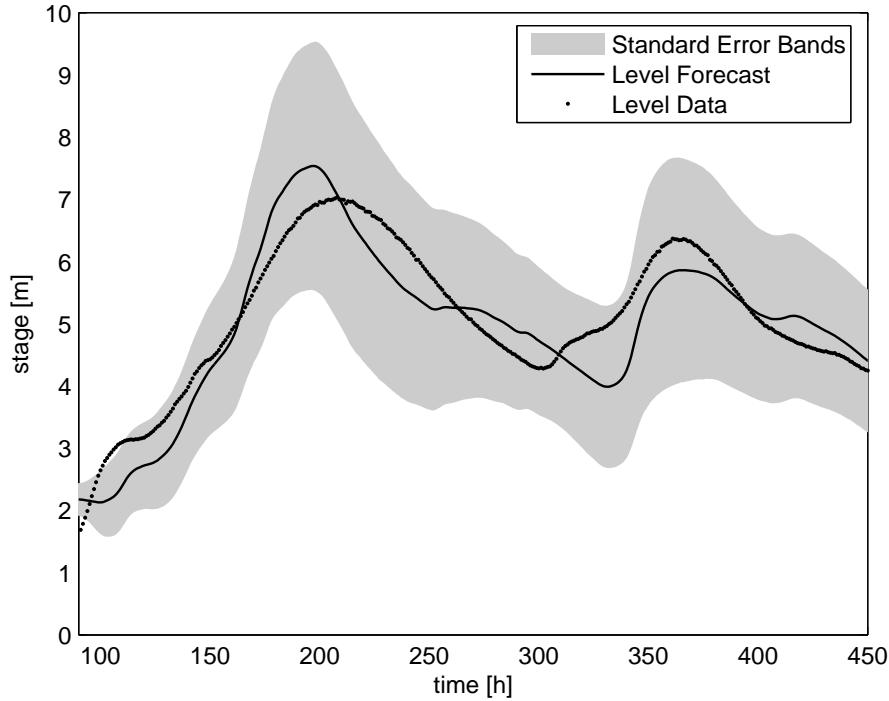


Figure 6. Buildwas: 35-hour validation forecast, 24th October 2000

Table 2. Model Structure Identification Results: Nonlinear Routing

Model Type	Location	Model Structure	Forecast Lead [h]	R^2_T Calibration	R^2_T Validation
nonlinear	Buildwas	[1 1 8]	8	0.997	0.996
nonlinear	Bridgenorth	[1 1 2]	10	0.997	0.996
nonlinear	Bewdley	[1 1 4]	14	0.998	0.989

nonlinearity is then parameterized using a *Radial Basis Function* (RBF) approximation (although any alternative, flexible parameterization would be suitable†) and a 10 element RBF is sufficient for all three models. In the final estimation phase of the modelling, the RBF parameters are re-optimized concurrently with the associated STF parameters, again using a similar optimization procedure to that used for the rainfall-water level modelling. The results from the RIV/SDP analysis of the DBM models for Buildwas, Bridgenorth and Bewdley, as well as their diagnostic performance measures are summarized in Table 2.

† The RBF is often portrayed as a ‘neural’ function but this can be misleading: as used here, the RBF is simply composed of Gaussian-normal shaped basis functions that, when combined linearly using optimized parameters (‘weights’), can approximate well smooth nonlinear curves, such as the SDP-type nonlinearity.

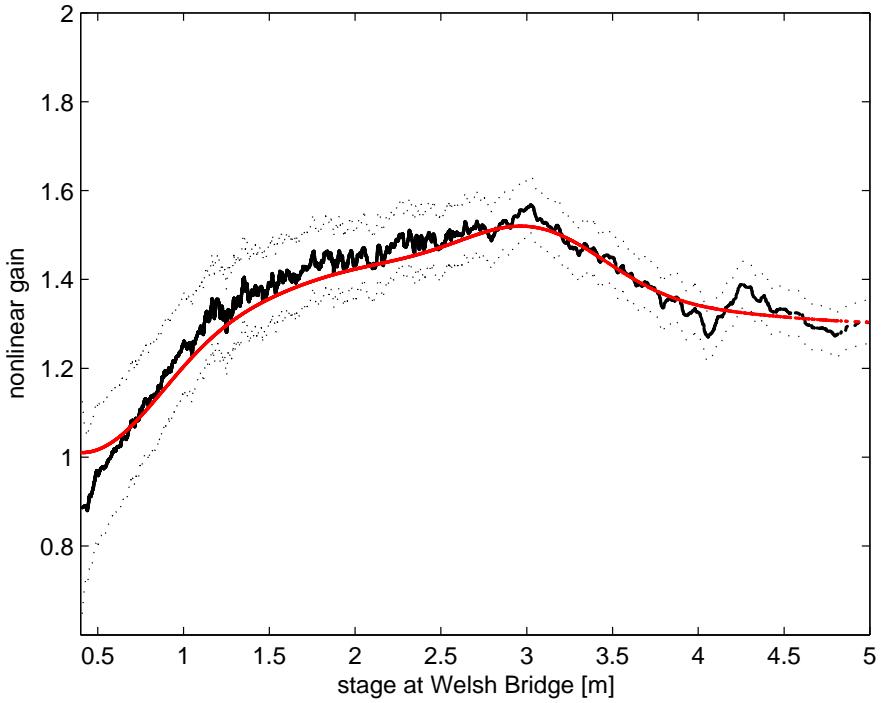


Figure 7. The estimated SDP nonlinearity for the Welsh Bridge–Buildwas routing model: the non-parametric estimate is shown as the black, full line, with its standard error bounds shown dotted; the red line is the optimal RBF estimate (see text).

(e) Nonlinear Water Level Routing for Welsh Bridge–Buildwas

The linear water level-routing model for Welsh Bridge–Buildwas is presented in Section 6(d) but the same reach can be modelled using the nonlinearly transformed water levels at Welsh Bridge as an input to a linear first order transfer function. The nonlinear relation is parameterized using 10 radial basis functions as explained above and Figure 7 compares the RBF parameterized nonlinearity (red line) with the initial non-parametric estimate (black line). Note that this red line is not estimated as a RBF approximation to the non-parametric black line; it is the finally optimized RBF function and is plotted here to show that it compares well with the initial non-parametric estimate. Note also how the state-dependent gain defined by this nonlinear curve reduces substantially at water levels greater than 3 m, possibly suggesting that over-bank flow is occurring above this level.

The best identified model structure for Welsh Bridge–Buildwas reach, incorporating this nonlinearity, has the form:

$$y_{5,k} = \frac{0.4683}{1 - 0.5224z^{-1}} f_4(y_{4,k-8}) + \xi_k \quad (1.22)$$

where $f_4(y_{4,k-8})$ denotes the nonlinearly transformed input water level at Welsh Bridge delayed by 8 hours and $y_{5,k}$ denotes water level at Buildwas. The noise ξ_k

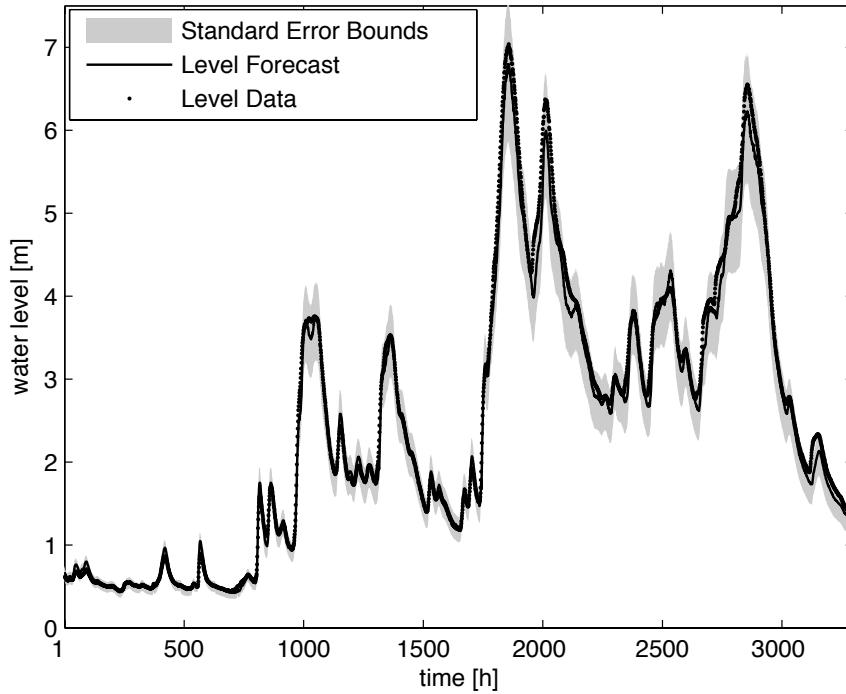


Figure 8. Buildwas: 8-hour-ahead validation forecast using the nonlinear SDP routing model.

is identified by the AIC criterion as AR(13) process. The model residence time is equal to 1.5 hours.

The 8-hour-ahead forecast for Buildwas explains 99.42% of the output water level variation for the validation period in November 2000. The results of validation are shown in Figure 8. The validation of the same model on the February 2002 flood data results in 99.62% explanation of the data.

(f) Nonlinear Water Level Routing for Buildwas–Bridgenorth

The best identified model structure for the Buildwas–Bridgenorth reach has the form:

$$y_{6,k} = \frac{0.6692}{1 - 0.3616z^{-1}} f_5(y_{5,k-2}) + \xi_k \quad (1.23)$$

where $f_5(y_{5,k-2})$ denotes the nonlinearly transformed input water level at Buildwas delayed by 2 hours and $y_{6,k}$ denotes water level at Bridgenorth. The noise ξ_k is identified by the AIC criterion as AR(11) process. The model residence time is equal to 1.0 hours.

The 2-hour-ahead forecast for Buildwas explains 99.99% of the output water level variation for the validation period in 2002. However, as the forecast is only 2 hours ahead, it is useful to extend it using upstream forecasts. Also, the validation

forecasts so far, as shown in Figures 3 to 8, have illustrated the overall performance of the forecasting system. In practice, however, the multiple-step-ahead forecasts, from a few hours ahead to the maximum forecast horizon, are required on demand at any time. Here, therefore, the results are presented in this operational mode of operation. Figure 9 shows a series of six such operational forecasts over the major flood peak. The numbered circle with an interior cross mark is the forecasting origin in each case: all the forecasts are plotted as red lines over a period of between 3 and 14 hours ahead, together with their associated standard error bounds. The water level before the first forecast, at point 1, has declined from the previous flood peak and has levelled out. This is the first forecast where an increase in water level is predicted and eventuates. At point 2, the forecast shows the water level continuing to rise sharply and so another, overlapping, forecast is shown at point 3, which predicts a still further rise but with the first sign of flattening out at the flood peak (these two forecasts tend to merge and are not easy to separate on the graph). Before point 4, the measured water levels have not been changing much around their peak values for about 12 hours, but the latest water level measurements at this point suggest a possible forthcoming decline and this is, indeed, confirmed by the forecast. Finally at points 5 and 6, the forecasts predict the continuing decline to the end of this particular data set.

(g) Nonlinear Water Level Routing for Bridgenorth–Bewdley

The best identified model structure for the Bridgenorth–Bewdley reach has the form:

$$y_{7,k} = \frac{0.4923}{1 - 0.4496z^{-1}} f_6(y_{6,k-4}) + \xi_k \quad (1.24)$$

where $f_6(y_{6,k-4})$ denotes the nonlinearly transformed input water level at Bridgenorth delayed by 4 hours and $y_{7,k}$ denotes water level at Bewdley. The noise ξ_k is identified by the AIC criterion as AR(11) process. The model residence time is just greater than 1.0 hours.

The 4-hour-ahead forecast for Bewdley explains 99.1% of output water level variations over the validation period in 2002 (the same 2002 flood event as at Bewdley, but considering a different peak wave). As in the previous reach, this forecast can be combined with the 10-hour-ahead forecast from Bridgenorth, thus obtaining a total 14 hours forecast lead time. Figure 10 shows this 14-hour-ahead forecast obtained for the same 2002 event, which explains 98.87% of the water level variations at Bewdley for this validation period.

It should be noted that the percentage of the variance explained provides a good measure of the overall performance and the figures cited in this and previous Sections are based on the whole forecast period. In order to obtain a better idea of comparative performance, however, it is worth looking at shorter periods, for example over flood peaks. In the case of a 100 hour period covering the peak wave in 2002, for instance, the percentage explanation of the 14-hour-ahead forecast is 89.7%, while for the ‘naive’ forecast (the current water level projected 14 hours ahead), this drops to 27.4%.

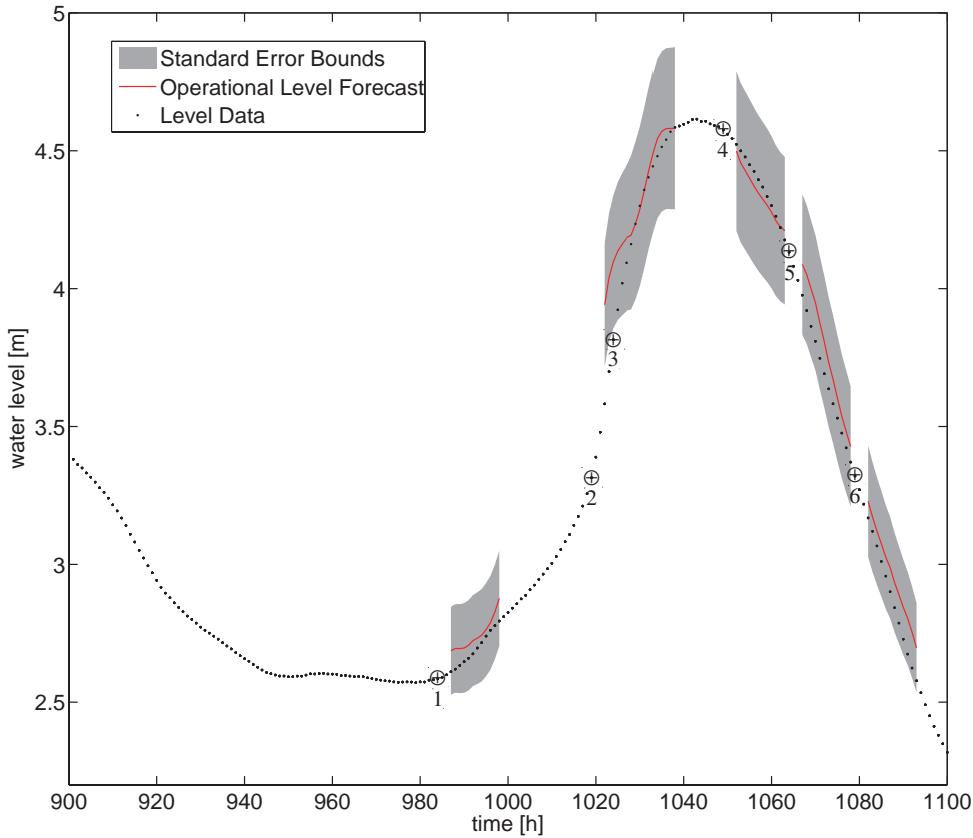


Figure 9. Bridgenorth: 14-hour-ahead operational forecasts using the nonlinear SDP routing model. The numbered circle with an interior cross marks the forecasting origin in each case (see text); the red line is the forecast; and the shaded bands are the estimated standard error bounds.

7. Incorporation into the DELFT-FEWS/NFFS

One useful aspect of the Study has been to demonstrate, with the help of Dr. Micha Werner of Delft Hydraulics, that the methodology described in this UFMO Report can be successfully incorporated into the *Environment Agency (EA) National Flood Forecasting System* (NFFS). The initial results obtained in this manner are promising and Figure 11 is a snapshot of the NFFS graphical user interface with the Severn System in place and yielding real-time forecasts. Unfortunately, Delft Hydraulics assistance in this connection has been essential but is not funded by the *Flood Risk Management Research Consortium* (FRMRC), and they have not been able to provide any further help, following the initial collaborative work. The funding limitations at Lancaster (where the research and development programme is funded on a part-time basis) will prevent any further work in this connection, unless it is strongly assisted by Delft Hydraulics. Funds are being sought elsewhere to continue this collaborative enterprise, but this has so far been unsuccessful. If the collaboration is continued, however, it will probably be based on a *Data-Based Mechanistic*

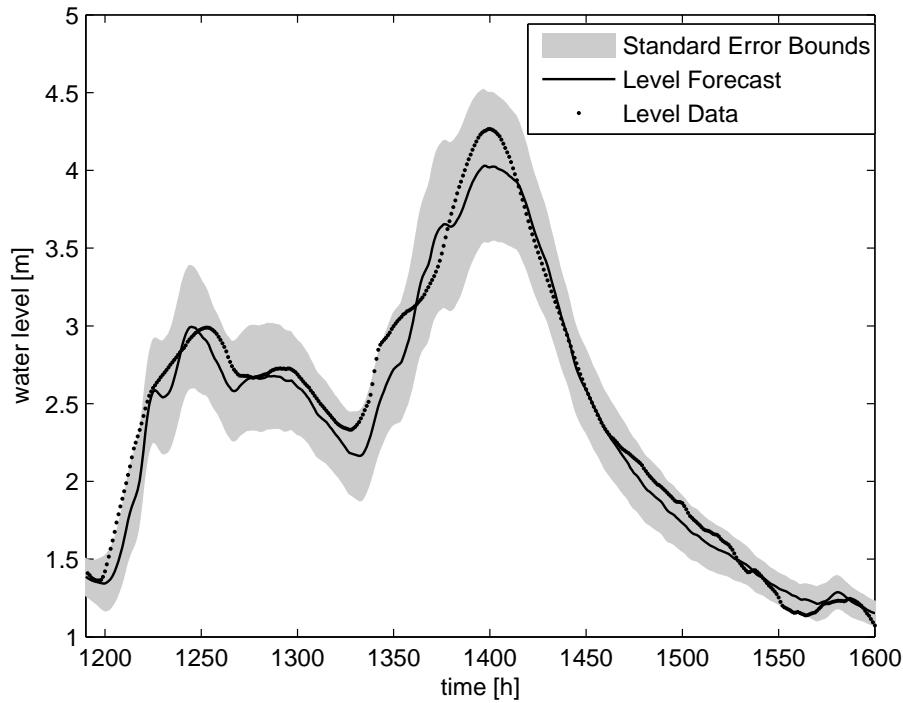


Figure 10. Bewdley: 14-hour-ahead validation forecast using the nonlinear SDP routing model.

DBM-type of forecasting system being developed for the River Dee by Jo Cullen, of the Welsh Division of the EA, as outlined in the next Section 8.

8. Associated Research on the River Dee

We have collaborated with Jo Cullen of the Environment Agency, Wales, on DBM modelling of the River Dee, with the objective of eventually incorporating this model into the NFFS. This research, is currently funded as a research studentship, with Jo Cullen registered for a PhD, degree at Lancaster, under the title '*Optimisation of the Flood Management System on River Dee*'.

The source of the River Dee is in Snowdonia, west of Bala in North Wales (altitude *circa* 700 m AOD). It then flows down through the deep gorge near Llangollen and through the Cheshire plain, reaching the sea at Chester. The total catchment area is 1816km² to the Chester weir at the head of the Dee estuary. The upper catchment is rural with the main land uses being farming and tourism; whereas further downstream, near Chester, some areas are heavily industrialised. The rainfall varies from *circa* 2000 mm per annum in the hills to *circa* 750mm per annum over the Cheshire plains. In the upper catchment, the river is steep and flows over impermeable rock, making it flashy in nature, responding quickly to rainfall events with an insignificant groundwater contribution.

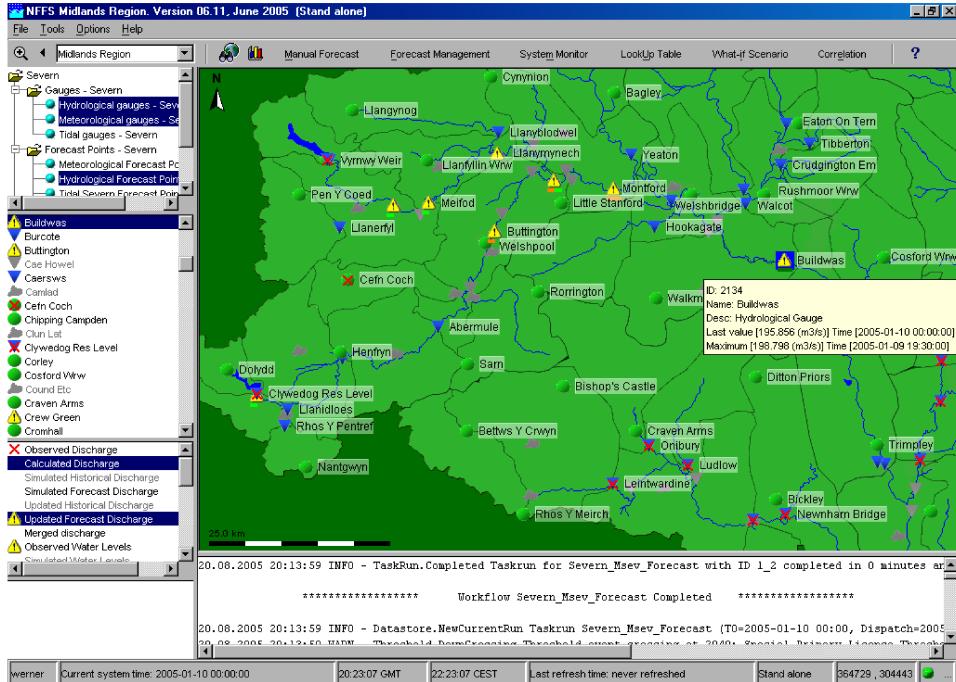


Figure 11. The River Severn Forecasting System in the NFFS.

The model developed so far consists of 10 subcatchments in the Upper Dee (upstream of Farndon), which were chosen in relation to the requirements for flood management: e.g. where target flows are set for issuing flood warnings; or where conditions affect the decision-making process for the flood management. Individual models have been then identified and estimated for each reach using the same DBM modelling approach and CAPTAIN Toolbox routines described in previous Sections of this Report. These have been combined into the final model but the full on-line forecasting system is still under construction.

Naturally, the scope of this research has been limited by the requirements of the Ph.D. degree and, so far, it has not allowed for any work on NFFS incorporation. Nevertheless, the DBM modelling and forecasting research is progressing well and Figure 12 shows a typical validation forecasting result in the lower part of modelled system using the latest optimized model. If additional funds can be obtained, this Study will be extended to include collaboration with Delft Hydraulics on NFFS related work.

9. Comments

The main aim of the Lancaster Real-Time Forecasting Study has been the derivation of a relatively simple and robust, on-line system for the forecasting of water levels in a river catchment, with the maximum possible lead-time and good real-time forecasting performance under high water level conditions. As a result, the analysis and forecasting system design is based on the water levels, rather than the

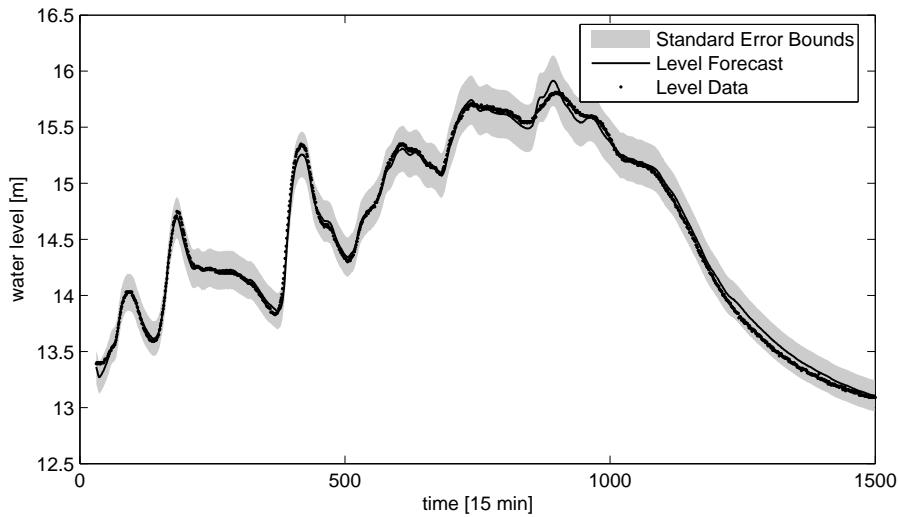


Figure 12. Bangor on Dee: 2.25 hours ahead validation forecast based on the water level measured at Manley Hall.

more conventional flow variables, in order to obtain superior long term forecasting performance. This removes the need to introduce the nonlinear water level-flow transformation, thus reducing the reliance on the prior calibration of this relationship and conveniently reducing the magnitude of the heteroscedasticity in the model residuals. In addition, improved forecasting performance is obtained by the introduction of real-time adaptive mechanisms that account for changes in both the system gain and the variance of the forecasting errors (heteroscedasticity).

An important contribution of the Study is the development of an adaptive forecasting and data assimilation system for a fairly large part of the River Severn catchment, based on a statistically estimated stochastic-dynamic, nonlinear DBM model composed of inter-connected rainfall-water level and water level routing modules. Although this adaptive forecasting system design is generic and could be applied to a wide variety of catchment systems, it has been developed specifically for the River Severn between Abermule and Bewdley, including the effects of the Vyrnwy tributary, using DBM models. As such, it is a quasi-distributed system: i.e. spatially distributed inputs but lumped parameter component models that consist of four main sub-models: two rainfall-water level models and five water level routing models for the river gauging stations downstream to Bewdley.

Without introducing external rainfall forecasts, the maximum length of the forecasting lead-time that can be handled successfully by this adaptive forecasting system depends on the advective delays that are inherent in the rainfall-water level dynamics; delays that depend on factors such as the changing speed (celerity) as the flood-wave moves along the river and the flood starts to inundate the flood plain. The gain adaptation can only off-set this nonlinearity in the effective time delay partially, but this still results in acceptable flood peak predictions. The result is a state/parameter updating system, where the parameter updating is limited to

the minimum that is necessary to achieve acceptable long term forecasting performance, combined with good potential for practical robustness and reliability. In this sense, the system represents a sophisticated development of the flood warning system for Dumfries (Lees *et al.*, 1993, 1994) that was operative over the 1990s.

The forecasting system exploits a development of the on-line updating methods developed by Young (2001c, 2002a). Forecasting is achieved through a sequential data assimilation procedure. Here, the available observations of rainfall and water levels at different locations along the river are sequentially assimilated into the Kalman filter-based forecasting engine, based on the off-line calibrated models, in order to derive the forecasts. These forecasts and the adaptive gains are updated recursively, in real time, as the new data become available from the remote sensors, so providing an adaptive capability that is better able to handle unforeseen changes in the catchment dynamics or lateral input effects.

The data assimilation involves sequential updating at each measurement location. As a result, the forecast uncertainty of this decomposed model will be different from the uncertainty of the entire system, unless the correlation between the observations is negligible. However, we decided to use the decomposed system for the model identification and parameter estimation phase of the analysis due to much better identifiability of this decomposed form and the associated higher robustness of the resulting model. Further work is being undertaken on the propagation of uncertainty in the entire forecasting system and initial results are presented in Romanowicz *et al.* (2006b). However, in order to check the estimates of the uncertainty bands of the forecasts, we applied an empirical approach based on the observed behaviour of the past forecast (Gilchrist, 1978), which confirmed that they are reasonable.

In order to achieve the main aim of the study, namely acceptable long-horizon flood forecasting, the research reported here has concentrated on a design that achieves good forecast accuracy at high water levels for long lead times. Our results show that the changes of water level dynamics for these high peak values can be predicted adequately using the recursively updated adaptive gain and variance parameters. As a flood event continues, the same methodology can be used to produce accurate forecasts with much smaller prediction variance for shorter lead times. However, there remain some differences in the forecast responses for low flow values that we feel could be reduced further and research is continuing to investigate this possibility.

10. Conclusions

The main conclusions of the Study described in this Report are summarized below,

- The main objectives of a real-time flood forecasting system are to guide decision making about whether flood warnings should be issued to the stakeholders and the public and to help avoid the issuing of false warnings. To this end, the forecasting system proposed here is able to provide accurate forecasts, based on real-time adaptive mechanisms for state and parameter updating, together with the estimates of uncertainties. This will allow the decision making process in the future to be based on an appropriate assessment of risk when issuing a warning.

- The Lancaster DBM model-based system is designed specifically to satisfy these objectives: its main aim is to process the on-line signals from the rainfall and water level sensors in a statistically efficient manner, in order to minimize forecasting errors.
- The DBM model-based state updating methods can be applied to any model that satisfies the Kalman Filter requirements (e.g. models such as IHACRES, PDM and HYMOD). However, large, physically-based models are normally over-parameterized and so suffer from inherent ambiguity (equifinality). As a result, both parameter estimation and updating is problematic: a subset of identifiable parameters has to be defined and the others constrained, either deterministically or stochastically, to assumed known values.
- The DBM model/Modified Kalman Filter approach can match, or improve upon, the performance of the currently popular but computationally very intensive, methods of numerical Bayesian analysis (e.g. the Ensemble Kalman Filter), yet it is computationally much more efficient, with updates taking only a few seconds.
- Research and development is continuing to further improve the forecasting system performance. This includes the reduction of the autocorrelation in the multi-step-ahead forecasting errors by extending the stochastic parts of the DBM model in the upstream reaches down to Buildwas.
- The initial studies carried out in collaboration with Delft Hydraulics on the incorporation of the Lancaster forecasting system into the NFFS have demonstrated that this is possible and have produced promising results. This work will be continued if additional funding can be found.
- The forecasting system has been developed with, and exploits, computational tools from the CAPTAIN Toolbox (e.g. Taylor *et al.*, 2006) for MatlabTM. A fully functional, 3-month trial version of this Toolbox can be dowloaded from <http://www.es.lancs.ac.uk/cres/captain/>.

Appendix 1: The Choice of Models for Flood Forecasting

Many different kinds of model have been suggested for flood forecasting applications: from simple, ‘black-box’ models at the one extreme; to complex, partial differential equation models that attempt to describe the full hydrodynamic behaviour at the other (see e.g. Wheater *et al.*, 1993; Beven, 2001). In general, the model used in any particular situation should match the objectives of the application being considered. Thus, if the main objective is to forecast river water level, in real-time and at multiple lead times, for the purposes of flood warning, then a relatively simple ‘dominant mode’ model that achieves this objective (see later) is more appropriate; while if it is desired to forecast inundation levels in detail, at any geographical locations where flooding may occur, then a more complex hydrodynamic model is more appropriate.

The choice of models for specified objectives is part of deeper philosophical and methodological considerations. For instance, there has recent increased interest in the so-called ‘top-down’ (or ‘holistic’) approach to modelling hydrological systems

(e.g. Jothityangkoon *et al.*, 2001, which follows from the earlier contributions of Klemes, 1983). Interest in top-down modelling has been revived largely because the alternative ‘bottom-up’ or ‘reductionist’ philosophy that dominated much research during the last century, has failed to solve the many problems of modelling natural environmental systems. Top-down modelling in hydrology has its parallels in the environmental (e.g. Young, 1978, 1983; Beck, 1983) and ecosystems (e.g. Silvert, 1981 and the prior references therein) literature of the 1970s and early 1980s.

In the twenty years since these earlier papers on top-down modelling were published, Young and his co-workers have sought to develop their approach within a more rigorous statistico-systems setting that Young has called *Data-Based Mechanistic* (DBM) modelling (this term is first used in Young and Lees, 1993, although it follows directly from Young and Minchin, 1991). Other recent publications that have concentrated more centrally on this topic and can be considered as adjuncts to the present report, in this more general regard, are: Young (1998a,b; 1999a); Young and Pedregal (1998,1999); Young and Parkinson (2002); Young *et al.*(1996); Shackley *et al.*(1998); Parkinson and Young, (1998).

With the above background in mind, let us first consider the types of model that are available. Wheater *et al.* (1993) have categorized rainfall-flow models in four broad classes.

- *Metric Models*, which are based primarily on observational data and seek to characterize the flow response largely on the basis of these data, using some form of statistical estimation or optimization (e.g. Wood and O’Connell, 1985; Young, 1986). These include purely black-box, time-series models, such as discrete and continuous-time transfer functions, neural network and neuro-fuzzy representations (e.g Jang *et al.*, 1997). Often, such models derive from, or can be related to, the earlier unit hydrograph theory but this is not always recognized 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). However, assumptions about catchment-scale response are not often included explicitly, notable exceptions being TOPMODEL (Beven and Kirkby, 1979) and the ARNO model (Todini, 1996). 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 optimize 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 discretization methods. A well known example is the *Système Hydrologique Européen* (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 discretization unit, particularly in re-

lation to sub-surface processes; and second, their complexity and consequent high dimensional parametrization. This latter problem makes objective optimization and calibration virtually impossible, since the model is normally so over-parameterized that the parameter values cannot be uniquely identified and estimated against the available data (see below).

- *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 characterize the observational data in statistical terms (the ‘principle of parsimony’ (Box and Jenkins, 1970); or the ‘Occam’s Razor’ of antiquity), 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 characterized by a large number of unknown parameters that need to be estimated ('optimized' or 'calibrated') in some manner against the observational rainfall-flow or water level 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-parameterized' and not normally identifiable, in the sense that it is impossible to estimate all of their parameters uniquely without imposing prior restrictions on a large subset of the parameter values prior to estimation, either deterministically or stochastically (see e.g. Young *et al.*, 1996). Young and his co-workers have addressed these problems of over-parameterization and poor identifiability associated with large environmental models many times over the past quarter century (see previous references). And more recently, Beven and his co-workers (e.g. Franks *et al.*, 1997) have revisited this idea within the hydrological context, using the term 'equifinality' rather than 'non-identifiability' to describe the consequences of such over-parametrization: namely the existence of many different parametrizations 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. Normally, when there is a reasonable amount of rainfall-flow data in a catchment, model identification and estimation is not affected by these considerations. However, 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.

Fortunately, as their name implies, these dominant modes define the characteristic 'signatures' of the catchment that are most important in forecasting terms, so that their identification and estimation allows for good forecasting performance. The importance of this dominant mode concept in model identification and estima-

tion is illustrated by appendix 1 of Young (2001b), which shows how the response of a 26th order flow-routing 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), Young (1998b) and Young and Parkinson (2002) 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 (Hasselmann *et al.*, 1997; Hasselmann, 1998). Moreover, these models can be validated in the sense that they are able to emulate the behaviour of the large model on data other than that used in their estimation.

In the above references, Young has stressed that dominant modal behaviour is a generic property of dynamic systems 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 he 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 man-made and specially designed cantilever beam (Young, 1998a), where the design and associated 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 for natural systems, 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.*, 1997a,b; Ye *et al.*, 1998) suggest that a typical set of rainfall-flow observations contain only sufficient information to estimate up to a maximum of six parameters within simple, nonlinear dynamic models of dynamic order three or less. In the rainfall-water level examples discussed in this Report, for instance, there is clear evidence in the data of only two dominant modes between the effective rainfall input and the flow response (as described by a second order transfer function model with only four parameters (see main text): a ‘quick’ mode with a residence time (time constant) of a few hours; and a ‘slow’ mode, with a residence time of many hours. For illustration, however, one higher order example is described here: a third order model of the Leaf River in the USA that is presented in Appendix 2.

By their very nature, both the metric and HMC approaches avoid many of these ‘large model’ problems. As a result, they provide a potentially attractive vehicle for real-time flood forecasting: they can be justified well in statistical terms and they are inherently simple in both structure and application. Such simplicity means that the forecasting system can be more easily optimized on a regular basis in order to ensure near-optimal performance. And, as we see in the case of the River Severn DBM model discussed in the main body of this report, it facilitates the incorporation of advanced features such as on-line state and parameter adaption.

Of the two approaches, however, the attractiveness and practical utility of the basic metric model as a vehicle for flood forecasting is marred by its lack of any clearly defined internal physical interpretation. For instance, neural network (e.g. Tokar and Johnson, 1999; Hsu *et al.*, 1993) and neuro-fuzzy models (e.g. Jang *et al.*, 1997) have attracted a great deal of attention in recent years but they are the

epitome of black box modelling, revealing very little of their internal structure that has any physical meaning (see the discussion in Young (2001d) on the paper by Hu *et al.*(2001) where a neuro-fuzzy model with 102 parameters can be replaced by a nonlinear transfer function model with only 15 parameters if the physically interpretable internal structure of the model is identified and taken into consideration using the DBM modelling methodology described in this Report). For this reason, many hydrologists tend to mistrust such a black box model as a basis for something as important as flood forecasting. Moreover, their lack of any obvious internal physical meaning means that metric models are difficult to interrogate and diagnose when errors are encountered. HMC models, on the other hand, do not suffer from these problems and, indeed, are often simpler in dynamic terms than the metric model.

This preference for HMC model should not be interpreted as a negative attitude towards neural-type models, which have a great capacity for modelling nonlinear mechanisms. Consequently, they can provide an excellent way of representing such mechanisms in HMC models. As can be seen in the cited references on DBM modelling, for instance, state-dependent parameters provide a description of nonlinear mechanisms identified within a DBM/HMC framework and neural techniques can be used to parameterize such SDP relationships. For instance, radial-basis functions are used to parameterize the SDP relationships in both the DBM rainfall-flow model for the Ceweeta catchment considered in Young (2001b) and in three of the water level-water level component models of the River Severn DBM model described in the main text. And it is clear that other neuro-fuzzy and neural procedures can be used in similar ways to this. Consequently, the preference for HMC models is because such models allow such useful but purely metric, black-box elements to be part of a more physically understandable representation of the hydrological system.

Within the category of HMC models two main approaches to modelling can be discerned. 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, as used in this Report, is basically inductive, in the sense that it tries to avoid theoretical pre-conceptions 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, it is inferred directly from the observational data in relation to a more general class of models. Only then is the model interpreted in a physically meaningful manner, most often (but not always) within the context of the current hydrological paradigm.

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 reasonable, physically meaningful terms. In this, the DBM 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.

Another important aspect of the DBM approach to rainfall-flow modelling re-

lates to the objectives of the modelling exercise in each case. We believe that a search for a single, all encompassing model of any dynamic system, appropriate to all requirements is not realistic. 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 the context of this UFMO, the primary objective is to obtain DBM models that perform well in a flood forecasting and warning context.

Appendix 2: Transfer Function Models

From a conceptual standpoint, most mathematical models of hydrological systems are formulated on the basis of natural laws, such as dynamic conservation equations, often expressed in terms of continuous-time linear or nonlinear differential equations. The objective of *Data-Based Mechanistic* (DBM) modelling (e.g. Young and Lees, 1993; Young, 1998b and the prior references therein) is to infer the nature and structure of such models directly from hydrological data, using powerful methods of statistical inference, and to then interpret the model equations in physically meaningful terms. One important generic model class that facilitates such DBM modelling studies is the *Transfer Function* (TF) family of models, which is the subject of this Appendix.

First, some of the the background to the use of TF models in hydrology is reviewed, concentrating on prior publications concerned with the modelling of rainfall-flow processes. This is followed by a tutorial Section that discusses the formulation of linear, constant parameter TF models in the derivative operator $s = d/dt$, which are simply the continuous-time (CT), transfer function form of ordinary differential equations. It then proceeds to develop and discuss the discrete-time (DT) equivalents of these CT models, namely transfer functions in the backward shift operator z^{-1} (see later), before outlining methods for the statistical identification and estimation of both CT and DT models from noisy time series data. In this manner, the models take on a natural stochastic form that is appropriate to their use in applications such as hydrological forecasting, uncertainty and risk analysis.

Finally, the Appendix shows that transfer function models can be extended to incorporate time variable and ‘state-dependent’ parameters, so allowing them to describe nonstationary and nonlinear stochastic systems, of which the nonlinear rainfall-flow model example that follows these sub-Sections is a good example. This helps to illustrate the DBM/TF modelling methodology and demonstrate its practical utility in a hydrological context.

A2.1 TF Models in Hydrology

The most common application of TF models in hydrology is connected with the modelling of *Rainfall-Flow* (RF) processes, where the objective is to characterize the dynamic relationship between rainfall and *total* measured flow in the river. Note that the term ‘rainfall-flow’ is used here, with an emphasis on the total flow in the river rather than the ubiquitous term *Rainfall-Runoff* (RR). As we shall see later, this is because the most recent work on the application of data-based TF models

in this context has shown how they are able to quantify other components of the flow; most importantly, those arising from groundwater processes that dominate the base flow in the river.

The characterization of the nonlinear dynamic relationship between rainfall and river flow is one of the most interesting and challenging modelling problems in hydrology. It has received considerable attention over the past forty years, with mathematical and computer-based models ranging from simple black-box representations to complex, physically-based catchment models. There are many books that consider it, either in whole, or in part: for example, Anderson and Burt (1985: see particularly the chapter by Wood and O'Connell); Shaw (1994); Singh (1995); and Beven (2001). But, in attempting to consider the historical context of this topic, we should recall Beven's comments in the latter book:

“It is now virtually impossible for any one person to be aware of all the models that are reported in the literature, let alone know something of the historical framework of the different initiatives.”

On this basis, it is clear that any treatment of such extensive and quite often controversial literature will tend to be somewhat subjective.

Following the model categorization of Wheater *et al.* (1993) discussed in Appendix 1, the HCM models are an attempt to combine the ability of metric models to efficiently characterize the observational data in statistical terms (the ‘principle of parsimony’ (Box and Jenkins, 1970); or the ‘Occam’s Razor’ of antiquity), with the advantages of *simple* conceptual models that have a prescribed physical interpretation within the current scientific paradigm. Transfer functions have become a very useful tool in HCM modelling: their outward ‘black box’ nature obscures an inherent ability to explain the more physically meaningful mechanisms that underlie this input-output description; mechanisms that can be revealed using the ‘system theoretic’ procedures of TF decomposition. In one important sense, TF models provide a rather natural model form for hydrologists because the impulse response of a continuous-time TF is equivalent to the *Instantaneous Unit Hydrograph* (IUH); while the impulse response of the discrete-time TF is equivalent the discrete-time UH (or TUH): see later Section A2.3(a).

System theoretic modelling ideas have had quite a strong influence in hydrology over many years: to name but a few contributions, for example, see Amorocho and Hart (1964); Salas *et al.*, (1988); Wood (1980); O’Connell and Clarke (1981); Sorooshian (1983); Gupta (1984); Bras and Rodriguez-Iturbe (1985); Singh (1988); Lees (2000a) and Lees (2000b). However, such models do not often attempt to represent the nonlinear dynamics inherent in the transformation of rainfall to runoff and, therefore, may not always perform well over long periods of time when the catchment storage and soil wetness is changing over a wide range. Sometimes, piece-wise linearity has been assumed to handle some aspects of the nonlinear behaviour (e.g. Natale and Todini, 1976); while, in other cases, the model parameters have been allowed to vary with time (Young, 1974; Whitehead and Young, 1975; Whitehead *et al.*, 1976; Young and Wallis, 1985; Young, 1986).

The latter *Time Variable Parameter* (TVP) approaches to TF estimation have led on to a more overt treatment of nonlinearity, sometimes by the use of nonlinear black-box models (e.g. the early example of Hsu *et al.*, 1993); and sometimes by the extension of TF models to allow for nonlinearity, as in the DBM models used

in this Report. As we shall see, this latter approach has the advantage of allowing for the easier inclusion of conceptual ideas and the retention of physical meaning within the estimated model structure.

This desire to associate a physical meaning with TF models has a rather natural appeal to hydrologists and was probably first adumbrated by Young (1974) and Whitehead and Young (1975). The idea of a *Physically Realizable Transfer Function* (PRTF: see Han, 1991) tackled this problem by ensuring that the estimated TF model maintained mass conservation and did not have any non-physical, oscillatory modes of dynamic behaviour. It was also the basis for the work of Jakeman *et al.* (1990) and provided the philosophical and methodological underpinning of the initial DBM approach to modelling RF processes (Young, 1993; Young and Beven, 1994).

Finally, it must be emphasised that TF models are not restricted to RF processes: since they provide a generic tool for modelling linear and nonlinear, stochastic dynamic systems, they can be applied to data-based modelling problems in many areas of science, engineering and the social sciences (see the wide variety of examples in Young 1998b). In the hydrological context, they have already been used for flow routing in river systems (see next Section) so that, together with rainfall-flow TF models, they allow for characterization of a whole river catchment. They have also been used successfully for the *Aggregated Dead Zone* (ADZ) modelling of pollution transport and dispersion in rivers and soils (e.g. Beer and Young, 1983; Wallis *et al.*, 1989; Beven and Young, 1988; Young and Wallis, 1994). Given this flexibility, it seems likely that they will be used even more widely in the future as a basic tool for modelling in the hydrological and wider environmental sciences.

A2.2 Linear Continuous-Time TF Models

In order to introduce TF models, let us consider first a conceptual catchment storage equation in the form of a continuous-time, linear storage (store, tank or reservoir) model: see, for example, the review papers by O'Donnell, Dooge and Young in Kraijenhoff and Moll (1986); or more comprehensive treatments, such as the recent books by Beven (2001) and Dooge and O'Kane (2003). Here, the rate of change of storage in the channel is defined in terms of water volume entering the linear storage element (e.g. river reach) in unit time, minus the volume leaving in the same time interval, i.e.,

$$\frac{dS(t)}{dt} = GQ_i(t - \tau) - Q_o(t) \quad (\text{A2.1})$$

where $Q_i(t - \tau)$ represents the input flow rate delayed by a pure time or 'transport' delay of τ time units to allow for pure advection; and G is a gain parameter inserted to represent gain (or loss) in the system. Making the reasonable and fairly common assumption that the outflow is proportional to the storage at any time, i.e.,

$$Q_o(t) = TS(t)$$

and substituting into (A2.1), we obtain,

$$T \frac{dQ_o(t)}{dt} = GQ_i(t - \tau) - Q_o(t); \quad (\text{A2.2})$$

This equation is a first order, linear differential equation model whose response, from an initial steady flow condition, to a unit impulsive change Q_i^{imp} of the input flow at time $t = t_0$, is given by

$$Q_o(t - \tau) = Q_e + Q_i^{imp} e^{-(t-t_0)/T},$$

where Q_e is the initial steady flow level. This has a typical hydrograph recession shape, with a decay *Time Constant*, T , that defines the *Residence Time* of the model. As we shall see later, combinations of two or more such first order models, exhibit a typical unit hydrograph form (e.g. Dooge, 1959; Beven, 2001).

By introducing the derivative operator s , i.e. $s = d/dt$, and collecting like-terms together, it is easy to see that equation (A2.2) can be written as†,

$$(1 + Ts)Q_o(t) = GQ_i(t - \tau)$$

so that, dividing throughout by $1 + Ts$, we obtain the following continuous-time TF form of equation (A2.2),

$$Q_o(t) = H(s)Q_i(t - \tau) \quad (\text{A2.3})$$

where,

$$H(s) = \frac{G}{1 + Ts}$$

represents the TF in terms of the derivative operator s .

(a) Physically Interpretable Parameters

The TF model (A2.3) is characterized by three parameters: G , T and τ . However, there are five, physically interpretable model parameters associated with the model that are worth discussing. The *Steady State Gain* (SSG), denoted by G , is obtained by setting the s operator in the TF to zero (i.e. $d/dt = 0$ in a steady state). It shows the relationship between the equilibrium output and input values when a steady input is applied. For this reason, *if the input and output have similar units*, G is ideal for indicating the physical losses or gains occurring in the system. In the case of a flow-routing model, for example, it indicates whether water has been added ($G > 1$) or lost ($G < 1$) between the upstream and downstream boundaries; and the percentage of water lost or gained can be defined by *Loss Efficiency* $LE = 100(1 - G)$, which will be negative if $G > 1.0$. As pointed out above, the *Residence Time* or *Time Constant* T is the time required for the storage element output to decay to e^{-1} or 0.3679 of its maximum value in response to an impulsive input. Finally the pure *Advection Time Delay* τ indicates the time it takes for a flow increase upstream to be first detected downstream; and $T_t = T + \tau$ defines the *Travel Time* of the system. These five parameters typify the equilibrium and dynamic characteristics of the TF model and provide a physical interpretation of the TF model in terms of its mass transfer and dispersive characteristics.

† The same letter s (or sometimes p) is used to represent the related Laplace transform operator. Considered in these Laplace transform terms, it is possible to utilize Laplace transform methods to handle initial conditions on the variables in the model and analytically compute its response (here $Q_o(t)$) to variations in input variable (here $Q_i(t)$). However, this is not essential in the present context, although the interested reader should find that this Appendix is a good primer for the deeper study of Laplace transform methods (e.g. in a text such as Schwarzenbach and Gill, 1979).

(b) *TF Manipulation and Block Diagrams*

The first order TF model (A2.3) is often written in the form,

$$Q_o(t) = \frac{g_0}{s + f_1} Q_i(t - \tau) \quad i.e. \quad H(s) = \frac{g_0}{s + f_1} \quad (\text{A2.4})$$

where,

$$g_0 = \frac{G}{T}; \quad f_1 = \frac{1}{T}$$

because this is the form in which the model is normally estimated (see later). Typically, a Channel or *Flow Routing* model for a river catchment will contain a number of elemental models, such as (A2.3) or (A2.4), connected in a manner that relates to the structure of the catchment. For instance, a serial connection of n such elements constitutes the lag-and-route model of a single river channel (Meijer, 1941; Dooge, 1986) and, with $\tau = 0$ and all elements identical, it becomes the well known ‘Nash Cascade’ model (Nash, 1959). More complex river systems can be represented by a main channel of this type, with tributaries modelled in a similar manner. Also, a typical TF model between effective rainfall and flow often contains a parallel connection of two or more such storage elements (see e.g. Young, 1992, 2001b,c, 2002a, 2003). Related serial and parallel arrangements characterize the mass conservation equation of the *Aggregated Dead Zone* (ADZ) model for the transport and dispersion of a solute in a river channel (e.g. Wallis *et al.*, 1989 and the prior references therein). And ADZ-type models can lead to more complex interactive water quality models, including chemical and biological interaction, such as DO-BOD models (e.g. Beck and Young, 1975; Whitehead and Young, 1975; Young, 1999b).

The TF formulation allows for the visual representation of a total system model in the form of a ‘*Systems Block Diagram*’. Figure 13 is a typical example of such a diagram that represents a catchment model consisting of a effective rainfall-flow sub-model involving two *different* first order TFs of the form (A2.3) with $\tau = 0$,

$$H_1(s) = \frac{G_1}{1 + T_1 s}; \quad H_2(s) = \frac{G_2}{1 + T_2 s},$$

that are connected in parallel. The flow output of this sub-model forms the input to a flow-routing sub-model composed of two *identical*, first order TFs,

$$H_3(s) = \frac{G_3}{1 + T_3 s},$$

again of the form (A2.3) with $\tau = 0$, but this time connected in series as a ‘Nash Cascade’. The upstream input to this complete system is an effective rainfall measure, represented by $u(t)$, that is generated from the gauged rainfall $r(t)$ (not shown) by a nonlinear relationship $N(s)$ involving a measure of the catchment wetness (see later example). The downstream output of the complete system is denoted by $y(t)$.

One advantage of the TF formulation of the model shown in Figure 13 is that it allows for the computation, using ‘*Block Diagram Algebra*’, of a single, multi-order TF that represents the total system. Here, TFs connected in parallel are additive; while those connected in series are multiplicative. Consequently, in this case, the two sub-models can be represented by the following composite TFs:

$$H_{rf}(s) = H_1(s) + H_2(s); \quad H_{ff}(s) = H_3(s) \cdot H_3(s)$$

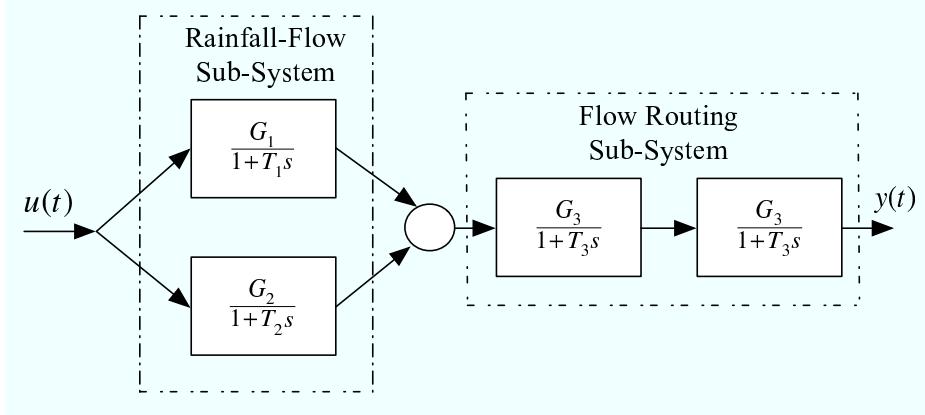


Figure 13. Block diagram of a hypothetical catchment model consisting of a parallel pathway, rainfall-flow sub-system in series with a two reach, flow-routing sub-system.

So that, with the above definitions of $H_1(s)$, $H_2(s)$ and $H_3(s)$,

$$H_{rf}(s) = \frac{G_1}{1 + T_1 s} + \frac{G_2}{1 + T_2 s} = \frac{(G_1 + G_2) + (G_1 T_2 + G_2 T_1)s}{(1 + T_1 s)(1 + T_2 s)}$$

and

$$H_{ff}(s) = \frac{(G_3)^2}{(1 + T_3 s)(1 + T_3 s)}$$

Now, since $H_{rf}(s)$ and $H_{ff}(s)$ are connected in series, the TF of the total system $H(s)$ is obtained as the multiplication of these two composite TFs: i.e.,

$$H(s) = H_{rf}(s) \cdot H_{ff}(s) = \frac{(G_1 + G_2) + (G_1 T_2 + G_2 T_1)s}{(1 + T_1 s)(1 + T_2 s)} \cdot \frac{(G_3)^2}{(1 + T_3 s)(1 + T_3 s)}$$

Multiplying out these expressions, we see that the complete $H(s)$ is a 4th order TF that can be manipulated to the form:

$$H(s) = \frac{g_0 + g_1 s}{s^4 + f_1 s^3 + f_2 s^2 + f_3 s + f_4} \quad (\text{A2.5})$$

where we will leave the definition of the parameters $f_i, i = 1, 2, \dots, 4$ and $g_j, j = 0, 1$ in (A2.5), as an exercise for the reader (*hint*: carry the above analysis with the TF representation (A2.4) rather than (A2.3): then it will be clear why the former representation is better for analysis, although it lacks the direct physical interpretation of the latter, which provides a better form for the block diagram representation).

(c) Stochastic Transfer Function Models

In this UFMO, transfer functions are utilized as elements in *Data-Based Mechanistic* (DBM) models that are inherently stochastic in form, so allowing for the quantification of uncertainty in the model output and any associated forecasts, as well as estimation of the associated uncertainty in the DBM model parameters (see

later, Section A2.4). Such *Stochastic Transfer Function* (STF) models are characterized by the presence of unobservable noise terms that represent that part of the data not explained by the model. The noise can be quantified in various ways: most simply by its variance, or its variance relative to the variance of the model output, using the well known coefficient of determination; by a stochastic model, if such a model is applicable; by its probability distribution; or by its spectral (frequency domain) properties; etc. Of course, it can be due to a variety of different reasons (measurement inaccuracies; limitations in the model as a representation of the data; the effects of unmeasured inputs; etc). However, it is conventional to lump the effects of all noise entering the system in terms of their combined effect on the model output variable (or variables); in the present context the flow or water level in the river at a specified location. For instance, in the case of the TF model (A2.5), the *Stochastic Transfer Function Model* (STF) model between $u(t)$ and $y(t)$ is written in the form:

$$y(t) = \frac{g_0 + g_1 s}{s^4 + f_1 s^3 + f_2 s^2 + f_3 s + f_4} u(t) + \xi(t) \quad (\text{A2.6})$$

where $\xi(t)$ represents the noise term in this STF. Alternatively, (A2.6) can be written as:

$$x(t) = \frac{g_0 + g_1 s}{s^4 + f_1 s^3 + f_2 s^2 + f_3 s + f_4} u(t) \quad (\text{A2.7})$$

$$y(t) = x(t) + \xi(t) \quad (\text{A2.8})$$

where now $x(t)$ is the hypothetical ‘noise free’ output that represents the part of the measured output that is defined by the model as the result of the input perturbation $u(t)$.

(d) The General, Multi-Order STF Model

It is clear from the above example that, in general, serial, parallel (or even feedback†) connections of elemental first order TF models, such as (A2.3) or (A2.4), lead to a multi-order TF model that takes the general TF form:

$$x(t) = \frac{G(s)}{F(s)} u(t - \tau) \quad y(t) = x(t) + \xi(t) \quad (\text{A2.9})$$

where $F(s)$ and $G(s)$ are polynomials in s of the following form:

$$\begin{aligned} F(s) &= s^p + f_1 s^{p-1} + f_2 s^{p-2} + \dots + f_p \\ G(s) &= g_0 s^q + g_1 s^{q-1} + g_2 s^{q-2} + \dots + g_q \end{aligned}$$

in which p and q can take on any positive integer values. Here $u(t)$ and $x(t)$ denote the deterministic input and output signals of the system at its upstream and downstream boundaries, respectively; τ is a pure advective time (transport) delay affecting the input signal $u(t)$; and $y(t)$ is the observed output, which is assumed to be contaminated by a noise or stochastic disturbance signal $\xi(t)$. This noise is assumed to be independent of the input signal and it represents the aggregate effect,

† The block diagram algebra for a feed back connection is a little more complicated but, since it is not particularly relevant in the current context, the interested reader should consult a standard text on the subject (e.g. Schwarzenbach and Gill, 1979) to find the details.

at the down stream boundary, of all the stochastic inputs to the system, including distributed unmeasured inputs, measurement errors and modelling error. Multiplying throughout equation (A2.9) by $F(s)$ and converting the resultant equation to alternative ordinary differential equation form, we obtain:

$$\frac{d^p y(t)}{dt^p} + f_1 \frac{d^{p-1} y(t)}{dt^{p-1}} + \dots + f_p y(t) = g_0 \frac{d^q u(t-\tau)}{dt^q} + \dots + g_q u(t-\tau) + \eta(t) \quad (\text{A2.10})$$

where $\eta(t) = F(s)\xi(t)$ is a modified noise signal generated by the manipulation of the equation. The structure of this model, in either form (A2.9) or (A2.10), is defined by the triad $[p \ q \ \tau]$.

If the noise $\xi(t)$ can be assumed to have specific statistical characteristics then this can help in obtaining low or minimum variance estimates of the TF model parameters. But, as we see later when discussing the identification and estimation of TF models, such assumptions are not an essential requirement of statistical estimation and good, low variance parameter estimates can be obtained without invoking them. Also, depending on the objectives of the modelling study, it may be necessary, in a complete system consisting of many sub-elements such as (A2.3) or (A2.4), to consider noise inputs *within* the system, associated with collections of sub-elements that have distinct physical meaning: e.g. stochastic lateral inflows.

A2.3 Linear Discrete-Time TF Models

To date, the most popular form of TF modelling has been carried using the discrete-time (DT) equivalents of the model (A2.9). If we consider first (A2.4), which is the differential equation form of a first order TF equation in CT, i.e.,

$$T \frac{dQ_o(t)}{dt} = GQ_i(t-\tau) - Q_o(t); \quad (\text{A2.11})$$

then, at a uniform sampling interval of Δt time units, an approximate discrete-time form of this model can be obtained in the following manner by approximating the first order derivative and introducing sampled variables:

$$T \frac{Q_{o,k} - Q_{o,k-1}}{\Delta t} \approx GQ_{i,k-\delta} - Q_{o,k-1}; \quad (\text{A2.12})$$

Here $Q_{o,k}$ is the sampled value of $Q_o(t)$ at the k^{th} sampling instant, i.e. after $k\Delta t$ time units; and δ is the advective time delay, normally defined as the nearest integer value of $\tau/\Delta t$ (thus incurring a possible approximation error). Collecting terms in this equation, it can be written as,

$$Q_{o,k} \approx -a_1 Q_{o,k-1} + b_0 Q_{i,k-\delta} \quad (\text{A2.13})$$

where $a_1 = -(1 - \Delta t/T) = -(1 - f_1 \Delta t)$ and $b_0 = G(\Delta t/T) = g_0 \Delta t$. This reveals that, as a first approximation in discrete-time, the flow $Q_{o,k}$ at the k^{th} sampling instant is a proportion $-a_1$ (note that, in the present context, a_1 will be a negative number less than unity, so that this is a positive proportion) of its value $Q_{o,k-1}$ at the previous $(k-1)^{th}$ sampling instant, plus a proportion b_0 of the delayed upstream flow input $Q_{i,k-\delta}$ measured δ sampling instants previously.

Although equation (A2.13) is an approximate expression, depending on the size of the sampling interval ΔT and the definition of the sampled variables, it can be shown that it has the same form as a more accurate discrete-time equivalent of (A2.11). In this alternative discrete-time representation, the values of the parameters a_1 and b_0 in equations (A2.13) can be related to the parameters of the model (A2.4) in various ways depending upon how the input flow $Q_i(t)$ is assumed to change over the sampling interval between the measurement of $Q_{i,k-1}$ and $Q_{i,k}$ (since it is not measured over this interval). The simplest and most common assumption is that it remains constant over this interval (the so-called zero-order hold, ZOH, assumption), in which case the relationships are as follows:

$$a_1 = -\exp(-f_1 \Delta t) \quad b_1 = \frac{g_0}{f_1} \{1 - \exp(-f_1 \Delta t)\} \quad (\text{A2.14})$$

We will leave the reader to show that the expressions for a_1 and b_0 in (A2.13) are approximations of these more accurate expressions. Note also that, because these relationships are functions of the sampling interval Δt , for every unique CT model such as (A2.4), there are infinitely many DT equivalents (A2.15), depending on the choice of Δt , all with different parameter values defined in (A2.14).

With the definitions of equation (A2.4), the equivalent discrete-time TF version of the model (A2.13) (now with an equality sign) takes the form:

$$Q_{o,k} = \frac{b_0}{1 + a_1 z^{-1}} Q_{i,k-\delta} \quad (\text{A2.15})$$

where z^{-1} is the backward shift operator; i.e. $z^{-1} Q_{o,k} = Q_{o,k-1}$ or, in general terms, $z^{-r} Q_{o,k} = Q_{o,k-r}$. Following from the definition of this first order DT model at the chosen Δt , the general multi-order equivalent of the general CT model (A2.9) is defined by the following discrete-time STF model:

$$x_k = \frac{B(z^{-1})}{A(z^{-1})} u_{k-\delta} \quad y_k = x_k + \xi_k \quad (\text{A2.16})$$

where,

$$\begin{aligned} A(z^{-1}) &= 1 + a_1 z^{-1} + a_2 z^{-2} + \dots + a_n z^{-n} \\ B(z^{-1}) &= b_0 + b_1 z^{-1} + b_2 z^{-2} + \dots + b_m z^{-m} \end{aligned}$$

Normally $n = p$ but m may be equal or greater than q . The structure of this DT model is defined by the triad $[n \ m \ \delta]$. Note that the general TFs in both DT, i.e. (A2.16), and CT, i.e. (A2.9), are composed of ratios of polynomials (in z^{-1} and s respectively), so they are sometimes referred to as *Rational Transfer Functions*.

In practice, a numerical algorithm, such as the *c2dm* routine in the MatlabTM numeric computation software is used to convert from a CT model of the form (A2.9) to a DT model such as (A2.16). For example, consider a [2 3 0], second order CT model, as estimated from a set of daily effective rainfall-flow data from the River Canning in Western Australia (Young, 2006a), with the parameters:

$$f_1 = 0.457 \quad f_2 = 0.0248 \quad g_0 = 0.0138 \quad g_1 = 0.0505 \quad g_2 = 0.0046$$

The *c2dm* routine in Matlab converts this to a [2 3 0] model with parameters:

$$a_1 = -1.6133 \quad a_2 = 0.6332 \quad b_0 = 0.0138 \quad b_1 = 0.0149 \quad b_2 = 0.0250$$

However normally, if data are available, such a DT model would be obtained by direct estimation from the data. This yields the daily data model with parameters:

$$a_1 = -1.6034 \quad a_2 = 0.6244 \quad b_0 = 0.0140 \quad b_1 = 0.0151 \quad b_2 = 0.0252$$

It will be noted that the parameters in these converted and estimated TFs are similar but not exactly the same. This is because conversion is made under the (normally) approximate assumption that the input signal is constant between samples (i.e. the ZOH, see earlier). However, the estimated model requires no such assumption: it produces a model that provides a best explanation of the data at the sampling points (indeed, in the case of zero noise on the data, it provides a perfect fit to the data). Consequently, if a DT model is required and data are available, as here, it is best to obtain it by direct identification and estimation from the data, using the methods discussed later.

Finally, if the sampling interval is changed to an hour, rather than a day, the DT model parameters produced by *c2dm* are as follows:

$$a_1 = -1.9811 \quad a_2 = 0.98114 \quad b_0 = 0.0138 \quad b_1 = -0.0255 \quad b_2 = 0.0117$$

showing how, as pointed out previously, the DT model parameters are a function of the sampling interval ΔT . Note also that, here, the roots of the $A(z^{-1})$ polynomial (the eigenvalues), at this faster sampling rate, are 0.99738 and 0.98371 and that these are very close to the unit circle in the complex z -plane, where the dynamics in discrete-time are much less well defined. For example, 0.99738 is very close to unity and an eigenvalue at unity would represent a pure integrator (infinite residence time). As a result, the eigenvalue (and associated residence time) can be sensitive to uncertainties in the parameter estimates: e.g. an increase of 0.001 in the eigenvalue at 0.99738 associated with this hourly data DT model, produces an increase in the residence time of 9.817 hours; while a similar change in the eigenvalue at 0.9390 associated with the daily data DT model, produces an increase of only 0.273 hours.

(a) The Unit Hydrograph and Finite Impulse Response TF Models

The reader can verify that the division of the numerator polynomial $B(z^{-1})$ by the denominator polynomial $A(z^{-1})$ in the TF model (A2.16) normally results in a infinite dimensional polynomial $G(z^{-1}) = g_0 + g_1 z^{-1} + g_2 z^{-2} + \dots + g_\infty z^{-\infty}$, so that the equation can also be written in the alternative form:

$$y_k = \sum_{i=\delta}^{\infty} g_i u_{k-i} + \xi_k; \quad g_j, j = 0, 1, \dots, \delta - 1 = 0 \quad (\text{A2.17})$$

This will be recognized as the discrete-time form of the convolution integral equation associated with the solution of differential equations (here with a pure time delay of δ sampling intervals or $\delta\Delta t$ time units) and, once again, we see that the TF model is simply a discrete-time equivalent of a continuous-time differential equation model.

Equation (A2.17) has important connotations in hydrology because, if the noise $\xi_k = 0$ for all k , then its unit impulse response, i.e. the response of the equation to a unit impulse input: $u_k = 1.0$ for $k = 1$; $u_k = 0$ for all $k > 0$), is equivalent to the hydrological unit hydrograph. Sometimes, indeed, the equation (A2.17) is referred

to as a TF model, although its infinite dimensional nature is an obvious restriction. Despite this disadvantage, some hydrologists have used the equation directly in RF modelling by considering it in a *Finite Impulse Response* (FIR) form, in which the upper limit of the summation is set to some value $r < \infty$ where it is considered that the ordinates of the impulse response have become small enough to be ignored.

Unfortunately, it can be shown that the number of FIR model parameters (or ‘weights’), g_i , $i = 1, 2, \dots, r$, is nearly always much larger than the number of parameters in the rational TF form (A2.16). As a result, the statistical estimates of these parameters will normally have unacceptably high variance and have to be constrained in some manner. For instance, Natale and Todini (1976) use quadratic programming to compute the constrained least squares estimates of the FIR parameters in order to ensure that they are all positive and, if necessary for conservation purposes, they all sum to unity (i.e. the model has unity steady state gain). Even with this approach, however, it is difficult to recommend the FIR model because the rational TF model (A2.16), normally with far fewer parameters, is not only entirely equivalent to the infinite dimensional IR model, without any approximation, it is also easier to estimate from rainfall-flow data using the methodology discussed in the next Section A2.4.

A2.4 Statistical Identification and Estimation of TF Models

One consequence of the STF model formulation is that, because of the uncertainty injected into the model by the presence of the additive noise variable $\xi(t)$, in the CT case, or ξ_k , in the DT case, the associated model parameters are themselves uncertain and not known exactly. So, as we shall see, the vector of STF model parameters is defined by its probability distribution which, in the case where the $\xi(t)$ or ξ_k are assumed to be normal Gaussian random variables, is defined by the mean values of the parameter estimates and the covariance matrix that defines their joint variance-covariance properties.

In statistical terms, the modelling of a system using a STF model is a problem of time series analysis (e.g. Box and Jenkins, 1970; Young, 1984) that involves identification and estimation of the model from time series data. Here, *Identification* means the definition of the most appropriate model structure: in particular the values of the elements in the triads $[p \ q \ \tau]$ and $[n \ m \ \delta]$. *Estimation* is then the estimation of the parameters that characterize this structure (f_i , $i = 1, 2, \dots, p$; g_j , $j = 0, 1, \dots, q$; and τ in the CT case; a_i , $i = 1, 2, \dots, n$; b_j , $j = 0, 1, \dots, m$; and δ in the DT case). Much has been written about the identification and estimation of the DT model (A2.16) but much less on the CT model (A2.9). This is almost certainly for two reasons: first, it is easier to analyze the DT model in statistical terms; second, in these days of digital instrumentation and computers, the DT model provides a more convenient model form. For these reasons, attention will be concentrated initially on the DT model (A2.16) and we will return to the more physically transparent CT modelling later.

(a) Discrete-Time TF Model Identification and Estimation

Much has been written on the identification and estimation of discrete-time TF models and the reader is advised to consult one or more of the many texts on the

1. In the case of the full Box-Jenkins model (A2.18) and following from an important theorem by Pierce (1972), the estimates of the ‘system’ parameters in $A(z^{-1})$ and $B(z^{-1})$ are asymptotically independent of those for the ‘noise’ parameters in $C(z^{-1})$ and $D(z^{-1})$. This has important consequences on parameter estimation (Jakeman and Young, 1981, 1983) that justify the RIV estimation of the TF model (A2.18).
2. Like all instrumental variable methods (see e.g. Young, 1984), the RIV approach does not necessarily require the concurrent estimation of a noise model and, indeed, remains statistically efficient (i.e. the parameter estimates are optimal in the sense that amongst all estimates, they have the minimum variance) if the noise ξ_k is itself white (i.e. $C(z^{-1}) = D(z^{-1}) = 1.0$). Used in this manner, the RIV algorithm is, for obvious reasons, called the *Simplified RIV* (SRIV) algorithm (Young, 1985).
3. The SRIV algorithm is a particularly important algorithm in the context of hydrology because its exploitation of instrumental variables (see e.g. Young, 1984) makes it robust in the situation when the noise ξ_k violates the assumption of rational spectral density and is not modelled well by an ARMA-type process. This is often the case in practice because the noise (recall that, in the present context, this is the unexplained part of the measured flow or water level) can contain odd effects, such as small, measured flow components that are not associated with the measured rainfall; or measured rainfall events that do not correspond to any measured flow perturbation. This is most often associated with the heterogeneity of the rainfall over the catchment and the inability of the rainfall sensors to fully capture this pattern of behaviour. Also, the noise tends to be ‘heteroscedastic’: i.e. its variance changes with the changes in the magnitude of the flow or water level, often being higher for larger flows or water levels.
4. As pointed out by Wellstead (1978) and considered further by Young *et al.* (1980) and Young (1989), model structure identification (definition of the triad $[n \ m \ \delta]$) is greatly facilitated by the special properties of the *Instrumental Product Matrix* (IPM) that is a fundamental component of IV estimation and has optimal statistical properties in the case of RIV/SRIV estimation. This has been exploited in the development of the YIC order identification criterion mentioned later.
5. The RIV/SRIV algorithms for DT models utilize a special form of adaptive prefiltering. This is further exploited in the RIV method for continuous-time systems (the RIVC algorithm: Young and Jakeman, 1980; Young, 2002b) to by-pass the need for direct differentiation of the input and output signals. This algorithm is discussed further in (b) below.

Finally, note that the RIV algorithm provides the estimation results in the form of an estimate $\hat{\mathbf{p}}$ of the STF model parameter vector \mathbf{p} and its estimated covariance matrix. Here, \mathbf{p} is defined as:

$$\mathbf{p} = [a_1 \ a_2 \ \cdots \ a_n \ b_0 \ b_1 \ \cdots \ b_m]^T$$

In the case where the ARMA noise model is also estimated, the estimates of its parameter vector and associated covariance matrix are also provided.

(b) Continuous-Time STF Model Identification and Estimation

Following on the point 4. in the previous sub-Section, the statistical estimation of the CT model (A2.9) is straightforward if completely continuous-time data are available. However, the hydrologist is normally confronted by discrete-time, sampled data and the problem of modelling continuous-time models such as this, based on discrete-time, sampled data at sampling interval Δt , is not so obvious. This problem can be approached in two main ways.

- *The Indirect Approach:* here, the identification and estimation steps are first applied to the DT model (A2.16) or (A2.18). This estimated model is then converted to the CT model (A2.9), again using some assumption about the nature of the input signal $u(t)$ over the sampling interval Δt . In the first order, ZOH case, this conversion is given by the relationships in equation (A2.14) but, in more general terms, the multi-order conversion must be carried out in a computer, using a conversion routine such as the *d2cm* algorithm in the Matlab Control Toolbox.
- *The Direct Approach:* here, the RIVC algorithm (Young and Jakeman, 1980; Young *et al.*, 2006), together with an appropriate order identification criterion (see below), is used to identify the most appropriate, identifiable CT model structure defined by the triad $[p \ q \ \tau]$; and then estimate the TF parameters f_i , $i = 1, 2, \dots, n$, g_j , $j = 0, 1, \dots, m$ and τ that characterize this structure. Of course, some approximation will be incurred in this estimation procedure because the inter-sample behaviour of the input signal $u(t)$ is not known and it must be interpolated over this interval in some manner (see previous discussion).

In the latter, direct estimation case, the RIVC algorithm provides the estimation results in the form of an estimate $\hat{\mathbf{p}}$ of the STF model parameter vector \mathbf{p} and its estimated covariance matrix. In this CT situation, \mathbf{p} is defined as:

$$\mathbf{p} = [f_1 \ f_2 \ \cdots \ f_p \ g_0 \ g_1 \ \cdots \ g_q]^T$$

In the case where the ARMA noise model is also estimated, normally in its discrete-time form (making the combination of system and noise models then represent a ‘hybrid BJ’ model: see Young *et al.*, 2006), the estimates of its parameter vector and associated covariance matrix are also provided.

(c) Model Structure Identification

Finally, as mentioned above, an important aspect of TF modelling, in both continuous and discrete-time, is *Model Structure Identification* (the definition of the model structure triads). This can be approached in various ways. For example, Box and Jenkins (1970) discuss the topic at length and Akaike (1974) suggested an alternative approach that has since spawned several other, related methods.

Within the context of the instrumental variable methods discussed above, however, model structure identification is based conveniently on two statistical criteria. First, the *Coefficient of Determination*, R_T^2 , a normalized measure based on the variance of the error between the sampled output data y_k and the simulated (CT or DT) model output at the same sampling instants (this is similar to the well known *Nash-Sutcliffe Efficiency* measure (Nash and Sutcliffe, 1970); and $100 \times R_T^2$ is the percentage of the variance of the output data explained by the model). Note that R_T^2 should not be confused with its well known relative R^2 , as used in classical regression and time series analysis, which is defined in terms of the one-step-ahead prediction errors. In general, R_T^2 is a more discerning measure of model adequacy in a dynamic systems context than R^2 since it quantifies the ability of the model to explain the whole of the output data from the input data, without any reference to the output data. In contrast, R^2 only measures the ability of the model to predict one-step-ahead on the basis of the latest input and output data. The second statistic is the *Young Information Criterion* (YIC) which is a heuristic measure of model identifiability and is based on the properties of the IPM matrix (see above). These statistics are discussed in more detail in Young (1989) and Appendix 3 of Young (2001b).

A2.5 Nonstationary and Nonlinear TF models

Nonlinearity in rainfall-flow and water level models is very important because it defines the way in which the model responds under different catchment wetness conditions. So, in general, it is necessary to consider extensions to the constant parameter, linear TF model that allow for the consideration of more complex hydrological processes such as this. Fortunately, it is possible to extend TF models to handle ‘nonstationary’ situations described by *Time Variable Parameter* (TVP) models; or ‘nonlinear’ situations characterized by *State-Dependent Parameter* (SDP) models. The latter model class encompasses a wide variety of nonlinear, stochastic, dynamic phenomena, including chaotic systems.

Although such TVP and SDP models are beyond the scope of this Appendix, they are introduced briefly below. Both types of model can be considered in either continuous or discrete-time. However, since statistical estimation is more straightforward in the DT case, it often provides the more practical approach. Consequently, the brief descriptions that follow are limited to this DT situation.

(a) Nonstationary Time Variable Parameter (TVP) Models

In the DT case, the TVP form of the TF model (A2.16) can be written as follows:

$$x_k = \frac{B(k, z^{-1})}{A(k, z^{-1})} u_{k-\delta} \quad y_k = x_k + \xi_k \quad (\text{A2.19})$$

where,

$$\begin{aligned} A(k, z^{-1}) &= 1 + a_{1,k}z^{-1} + a_{2,k}z^{-2} + \dots + a_{n,k}z^{-n} \\ B(k, z^{-1}) &= b_{0,k} + b_{1,k}z^{-1} + b_{2,k}z^{-2} + \dots + b_{m,k}z^{-m} \end{aligned}$$

Here, all the parameters are assumed to be functions of the time index k , i.e. it is assumed that they may vary over time in an unknown manner that needs to be estimated from the data.

Some of the latest research on TVP estimation is reported in Young (1999b, 2000, 2004b) where the reader will find a complete description of the recursive estimation algorithms that allow for the estimation of the time variable parameters. A simple example would be a model such as (A2.15) in which the ‘gain’ parameter $b_0 = b_{0,k}$ is assumed to vary over time in order to reflect any changes in the dynamic behaviour of the channel that may occur over a wide range of flow conditions. An approach similar to this is suggested by Cluckie (1993), who refers to the gain as a ‘model scaling factor’ and points out that it is analogous to the ‘variable proportional loss method’ of defining effective rainfall. An example of adaptive gain adjustment that has been implemented in practice is the adaptive flood warning system for the River Nith at Dumfries, in S.W. Scotland (Lees *et al.*, 1993, 1994). Here, a recursive estimation algorithm has been used for over a decade to continually update a gain parameter, based on telemetered data from the catchment, in order to provide an adaptive capability. In this case, however, the adaptive gain parameter is only required to ‘fine-tune’ an *already computed* effective rainfall input generated from the measured rainfall by a ‘state-dependent parameter’ nonlinearity, as discussed in the next Section.

(b) Nonlinear State-Dependent Parameter (SDP) Models

Again in the discrete-time case, the SDP form of the TF model (A2.16) can be written as follows:

$$x_k = \frac{B(\mathbf{w}_k, z^{-1})}{A(\mathbf{v}_k, z^{-1})} u_{k-\delta} \quad y_k = x_k + \xi_k \quad (\text{A2.20})$$

where,

$$\begin{aligned} A(\mathbf{v}_k, z^{-1}) &= 1 + a_1(v_{1,k})z^{-1} + a_2(v_{2,k})z^{-2} + \dots + a_n(v_{n,k})z^{-n} \\ B(\mathbf{w}_k, z^{-1}) &= b_0(w_{0,k}) + b_1(w_{1,k})z^{-1} + b_2(w_{2,k})z^{-2} + \dots + b_m(w_{m,k})z^{-m} \end{aligned}$$

Here, the possibility that the parameters may be functions of other ‘state’ variables is investigated. In other words, it is assumed that any parameter in the model may vary over time as a function of one or more other variables (e.g. the input u_k or output y_k and their past values), so introducing nonlinear behaviour into the model. In the SDPTF model (A2.20), these variables are denoted by $v_{i,k}, i = 1, 2, \dots, n$ and $w_{j,k}, j = 0, 1, \dots, m$ and they are, respectively, the elements of the vectors \mathbf{v}_k and \mathbf{w}_k .

The first applications of SDP estimation in hydrology are described in Young (1993); and Young and Beven (1994); while the latest research on SDP estimation is reported in Young (2000, 2001a,b,c, 2002a, 2003, 2006a) and Young *et al.* (2001). This later research exposes a special example of the SDP model that is particularly important in a hydrological context. This is the ‘Hammerstein’ model, where the SDP nonlinearity only affects the numerator parameters in the SDPTF model (A2.20) and is of a form where it can be factored out of the model and form a single, input nonlinearity that converts the measured rainfall into an ‘effective rainfall’ (see next Section A2.6). This model can be written in the form:

$$x_k = \frac{B(z^{-1})}{A(z^{-1})} f(u_{k-\delta}) \quad y_k = x_k + \xi_k \quad (\text{A2.21})$$

where $f(u_{k-\delta})$ represents the SDP effective rainfall nonlinearity. This is discussed further in the next Section A2.6.

A2.6 A Practical Example

TF models can be applied in many areas of hydrology and provide a good basis for DBM modelling, as discussed in the main text. The typical example outlined in this Section is based on the analysis of daily rainfall-flow data from the Leaf River catchment, a humid watershed with an area of 1944 km^2 located north of Collins, Mississippi. The first step in such modelling is to evaluate whether a linear, constant parameter TF model is able to explain the data. In this case, identification and estimation based on the RIV algorithm in the CAPTAIN Toolbox, suggests a 3rd order TF model between the measured rainfall (mm/day) and flow (cumecs), with a scalar numerator gain and no pure time delay (i.e. a [3 1 0] structure). This model has a quite low coefficient of determination of $R_T^2 = 0.56$ (i.e. it explains only 56% of the flow variance). This suggests that the linear model is not an adequate representation of the rainfall-flow process.

At the next stage of modelling, the rainfall-flow data are investigated further, using the non-parametric SDP estimation algorithm in CAPTAIN, to see if there is evidence of nonlinearity that could help to improve the model's descriptive ability. The results of this SDP analysis identify that the main source of nonlinearity is affecting the input rainfall and the associated non-parametric estimate of the input SDP is plotted in Figure 14 as a function of y_k (full-line), with the estimated standard errors shown as dotted lines. The dash-dot line is a parametric function of the form $1 - e^{-\gamma y_k}$ that is able to mimic the non-parametric function and so provides the basis for subsequent parameterization of the model.

The model in this form has a single SDP input nonlinearity but is otherwise linear: it is, in other words, a 'Hammerstein' model form. It also has an emerging physical significance in DBM modelling terms as an 'effective rainfall' nonlinearity. In particular, it is clear that the flow variable y_k mirrors the changing storage of water in the catchment (the soil moisture and ground water). It is not surprising, therefore, that the effective rainfall, computed as the product of the measured rainfall with a parameter that has been identified as being dependent of the flow, should be involved in defining the effective rainfall. Of course, this relationship is not real: the flow is simply acting as a surrogate measure of the catchment storage and so, as it increases in Figure 14, so the effect of the rainfall increases until it reaches a saturation level at the high flows that indicate high catchment storage. In physical terms, the effect of rainfall is small when the catchment is dry because the water is utilised to wet the soils and replenish the groundwater resources; but when the catchment is wet, most of the rainfall contributes to 'run-off' and consequent increases in flow.

One important consequence of the non-parametric SDP estimation is that the effective rainfall can be generated as the input to the linear transfer function part of the model, so allowing for the better identification of its structure. When considered in this manner, the best identified TF model is the following [3 4 0] TF relationship,

$$y_k = \frac{b_0 + b_1 z^{-1} + b_2 z^{-2} + b_3 z^{-3}}{1 + a_1 z^{-1} + a_2 z^{-2} + a_3 z^{-3}} u_k + \xi_k$$

subject (e.g. Ljung and Söderstrom, 1983; Young, 1984; Norton, 1986). Here, we will not attempt to review this literature but simply refer briefly to a number of topics that are particularly pertinent to the use of TF models in hydrology.

(i) *The Box-Jenkins Model*

The best known work on the identification and estimation of the DT model (A2.16) is by Box and Jenkins (1970: see chapter 10), to which the reader is directed for a comprehensive description of how the model can be estimated using the *Maximum Likelihood* (ML) approach, under the assumption that the noise ξ_k has rational spectral density†. This assumption leads to the formulation of the following *Box-Jenkins* model:

$$y_k = \frac{B(z^{-1})}{A(z^{-1})} u_{k-\delta} + \xi_k \quad \xi_k = \frac{D(z^{-1})}{C(z^{-1})} e_k \quad e_k = N(0, \sigma^2)$$

or,

$$y_k = \frac{B(z^{-1})}{A(z^{-1})} u_{k-\delta} + \frac{D(z^{-1})}{C(z^{-1})} e_k \quad e_k = N(0, \sigma^2) \quad (\text{A2.18})$$

where,

$$\begin{aligned} C(z^{-1}) &= 1 + c_1 z^{-1} + c_2 z^{-2} + \dots + c_s z^{-s} \\ D(z^{-1}) &= 1 + d_1 z^{-1} + d_2 z^{-2} + \dots + d_r z^{-r} \end{aligned}$$

and e_k is defined as normally distributed ‘white noise’, defined in statistical terms as $N(0, \sigma^2)$: i.e. a zero mean, serially uncorrelated sequence of normally distributed random variables with variance (an additional unknown parameter) σ^2 . We see, therefore, that the ‘coloured’ noise ξ_k is assumed to be generated from the white noise e_k by passing it through a ‘filter’ that has a similar TF form to the system model, but with both polynomials in z^{-1} having leading unity elements (monic polynomials). This particular type of filter is called a *AutoRegressive, Moving Average* (ARMA) model (see Box and Jenkins, 1970). With the noise process defined in this manner, it is clearly necessary to identify the order of the noise model polynomials $C(z^{-1})$ and $D(z^{-1})$ and estimate the associated parameters $c_i, i = 1, 2, \dots, s$ and $d_i, i = 1, 2, \dots, r$ and σ^2 .

(ii) *Refined Instrumental Variable (RIV) Estimation*

One approach to TF model estimation that is simpler and more robust, because does not rely on the assumption that the noise has rational spectral density, is the *Refined Instrumental Variable* (RIV) method, which has proven particularly useful and robust in hydrological applications. The RIV approach (see Young, 1976; Young and Jakeman, 1979, 1980; Young, 1984) is based on the TF models (A2.16) and (A2.18) and was initially developed with environmental applications in mind, where robustness to the kinds on non-standard conditions met in the environment, including hydrology, is very important. The RIV method has a number of advantages that are pertinent to the discussion here.

† so-called because it is generated by passing white noise through a TF, here the ARMA model, that consists of a ratio of rational polynomials in z^{-1} .

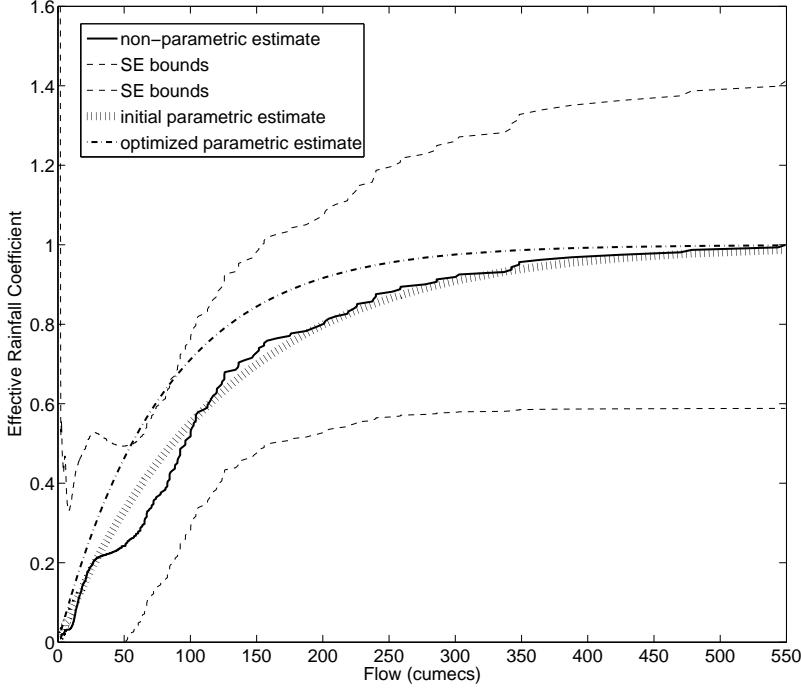


Figure 14. SDP estimation results.

with the following parameter estimates:

$$\begin{aligned} \hat{a}_1 &= -2.053(0.033) & \hat{a}_2 &= 1.452(0.057) & \hat{a}_3 &= -0.385(0.024) & \hat{b}_0 &= 2.691(0.141) \\ \hat{b}_1 &= -0.729(0.343) & \hat{b}_2 &= 0.321(0.420) & \hat{b}_3 &= 1.812(0.028) \end{aligned}$$

Here, the noise ξ_k identified as either an AR(5) or ARMA(3,2) process.

Although this model explains the data well with $R_T^2 = 0.86$, it is not satisfactory from a DBM standpoint because the TF poles are complex ($0.9533; 0.5500 \pm 0.3180j$) and there is no obvious physical explanation for such characteristics. In order to correct this problem, the model is parameterized with the three poles constrained to be real and with the SDP parameterized as the exponential function identified previously. Estimation of the model in this constrained form is achieved by an optimization routine in which the constrained poles of the model and the exponential function parameter γ are optimized using a nonlinear least squares cost function. Here, at each iteration of the optimization, the updated estimates of the poles are used to define the constrained denominator polynomial of the TF model and associated SRIV estimation then optimizes the numerator polynomial parameters. This novel constrained optimization strategy yields a nonlinear model of the form,

$$y_k = \frac{b_0 + b_1 z^{-1} + b_2 z^{-2} + b_3 z^{-3}}{(1 + \alpha_1 z^{-1})(1 + \alpha_2 z^{-1})^2} u_k + \xi_k \quad (\text{A2.22})$$

$$u_k = (1 - e^{\gamma y_k}) r_k \quad (\text{A2.23})$$

with the following parameter estimates:

$$\begin{aligned}\hat{\alpha}_1 &= -0.961(0.008) \quad \hat{\alpha}_2 = -0.443(0.01) \quad \hat{b}_0 = 0.068(0.004) \quad \hat{b}_1 = 0.015(0.009) \\ \hat{b}_2 &= 0.0125(0.009) \quad \hat{b}_3 = -0.084(0.004) \quad \hat{\gamma} = 0.0124(0.0005)\end{aligned}$$

The model explains the data as well as the unconstrained version (see the upper panel of Figure 15), with $R_T^2 = 0.86$ and, as before, the noise ξ_k is identified as an AR(5) or ARMA(3,2) process. The model is also well validated when applied, without re-estimation, to a different portion of the rainfall-flow data. This is shown in the lower panel of Figure 15, where the $R_T^2 = 0.89$, which is a little better than that obtained for the estimation data set.

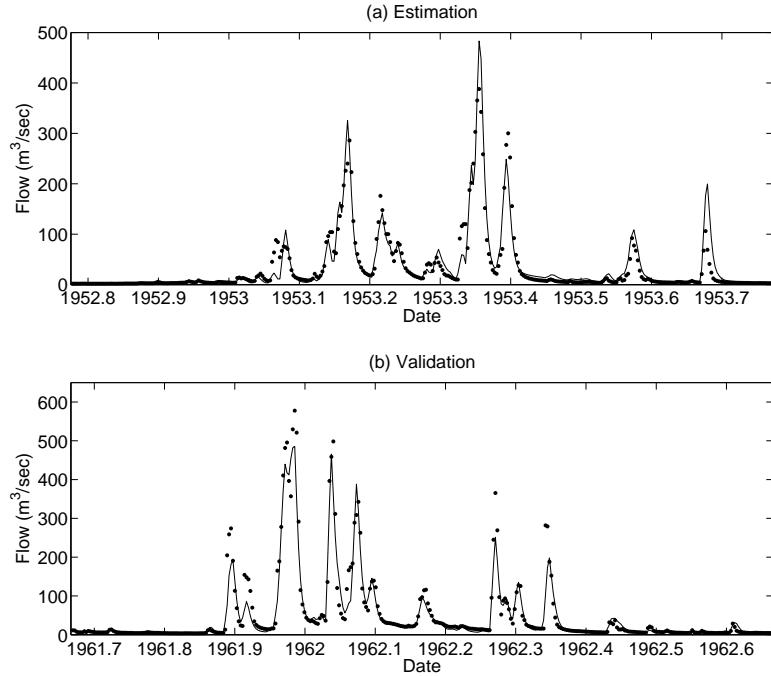


Figure 15. Estimation and validation results for the final parameterized DBM model
(For clarity, only part of the results are shown).

The physical nature of the TF model (A2.22) can be investigated by using partial fraction expansion to decompose it into a variety of forms. However, the most physically meaningful form obtained in this manner is shown as a block diagram in Figure 16, with the associated first order ‘store’ or ‘tank’ characteristics (SSGs, time constants and partition percentages) presented in Table 3.

A2.7 Stochastic Simulation Models

RIV estimated Linear TF models are in an ideal form for stochastic *Monte-Carlo Simulation* (MCS) studies because the parameter estimates are returned with their associated covariance matrix and the nature of the additive noise process is quantified. In the case on nonlinear SDPTF models, however, MCS may be prevented

Table 3. Parallel Decomposition of DBM Model

TF	Slow	Quick 1	Quick 2	Inst.
SSG	0.201	0.238	0.433	0.068
Partition %	21.4	25.3	46.1	7.2
Time Constant	24.8	1.23	2.46	0.0

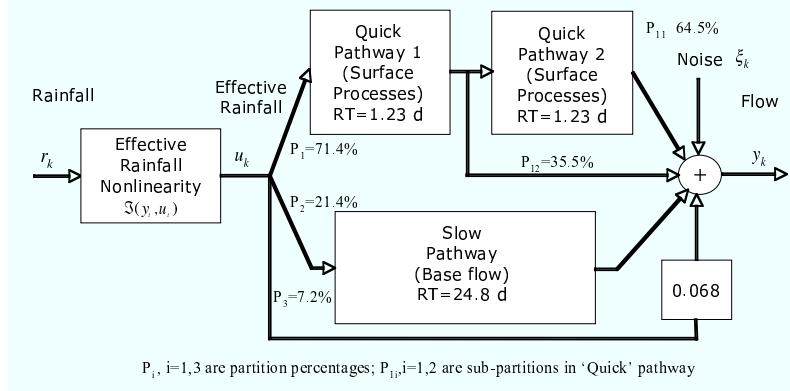


Figure 16. Physically meaningful decomposition of the DBM model.

in some cases if the nonlinearity, as in the DBM rainfall-flow model, utilizes a surrogate variable (here y_k) to replace a real but unobserved variable (here catchment storage), so preventing dynamic simulation. However, most nonlinear models that include TF elements, as in the case of the SDPTF, do not suffer from this limitation.

Even in cases where the limitation exists, it is always possible to introduce more speculative conceptual model elements to generate estimates of unobserved (or 'latent') variables. For example, in the case of rainfall-flow modelling, the SDP nonlinearity can be replaced by a more speculative catchment storage model whose output can then replace the surrogate measure y_k (see e.g. Young, 2001b, 2002a, 2003). In this stochastic simulation form, the model can then be used for various purposes, such as 'what-if' and 'regionalization' studies (see e.g. Kokkonen *et al.*, 2003). However, it is likely that the derived parameters of the model will be 'bulk' parameters that relate to the behaviour of the system at the catchment scale, rather than the kind of 'process' parameters used in more conventional 'physically-based' hydrological simulation models.

Even if they are not used as the basis for stochastic simulation studies themselves, however, it is clear that when suitable measured time series data are available, DBM/TF models should always provide a useful adjunct to simulation model synthesis because they identify well the 'dominant mode' behaviour of the system that is identifiable from the historical data. In this way, they can alert the 'physically-based' model builder to those aspects of the simulation model that are not well defined in relation to the available data and so are of a more speculative nature. An example which illustrates this approach is the modelling of the Leaf River in the USA, as considered in the previous sub-Section, where both conceptual and DBM models can be compared. In particular, the DBM model shown in

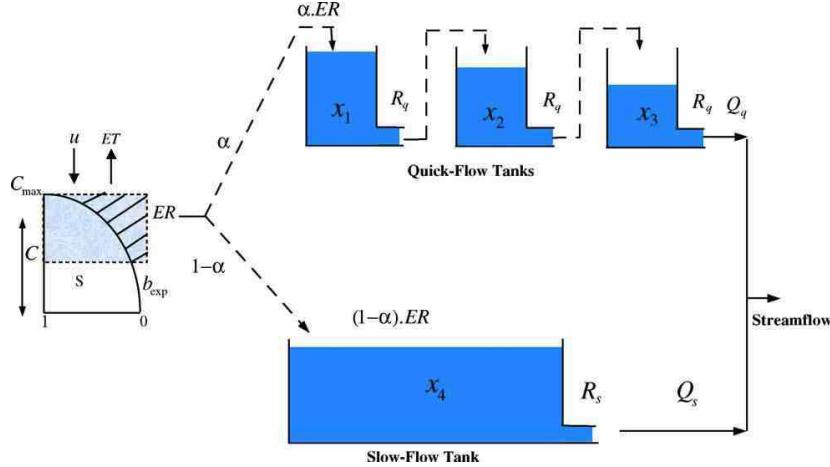


Figure 17. A conceptual model of the Leaf River: the higher order HYMOD model used in forecasting research by Vrugt *et al* (2002).

Figure 16 can be compared directly with the HyMOD model obtained by Vrugt *et al.* (2005) and shown in Figure 17, which was obtained from exactly the same data set.

Although identified by quite different means, there is clearly a close similarity between the two models: both contain an input nonlinearity and, although the DBM is third order and HYMOD is fourth order (four ‘tanks’), both exhibit a parallel pathway structure of quick and slow ‘tanks’. However, there are differences: the DBM model has an instantaneous pathway, indicating that there is an effect seen at the output within one sampling period (one day); and the input nonlinearities are different, with the data-based DBM nonlinearity replaced by the conceptual storage model in HYMOD. Both explain the rainfall-flow data well but the data-based identification stage in the DBM model development shows that only three ‘tanks’ are necessary and that the model should contain the instantaneous pathway. This information could suggest a simplifying modification to HYMOD, in which the fourth store, defined by two parameters, is replaced by the instantaneous parallel pathway, defined by one parameter.

Although, in this Leaf River example, the suggested changes are small, this is because the HYMOD model is of the HMC form and has been constructed with parsimony of parameterization in mind. DBM analysis would probably suggest much more significant changes in larger and less parametrically efficient, physically-based models. For instance, a number of publications (e.g. Young *et al.*, 1996; Young and Parkinson, 2002, Young, 2006b) have shown how the response of very large physically-based models, such as those describing the *Global Carbon Cycle* (GCC) model, and even larger models, such as the Hadley *Global Circulation Model* (GCM), can be emulated extremely well by much smaller dominant mode DBM models. Moreover recent, as yet unreported, research at Lancaster has shown that this is also possible in the case of the well known ISIS catchment model.

A2.8 CONCLUSIONS

At one level, transfer function models are simply elegant and convenient representations of continuous-time, stochastic differential equation models, or their discrete-time equivalents. This article demonstrates, however, that they are much more than this: they also provide a powerful, generic method of modelling hydrological systems. This method provides a useful block diagram interpretation of the input-output dynamics of the system under study that can be decomposed straightforwardly into physically meaningful sub-systems that are in an ideal form for data-based mechanistic modelling studies. The utility of the method is further enhanced by the powerful methods of statistical identification and parameter estimation that have been developed for such TF models over many years. These are not only robust in practical application, they also provide valuable information about the stochastic nature of the system and allow for the quantification of the uncertainty associated with the model parameter estimates and its output predictions. Moreover, these estimation methods are normally available in a recursive form that allows for their use in on-line, real-time applications, where they provide a natural basis for adaptive modelling and data assimilation. Recent developments in recursive time variable and state dependent parameter estimation have enhanced the utility of TF models still further, so that they are now able to characterize both nonstationary and nonlinear stochastic systems.

Finally, it should be emphasized that DBM models, in general, and data-based TF models, in particular, naturally require real time series data for their identification and estimation. Also, their primary use is for improving our understanding of the system dynamics and/or for implementing model-based prediction, as in flood warning and forecasting applications, where the main changes that are likely to occur in future relate to the input variables (measured rainfall and upstream flows). As we have seen in Section A2.7, however, they can also be utilized in stochastic simulation studies, provided they are in a suitable form for this. If not, the synthesis of a simulation model may necessitate the introduction of more speculative conceptual model elements to generate estimates of hidden (latent) variables (such as a catchment storage variable in the case of rainfall-flow modelling).

Appendix 3: Recursive Estimation and the Kalman Filter

Recursive estimation is the embodiment of real-time updating. In recursive estimation, either the estimate of a model parameter vector, or the estimate of a state variable vector, are updated at the k^{th} sampling instant based on the estimate obtained at the previous $(k - 1)^{th}$ sampling instant. This update also depends upon the model that describes the relationship between the parameters or state variables and the latest data received at the k^{th} sampling instant. So, for example, the state of a catchment model at a given k^{th} hour, as defined by the hourly flows at various locations in the catchment, is updated on the basis of the estimates of these flows at the previous $(k - 1)^{th}$ hour, the catchment model, and the latest flow measurements, as received remotely from flow gauges at the various locations at the k^{th} hour.

Recursive estimation was first developed by K. F. Gauss, sometimes before 1826. A translation and an interpretation of his recursive linear least squares regression algorithm, in modern vector-matrix terms, is available in Appendix 2 of Young (1984). Over one hundred and thirty years later, apparently without any knowledge of the Gauss algorithm, the systems theorist, Rudolf Kalman, developed a related algorithm for state variable estimation. This Kalman Filter (KF) algorithm, as it has come to be known in many areas of science and social science, is a special form of recursive linear least squares estimation where the constant parameters considered by Gauss are replaced by state variables generated by a dynamic linear system, in the form of a set of linear, stochastic state equations (a vector Gauss-Markov process). Such equations could, for example, be those of a linear catchment model.

The simplest way to derive the linear least squares regression algorithm of Gauss is to consider the well known problem of estimating of the set of n unknown, constant parameters $x_j, j = 1, \dots, n$, which appear in a linear ‘regression’ relationship of the form:

$$x_k = h_{1,k}x_1 + h_{2,k}x_2 + \dots + h_{n,k}x_n \quad (\text{A3.1})$$

where the measurement y_k of x_k is contaminated by noise , i.e.,

$$y_k = x_k + e_k = h_{1,k}x_1 + h_{2,k}x_2 + \dots + h_{n,k}x_n + e_k \quad (\text{A3.2})$$

while the $h_{j,k}; j = 1, 2, \dots, n$, are exactly known, linearly independent variables which are also statistically independent of the measurement noise on y_k .

Most readers will recognise this problem and will know that the minimization of the least squares criterion function for k samples, i.e.,

$$J_2 = \sum_{i=1}^k \left\{ \sum_{j=1}^n [y_i - h_{j,i}x_j]^2 \right\} \quad (\text{A3.3})$$

requires that all the partial derivatives of J_2 with respect to each of the parameters $x_j, j = 1, 2, \dots, n$, should be set simultaneously to zero. Such a procedure yields a set of n linear, simultaneous algebraic equations that are sometimes termed the ‘normal equations’ and which can be solved to obtain the *en-bloc* estimates $\hat{x}_j, j = 1, 2, \dots, n$, of the parameters $x_j, j = 1, 2, \dots, n$, based on the k data samples.

A simple and concise statement of the least squares results in the multi-parameter case can be obtained by using a vector-matrix formulation: thus by writing (A3.2) in the alternative vector form,

$$y_k = \mathbf{h}_k^T \mathbf{x} + e_k \quad (\text{A3.4})$$

where

$$\mathbf{h}_k^T = [h_{1,k} \ h_{2,k} \ \dots \ h_{n,k}]; \quad \mathbf{x}^T = [x_1 \ x_2 \ \dots \ x_n] \quad (\text{A3.5})$$

the superscript T denotes the vector/matrix transpose, and $\mathbf{h}_k^T \mathbf{x}$ is the vector inner product. With this notation, we are able to define J_2 as

$$J_2 = \sum_{i=1}^k [y_i - \mathbf{h}_i^T \mathbf{x}]^2 = \sum_{i=1}^k e_i^2 \quad (\text{A3.6})$$

Using the rules of vector differentiation, the partial derivatives of J_2 with respect to the vector of parameters \mathbf{x} are given by,

$$\frac{\partial}{\partial \mathbf{x}} \sum_{i=1}^k [y_i - \mathbf{h}_i^T \mathbf{x}]^2 = -2 \sum_{i=1}^k \mathbf{h}_i [y_i - \mathbf{h}_i^T \mathbf{x}] \quad (\text{A3.7})$$

so that the normal equations are obtained from,

$$\frac{1}{2} \nabla_{\mathbf{x}} (J_2) = - \sum_{i=1}^k \mathbf{h}_i y_i + [\sum_{i=1}^k \mathbf{h}_i \mathbf{h}_i^T] \mathbf{x} = 0 \quad (\text{A3.8})$$

where $\frac{1}{2} \nabla_{\mathbf{x}} (J_2)$ denotes the gradient of J_2 with respect to all the elements of \mathbf{x} .

(a) *The Recursive Least Squares Algorithm*

Now, provided that the matrix $[\sum_{i=1}^k \mathbf{h}_i \mathbf{h}_i^T]$ is non-singular†, then the solution to the normal equations (A3.8) takes the form:

$$\hat{\mathbf{x}}_k = [\sum_{i=1}^k \mathbf{h}_i \mathbf{h}_i^T]^{-1} \sum_{i=1}^k \mathbf{h}_i y_i \quad (\text{A3.9})$$

where $\hat{\mathbf{x}}_k$ is the estimate of \mathbf{x} based on the k data samples. This solution can be written as,

$$\hat{\mathbf{x}}_k = \mathbf{P}_k \mathbf{b}_k \quad (\text{A3.10})$$

where,

$$\mathbf{P}_k = [\sum_{i=1}^k \mathbf{h}_i \mathbf{h}_i^T]^{-1}; \quad \mathbf{b}_k = \sum_{i=1}^k \mathbf{h}_i y_i \quad (\text{A3.11})$$

and we see that \mathbf{P}_k^{-1} and \mathbf{b}_k can be obtained recursively from the equations:

$$\mathbf{P}_k^{-1} = \mathbf{P}_{k-1}^{-1} + \mathbf{h}_k \mathbf{h}_k^T; \quad \mathbf{b}_k = \mathbf{b}_{k-1} + \mathbf{h}_k y_k \quad (\text{A3.12})$$

A few lines on matrix manipulation (see e.g. Young, 1984, page 24 *et seq*) then produces the following recursive least squares algorithm for updating the estimate $\hat{\mathbf{x}}_k$ of \mathbf{x}_k from the previous estimate $\hat{\mathbf{x}}_{k-1}$:

$$\hat{\mathbf{x}}_k = \hat{\mathbf{x}}_{k-1} + \mathbf{P}_{k-1} \mathbf{h}_k [1 + \mathbf{h}_k^T \mathbf{P}_{k-1} \mathbf{h}_k]^{-1} \{y_k - \mathbf{h}_k^T \hat{\mathbf{x}}_{k-1}\} \quad (\text{A3.13})$$

where \mathbf{P}_k is obtained recursively from \mathbf{P}_{k-1} by the equation:

$$\mathbf{P}_k = \mathbf{P}_{k-1} + \mathbf{P}_{k-1} \mathbf{h}_k [1 + \mathbf{h}_k^T \mathbf{P}_{k-1} \mathbf{h}_k]^{-1} \mathbf{h}_k^T \mathbf{P}_{k-1} \quad (\text{A3.14})$$

It is interesting to note that, following a little more matrix manipulation, an alternative form of the recursion (A3.13) is the following

$$\hat{\mathbf{x}}_k = \hat{\mathbf{x}}_{k-1} + \mathbf{P}_k \{\mathbf{h}_k y_k - \mathbf{h}_k \mathbf{h}_k^T \hat{\mathbf{x}}_{k-1}\} \quad (\text{A3.15})$$

† The need for linear independence between the x_j now becomes clear since linear dependence would result in singularity of the matrix $C_k = [\sum_{i=1}^k \mathbf{h}_i \mathbf{h}_i^T]$ with $\det[C(k)] = 0$ and the inverse ‘blowing up’

This second form shows that the recursive update is in the form of a ‘gradient algorithm’, since $\{\mathbf{h}_k y_k - \mathbf{h}_k \mathbf{h}_k^T \hat{\mathbf{x}}_{k-1}\}$ is proportional to the instantaneous gradient of the squared error function $[y_k - \mathbf{h}_k^T \hat{\mathbf{x}}]^2$. However, the form (A3.13) is usually preferred in computational terms.

Equations (A3.13) and (A3.14) constitute the *Recursive Least Squares* (RLS) algorithm. It is interesting to note the simplicity of the above derivation in vector-matrix terms which contrasts with the complexity of Gauss’s original derivation (see Appendix 2 of Young, 1984) using ordinary algebra. Note also that the RLS algorithm provides a computational advantage over the stage-wise solution of the *en bloc* solution (A3.9). In addition to the now convenient recursive form, which provides for a minimum of computer storage, note that the term $1 + \mathbf{h}_k^T \mathbf{P}_{k-1} \mathbf{h}_k$ is simply a scalar quantity. As a result, there is no requirement for direct matrix inversion even though the repeated solution of the equivalent classical solution (A3.9) entails inverting an $n \times n$ matrix for each solution.

Since the RLS is recursive, it is necessary to specify starting values $\hat{\mathbf{x}}_0$ and \mathbf{P}_0 for the vector $\hat{\mathbf{x}}$ and the matrix \mathbf{P} , respectively. This presents no real problem, however, since it can be shown that the criterion function-parameter hypersurface is unimodal and so an arbitrary finite $\hat{\mathbf{x}}_0$ (say $\hat{\mathbf{x}}_0 = \mathbf{0}$), coupled with a \mathbf{P}_0 having large diagonal elements (say 10^6 in general), will yield convergence and performance commensurate with the stage-wise solution of the same problem. This setting is often referred to as a ‘diffuse prior’, which exposes the fact that the algorithm has obvious Bayesian interpretation, in the sense that the *a priori* estimate $\hat{\mathbf{x}}_{k-1}$ at the $k-1^{th}$ sampling instant is updated to the *a posteriori* estimate $\hat{\mathbf{x}}_k$ at the k^{th} sampling instant.

This Bayesian interpretation is enhanced still further if it is assumed that the noise e_k is a Gaussian white noise process with variance σ^2 , for then the estimate $\hat{\mathbf{x}}_k$ will also have a Gaussian distribution and the statistical properties of the estimate, in the form of the covariance matrix, are conveniently generated by the algorithm if it is modified slightly to the form:

$$\hat{\mathbf{x}}_k = \hat{\mathbf{x}}_{k-1} + \mathbf{P}_{k-1} \mathbf{h}_k [\sigma^2 + \mathbf{h}_k^T \mathbf{P}_{k-1} \mathbf{h}_k]^{-1} \{y_k - \mathbf{h}_k^T \hat{\mathbf{x}}_{k-1}\} \quad (\text{A3.16a})$$

$$\mathbf{P}_k = \mathbf{P}_{k-1} + \mathbf{P}_{k-1} \mathbf{h}_k [\sigma^2 + \mathbf{h}_k^T \mathbf{P}_{k-1} \mathbf{h}_k]^{-1} \mathbf{h}_k^T \mathbf{P}_{k-1} \quad (\text{A3.16b})$$

where now \mathbf{P}_k is the covariance matrix, i.e.

$$\mathbf{P}_k = E\{\tilde{\mathbf{x}}_k \tilde{\mathbf{x}}_k^T\}; \quad \tilde{\mathbf{x}}_k = \mathbf{x}_k - \hat{\mathbf{x}}_k \quad (\text{A3.16c})$$

so that the square root of the diagonal elements of \mathbf{P}_k quantify the estimated standard errors on the elements of the estimate $\hat{\mathbf{x}}_k$. It must be emphasized, however, that the Gaussian assumptions utilized for this Bayesian interpretation of the algorithm are not essential to its success as an estimation algorithm. The algorithm is robust to the violation of these assumptions in the sense that the estimate $\hat{\mathbf{x}}_k$ is still the minimum covariance linear unbiased estimator of the state vector \mathbf{x}_k (see e.g. Norton, 1986).

(e) The Kalman Filter (KF)

In the RLS algorithm, there is an implicit assumption that \mathbf{x}_k is time invariant; an assumption that can be made explicit by stating that,

$$\mathbf{x}_k = \mathbf{F} \mathbf{x}_{k-1}; \quad \mathbf{F} = \mathbf{I}_n \quad (\text{A3.17})$$

where \mathbf{I}_n is the identity matrix (a purely diagonal $n \times n$ matrix with unity diagonal elements).

Kalman (1960), using orthogonal projection theory, extended this assumption by considering the situation when \mathbf{x}_k is not a vector of constant parameters, as in the RLS algorithm, but a vector of time-variable stochastic variables generated by the following stochastic state equations (a ‘Gauss-Markov process’):

$$\mathbf{x}_k = \mathbf{F}\mathbf{x}_{k-1} + \boldsymbol{\zeta}_k \quad (\text{A3.18})$$

where \mathbf{F} is a ‘state transition matrix’ that defines the dynamic behaviour of \mathbf{x}_k and is not, therefore, an identity matrix. This equation is obviously a generalization of (A3.17), allowing \mathbf{x}_k to vary over time in a stochastic-dynamic manner, where the stochasticity arises from the input $\boldsymbol{\zeta}_k$, which is assumed to be a vector of zero mean, white noise inputs with covariance matrix \mathbf{Q} .

In practice, we might expect that, if \mathbf{x}_k is a physically meaningful state vector, then it may be affected by one or more input variables. For instance, if the state variables are both observed and unobserved flows occurring at locations along a river, then these flows will be caused by the variations in the rainfall. Also, we might expect that not all the flows will be observed (e.g. some could be flows defined by the TF decomposition analysis discussed in Appendix 2, which separates the observed flow into unobserved quick and slow components). Consequently, it is necessary to specify how the observed (measured) variables are related to the state variables by introducing a ‘measurement equation’ that accounts also for any noise on these measured variables.

In the case of a single input variable $u_{k-\delta}$, delayed by δ samples (which is relevant to the rainfall-flow models considered in this Report, where $u_{k-\delta}$ is the delayed effective rainfall), these additional factors can be introduced quite straightforwardly by extending the model (1.9) to the form:

$$\mathbf{x}_k = \mathbf{F}\mathbf{x}_{k-1} + \mathbf{G}u_{k-\delta} + \boldsymbol{\zeta}_k \quad (\text{A3.19a})$$

$$y_k = \mathbf{h}^T \mathbf{x}_k + e_k \quad (\text{A3.19b})$$

Here, the second equation (A3.19b) is the measurement equation and it is very similar to the regression equation (A3.4), except that it will be noted that the subscript k on \mathbf{h} has been removed, showing that it is composed of constant elements. Although the elements of \mathbf{h} could vary, if this is required, it is more usual, within this dynamic systems setting, that they will be constant since the relationship between the observed variable y_k and the state vector \mathbf{x}_k will normally remain fixed. For example in the case of state equations (1.9) in the main body of this report, the measured water level is sum of the quick and slow components, so that $\mathbf{h} = [1 \ 1]$.

Given the stochastic state equations (A3.19a) and (A3.19b), the recursive equations of the Kalman Filter can be written in the following prediction-correction form:

***A priori* prediction:**

$$\hat{\mathbf{x}}_{k|k-1} = \mathbf{F}\hat{\mathbf{x}}_{k-1} + \mathbf{G}u_{k-\delta} \quad (\text{A3.20a})$$

$$\mathbf{P}_{k|k-1} = \mathbf{F}\mathbf{P}_{k-1}\mathbf{F}^T + \mathbf{Q} \quad (\text{A3.20b})$$

A posteriori correction:

$$\hat{\mathbf{x}}_k = \hat{\mathbf{x}}_{k|k-1} + \mathbf{P}_{k|k-1} \mathbf{h} [\sigma^2 + \mathbf{h}^T \mathbf{P}_{k|k-1} \mathbf{h}]^{-1} \{ (y_k - \mathbf{h}^T \hat{\mathbf{x}}_{k|k-1}) \} \quad (\text{A3.20c})$$

$$\mathbf{P}_k = \mathbf{P}_{k|k-1} - \mathbf{P}_{k|k-1} \mathbf{h} [\sigma^2 + \mathbf{h}^T \mathbf{P}_{k|k-1} \mathbf{h}]^{-1} \mathbf{h}^T \mathbf{P}_{k|k-1} \quad (\text{A3.20d})$$

$$\hat{y}_k = \mathbf{h}^T \hat{\mathbf{x}}_k \quad (\text{A3.20e})$$

The derivation of these equations is straightforward (e.g. Young, 1984) but, in any case, they make intuitive sense:

- Since the stochastic inputs ζ_k and e_k both involve only zero mean, white noise variables, the state prediction equation (A3.20a) provides a logical prediction of the state vector \mathbf{x}_k , given the equation (A3.19a) for its propagation in time, because the expected values of these random inputs is zero and the dynamic system is assumed to be stable. Here, the subscript notation $k|k-1$ denotes the estimate at the k^{th} sampling instant (in the main text one hour), based of the estimate at the previous $(k-1)^{th}$ sampling instant.
- The state update equations (A3.20c) and (A3.20d) follow directly from their equivalent equations (A3.16a) and (A3.16b), respectively, in the RLS algorithm.
- The covariance matrix prediction in equation (A3.20b) is not quite so obvious but, if we consider the estimation error $\tilde{\mathbf{x}}_k = \mathbf{x}_k - \hat{\mathbf{x}}_k$ then,

$$\tilde{\mathbf{x}}_k = \mathbf{F}\mathbf{x}_{k-1} - \mathbf{F}\hat{\mathbf{x}}_{k-1} + \zeta_k = \mathbf{F}\tilde{\mathbf{x}}_{k-1} + \zeta_k$$

because the effects of the input term $\mathbf{G}u_{k-\delta}$ cancel out. Consequently, the covariance matrix $\mathbf{P}_{k|k-1}$, which is the expected value of $\tilde{\mathbf{x}}_k \tilde{\mathbf{x}}_k^T$, is given by:

$$\mathbf{P}_{k|k-1} = E\{\tilde{\mathbf{x}}_k \tilde{\mathbf{x}}_k^T\} = E\{\mathbf{F}[\tilde{\mathbf{x}}_{k-1} \tilde{\mathbf{x}}_{k-1}^T] \mathbf{F}^T\} + E\{\zeta_k \zeta_k^T\} = \mathbf{F}\mathbf{P}_{k-1}\mathbf{F}^T + \mathbf{Q}$$

Here, use is made of the matrix identity $[\mathbf{F}\tilde{\mathbf{x}}_{k-1}]^T = \tilde{\mathbf{x}}_{k-1}^T \mathbf{F}^T$, associated with a matrix product; as well as the fact that the expected value of the cross-products between $\tilde{\mathbf{x}}_{k-1}$ and ζ are zero because they are uncorrelated.

- The estimate \hat{y}_k of the underlying ‘noise-free’ output (see later comment), i.e. $\dot{y}_k = \mathbf{h}^T \hat{\mathbf{x}}_k$, is simply a combination of the state estimates defined by the known measurement equation vector \mathbf{h} (e.g. in the case of the state space model (1.9) in the main text, $\mathbf{h}^T = [1 \ 1]$ and the estimate is the sum of the two state variables, in this case the ‘quick’ and ‘slow’ component water level estimates).
- Like its simple RLS relative, the KF can be considered in Bayesian terms. It is important to note, however, that KF algorithm is robust to the violation of the Gaussian assumptions required for Bayesian interpretation, in the sense that the estimate $\hat{\mathbf{x}}_k$ remains the minimum covariance linear unbiased estimator of the state vector \mathbf{x}_k in the face of such a violation (see e.g. Norton, 1986).

In the context of the present Report, the main reason for using the KF algorithm is forecasting water level or flow. The N -step-ahead forecasts are obtained by simply

repeating the prediction steps in (A3.20a) and (A3.20b) N times, without correction (since no new data over this interval are available). The N -step ahead forecast variance is then given by:

$$\text{var}(\hat{y}_{k+N|k}) = \hat{\sigma}_k^2 + \mathbf{h}^T \mathbf{P}_{k+N|k} \mathbf{h} \quad (\text{A3.20f})$$

where $\mathbf{P}_{k+N|k}$ is the error covariance matrix estimate associated with the N -step ahead prediction of the state estimates. This estimate of the N -step ahead prediction variance is used to derive approximate 95% confidence bounds for the forecasts, under the approximating assumption that the prediction error can be characterized as a nonstationary Gaussian process (i.e. twice the square root of the variance at each time step is used to define the 95% confidence region).

It is important to note one important aspect of the stochastic formulation of the KF in relation to flood forecasting: namely the assumption that the measured water level (or flow) variable is subject to error and uncertainty. The objective of the KF is to provide an *estimate* of this variable so, at each recursion, the state update equation (A3.20c) adjusts the estimate of the state vector \hat{x}_k to its most likely value, based on the past estimates and the latest noisy measurement. The associated estimate of the water level \hat{y}_k in equation (A3.20e) is adjusted accordingly and it will not, in general, be equal to the measured water level.

This means that the forecast generated by the KF should not be considered a forecast of the *measured* water level variable but an estimate of the underlying ‘noise-free’ variable \dot{y}_k (see above), together with a quantification of the uncertainty associated with this estimate. It is important to stress this point, since there is a tendency to judge the quality of a forecast by how close it forecasts the measured water level. In fact, the forecast is the mean of an estimated random variable defined by this mean value and the associated confidence bounds, so that a good forecast is one in which, most of the time, the measured water level falls within the 95% confidence interval associated with the forecast.

Finally, it should be mentioned that other, more complex recursive algorithms have been developed for special problems: for instance, the recursive form of the *Refined Instrumental Variable* (RIV) algorithm discussed in Appendix 2 and used in the main part of the Report for DBM modelling (see Young, 1984), which involves iteration as well as recursion.

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