PRACTICAL SOLUTION OF SOME FORWARD AND INVERSE PROBLEMS IN HYDROLOGY

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1. INTRODUCTION

What is the need for solving inverse problems in hydrology? The basic answer to this question is that many laws in hydrology invoke parameters that are not easily measured or even observed. This means that modelling will require at the very least a calibration of parameters from observation of other variables, often termed indirect observations. For example the transmissivity or rate at which water is transmitted through an aquifer depends on the physical properties of the medium and these properties are reflected partly in the observations of aquifer water level. Often hydrologic models require additional knowledge of the specific functional forms of system dependent terms within the general model structure. For example, the functional approximation of hydraulic conductivity in Richards equation for transport in unsaturated soil depends on the soil properties. These model structure identification and parameter estimation problems from indirect observations and other prior knowledge represent fundamental inverse problems.

Why in the title of the paper, qualify the solution of inverse problems with the word 'practical' and why include 'forward' with 'inverse' problems? Practical solution implies that the forward modelling task has a specific purpose, perhaps ranging through simple investigatory analysis, on-line operational or off-line management and planning to improved scientific understanding of natural processes. The inclusion of forward with inverse problems is necessary because solving an inverse problem requires awareness of the forward modelling aspects. In practice, the motivation for solving an inverse problem, and the formulation eventually selected, is dependent on the forward problem of interest.

An indicative but by no means comprehensive range of examples of forward modelling problems in hydrology, which require inversion treatment, can be given by a citation of some of the research carried out separately at the Centre for Resource and Environmental Studies and in collaboration with the Centre for Mathematical Analysis at the Australian National University and the Institute of Hydrology in the United Kingdom. The recent research output includes treatment of the following flow and transport problems. In the atmospheric component of the hydrological cycle, the research program includes prediction of the global distribution of trace gases in the troposphere [25] and simulation of weather variables such as rainfall [13] and cloud [3]. In humid catchments, attention has been given to simulation of streamflow from rainfall [16] and prediction of the distribution of surface soil water content in response to topography and other factors [22]. Within streams, Dietrich et al. [6, 8] have considered forecasting the downstream concentration of conservative pollutants from upstream concentration and discharge measurements and predicting the transport of salinity in streams subject to groundwater interaction. Another water quality problem being addressed is predicting the extremes of stream acidity variables [17]. Subsurface problems for which simulation models were constructed involve control of groundwater behaviour in aquifers by interception pumping and irrigation reductions [9, 10] and assessment of saline intrusion in coastal aquifers [11].

Partial differential equations (PDEs) are recognised as the basic model descriptions of flow and transport in hydrology and more generally for natural environmental processes. Steffen and Denmead [24] for example contains state-of-the- art surveys of the mathematical formulations associated with many of these processes. Despite increasing process knowledge from experiments (often incorporated in the form of PDEs), improved and more specialised physical theories and recognition of and attention to the stochastic nature of some of the associated variables, large uncertainty continues to surround the modelling of many hydrological systems. While our process-based knowledge can be very detailed and sophisticated, the amount of irreducible or inherent uncertainty can be and may remain quite large.

The reasons for having to accept a minimum amount of uncertainty as the norm are discussed in the next section. These include: the idealised nature of process-based models such as PDE equation formulations which are only applicable at scales where underlying assumptions about the system properties apply; the ill-posed character of certain aspects of the modelling exercise; the sampling and measurement errors associated with observations; and the amount of information in or representativeness of the available observations both in space and time.

This said, the paper illustrates that in hydrology practically useful solution of forward and inverse problems associated with flow and transport is still often very possible despite high levels of uncertainties. With two representative examples, it is demonstrated how useful information was extracted from the modelling exercise. This extraction requires a systematic and contextual approach, addressing carefully and perhaps iteratively all steps in the model construction procedure in relation to the specific problem of interest and its setting. Emphasis is given to deciding what are achievable objectives and to specification of a comprehensive range of prior information that can be imposed and/or tested. It is also illustrated how it can be crucially important to select an estimation procedure and numerical algorithm with desirable mathematical and statistical properties.

Section 2 attempts to explain the major features of problems requiring solution in hydrology and the mathematical implications. Section 3 indicates the partial differential equation nature of flow and other mass transport problems in hydrology. In particular, it deals with problems of advection- diffusion type, characterises associated ill-posed problems and the ensuing difficulties created in a hydrological problem context where indirect observations and prior knowledge of solution values are limited and models contain their own errors.

Section 4 introduces the major considerations in practice for obtaining (inverse) solutions to such problems. The next two sections discuss the first two of these with section 5 emphasising that what can be accomplished by modelling is very much a function of the level of prior knowledge and the objective. Section 6 categorises the form that prior knowledge can take.

Sections 7 - 8 illustrate the application of these considerations to two problems. The first, presented in section 7, involves rainfall-runoff modelling at catchment scale. Here the objectives and prior information allow simplification of the formulation to one which remains dynamic but dispenses with the added dimensionality required by use of spatially distributed parameters. The second problem, presented in section 8, involves use of the groundwater flow equation in a confined aquifer so that the standard PDE is retained as the formulation for which an inverse solution is required. In this case, most attention is paid to the imposition of prior assumptions and constraints on model simulation performance to obtain the range and covariation of parameter values which yield acceptable performance. For the inverse problems in sections 7 - 8, the numerical techniques used are important contributors to the success of both modelling exercises, although for different reasons.

2. FEATURES OF HYDROLOGIC SYSTEMS

2.1 Coupled subsystems of storages and pathways

Figure 1 from Chapman [2] is a typical conceptual framework used to represent the hydrologic system of a catchment. Such a system consists of a set of storages (subsystems) linked by flow pathways (inputs and outputs) and the precise detail and configuration of the subsystems depend on the problem of interest. Conservation of mass, known as the water or material balance, can be applied to each of the storages or over a group of storages.

2.2 Time and space scales

There is no single common time or space scale for modelling hydrologic systems. The time taken to turnover mass within a storage can vary from a few minutes for overland flow to years for groundwater systems while travel distances of interest can range from metres to hundreds of kilometres [2]. Therefore, it very often occurs that a modelling problem in hydrology involves interconnected systems of different scales.

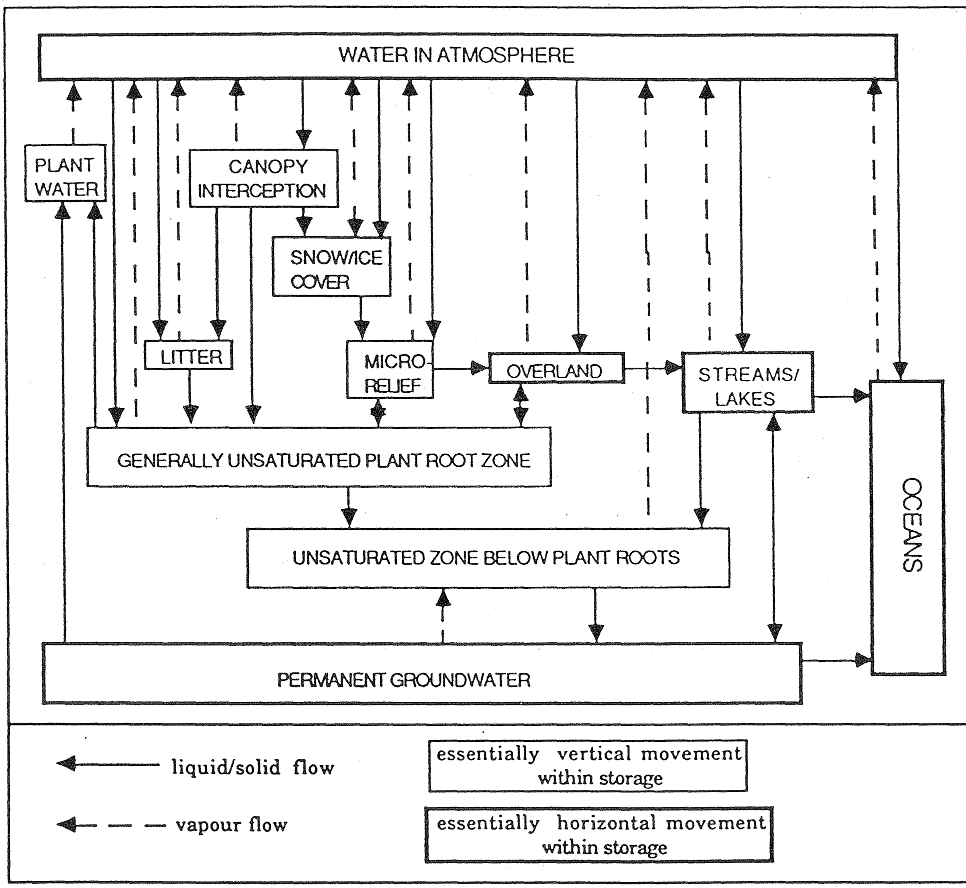

Figure 1: Hydrological system for a catchment [2]

2.3 Processes - multidimensional and dynamic

The phenomena (inputs, outputs and internal states) in hydrology evolve in three-dimensional space, although sometimes vertical or horizontal flows dominate. Generally, the processes need to be modelled dynamically but some components may be modelled in steady state. In other words, hydrologic phenomena can be non-steady and driven by multi-dimensional velocity fields.

2.4 Processes - physical, chemical and biological

Many processes such as the flow of water in an aquifer are merely physical. Other processes such as the transport of reactive pollutants are chemical or biological as well. One of the most difficult problems in hydrology is manifested in the current inability to incorporate biochemical processes in descriptions of flow and transport in soils. Plants and their associated soil flora and fauna often critically control mass transport in surface soil [5].

2.5 Phenomena essentially episodic and uncontrollable

There can be long periods of quiescence between some of the storages, particularly in semi-arid to arid environments. Chapman [2] points out that most of the transport of surface and near-surface water occurs during hydrological events. The range of excitations over which a subsystem is perturbed is dictated mainly by climatic events so that planned experiments cannot be performed to improve the information content in indirect observations from which models are constructed. These features have implications for the design of monitoring schemes to obtain indirect observational data.

2.6 Heterogeneity of transport media

The storages or media which provide transport of mass are heterogeneous at many scales. This causes problems for the characterisation of effectively homogeneous scales for modelling and for measurement of parameters. Some of the more acute problems in flow variability relate to preferential transport pathways such as is caused by macropores and fissures.

2.7 Expense and sampling and measurement errors of monitoring

It is often too impractical and costly to obtain a good spatial and temporal coverage of indirect observations and especially of point parameters. To compound this sampling error problem, much instrumentation is not precise and associated data are therefore prone to measurement error.

2.8 Implications for mathematical modelling

The foregoing characterisation of the features of modelling hydrologic systems can be summarised from a mathematical modelling point of view in the following way. First, the basic formulations, which include PDEs, tend to be highly idealised. Typical among these PDEs are advection-diffusion descriptions. It is now recognised that even in homogeneous media diffusion approximations are 'only asymptotically true, being valid only if the time and length scales of the transport process are large enough for a typical tracer particle to have experienced the full range of variations in the velocity field' [20]. Stochastic process descriptions can be helpful, but these do not obviate the need for measurements and determining relationships between major forcing functions and behavioural outputs. Second, some aspects of modelling represent ill-posed problems and these need to be translated into well-posed formulations by the imposition of sufficient prior information. Third, the information content associated with indirect observations and direct parameter values is rarely adequate on its own to counteract the ill-posedness. Observations contain measurement and sampling error and the observation period may not span all conditions under which the model is intended to be used. In the next section, these points are given an expanded treatment.

3. SOME ASPECTS OF MASS TRANSPORT IN THE ENVIRONMENT

Mass transport phenomena represent an important class of problems associated with understanding and managing the natural environment. Indeed, from the small scale movement of pollutant in underground porous media to large scale atmospheric circulation of gases, the environment offers a variety of challenges to modellers keen to use PDEs to describe transport phenomena. However, as indicated in the previous section, the physics of the environment deals with interconnected and complex processes that may take place at vastly different spatial and time scales. This means that the associated mathematics can be expected to be tricky if not intractable. To illustrate some of the difficulties that environmental modellers may face, we shall consider here solute transport in a groundwater system.

At a sufficiently small scale, solute transport depends on the microscopic properties of the supporting porous medium and the flow equations usually invoke mass, momentum and energy conservation principles.

To simplify the exposition, we shall assume that some suitable averaging has taken place so that essentially transport will be the result of a mass balance between the time and spatial rate of changes of relevant solute attributes. Such a simplification yields an equation of the form

$$\frac{\partial c}{\partial t} + \nabla \cdot \boldsymbol{j} = -s \tag{1}$$

where c is the solute concentration; j is the solute mass flux; and s is a source term. We shall assume that j is caused by the presence of an advective velocity field and a concentration gradient. In other words $j = c\boldsymbol{u} + K\nabla c$ where $\boldsymbol{u}$ is the advective velocity and K is a diffusivity tensor. If the fluid is incompressible, $\boldsymbol{u}$ is divergence free, and (1) becomes the classical advection-diffusion equation

$$\frac{\partial c}{\partial t} + \boldsymbol{u} \cdot \nabla c + \nabla \cdot K\nabla c = -s \tag{2}$$

Associated with the solute transport equation (2) is the transport equation for the fluid, here water. In its simplest form it is given by

$$S\frac{\partial h}{\partial t} + \nabla \cdot T\nabla h = -q \tag{3}$$

where h is the water potential; S is the storativity; T the transmissivity; and q a source term. The link between (3) and (2) is provided by Darcy's law, i.e.

$$\boldsymbol{u} = T\nabla h \tag{4}$$

With this, equations (2) to (4) yield an uncoupled system of partial differential equations that can be used to model, for example, the movement of a pollutant plume in a groundwater system.

A first point to note is that the advective velocity u required in (2) is going to be obtained from (3) and (4) via differentiation of the water potential h. This means that the forward problem (3) will need to be solved with sufficient accuracy to avoid large error magnification associated with numerical differentiation.

An additional point is that in most practical cases, only partial information will be available on the physical parameters, sinks, boundary and initial conditions appearing in the transport equations. In the particular example of a groundwater system, it is very likely that essentially the available data will be point measurements of the solute concentration c and the water pressure potential h since such data are relatively easy and inexpensive to gather. On the other hand, data on the physical parameters will be scarce, comprising only few scattered and noisy measurements.

This indicates that prior to solving the forward problems (2) and (3), some (possibly non-linear) inverse procedures are to be used so as to recover information on parameters from measurements of the dependent variables. For example, consider (3) with the potential h being the dependent variable. Use of the PDE with measurements of the potential h to recover information of the sink term q is going to involve two differentiations of data and thus be quite ill- posed. The situation is even worse for transmissivity T. In this case, the inverse problem is non-linear while its degree of ill-posedness can be expected to be equivalent to two differentiations of the measurements of h. This can be seen by noting that transmissivity values in the neighbourhood of a point P with $\nabla h(P) = 0$ will depend on $\nabla h(P)$ [7].

The well-known difficulties associated with such inversions are compounded when available data are likely to be noisy and made on a scale that is not truly that of the hypothesised mathematical model. Under those circumstances, one may wonder if it is practically feasible to model such a poorly defined system. The answer is a cautious and qualified 'yes'. As discussed in the next section, environmental modelling is an iterative procedure through which a balance among the modelling objectives, the degree of resolution in the available prior knowledge, and the complexity of the hypothesised mathematical model needs to be found. Thus given some modelling objectives, lack of prior knowledge at a degree of resolution commensurate with the mathematical model hypothesised requires that additional prior information be sought and/or some form of aggregation be imposed on the model. Alternatively, or in addition, the modeller may have to pursue a less demanding objective.

4. MAJOR CONSIDERATIONS FOR PRACTICAL MODELLING

A quantitative model construction exercise in hydrology involves consideration of the forward problem with associated inverse problems. While the major steps in such an exercise tend to be iterative and interconnected, they bear explicit recognition here. They can be of crucial importance when dealing with the solution of practical problems where: the underlying representations are idealised and (with respect to the inverse component of the exercise) are ill-posed; and indirect observations are of limited availability and contain errors. These steps are:

i. Define the range of useful objectives for the forward modelling component (including general purposes and model response properties and scales of interest).

ii. Specify and obtain prior knowledge for the forward and inverse components (including basic physical laws, observational data, parameter values, errors); assume more if necessary and test validity as far as possible for the inverse component.

iii. Incorporate (i) and (ii) in selection of a model family (level of determinism and stochasticity, spatial dimensionality, static or dynamic formulation).

iv. Discriminate among alternative parameterisations, identify order of parameterisation, estimate parameters and uncertainty, perform diagnostic checks on models.

The examples in sections 7 and 8 of the paper are used to indicate the importance of all these steps, although there is no attention given to discrimination among alternative parameterisations. Suffice it to say here that one should be eclectic with respect to the breadth of models tested and discrimination should involve evaluation of as wide a range of criteria as is necessary.

5. DEFINITION OF OBJECTIVES

In this and the following section, it is worth some attempt at qualitative elucidation of the sorts of decisions that need to be made in steps (i) and (ii) of a model construction exercise for problems associated with mass transport in the natural environment. The main emphasis is given to step (i). The importance of and considerations in this step are seldom stressed. The considerations developed will also be helpful in presenting the examples. Jakeman [14] contains more detail on the other steps.

Figure 2 aims to convey the degree of difficulty with respect to objectives in solving the class of inverse problems which relates to model calibration of mass transport phenomena. While the focus here is on the three axes shown, other factors may influence the degree of difficulty. These other factors include the level of discretisation sought, the spatial dimensionality and the transport medium or storage zone(s) of interest. In the latter case, for example, the unsaturated zone tends to be more difficult to model than the saturated, while root zone processes are even more complex.

In the following discussion, it is simpler to restrict attention to one medium. Each axis in Figure 2 represents an element of the specification to be made in step (i). Each annotation on an axis represents the marginal degree of difficulty imposed by that element. A coordinate in 3-space can be plotted for a given modelling problem which has a characteristic value or position on each of the three axes. The joint degree of difficulty is notionally some function of distance of the coordinate from the origin. However, it must be appreciated that the degree of difficulty is conditional on the level of prior knowledge. If two

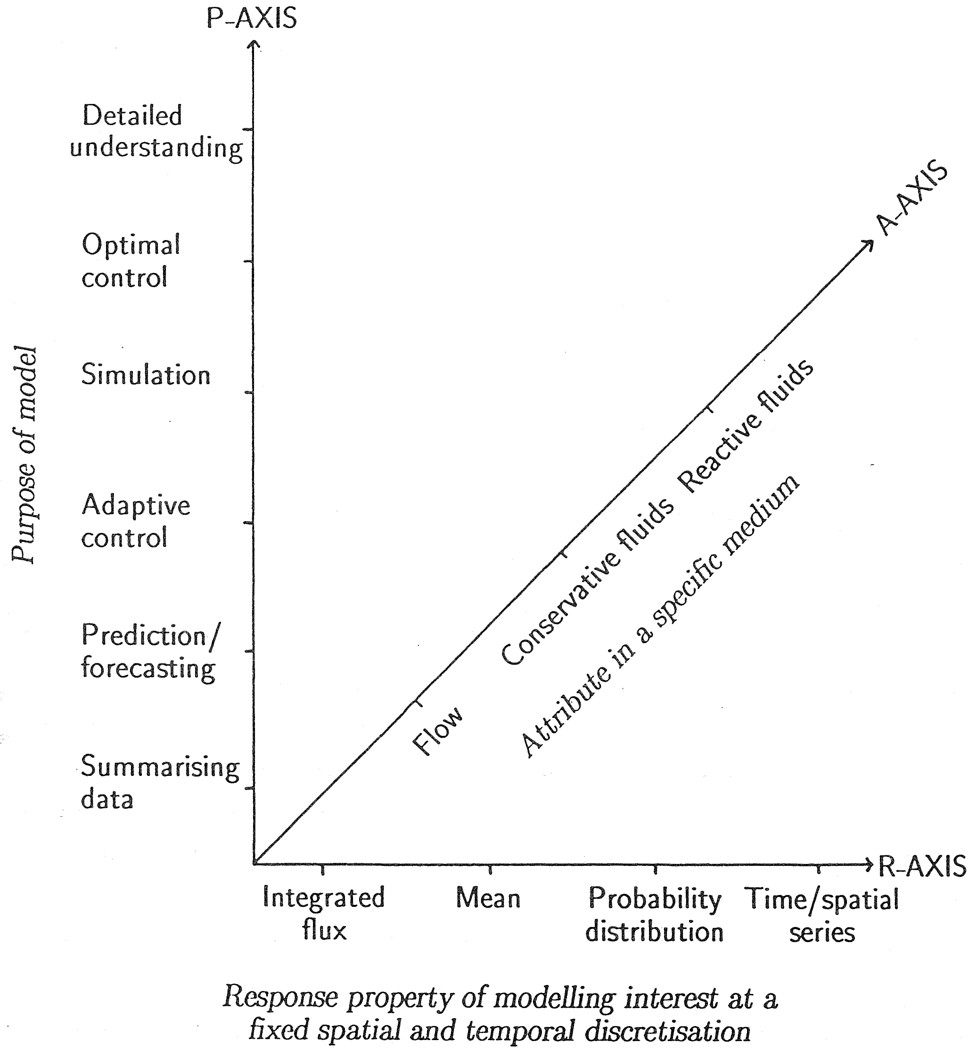

Figure 2: Degree of difficulty with respect to objectives in calibration of a model is some (increasing) non-linear function of distance from the origin.

modelling problems occupy the same point in the space, the one with a superior level of indirect observations, prior parameter estimates and representative observation period will generally yield a more certain solution. Thus the degree of difficulty can be considered as a marginal or inherent uncertainty.

The axes have been labelled A-, P- and R- axes, with axes for D (dimensionality), I (interval of discretisation) and M (medium) not shown. The A- or Attribute-axis can be used to locate the attribute or variable of modelling interest, the one the model is being constructed to summarise, simulate, forecast or control. Thus for a specific medium, the forward modelling of a flow attribute is easier than that of concentration of a conservative solute and this in turn is less difficult than modelling the concentration of a reactive fluid in that medium. In addition to knowledge of the physics of conservative fluids, the modelling of reactive fluids requires some description of the chemical processes, while for the modelling of any solute concentration, knowledge of the flow field is required.

The D- or Dimensionality-axis (not shown in Figure 2) indicates the most obvious point that a higher dimensional problem is usually more difficult to model than a lower dimensional one. However, a point to note is that if the problem in hand is difficult only because it requires solution of an inverse problem, then the degree of ill-posedness and the degree of difficulty associated with it, may be less in higher dimensions. For example, under appropriate assumptions the eigenvalues of the inverse of the Laplace operator ∇ decay essentially like $k^{-2/d}$ where d is the dimension of the problem. Inversion of ∇ in two or higher dimensions is therefore less ill-posed than in one dimension. This said, in practical environmental problems data are more scarce in higher dimensions, and this may be the feature that eventually dominates the degree of difficulty in the modelling exercise.

The P- or Purpose-axis says that it is easier to construct a model for summarising data, where many abstract formalisms may suffice for the model representation than it is to forecast a few time steps ahead or to extrapolate spatially. Like adaptive control the latter requires at least constructing some stochastic formalism which holds the recent memory of the historical observations of the attribute of interest or relates the attribute to other causal variables. Simulation and optimal control are even more difficult since these objectives require the model to be able to reproduce the system behaviour in response to changes in model inputs and boundary conditions, perhaps beyond those experienced in the observation period used to calibrate the model.

The R-axis represents the response property of forward modelling interest. Thus, at a fixed spatial and temporal discretisation, an integrated flux of some mass transport phenomena, a zeroth moment, tends to be less demanding a response property than the mean, the first moment. The probability distribution of a response variable requires further information, usually at least the second moment. Finally, reproduction of the individual time series and/or spatial series realisations of the response variable may require still more demanding model construction.

In order to obtain a modelling result with an acceptable level of uncertainty, a balance has to be struck among the modelling objectives and the level of prior knowledge. The further the objectives place the modelling problem from our origin (in the context of our experience or literature appreciation), the more prior knowledge that must be sought or imposed as an assumption. An alternative or additional approach to reduce the uncertainty is to seek a less demanding objective and hence degree of difficulty. This can be achieved by locating one or more of the characteristics on the axes of our conceptual diagram closer to the origin.

6. PRIOR KNOWLEDGE

The term 'prior' knowledge is used in this paper to denote knowledge or information about the model structure, parameter values, direct and indirect observational data. This knowledge may be derived from theory, empirical analysis, or it may be assumed and only partly tested.

Knowledge about parameter values may come in one of several forms, for example, point estimates (as obtained from measurements), constraints such as bounds (from literature values or physical arguments), or probability distributions.

Knowledge about the data may also come in the form of constraints or probability distributions. Other knowledge about the properties of the measurement and sampling errors in the data may also be available and can be helpful in selecting discretisation intervals, parameter estimation technique and model performance evaluation.

Knowledge about model structure can be determined in different ways. Take the two examples to follow. For the groundwater flow example, a bottom-up approach is taken in the sense that the well known idealised PDE is invoked as the basic formulation. The classical PDE for flow in a confined aquifer is used and the ill-posedness of its inversion is controlled by imposing a wealth of prior information on unknown parameters. For the rainfall-streamflow example, a top-down approach is used in the sense that few physically-based assumptions are invoked. A spatially lumped representation of the convolution integral is proposed. It is found to be an adequate basic model structure provided a low parameterisation is used to approximate the solution of the inverse problem.

7. RAINFALL-STREAMFLOW MODELLING

One of the most considered problems in the hydrological literature continues to be the estimation of streamflow or discharge at some point in a catchment. Such a discharge represents the final output of a myriad of flow processes following the fall of precipitation on the surface of a catchment. Models of streamflow are constructed in practice to satisfy one or more of a number of purposes including:

P1: Interpolation or real-time forecasting of streamflow levels at a particular location (e.g. to fill in missing records or for operational decisions).

P2: Simulation of streamflow in response to weather inputs such as rainfall and temperature (e.g. for water quality modelling).

P3: Understanding of catchment-scale dynamics of streamflow response in response to rainfall events and in particular baseflow component separation (e.g. to assess the effect of future climatic scenarios on streamflow or the effect of past and present land use on hydrology).

P4: Understanding of hydrological response in different parts of a catchment (e.g. to simulate streamflow in response to land use and catchment management options and weather inputs).

There is certain general prior knowledge which is available for tackling these forward problems. This knowledge is critical in the design of the inverse procedure to construct a model of streamflow. Model types used and their information requirements are considered below.

- Differential equations discretised in time and space have been employed to represent subsystems of a catchment. These express conservation of mass and momentum for each subsystem. The subsystems are linked by matching mutual boundary conditions at each time step [26]. Large amounts of observational data and prior parameter estimates are required to calibrate and run these models. The few well-documented accounts of the performance of these models reveal large uncertainties.
- Aggregated conceptual models of catchment behaviour predict runoff by accounting for the processing of moisture through the soil column and channel system. They tend to be distributed in time but may be lumped in space. Several storage zones are hypothesised to account for the various storage mechanisms on an aggregated basis. The functions describing exchange of storage contents can be highly nonlinear [21]. Observational data and prior parameter values associated with storage zones in the above conceptual models are usually scant. Optimisation of parameters is required leading generally to dependence of the calibration on only a few key parameters, most others being insensitive.
- The unit hydrograph concept assumes there is a linear convolution integral relating rainfall excess $u(t)$ and streamflow $x(t)$ (e.g. [4]). The kernel or impulse response function $k(t-s)$ in the integrand is known as the instantaneous unit hydrograph and is the function sought in the model calibration exercise. Rainfall excess is that

rainfall not lost to evapotranspiration and able to contribute to streamflow. Thus

$$x(t) = \int_{-\infty}^{t} k(t-s)\ u(s)\,ds$$

Identification and calibration of the convolution integral requires rainfall and streamflow time series data. Finite representations of the kernel use approximations and/or smoothness constraints on the unit hydrograph. Modelling efforts using a rational polynomial approximation of the unit hydrograph, at least on humid catchments, appear very promising [16]. The non-linear relationship between rainfall and rainfall excess can also be modelled in a lumped fashion. While this problem can itself be very difficult, simple parameterisations can work very well (e.g. [27], [16]).

- Purely stochastic time series models, for example of autoregressive-moving average type, have been used to characterise streamflow (e.g. [18]). The only prior knowledge needed for these models, which do not postulate a causal relationship, is streamflow measurements. However, stationarity of the latter is required.

Which modelling approach is taken to estimate streamflow depends on the objective and prior knowledge. It may also depend on the input data available in practice to run a model forward as well as a good numerical algorithm. If the purpose is real-time forecasting or streamflow interpolation (P1), then little prior knowledge may be needed. If the attribute of interest is just a mean prediction over a long enough time step, an assumption of stationarity in the historical streamflow data may be sufficiently valid. A stochastic model may then be capable of identifying predictably regular statistical patterns in the observations.

However, if simulation under changing rainfall conditions is the purpose (P2) or forecasting is required in a situation where stationarity does not apply, additional prior knowledge must be injected to deal with the relationship between key variables, such as rainfall and streamflow.

This is where the unit hydrograph concept can be useful. Note that, like the purely stochastic approach, it also keeps the degree of difficulty low by not using a spatial distribution of parameter values. Most unit hydrograph approaches simplify the problem further by intuitively removing the base flow component of streamflow observations so that the convolution integral represents only the short term dynamic relationship between rainfall excess and streamflow.

If the purpose is more demanding, such as understanding hydrological response to land use or climate change (P3 or P4), then more prior knowledge must be injected. If only aggregate catchment scale understanding is required, then the dimensionality can be kept down. An approach that has proven successful is to hypothesise a configuration of linear reservoirs, usually in parallel, in order to parameterise the unit hydrograph efficiently, and to allow part of the configuration to represent the slower baseflow processes. In mathematical terms, this configuration is equivalent to postulating approximation of the unit hydrograph by a sum of exponential decays. Associated tools are then required to identify the number of terms in the summation and to estimate the parameters.

Jakeman et al. [16] stress the importance of selecting a numerical algorithm which is robust to even very small model and data errors. This was demonstrated for rainfall-streamflow data from a catchment in Wales. The model identified between rainfall r_k, at hour k, rainfall excess, u_k and streamflow x_k for this particular catchment is

$$s_k = s_{k-1} + (r_k - s_{k-1})/86, \qquad s_0 = 0$$

(5)
$$u_k = const.\ r_k\, s_k$$

$$x_k = \frac{18.8796}{1-0.7947z^{-1}}\, u_k + \frac{1.5521}{1-0.9890z^{-1}}\, u_k$$

where z^{-1} is the backward shift operator. Note that the term const. is estimated independently but its value is not required. It can be incorporated in estimation of the parameters in the numerator of (5). The two transfer functions in (5) are the identifiable components of a rational polynomial approximation of a discretised version of the convolution integral.

The need for careful selection of an estimation algorithm may be appreciated from recognising the possibility that one of the transfer functions may possess a polynomial denominator with a root near the unit circle, as is the value of 0.9890 in (5). Values close to unity occur when streamflow has a slowly decaying baseflow component following the cessation of rainfall. Another factor influencing selection of the estimation algorithm is the closeness of baseflow to zero. The closer baseflow is to zero the more difficult the estimation of the associated polynomial root. To minimise both estimation problems, a simple refined instrumental variable (SRIV) algorithm was applied in Jakeman et al. [16]. It has the properties of being consistent and relatively efficient statistically. It also applies a linear filter to the rainfall excess and streamflow series, which has the effect of increasing low baseflow (and rainfall excess) values. Such a linear transformation does not affect the relationship between rainfall excess and streamflow. SRIV estimation is also optimal in that it minimises the sum of squared errors between x_k and the model estimate of x_k.

These points are stressed because the usual algorithms prove inadequate for this problem. Both a so-called least squares (LS), used for example by Rao and Mao [23], and a basic instrumental variable (BIV) algorithm, usually adequate for most engineering modelling purposes, fail to extract the second component from the transfer function representation. Figures 3 and 4 illustrate the performance of the BIV and SRIV algorithms on 400 hours of data from the catchment in Wales. The LS performance is visually similar to that of BIV. Table 1 gives the parameter values estimated by the three algorithms when a second order approximation is assumed. Notice that LS and BIV estimate that the denominator parameter of the second order component is close to zero.

When the purpose of the modelling exercise is to simulate streamflow in relation to postulated land use and land cover characteristics (P4),

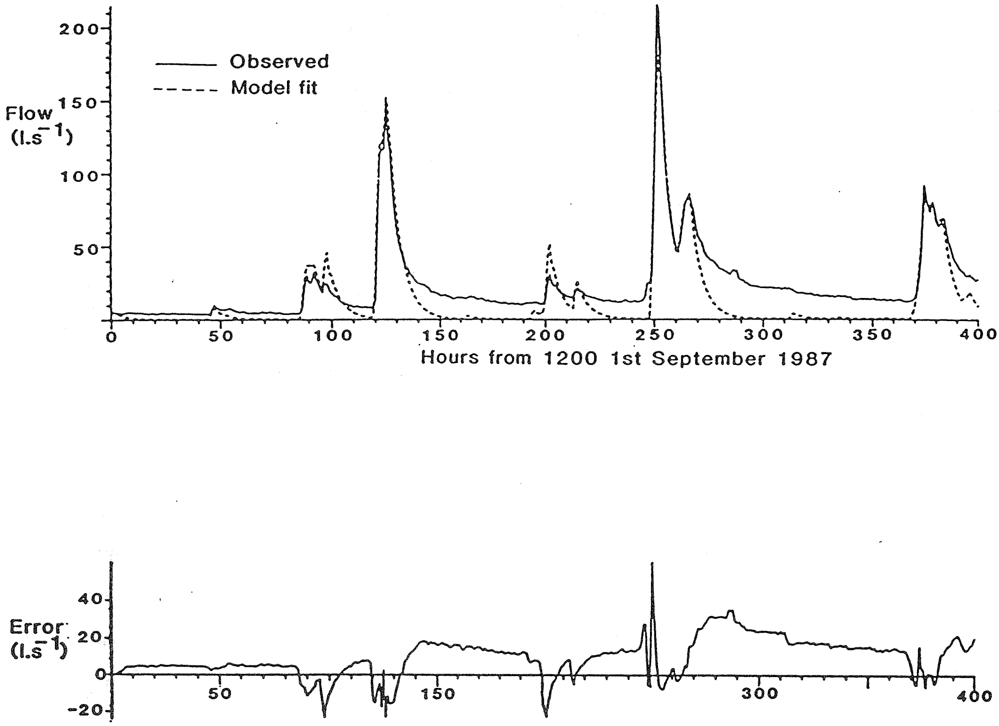

Figure 3: Fit of model using BIV estimation to 400 hours of streamflow from a catchment in Wales.

Table 1: Estimation results using LS, BIV and SRIV.

	Denominator parameters		Numerator parameters		R^2 fit
LS	-0.8804	0.0424	15.3466	6.9673	0.7916
BIV	-0.7733	-0.0381	15.2651	8.7720	0.7947
SRIV	-0.7947	-0.9890	18.8796	1.5521	0.9455

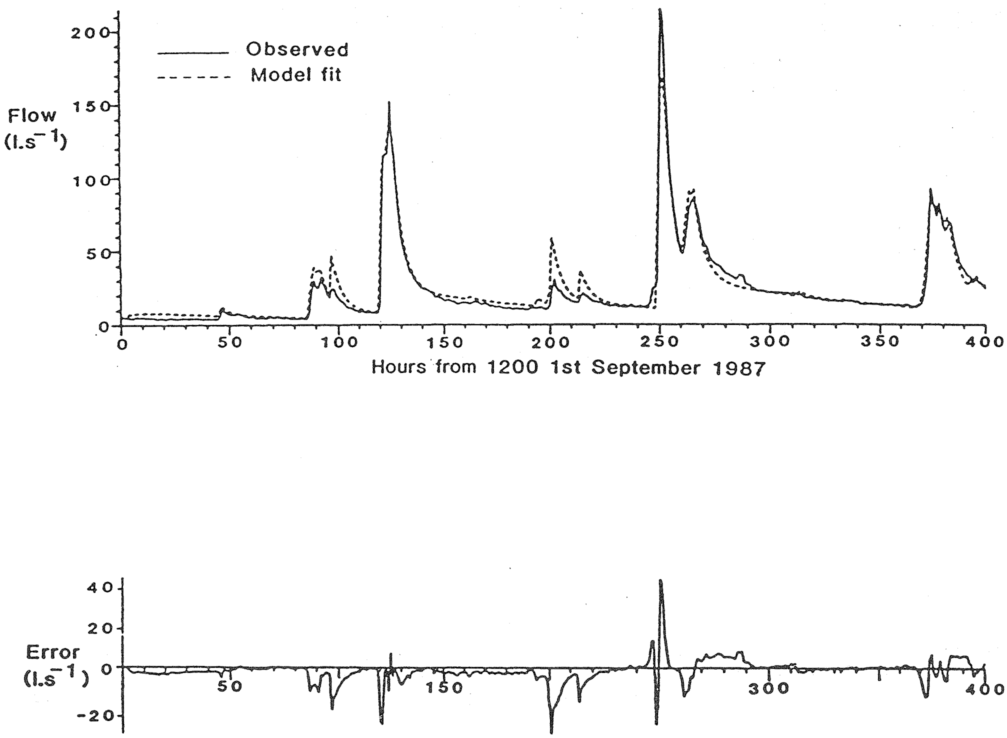

Figure 4: Fit of model (5) obtained using SRIV estimation to same streamflow data as in Figure 3.

possibly different in various parts of the catchment, so-called physically-based models have been promoted. The argument is that only by discretising the catchment into effectively homogeneous elements and using the appropriate conservation equations, with separate parameter values for each element, can such simulation be successful Unfortunately, progress in this area is slow. Satisfactory results will require model structure simplifications which are consistent with the level of observational information available to calibrate parameters.

It can be argued that the previous desire of hydrologists to make point measurements of 'physical' parameters (such as infiltration, transmissivity) and insert them in finely discretised physically-based models for simulation purposes was always ill-fated. This is now recognised in many quarters so that the basic paradigm has shifted from one based almost entirely upon physical determinism to recognition of uncertainty and the need for model calibration of parameters (e.g. [21]). However, it has not shifted far enough. Calls continue to be made for validation of models and characterisation of uncertainty [19] and this will eventually become the next operational paradigm. More revolutionary is the call, for example, by Beven [1], for a new paradigm involving "a macroscale theory that deals explicitly with the problems posed by spatial integration of heterogeneous, non- linear interacting processes ... Such a theory will be inherently stochastic and will deal with the value of observations and qualitative knowledge in reducing predictive uncertainty; the interactions between parameterisations and uncertainty; and the changes in hydrological response to be expected as spatial scale increases".

8. GROUNDWATER EXAMPLE

The problem here relates to groundwater flow in an area near Mildura in Australia. The area of interest is shown in Figure 5. It is subject to different forms of land use as indicated. In particular, commercial crops are irrigated in part of the area and over several decades this has resulted in a rise in the underlying water table which is saline. Consequently, the increased gradient of groundwater has caused larger fluxes of salt to the river on the northern boundary. An interception scheme was installed to pump groundwater away from the river to evaporation basins. The scheme lowers this gradient and reduces the accessions of salt to the river in order to afford protection to downstream uses. The location of present pump sites is also shown in Figure 5.

The purpose of the associated modelling exercise [9, 10] was:

P1: Simulate salt load to the river boundary to assess the efficiency of the interception scheme and to recommend improvements.

P2: Quantify the contribution of irrigation to groundwater levels.

The prior knowledge available for these purposes was the following:

- Basic model structures available are the relevant PDEs of soil infiltration, groundwater flow and conservative solute transport.
- Point estimates of aquifer parameters, adjacent to the river only.
- Monthly irrigation in relation to land use and rainfall data.
- Daily aquifer pumping rate data for the interception bores.
- Point estimates of monthly groundwater levels.
- River height measured daily as a boundary condition along a portion of the aquifer.

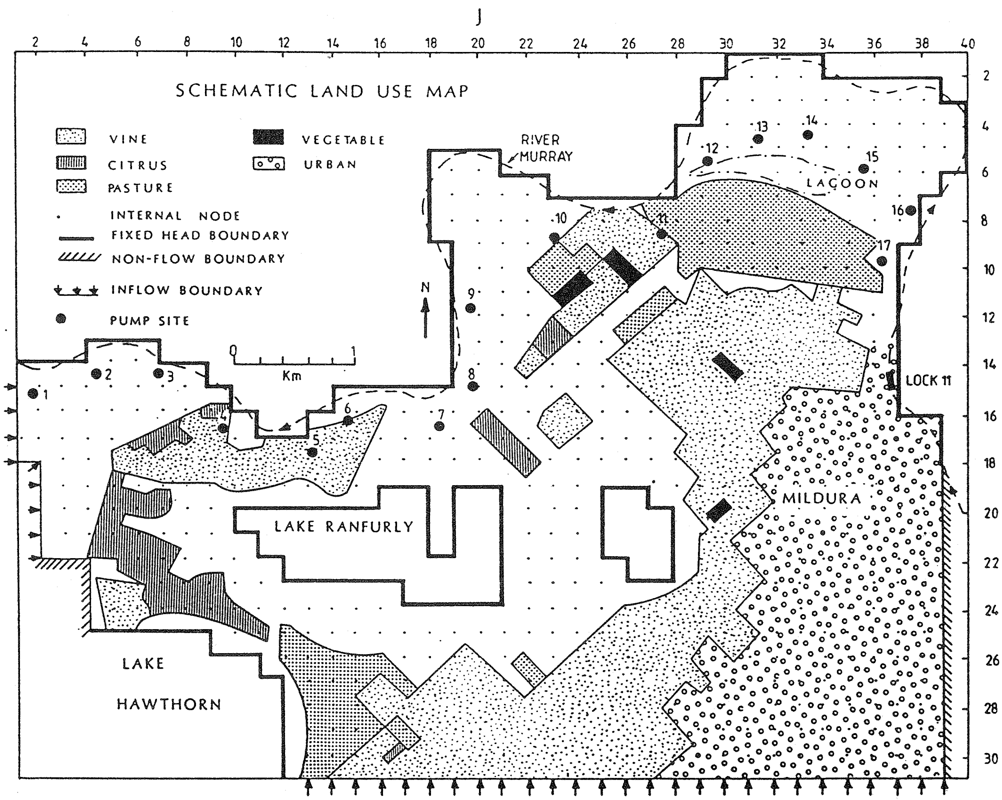

Figure 5: Land use map of Mildura study area, also showing location of interception pumps, discretisation of aquifer and boundary conditions adopted.

Other assumptions were also necessary to simplify the task. These were:

- The aquifer is isotropic, confined and two-dimensional.
- Aquifer salinity is temporally constant at river nodes (point estimates in space are available at two points in time three years apart).
- Groundwater level (piezometric) contours were hand-drawn by reference to the hydrogeologic data.
- Simple no-flow boundary conditions were adopted.

There were insufficient prior parameter estimates and observational data to warrant calibration of a model of soil infiltration. In its place a simple assumption was made that:

- Monthly accessions to the aquifer from rainfall and irrigation were a proportion of rainfall and irrigation applied.

Only two constants of proportionality, one for rainfall and one for irrigation, were calibrated for each land use zone.

The assumption that aquifer salinity is temporally constant at river nodes also allowed us to dispense with modelling solute transport throughout the aquifer. Since one major purpose was to simulate salt load to the river boundary, a (two- dimensional) model of groundwater flow (in a confined aquifer) with attendant assumptions about aquifer salinities at the river boundary was considered a useful simplification. The model used is therefore

$$\nabla \cdot T\nabla h = q + S\frac{\partial h}{\partial t} \qquad (6)$$

where T represents transmissivity, S storativity, h the groundwater levels and q source terms.

Since the purposes of our modelling (P1 and P2) are fixed, they cannot be narrowed further to obviate the need for a distributed parameter model. The A-axis characteristic value has been reduced to flow while the D-axis characteristic has been lowered to a value associated with two-dimensional modelling. The P-axis is fixed for simulation. Likewise, the R-axis characteristic value is demanding, requiring a time series, although the annotation on the characteristic M-axis, the media modelled, has been reduced considerably by lumping the model of infiltration through the root and unsaturated zones as one of simple proportionality of rainfall or irrigation applied. In addition, the I-axis, the intervals of spatial and temporal discretisation were aggregated. A monthly time step was considered necessary as it was almost the maximum desirable for testing the simulation performance of the model on historical data and the minimum interval at which much of the input data was available. Discretisation of the problem was by finite difference. A square mesh interval of 200 m was chosen because it was judged a compromise between being able to evaluate pump site options sensitively and the minimum distance that could be tolerated for interpolating hand drawn piezometric contours. Seven zones of constant transmissivity were assumed for the aquifer.

Clearly, there are many assumptions needed to achieve the above simplification of the modelling problem when it is not desirable to refine the modelling purpose further. The uncertainty or sensitivity of the model parameters and hence simulation results to these assumptions must be evaluated to assess the credibility of the results. To calibrate the parameters and to obtain a feel for this uncertainty, a technique known as generalised sensitivity analysis (GSA) was used. The technique was originally derived by Hornberger and Spear [12] to identify in a preliminary or exploratory manner, important parameters and processes in models of environmental flow and transport phenomena. We adopted GSA for the example here as a conceptually simple and flexible approach to the calibration of parameters and their uncertainty in a traditional model of the process of groundwater flow.

For a given mathematical model of a system, the essential steps in GSA are the following:

(a) Specify probability distributions for the parameters of the model.

(b) Impose acceptable model behaviour or performance in terms of constraints on objective functions.

(c) Perform Monte Carlo simulation runs, each run taking a random sample from the parameter distributions and driving the model to yield model behaviours.

(d) Classify each simulation run in terms of acceptable or unacceptable behaviour.

(e) Analyse statistical relationships between the parameters in both acceptable and unacceptable classes to obtain a sensitivity ranking and the covariation of parameters responsible for the acceptable model behaviour.

The application of this procedure was demonstrated for a steady state model of the system (S = 0 in equation 6) in Jakeman et al. [15]. The uncertainty of the model in terms of mean error of groundwater levels throughout the aquifer and salt load to the river was calculated. The variability in both quantities suggests the model is a useful tool to investigate the effects of groundwater interception options. For example, almost all the variability in salt load is contained within bounds about 10 per cent either side of the simulated mean. Ghassemi et al. [9] have demonstrated that this variability is about one-fifth the deterministic reduction in salt load simulated from improvements to practicable pump placements and rates.

Whether or not the model needs improvement requires further analysis since the variability above was assessed for the aquifer transmissivity parameters only. All boundary conditions, including accession parameters from rainfall and irrigation, were kept at fixed values. Sensitivity of simulations to these conditions is also required. On the one hand, this means that the salt load variability calculated already is the minimum that could be expected. On the other hand, it is quite probable that uncertainties in parameter estimates could be reduced further by performing generalised sensitivity analysis on a transient form of the model for which appropriate indirect observational data (i.e. groundwater levels) are available. In this way, the parameter space of acceptable solutions could be further constrained (by imposing that model behaviour conform to observations over the transient period) to reduce uncertainty.

This example illustrates that there are several potential advantages of using GSA for general model calibration. As indicated and referred to above, uncertainty estimates are a byproduct of the analysis. In addition, there is no need to use mathematical methods of calculus and algebra to derive an optimisation algorithm as the power of the computer is used to sample the parameter space for optima. Traditional algebraic approaches minimise an objective function, such as a least squares criterion, perhaps subject to bounds or smoothing constraints on parameter values. The GSA technique allows straightforward incorporation of prior knowledge and hypothesis testing in almost any form without significant addition to the level of computational complexity. The procedure is robust in the sense that numerical problems such as stability and convergence that are associated with the algebraic optimisation approach to the solution of inverse problems are avoided. In summary, the approach seems well suited to the practitioner without a strong mathematical or computational background. Assumptions can be tested in a direct way by specifying diffuse probability distributions for model parameters and fine-tuning these by imposing any behaviour criteria deemed important and calculating the parameter covariation which yields this behaviour. The approach can be built around forward simulation models of model behaviour, which are available as computer packages for many physical modelling problems. The main constraint to its use is that sufficient computer time and resources can be obtained to generate a large number of forward model runs.

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