'Blueprint' for the UP Modelling System for Large Scale Hydrology

John Ewen

Water Resource Systems Research Laboratory, University of Newcastle, Newcastle upon Tyne, UK NE1 7RU

Abstract

There are at least two needs to be met by the current research efforts on large scale hydrological modelling. The first is for practical conceptual land-surface hydrology schemes for use with existing operational climate and weather forecasting models, to replace the overly simple schemes often used in such models. The second is for models of large scale hydrology which are properly sensitive to changes in physical properties and inputs measured (or predicted) over a wide range of scales, from the point-scale upwards, yet are simple enough in structure to be coupled to climate and weather forecasting models. Such models of large scale hydrology are needed for studying the environmental impact of pollution and changes in climate and land-use, especially the impact on water resources. The UP system (name derived from Upscaled Physically-based) is an attempt to satisfy the second need. It uses a physically-based approach and has a simple structure, yet incorporates sufficient information on sub-grid behaviour to make it a useful tool for the study of environmental impacts over a wide range of scales. The system uses a new approach to large scale modelling, giving physically-based predictions of hourly flows, storages, saturated areas, etc., for regions covering hundreds of thousands of square kilometres. The basic component of the system is the UP element. This has seven water storage compartments (one each for the snowpack, vegetation canopy, surface water, root zone, unsaturated percolation, interflow and groundwater) and allows all the main processes of the terrestrial phase of the hydrological cycle to be represented. A region is modelled as a collection of UP elements, linked by a river routing scheme. Each compartment represents a fixed zone within the area covered by the UP element, and each is related to a physical process such as groundwater flow. Most of the parameterizations for the compartments are in the form of look-up tables, linking the outputs from the compartments to state variables such as the current storage in the compartment. These parameterizations are, in the main, derived from results from physically-based, distributed models applied to the zones (e.g. a groundwater compartment is parameterized using a groundwater model). For large regions modelled using many UP elements, the UP parameters are regionalized using a classification scheme, thus reducing the overall effort spent in parameterization. The development of the UP system is a long-term project involving research into physically-based parameterization of large scale hydrology models, including the effects of sub-grid spatial variations. The first stage involved developing a 'blueprint' for the UP element, based on experience with physically-based, distributed river basin modelling and reviews of existing techniques and modelling approaches for large scale and linked atmosphere-hydrology modelling. This paper describes the UP element and the concepts and ideas behind the development of the UP system and, briefly, describes some of the research and development work currently in progress on UP and its parameterization.

Introduction

There is worldwide concern about the way human actions are altering global-scale environmental properties and processes and research on the global environment has been initiated in many countries and by many organisations. In the UK, for example, the Natural Environment Research Council sponsored the Terrestrial Initiative In Global Environmental Research (TIGER) (NERC, 1993), which contributed to the development of the UP system (the name derives from Upscaled Physically-based), and a UK national strategy for global environmental research has been published (IACGEC, 1996). One general goal of this strategy is 'the better representation and integration of processes occurring over a wide range of spatial . . . and temporal . . . scales', and one named concern is the availability and quality of water resources.

The link between the atmosphere and terrestrial

hydrology must be considered when assessing the impact of global change on water resources and design concepts for linked atmosphere-hydrology models at the macro-scale have been discussed (e.g. Vörösmarty et al., 1993). For atmospheric modelling, the main requirement of a linked hydrology model is that it gives the correct balance between sensible and latent heat exchange between the ground and atmosphere, so that the boundary fluxes for the atmosphere model are correct. In contrast, for hydrological modelling, the main interest is in the distribution of surface and subsurface water storages and flows. The UP system is designed both as a stand-alone hydrology model, giving distributions of surface and subsurface water storages and flows, and for linked atmosphere-hydrology modelling, for which it is being coupled to the United Kingdom Meteorological Office's Unified (forecasting and climate) Model. The emphasis in the development of the system is on the link between the point-scale and grid-scale, and the representation of the physical processes known to be important in temperate climates, such as soilwater storage and flow, groundwater storage and flow, interflow, surface runoff, canopy storage, transpiration and evaporation.

The development of the UP system is a long-term project (not aimed at meeting immediate needs for improved land-surface hydrology schemes for operational climate and weather forecasting models), involving research into physically-based parameterization of large scale hydrology models, including the effects of sub-grid spatial variations. The aim is to develop a large scale modelling system which is properly sensitive to changes in physical properties and inputs measured (or predicted) over a wide range of scales, from the point scale upwards, yet is simple enough in structure to be coupled to climate and weather forecasting models. It is intended that this system will be used to study the environmental impact of pollution and changes in climate and land use, especially the impact on water resources.

The first stage of work involved developing a 'blueprint' for the UP element, which lies at the heart of the UP system, starting from a consideration of existing physically-based, distributed river basin models and existing large scale and linked atmosphere-hydrology models. This paper describes the UP element and the concepts and ideas behind the development of the UP system, and some of the research and development work currently in progress on UP and its parameterization.

Existing models, sub-grid variability and the physically-based approach

In the early days of numerical weather prediction (Richardson, 1922) surface and subsurface water storage and flow were seen as important, and detailed physically-

based modelling was proposed. In current atmospheric models, however, it is quite usual for the modelling of hydrology to be trivial, with less than 1% of the model run time spent on calculations of the hydrology. Recent reports on the representation of runoff and soil moisture storage in the land-surface schemes of current operational GCMs (Polcher et al., 1996) show that some progress has been made from the previous generation of schemes, in which the 'Budyko bucket' (Manabe et al., 1965) was ubiquitous. However, from a hydrological point of view (and when considered alongside the very detailed schemes for, say, radiation exchange used in the GCMs), the new representations of runoff and soil moisture storage are still very basic. At the other extreme, some of the newer land-surface schemes being developed for smaller-scale atmospheric modelling describe vertical exchanges in great detail, but neglect sub-grid variations in storage and flow. Schemes based on the detailed modelling of momentum, heat and moisture transfer in the vegetation canopy, such as the BATS model of Dickinson et al. (1986) and the SiB model of Sellers et al. (1986), fall into this category.

In a large scale hydrology model, it is important to account for the effects of sub-grid variability in physical parameters and water storages, as well as for the effects of sub-grid lateral flows. This involves moving up in scale (Fig. 1), in the sense that some sub-grid information is retained in moving to the grid scale. Moving down in scale can also be important. For example, the analysis of the impact of an event modelled at the large scale (an extreme storm, say) might require that the response at the sub-grid scale is inferred from the simulated response at the grid scale. Ideally, therefore, moving both up and down in scale should be possible within a single modelling system for large scale hydrology.

In the nomenclature of Sivapalan (1993), the general problem in accounting for sub-grid variability involves finding vector G, which represents grid-scale hydrologi-
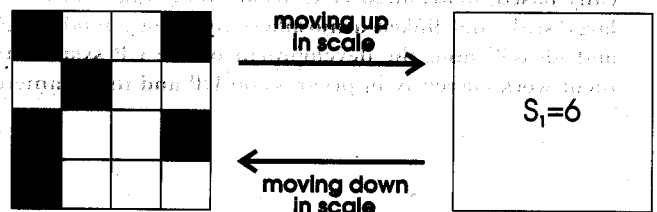

Fig. 1 Simple illustrative example of moving up and down in scale. Moving up in scale, the fact that six sub-grid blocks are saturated (indicated by shading) might be represented at the grid scale by the state variable S_1 taking the value 6. For moving down in scale, given that $S_1 = 6$ (this could be a simulation result from grid-scale modelling in which the sub-grid blocks are not explicitly represented), the ideal involves knowing that this value indicates that an area equal to six sub-grid blocks is saturated, and being able to determine the locations of the saturated blocks.

cal responses, so the output vector O at the grid-scale can be found:

$$O(X, T) = G\{S(X, T):\Theta(X, T):I(X, T)\} \qquad (1)$$

where X and T are the spatial coordinates and time, respectively, and S, Θ and I are the vectors of state variables, parameters and inputs, respectively. The corresponding equation at the point-scale is:

$$o(x, t) = g\{s(x, t):\theta(x, t):i(x, t)\}. \qquad (2)$$

An indirect approach to the problem of finding G involves the concept of parameter scaling [i.e. $\theta(x,t)\rightarrow\Theta(X,T)$]. This has been discussed at length in the literature (e.g. King, 1991; Levin, 1992; Rastetter *et al.*, 1992; Chen *et al.*, 1993; Sivapalan, 1993; Beven, 1995; Blöschl and Sivapalan, 1995; Wen and Gómez-Hernández, 1996). The main conclusion from this discussion is that procedures for scaling parameters (i.e. to get 'effective' parameters) are not generally practical unless the system is linear so that the scaled parameters are simply weighted averages of the point-scale values. A more direct and promising approach is to develop (reduced) schemes based on:

$$O(T) = G\{S(T):\Theta(T)\}; \ T=t \qquad (3)$$

$$o(x) = g\{s(x):\theta(x):i\}. \qquad (4)$$

For example, if S has one component, the grid-scale storage, and O has one component, the grid-scale runoff, Equation 3 is simply a storage-runoff equation. Two types of such schemes have been described in the literature. Schemes of the first type are based on spatial distribution functions, such as the schemes of Dümenil and Todini (1992) and Wood *et al.* (1992), both of which are based on the Xinanjiang water balance model of Zhao (1980), and the scheme used by Johnson *et al.* (1993) which is based on the probability distribution function model of Entekhabi and Eagleson (1989). For these schemes, the grid-scale behaviour depends only on spatial distribution functions of point-scale properties (the point-scale soilwater storage capacity in the case of Xinanjiang-based schemes), so information on the spatial patterns of the point-scale state variable s and point-scale parameters θ is not used in defining G. The runoff-production part of the equation for G in Xinanjiang-based schemes was developed by Zhao (1980). It is an empirical equation with two parameters and, in operational land-surface schemes, these parameters are calibrated against measured storage-runoff data, which means that no information whatsoever on s and θ are used in defining G.

Schemes of the second type are typified by the patch scheme of Beven (1995), which is based on the TOP-MODEL approach of Beven and Kirkby (1979), which does not need an equation to be specified for G; rather a set of (O,S) vector pairs can be found and G represented by charts or look-up tables. The scheme is based on Darcy flow driven by topographic gradients defined from a digital elevation model (DEM), and, effectively, involves working with sets of steady two-dimensional (2D) flow fields, each field being consistent with a given steady infiltration rate (and consistent with Darcy's law, the DEM, and simple assumptions about the DEM-pixel-scale soil hydraulic conductivity). One (O,S) pair is determined from each field, by summing the discharge, saturated area, storage, etc., over the pixels.

For TOPMODEL-based schemes, it is usual for the O vector to have two components, discharge and saturated area, and for runoff production to be simulated as the result of both water discharge from the subsurface and direct runoff of rain falling on the saturated area. For schemes of this type, there is, implicitly, lateral interaction within the sub-grid area and the patterns of both s (storage) and θ (slope and conductivity) are used in defining G. Sivapalan (1993) showed that the TOP-MODEL-based approach can be used both to obtain G and to distribute soil moisture in the sub-grid area [i.e. to move down in scale from S(T) to s(x,t)].

TOPMODEL-based schemes can be seen to have a physical basis, since they use Darcy's law and small-scale hydraulic conductivities. In theory, models which are parameterized using physical properties such as hydraulic conductivity are more suitable for studying the effect of changes in land use, climate, etc., than conceptual models parameterized by calibrating their output against field observations. The consequences of measured or expected changes in physical properties can be mirrored by changing the parameters in the model, and the impact of the changes can be assessed by running the model with its old and then its new parameters. At the river-basin scale, there has been nearly 30-years of development of a distributed physically-based approach to modelling, starting with the model 'blueprint' of Freeze and Harlan (1969). One of the main modelling systems is the Système Hydrologique Européen, SHE (Abbott *et al.*, 1986ab). This is a three-dimensional model, based on finite-difference solutions of the differential equations describing the surface and subsurface flows in a basin, and the main parameters are the point-scale physical properties of the vegetation, ground surface, river channels and subsurface porous media. It has been updated to allow for 3D variably-saturated subsurface flow, and extended to model the transport of sediment and solute (Ewen, 1995; Ewen *et al.*, in preparation). At larger scales, physically-based modelling has not progressed as far as at the river-basin scale, but outline concepts have been developed (e.g. Vörösmarty *et al.*, 1993).

There has been much debate over several years about whether physically-based models are in practice more

useful in hydrological modelling than conceptual models (Abbott *et al.*, 1986a; Beven, 1989; Bathurst and O'Connell, 1992; Blöschl and Sivapalan, 1995; Grayson *et al.*, 1992 and 1994; Loague, 1990; Smith *et al.*, 1994; and O'Connell and Todini, 1996). Recently a scientific approach involving 'blind' testing and uncertainty bounds has been developed to test some of the claims made for physically-based river basin models (Ewen and Parkin, 1996; Parkin *et al.*, 1996). It is clearly far more difficult to parameterize a hydrological model in a way that is consistent with both grid-scale storage and flow and point-scale physical properties than it is simply to make it consistent only with the grid-scale storage and flow. There is, therefore, a more substantial cost in time and effort in searching for and using 'physically-based' parameterizations (such as are used in UP) than is necessary in calibrating a Xinanjiang-based scheme, for example.

Physically-based, distributed modelling usually requires extensive sets of data on the physical properties of the catchment, sets which are often not readily available. This has led some to argue that data availability is a fundamental limitation on physically-based, distributed modelling, rendering it impractical. Others take the view that physically-based, distributed modelling holds much promise, has already achieved much success, and should continue to be investigated and tested thoroughly.

Design Requirements

The first stage in the design of the UP system is to draw up a list of requirements to be met.

Requirement 1. The system should be physically based, and sensitive to changes in sub-grid physical properties.

Requirement 2. It must be possible within the system to move both up and down in scale, to ensure the system has a powerful capability for use in impact assessment.

Requirement 3. The approach used should be applicable at all scales above the plot scale. It is an attractive idea that there are natural scales in hydrology, as models could then readily be built at these scales. However, the idea of natural scales appears to have limited usefulness, especially where there are systematic multi-scale variations in geology and land cover.

The river basin is a natural unit and is an obvious choice whenever mass balance calculations are involved. For flexibility, therefore, the UP system should be applicable to regions discretised either by division into sub-basins or into grid-squares. (The terms grid and grid-square will be used hereafter, for convenience.)

Requirement 4. As well as the processes usually considered in hydrological soil-vegetation-atmosphere modelling, groundwater flows and large scale flows of surface water should be represented. These can have very significant effects on the water balance in an area, yet have been almost entirely neglected in large scale hydrological modelling.

Requirement 5. The timestep should be fixed at 1 hour. This is short enough for rainfall and flooding events to be simulated in some detail.

Requirement 6. The main purpose is to simulate the behaviour in all the grid-squares contained within the modelled region, so each grid-square must have state variables associated with it. The natural choice for the main state variables are the storages of water in the grid-square. The basic building blocks for modelling should therefore be input-storage-output conservation compartments (Fig. 2). This building block was chosen as it can be applied at any scale (it is equally useful for a 10 cm cube of soil, for a 5 km^2 river basin, or a 50 km $\times$ 50 km $\times$ 100 m deep block in a continental-scale model), and it also reflects the central importance of mass conservation in the system. Since the basic building blocks are conservation compartments, the main coupling between the compartments will be via inter-compartment transfers of water.
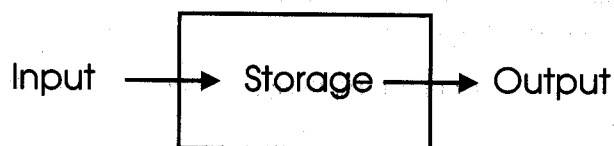

Input ⟶ Storage ⟶ Output

Fig. 2 *Schematic of an input-storage-output conservation compartment. The rate of change of storage is equal to the rate of input minus the rate of output.*

Input-output transfer functions are widely used in hydrology (e.g. *see* Shaw, 1988), and are a natural choice to describe some flows, such as surface water flow, so the use of transfer functions to parameterize compartments should be allowed. For use in the UP system, an input-output transfer function is simply a list giving the output (e.g. depth of discharge) during the 1st, 2nd, 3rd, etc., hours after an input of, say, 1mm of water. Using the function, the output for a given timeseries of input depths is calculated using superposition: for a given hour, the output is simply the sum of the contributions to output associated with the inputs which took place during the current and all previous hours. As output is calculated directly from input, a compartment parameterized using a transfer function need not have storage as a state variable. If the storage must be known for another purpose, however, it can readily be calculated using mass balance, as the rate of change of storage is simply the rate of input minus the rate of output.

Requirement 7. To make it possible to use existing techniques for physically-based, distributed modelling in

the parameterization of compartments, each compartment in a grid-square should be associated with a fixed zone within the grid-square, and be associated with a named physical process, such as groundwater flow. (It may be inevitable that there will be some overlap between zones, which has to be handled carefully to ensure mass conservation.) With this approach, inter-compartment transfers will be associated with named physical processes, such as groundwater recharge or exfiltration to the ground surface.

Requirement 8. To ensure the system runs quickly enough to make linked atmosphere-hydrology modelling practical, each grid-square should be represented by only a few compartments, and the state of each compartment should be described using only one or a few state variables. This also makes calibration and data assimilation practical, as would be required if UP were to be used in operational modelling.

Design

To meet the requirements above, the UP system comprises two parts: a fast-running simulation model and a set of physically-based, distributed parameterization models. The simulation model is the model of large scale hydrology and it is this which is coupled to an atmospheric model in linked atmosphere-hydrology modelling. In the simulation model, each grid-square is modelled as a single UP element (Fig. 3), and each UP element has seven water storage compartments: one each for the

snowpack, vegetation canopy, surface water, root zone, unsaturated percolation zone, interflow zone, and groundwater zone.

The basic concept behind the parameterization of UP elements is that for each compartment there is a physically-based, distributed parameterization model and the compartment is parameterized using results produced by running the parameterization model. In this way, the parameterization of the compartment has a physical basis, and is sensitive to the point-scale property data used in the parameterization model. It is time consuming to parameterize UP elements, so when parameterizing UP for a large region modelled using many grid-squares, it is usual to regionalize some of the UP parameters. This works in the following way. A small subset of the region's grid-squares is chosen, each member of the subset being representative of a different type of area within the modelled region, and the UP elements for these are parameterized using the parameterization models. Those grid-squares not included in the subset are then parameterized based on the parameterizations for the grid-squares in the subset, using a classification system, within a GIS.

The seven compartments were chosen to represent hydrologically distinct zones (as distinct, at least, as is practical if the total number of compartments is limited to seven). The choices made for the seven zones should appear natural to many with experience in hydrological modelling, since they are often used in modelling, mainly because they each have a clear, distinct role in runoff
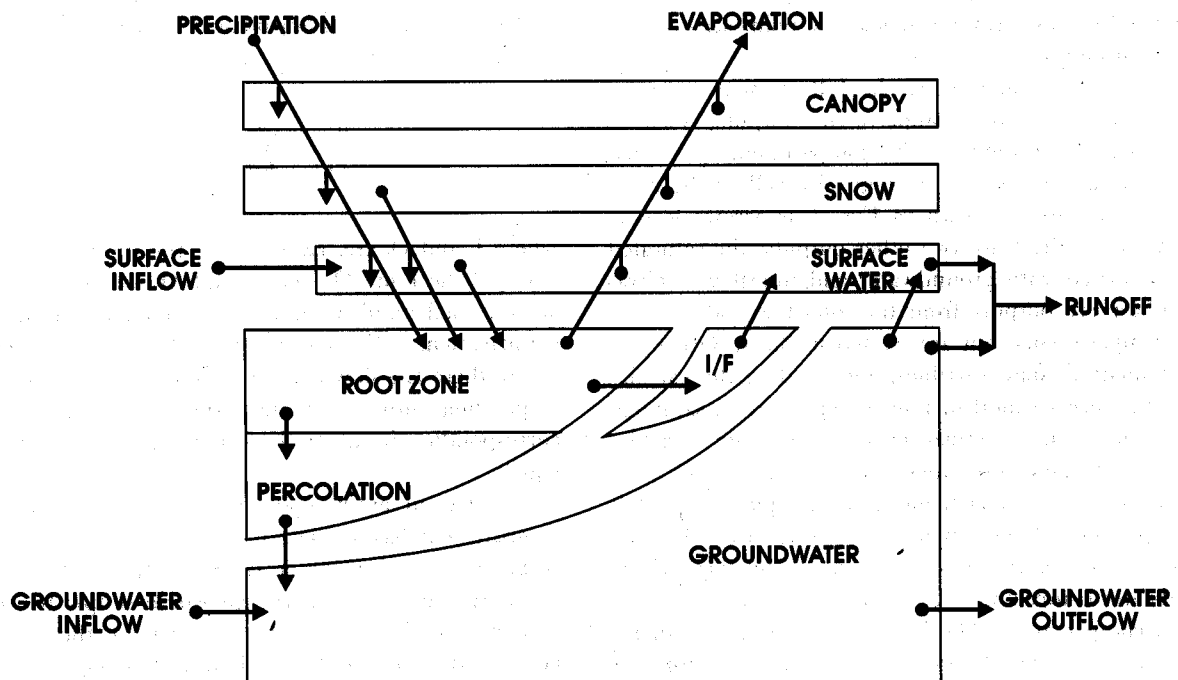

Fig. 3 *'Blueprint' for an UP element, showing the seven compartments and the flows between them (I/F denotes interflow). The canopy can have up to three vegetation types. There is canopy throughfall, but not canopy drainage. Evaporation is calculated using a Penman-Monteith approach. Drainage from interflow to groundwater is not allowed.*

generation and a different timescale for response. All the flows between the compartments can be given recognizable names, such as recharge from the percolation compartment to the groundwater compartment, and the exfiltration of groundwater to surface water. The direct output from the groundwater compartment to runoff (at the top right hand side of the groundwater compartment in the UP 'blueprint') is direct groundwater discharge to the main channel network. This main channel network receives all the runoff from all the UP elements, and routes it out of the modelled region using a scheme based on Naden (1992), with network-width-functions to account for the spatial distribution and dendritic nature of the main channel network. The groundwater inflow and outflow shown in the UP 'blueprint' are usually both zero, and are non-zero only when there are very strong regional flows of groundwater, requiring flow between grid-squares to be simulated. The surface inflow shown in the 'blueprint' is zero except when there is major flooding, in which case the inflowing water is flood water from the main channel.

The approach taken in parameterizing UP elements is an extension of the approaches discussed earlier. In general, for each compartment, it can be represented by:

$$O(T) = G\{S(T){:}\Theta\{S(T){:}\Theta(T){:}I(T)\}I(T)\}; \quad T=t \quad (5)$$

$$o(x, t) = g\{s(x, t){:}\theta(x){:}i(x, t)\}. \quad (6)$$

The main differences from the approaches discussed earlier are that the vector of state variables, S, sometimes has more than one component, and the parameterizations can depend on non-steady states at the point-scale: i.e. o, s and i can be time dependent.

The aim in parameterizing the UP element compartments is to relate the compartment outputs, such as groundwater exfiltration, to the compartment state variables, such as groundwater storage. As well as the compartment discharges, shown in Fig. 3 as arrows leaving compartments, there are two other outputs: the saturated areas associated with groundwater and interflow exfiltration. These are outputs from the interflow and groundwater compartments, but are treated in the surface water compartment as state variables, and used in the calculation of the direct runoff of rain falling on areas saturated by exfiltration. In a similar fashion, the state variables simulated for one compartment can be used as state variables in another compartment. For example, as a result of the influence of the phreatic surface level on the plan area and depth of the percolation zone, the state of the groundwater compartment can affect the state of the percolation compartment. The groundwater storage is therefore sometimes used as an additional state variable for the percolation compartment, in which case the parameterization of the percolation compartment is based on both the storage in the percolation compartment and the storage in the groundwater compartment.

The surface water, interflow and groundwater compartments are parameterized using parameterization models which simulate lateral sub-grid flow on a sub-grid computational mesh, often based on a DEM (typically with pixels in the range 100 m–1 km in size). The other compartments are parameterized using parameterization models which simulate vertical flow on sub-grid patches. The parameterization procedure is the same in all cases, however. The first step involves creating quasi-steady or transient data sets by running the parameterization models using forcing data, often the actual forcing data to be used in the UP simulation. Grid scale input-storage-output data sets are then created by adding up the inputs, storages and outputs across the sub-grid mesh or patches. The next step involves using the grid-scale data to create look-up tables or input-output transfer functions for the UP element compartment. For example, if one of the grid-scale outputs is strongly related to grid-scale storage, a look-up table would be created which simply lists storage and output pairs [e.g. pairs such as (30 mm, 0.213 mm hr^{-1})] covering the full range of storage likely to be met during an UP simulation. This table would form the whole (if there is only one output) or part (if there is more than one output) of the parameterization for the UP element compartment, and would be loaded into the UP system and used in the UP simulations.

The governing equations for an UP element are a coupled set of ordinary differential equations (ODEs). The main equation for each compartment is usually the water mass balance equation, which, as noted earlier, can be applied even if the compartment is parameterized using an input-output transfer function:

$$\frac{dS_i}{dT} = \sum_{i=1}^{M} I_i - \sum_{j=1}^{N} O_j \quad (7)$$

where I_i and O_j are, respectively, the ith and jth components of the I and O vectors, and M and N, respectively, are the total numbers of water inputs and outputs to the compartment. To ensure overall mass conservation, where there is a flow between two compartments the corresponding output from the losing compartment and the corresponding input to the gaining compartment are set equal.

To give an example of the use of Equation 7, if a compartment has a single input and a single output and is parameterized using a storage-output look-up table, the storage in the compartment would simply be updated hour-by-hour by an amount equal to the difference between the input and output, where the output is calculated from the storage using linear interpolation between the data pairs in the look-up table.

SIZE OF GRID-SQUARES

The length scales for the grid-squares will depend on the application, but the basic scale is (nominally) 10 km. This is large enough so substantial regions can be modelled, yet small enough so the representation of the sub-grid distribution of rainfall can be simple (usually assumed uniform at this scale). In practice any grid size can be used in a simulation, and the system has been designed so that any geometry of 'grid' can be used, thus making it is possible to model a region as a collection of contiguous sub-basins, as is often convenient in hydrological modelling.

The idea that the basic scale of the UP system is 10 km is little more than a handy shorthand, to give an indication of the typical grid scale appropriate for the system. In a similar manner, a grid scale of 50 km would be appropriate if the UP system is to be run coupled to a regional climate model. At this scale, an algorithm is required for the sub-grid redistribution (disaggregation) of the grid-average rainfall predicted by the climate model (the development of such an algorithm is not a trivial task), but important sub-regions within the modelled region can be modelled using a nested 10 km grid, giving better spatial descriptions of the behaviour in the sub-regions.

At the 10 km scale and above, it is usual for the direct, land-based interaction between the runoff conditions at any two given points on a river system to be very weak, so interaction between UP elements can usually be neglected in the main channel routing scheme. There is interaction, however, when a substantial flood plain in one grid-square is flooded by river runoff from upstream grid-squares, in which case the parameterization of the UP element for the flooded grid-square must take account of the flooding, and the routing scheme must be modified.

Parameterization models

To parameterize the surface flow compartment for a range of saturation and flow conditions, a set of grid-scale transfer functions is created on a GIS. The transfer functions are generated by releasing packets of water (separate packets, giving separate transfer functions, for direct rainwater runoff, interflow exfiltration runoff and groundwater exfiltration runoff) and tracking them through the GIS to find the time each packet takes to reach the main channel, which marks the hand-over point for transferring sub-grid runoff to the main channel routing scheme.

The interflow compartment is parameterized using a method closely based on TOPMODEL. Some complications arise in handling the interaction between the interflow compartment and the other compartments. For example, both interflow and groundwater cause surface saturation and runoff, so the interflow and groundwater compartments must be treated in a consistent fashion. The greatest problem in parameterizing the interflow compartment, however, as yet unsolved, is to develop a method for determining which part of the sub-grid area is associated with interflow, as this affects the partitioning of the discharge from the root zone into the percolation and interflow compartments.

Analytical transfer functions and 2D Boussinesq and 3D variable-saturated finite-difference models have been used to parameterize the groundwater compartment. The main problem faced in modelling groundwater is lack of data on the hydrogeological structure and physical properties of the porous media. Groundwater and geology maps do exist for some areas, but even in 'well mapped' areas the information tends to be sparse and approximate. Despite this problem, research has been undertaken into the parameterization of the groundwater compartment to see what progress can be made from a physically-based starting point.

One of the reasons for using a parameterization method based on physically-based, distributed modelling is that the parameterization models can be used to move down in scale, for use in the assessment of impact. To give an example of the use of such an approach, in recent experiments the subsurface in a small river basin was modelled using a 3D physically-based variably-saturated parameterization model, and UP compartments were parameterized for groundwater flow, interflow and unsaturated flow. During the parameterization process, a set of 3D velocity fields was derived from the results from the 3D model (run for 30 years, the longest time practical). This was done in such a way that each field in the set was associated with a different set of values for the UP state variables. A two hundred and fifty year UP simulation was then run for water storage and flow (in a few minutes of computer processing time) and a time-series of 3D velocity fields created by picking a series of fields from the set, based on the simulated UP state variables. This timeseries of 3D velocity fields was then used in impact studies involving the detailed study of the long-term transport of solute.

The percolation compartment is an example of a compartment with no lateral sub-grid flow, parameterized using a model of vertical flow. Where the water-table is deep, there can be considerable storage in the unsaturated region lying below the root zone, and the water residence times in the zone can be quite long. In most cases, the main direction for flow in this zone is vertically down and, if the primary flow is matrix flow rather than macropore flow, the point-scale behaviour can be described by the 1D Richards' equation (Klute, 1952). For convenience, this is presented here in a mixed form in terms of both moisture content, w, and matric potential, ψ:

$$\frac{\partial w}{\partial t} = \frac{\partial}{\partial z}\left(K\frac{\partial \psi}{\partial z} + K\right) \qquad (8)$$

where z is the elevation and K the unsaturated hydraulic conductivity.

Before a numerical solution can be found for Equation 8, the hydraulic property functions $\psi(w,z)$ and $K(w,z)$ must be known, and initial and boundary conditions specified. In research into the development of a technique for parameterizing the percolation component of UP elements, Pimentel da Silva (1997) used an implicit finite-difference solution for Equation 8, a no-flow initial condition, a fixed water-table elevation, and a time-varying infiltration rate. She found that the output (i.e. the discharge to the water-table) can, in general, in layered soils, be approximated by $O(T)=\alpha S^{T-\beta}$, where α and β can readily be calibrated against the numerical results, and $S^{T-\beta}$ indicates the total storage in the zone at time $T-\beta$ (so β is a time delay).

The parameterization procedure developed by Pimentel da Silva (1997) involves approximating Equation 8 using a linear advection-dispersion equation which has two parameters, and determining these two parameters directly (i.e. using analytic techniques, not involving numerical simulation) from $\psi(w,z)$ and $K(w,z)$. Since the approximate equation is linear, the relationship between input and output for the zone is given by a transfer function, and the effects of the spatial distribution of the hydraulic property functions and the depth to the water-table can be accounted for by superposition of transfer functions. To parameterize a grid-square, the grid-square is divided into patches, a transfer function is created for each patch, and superposition is used to obtain a single transfer function for the grid-square. This single transfer function can be used directly as the parameterization for the grid-square's percolation compartment. However, if a fast-running scheme is required, the transfer function can be used to calibrate grid-scale values for α and β, and the simple delay function can then be used to parameterize the percolation compartment as an input-storage-output conservation compartment. In grid-squares where the water-table depth varies greatly with time, more than one (α,β) pair can be used. For such a case, the storage in the groundwater compartment is used as a second state variable for the percolation compartment, and the choice of which (α,β) pair to use at a given time is based on the current value of this state variable.

Hysteresis and second state variables

The aim in parameterizing an UP element compartment is to create a compartment model which behaves in a way consistent with the physically-based, distributed parameterization model of that compartment. This means that the grid-scale input-storage-output data set created using the parameterization model must be consistent with the parameterization model, and the main features of that data set must be well represented in the look-up tables or transfer functions which are derived from it. Many hydrological systems exhibit hysteresis at all scales, from the point scale upwards, and one challenge in parameterization is to represent this hysteresis. At the point scale, hysteresis in storage-flow behaviour results when the point-scale flow is not a single-valued function of point-scale storage. This in turn results in the grid-scale storage not being adequate as a single state variable controlling grid-scale discharge. To give an example, Fig. 4 shows hysteresis in the storage-discharge curve of the infiltration-pulse response for the top 50 cm (the root zone) of a 1D vertical homogeneous unsaturated soil column. The infiltration rate is initially 1 mm hr^{-1}. It rises to 9 mm hr^{-1} and stays at this level until steady flow is achieved, then falls back to 1 mm hr^{-1}. The discharge in this case is the loss of water through the base of the zone. The hysteresis is associated solely with the dynamics of the point-scale storage-discharge relationships, so should not be confused with capillary hysteresis (Jaynes, 1985) or the hysteretic effect associated with upscaling heterogeneous fields of parameters (Mantoglou and Gelhar, 1987). A general parameterization involving a single quasi-steady storage-discharge curve (and hence, one state variable, namely, storage) can readily be created for the zone, using an analytic solution for the steady distribution of moisture content under steady infiltration. Clearly, however, this will not be adequate to capture the hysteretic response of the zone.

For similar reasons, if a TOPMODEL-based approach is used to parameterize a groundwater compartment [e.g. using a characteristic shape of the water table to define hydraulic gradients (see Quinn et al., 1991)] the parameterization will break down whenever the gradients in groundwater potential are strongly time-dependent, either between storms or between seasons of the year. The need to model hysteresis in groundwater behaviour can be seen in Fig. 5. This is a plot of instantaneous data from a 3D groundwater model, run for the parameterization of a groundwater compartment. Each data point on the figure represents a storage-discharge pair, each giving the total storage in the groundwater zone and the total rate of discharge from the zone to the ground surface and surface waters (the totals were calculated from 3D fields of moisture content and flow velocity). It can be seen that the behaviour of the groundwater system is complex, and there is clear evidence of annual hysteresis in the storage-discharge relationship.

It has been known for a long time that simple storage-discharge curves are not adequate to represent the responses of hydrological systems, and a great deal of effort has been expended in parameterizing, say, rainfall-runoff models based on field data (O'Connell, 1991).
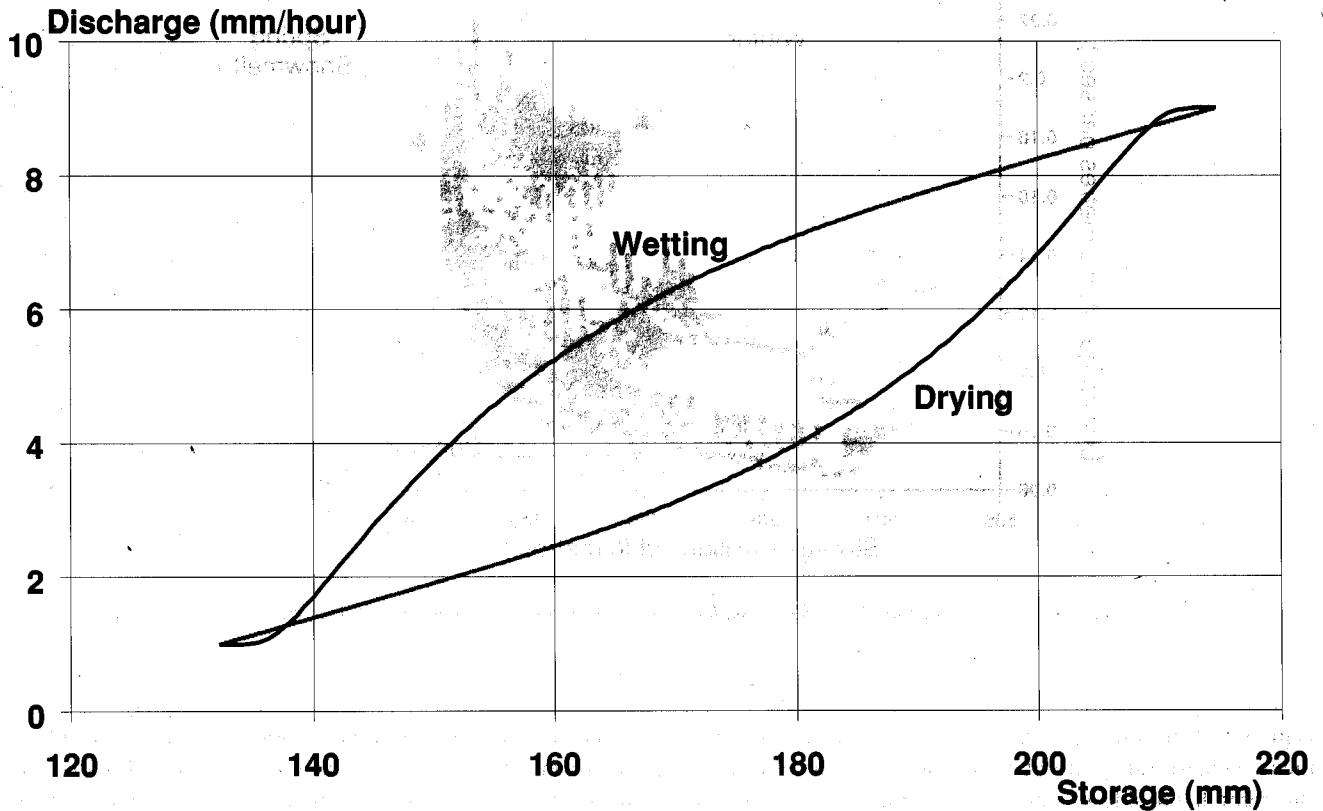
Fig. 4 *At-a-point storage–discharge hysteresis for a root zone, calculated using the analytic 1D Richards' equation solution of Srivastava and Yeh (1991). The water table is at 2 m, the soil is homogeneous with a saturated hydraulic conductivity of 1 cm hr^{-1} and a porosity of 0.45, and the root zone is 50 cm thick.*

There are at least two approaches to improving on single storage–discharge curves, both involving the introduction of further state variables. The first approach is partitioning, where the compartment is broken into two or more sub-compartments, and the storage in each sub-compartment is treated as an independent state variable. The second approach (not commonly attempted) is to leave the compartment unpartitioned and to introduce further state variables which apply to the compartment as a whole. This second approach is being studied in research aimed at improving the parameterizations of UP elements.

The usual way to represent hysteresis in UP parameterizations is to use a two dimensional look-up table, each value in the table corresponding to given values for the first and second state variables. This was the approach taken in successfully parameterizing a groundwater compartment using the grid-scale storage–output data in Fig. 5. The second state variable in this case was time-of-year. Five values of storage and ten values of time-of-year were used in the look-up table, so the table size was five by ten. To capture the effect of annual hysteresis, the table value for a given storage is higher for a time-of-year falling during autumn, say, than for a time-of-year falling during summer.

One new type of state variable being studied, so far with mixed success, is age (i.e. a variable associated with how long the water has been in the compartment). A governing differential equation for the age of the water in any input-storage-output compartment can be written down once assumptions have been made about the mixing behaviour of age. For example, if it is assumed that age mixes fully within a compartment, a conservation equation for the product of storage and age is:

$$\frac{d(S_1 S_2)}{dT} = S_1 - O_1 S_2 \qquad (9)$$

where S_1 is the compartment storage, S_2 the age of the water in the compartment, and O_1 the total rate of output from the compartment. For conservation of mass, if the total rate of input of water is I_1, then $dS_1/dT = I_1 - O_1$ and Equation 9 can be rearranged to:

$$\frac{dS_2}{dT} = 1 - S_2 I_1 / S_1 \qquad (10)$$

Three assumptions are implicit in Equations 9 and 10. First, all the water entering the compartment has zero age; this has the consequence that I_1 does not appear in
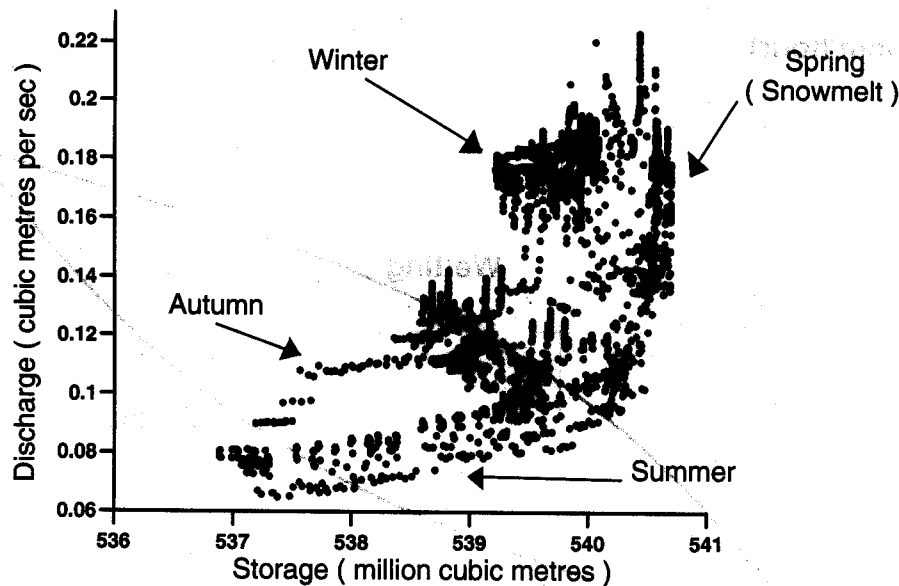
Fig. 5 *Grid-scale groundwater zone storage-discharge hysteresis for 3 years of groundwater flow in a 46 km² river basin.*

Equation 9. Second, the age of the water in the compartment increases at a rate of unity; hence the first term on the right hand side of equation 9, which is the term for aging, is the product of the total storage and the rate of aging. Third, the age of all outflowing water is S_2; hence the second term on the right hand side of Equation 9, which is the term representing losses of the product of storage and age, is the product of the rate of loss of storage, O_1, and the age of the lost material, S_2.

Basically, the role of a second state variable like age is to describe the effect of the spatial pattern of storage on the rate of discharge, and thus to improve the modelling of hysteretic and other types of non-linear compartments. Age is therefore, in some respects, a surrogate for a variable which describes the spatial pattern in a direct manner, and .works in the sense that old water tends to be distributed in a more 'equilibrium-like' fashion than new water. Age also allows the recent history of inputs to affect the outputs strongly, without the use of transfer functions, which are expensive in computer processing time if the output resulting from a given input lasts for more than a few hours.

For the few numerical experiments which have been run to date, it has been found that inverse age (which has been given the name youth) is often a good choice for a second variable. In one experiment, a 1D physically-based soil-vegetation-atmosphere model was used to create a one-year, 4-hourly, input-storage-output data set for a 50 cm root zone. The storage did not drop below 55 mm during the year, and all the calculations were performed on adjusted storage, where the adjustment involved subtracting 45 mm from actual storage.

The data set was divided into a 3200 hour calibration period and a 5560 hour validation period. Two calibrations were performed. A look-up table was calibrated for output (in mm per hour) against storage (in mm), giving the following look-up table pairs, each pair in the order storage then output rate: (40,-0.0128); (55,-0.0128); (75,0.0808); (100,1.43); (135,23.5). Note, the first two output rates are equal as a result of a restriction enforced during the calibration procedure to ensure that output increases monotonically with storage.

Fig. 6 shows the storage-output data for the calibration period. It can be seen that the output for a given storage can vary widely, between 0.2 and 0.9 mm hr⁻¹ at a storage of 40 mm, for example.

Fig. 7 shows cumulative input and output, and also the cumulative output derived using the look-up table to calculate output from storage. These curves are not monotonic since the input includes losses by evaporation (the soil is bare) and the output includes gains by capillary rise.

The second calibration was for youth versus storage (Fig. 8), giving storage $= 9.965 + 3794 \times$ youth. Youth is inverse age so has the units of hr⁻¹. For this calibration, age is calculated using Equation 10, with the values for I_1 and S_1, for input and storage, respectively, taken directly from the calibration data set. The initial youth was not calibrated, but calculated from the average input and storage for the calibration period. It can be seen in Fig. 8 that the calibrated equation based on youth gives a good estimate of storage. The quality of the estimate improves markedly with time, and is very good during the second half of the calibration period. This improvement is partly the result of the decay of the effect of the initial condition through time, but more to do with there
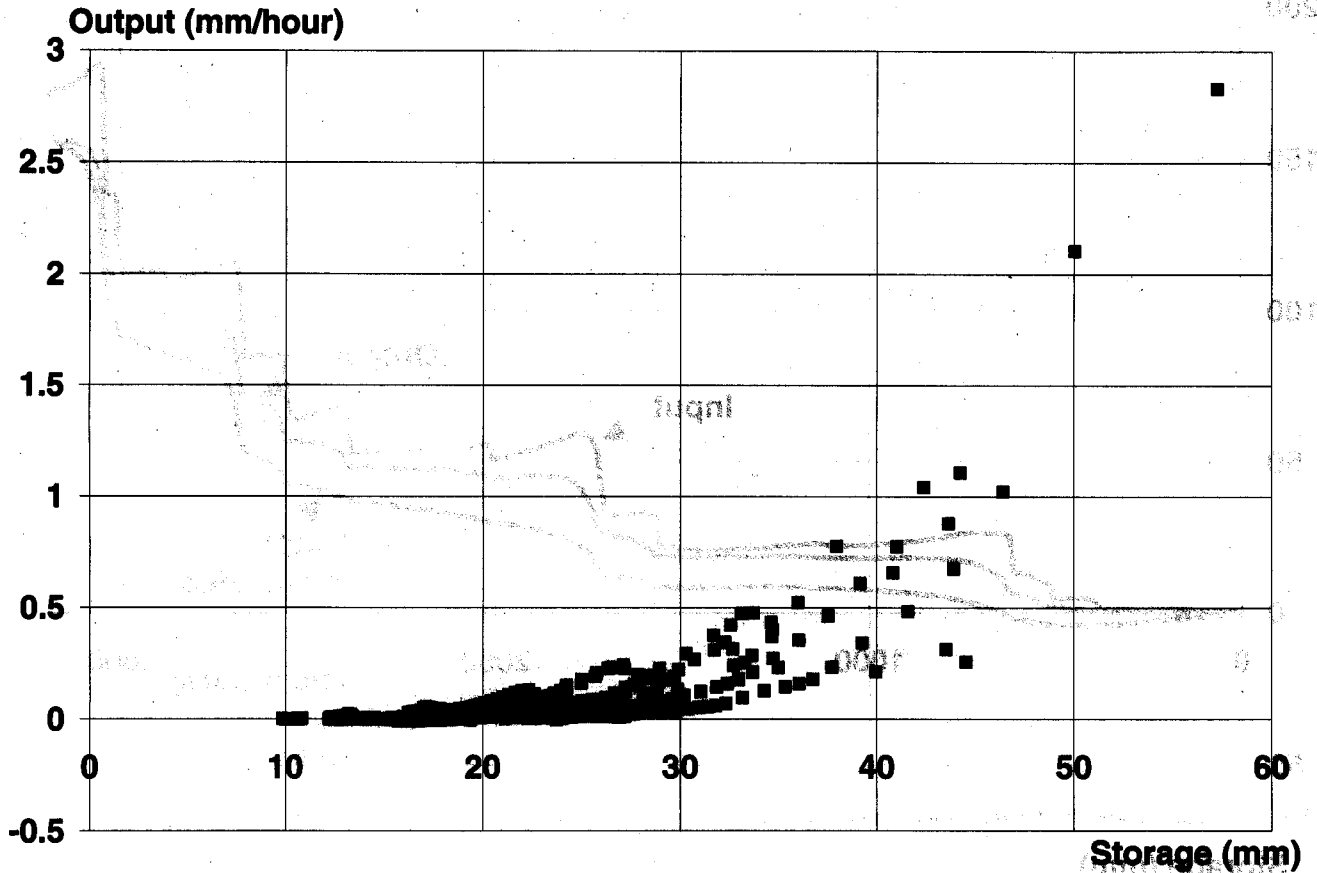
Output (mm/hour)

Storage (mm)

Fig. 6 *Output-storage plot for the root zone for the calibration period in the youth experiment. (Storage is given as adjusted storage; add 45 mm to get actual storage.)*

being more storms in the second half of the calibration period, adding more youth to the compartment and strengthening the link between input and output.

Two parameterizations were used to simulate the dynamics of the storage over the validation period (Fig. 9). The first involved the use of the look-up table for output, and gave an r.m.s. error fit to storage of 5.34 mm. For the second parameterization, the basic simulation using the look-up table is run exactly as it is for the first parameterization and calculates exactly the same values for storage. At each timestep, however, youth is updated based on this storage, using Equation 10. The predicted storage is then calculated from youth using the calibrated storage-youth equation. This approach, although a little unorthodox, is successful in improving the prediction of storage: the r.m.s. error is 3.38 mm, which is substantially lower than for the first parameterization. The storages predicted using both parameterizations are shown in Fig. 9.

The ultimate aim of the parameterization of the root zone is the prediction of output. For the second parameterization, the output is calculated from the input and the predicted storage, using mass balance. The r.m.s. error in the predicted output for the validation period is

0.297 mm hr^{-1}, compared to 0.433 mm hr^{-1} for the first parameterization.

Conclusions

There is a need for models of large scale hydrology which can be coupled to climate and weather forecasting models, yet which contain sufficient information on sub-grid scale behaviour to make them useful in studies of environmental impacts over a wide range of scales. The UP system is being developed to meet this need. It comprises two parts. The first part is a fast-running model of large scale hydrology, which models a region as a collection of UP elements. Each UP element represents a sub-basin or grid-square, and the elements are linked by a river routing scheme which collects the runoff from the elements and routes it out of the modelled region through the main channel network. The second part is a set of physically-based, distributed models, the results from which are used to parameterize the UP elements.

Each UP element has seven water storage compartments (one each for the snowpack, vegetation canopy, surface water, root zone, unsaturated percolation,
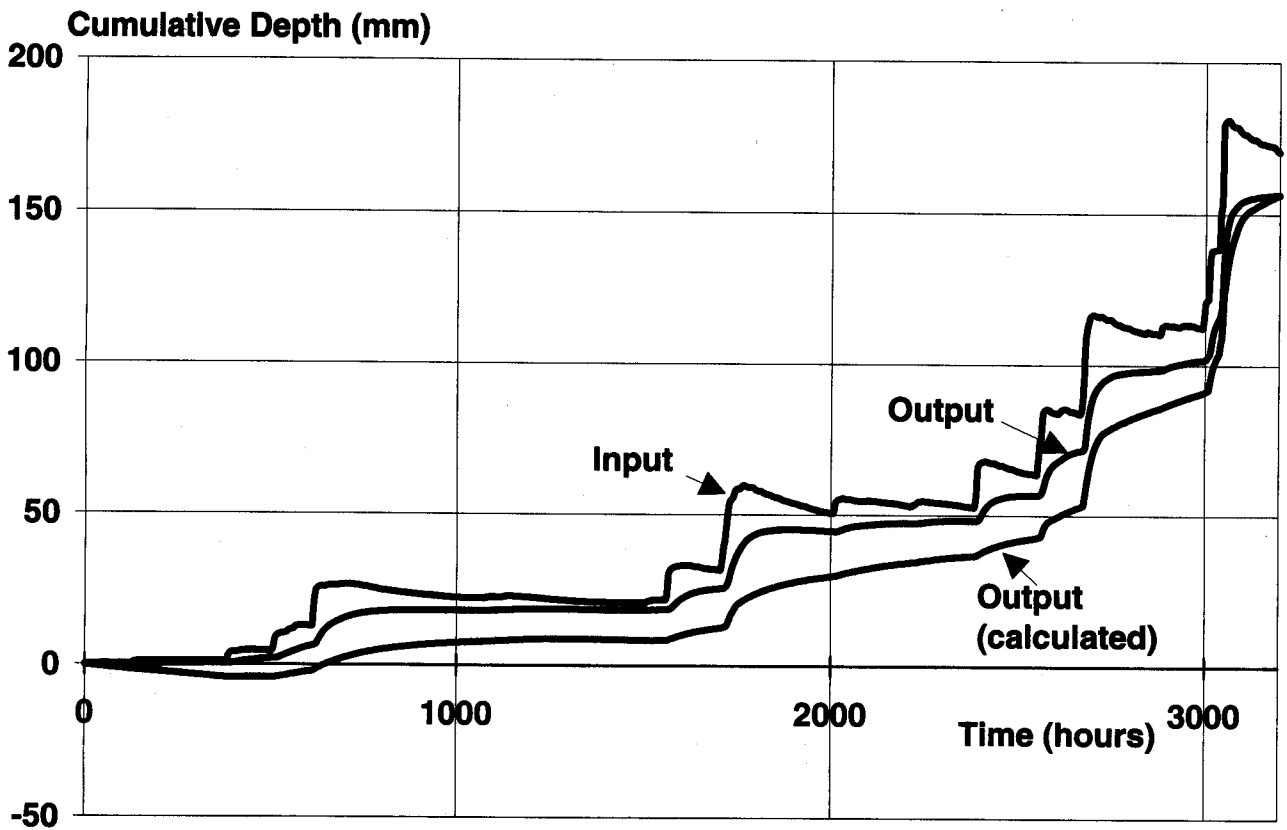
Cumulative Depth (mm)

Fig. 7 *Cumulative input and output depths for the root zone during the calibration period in the youth experiment.*
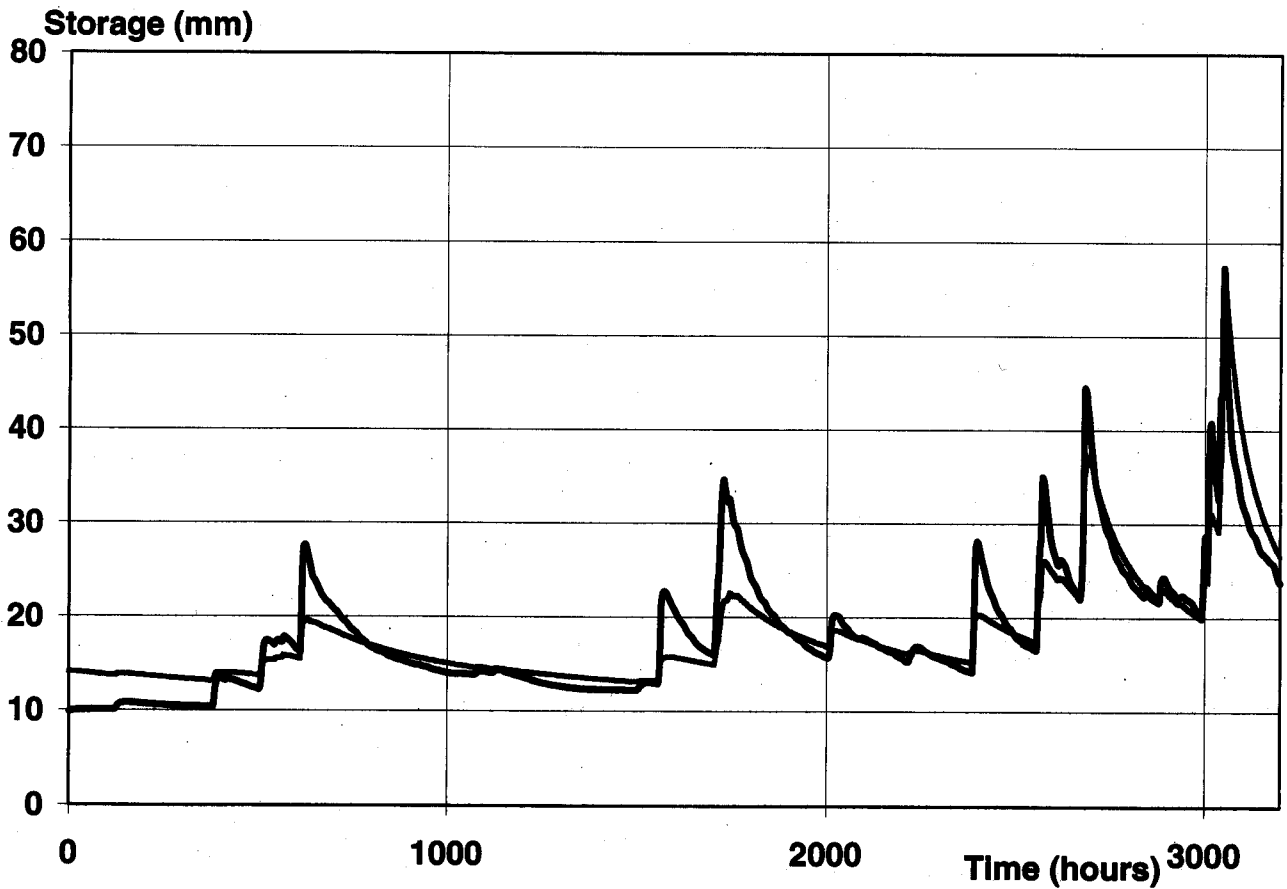
Storage (mm)

Fig. 8 *Storage in the root zone during the calibration period in the youth experiment. The light line is for the calibrated youth equation. (Storage is given as adjusted storage; add 45 mm to get actual storage.*
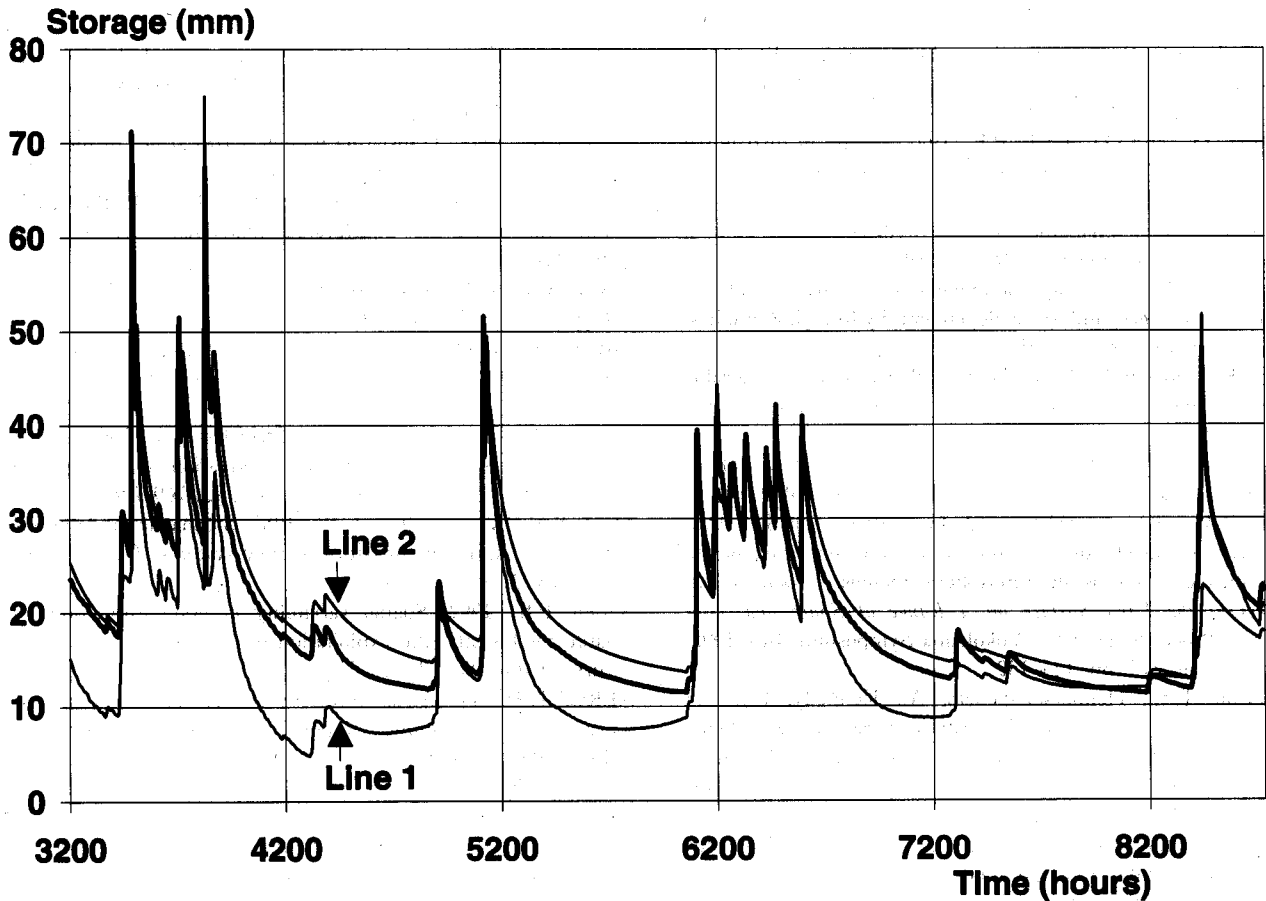
Fig. 9 *Storage in the root zone during the validation period in the youth experiment. Line 1 uses only the storage-output look-up table. Line 2 uses the storage-output look-up table and youth. (Storage is given as adjusted storage; add 45 mm to get actual storage.)*

interflow and groundwater), and allows all the main processes of the terrestrial phase of the hydrological cycle to be represented. Each compartment represents a fixed zone within the area covered by the UP element, and each is related to a physical process such as groundwater flow. Most of the parameterizations for the compartments are in the form of look-up tables, linking the outputs from the compartments to state variables such as the current storage in the compartment. These parameterizations are, in the main, derived from results from physically-based, distributed models applied to the zones (e.g. a groundwater compartment is parameterized using a groundwater model). For large regions modelled using many UP elements, the UP parameters are regionalized using a classification scheme, thus reducing the overall effort spent in parameterization.

The development of the UP system is a long-term project involving research into physically-based parameterization of large scale hydrology models, including the effects of sub-grid spatial variations. The first stage involved developing a 'blueprint' for the UP element, based on experience with physically-based, distributed river basin modelling and reviews of existing techniques and modelling approaches for large scale and linked atmosphere-hydrology modelling. This paper describes the UP element and the concepts and ideas behind the development of the UP system, and briefly describes some of the research and development work currently in progress on UP and its parameterization.

Acknowledgements

References

Abbott, M.B., Bathurst, J.C., Cunge, J.A., O'Connell, P.E. and J. Rasmussen, 1986a. An introduction to the European Hydrological System—Système Hydrologique Européen, 'SHE', 1: History and philosophy of a physically-based, distributed modelling system. *J. Hydrol.*, 87: 45–59.

Abbott, M.B., Bathurst, J.C., Cunge, J.A., O'Connell, P.E. and J. Rasmussen, 1986b. An introduction to the European

Hydrological System—Système Hydrologique Européen, "SHE", 2: Structure of a physically-based, distributed modelling system. *J. Hydrol.*, 87: 61–7.

Bathurst, J.C. and O'Connell, P.E., 1992. Future of distributed modelling: The Système Hydrologique Européen. *Hydrol. Process.*, 6: 265–277.

Beven, K., 1989. Changing ideas in hydrology—the case of physically-based models. *J. Hydrol.*, 105: 157–172.

Beven, K., 1995. Linking parameters across scales: subgrid parameterizations and scale dependent hydrological models. *Hydrol. Process.*, 9: 507–525.

Beven, K., and Kirkby, M.J., 1979. A physically based, variable contributing area model of basin hydrology. *Hydrol. Sci. Bull.*, 24: 43–69.

Blöschl, G., and Sivapalan, M., 1995. Scale issues in hydrological modelling: a review. *Hydrol. Process.*, 9: 251–290.

Chen, Z-Q., Kavvas, M.L. and Govindaraju, R.S., 1993. Upscaling of Richards equation for soil moisture dynamics to be utilized in mesoscale atmospheric models. *Exchange Processes at the Land Surface for a Range of Space and Time Scales*, Proceedings of the Yokohama Symposium, July 1993. IAHS Publ. 212, pp. 125–132.

Dickinson, R.E., Henderson-Sellers, A., Kennedy, P.J. and Wilson, M.F., 1986. Biosphere-atmosphere transfer scheme (BATS) for the NACR community climate model. Technical Note NCAR/TN 275+STR, *Natl. Cent. Atmos. Res.*, Boulder, CO, 69 pp.

Dümenil, L. and Todini, E., 1992. A rainfall-runoff scheme for use in the Hamburg climate model. In: J.P. O'Kane (Editor), Advances in Theoretical Hydrology, a Tribute to James Dooge. *Euro. Geophys. Soc. Ser. of Hydrol. Sci.*, 1. Elsevier, Amsterdam, pp. 129–157.

Entekhabi, D. and Eagleson, P.S., 1989. Land surface hydrology parameterization for atmospheric general circulation models including subgrid scale spatial variability. *J. Climate*, 2: 816–831.

Ewen, J., 1995. Solute transport component of the catchment modelling system SHETRAN. In: S.T. Trudgill (Editor), Solute Modelling in Catchment Systems. John Wiley and Sons, UK, pp. 417–441.

Ewen, J., Parkin, G. and O'Connell, P.E., in preparation. SHETRAN: a coupled surface/subsurface modelling system for 3D water flow and sediment and solute transport in river basins.

Ewen, J., and Parkin, G., 1996. Validation of catchment models for predicting land-use and climate change impacts. 1. Method. *J. Hydrol.*, 175: 583–594.

Freeze, R.A. and Harlan, R.L., 1969. Blueprint for a physically-based, digitally-simulated hydrologic response model. *J. Hydrol.*, 9: 237–258.

Grayson, R.B., Moore, I.D. and McMahon, T.A., 1992. Physically based hydrologic modeling 2. Is the concept realistic? *Water Resour. Res.*, 26: 2659–2666.

Grayson, R.B., Moore, I.D. and McMahon, T.A., 1994. Reply. *Water Resour. Res.*, 30: 855–856.

IACGEC, 1996. *UK National Strategy for Global Environmental Research*. Inter-Agency Committee on Global Environmental Change: Report of Expert Panel, 42 pp.

Jaynes, D.B., 1985. Comparison of soil-water hysteresis models. *J. Hydrol.*, 75: 287–299.

Johnson, K.D., Entekhabi, D. and Eagleson, P.S., 1993. The implementation and validation of improved land-surface hydrology in an atmospheric general circulation model. *J. Climate*, 6: 1009–1026.

King, A.W., 1991. Translating models across scales in the landscape. *Ecological Studies*, 82: 479–517.

Klute, A., 1952. A numerical method for solving the flow equation for water in unsaturated materials. *Soil Sci.*, 73: 105–116.

Levin, S.A., 1992. The problem of pattern and scale in ecology. *Ecology*, 73: 1943–1967.

Loague, K., 1990. Changing ideas in hydrology—the case of physically-based models—comment. *J. Hydrol.*, 120: 405–407.

Manabe, S., Smagorinsky, J. and Strickler, R.J., 1965. Simulated climatology of a general circulation model with a hydrological cycle. *Mon. Weather Rev.*, 93: 769–798.

Mantoglou, A. and Gelhar, L.W., 1987. Stochastic modelling of large-scale transient unsaturated flow systems. *Water Resour. Res.*, 23: 37–46.

Naden, P.S., 1992. Spatial variability in flood estimation for large catchments: the exploitation of channel network structure. *Hydrol. Sci.*, 37: 53–71.

NERC, 1993. Terrestrial Initiative in Global Environmental Research. Programme Report and Science Highlights 1990–1992. Natural Environment Research Council, London, UK, 63 pp.

O'Connell, P.E., 1991. A historical perspective. In: D.S. Bowles and P.E. O'Connell (Editors), Recent Advances in Modelling of Hydrologic Systems. NATO ASI Ser. C345. Kluwer, Dordrecht, pp. 3–30.

O'Connell, P.E. and Todini, E., 1996. Modelling rainfall, flow and mass transport in hydrological systems: an overview. *J. Hydrol.*, 175: 3–16.

Parkin, G., O'Donnell, G.M., Ewen, J., Bathurst, J.C., O'Connell, P.E. and Lavabre, J., 1996. Validation of catchment models for predicting land-use and climate change impacts: 2, Case study for a Mediterranean catchment. *J. Hydrol.*, 175: 595–613.

Pimentel da Silva, L., 1997. *Large-scale hydrological modelling: physical parameterisation for groundwater recharge*. PhD Thesis, University of Newcastle upon Tyne, Newcastle upon Tyne, UK, 212 pp.

Polcher, J., Laval, K., Dümenil, L., Lean, J. and Rowntree, P.R., 1996. Comparing three land surface schemes used in general circulation models. *J. Hydrol.*, 180: 373–394.

Quinn, P.F., Beven, K., Chevallier, P., and Planchon, O., 1991. The prediction of hillslope flow paths for distributed hydrological modelling using digital terrain models. *Hydrol. Process.*, 5: 59–79.

Rastetter, E.B., King, A.W., Cosby, B.J., Hornberger, G.M., O'Neill, R.V. and Hobbie, J.E., 1992. Aggregating fine-scale ecological knowledge to model coarser-scale attributes of ecosystems. *Ecological Applications*, 2: 55–70.

Richardson, L.F., 1922. *Weather Prediction by Numerical Process*. Cambridge University Press, pp. 104–114.

Sellers, P.J., Mintz, Y., Sud, Y.C. and Dalcher, A., 1986. A simple biosphere model (SiB) for use within general circulation models. *J. Atmos. Sci.*, 43: 505–530.

Shaw, E.M., 1988. *Hydrology in Practice*. Chapman and Hall, London, 539 pp.

Sivapalan, M., 1993. Linking hydrologic parameterizations

across a range of scales: hillslope to catchment to region. *Exchange Processes at the Land Surface for a Range of Space and Time Scales*, Proceedings of the Yokohama Symposium, July 1993. IAHS Publ. 212, pp. 115–123.

Smith, R.E., Goodrich, D.R., Woolhiser, D.A. and Simanton, J.R., 1994. Comment on physically based hydrologic modeling, 2, Is the concept realistic? *Water Resour. Res.*, 30: 851–854.

Srivastava, R. and Yeh, T-C. J., 1991. Analytical solutions for one-dimensional, transient infiltration towards the water table in homogeneous and layered soils. *Water Resour. Res.*, 27: 753–762.

Vörösmarty, C.J., Gutowski, W.J., Person, M., Chen, T-C. and Case, D., 1993. Linked atmosphere-hydrology models at the macroscale. *Macroscale Modeling of the Hydrosphere*, Proceedings of the Yokohama Symposium, July 1993. IAHS Publ. 214, pp. 3–27.

Wen, X-H. and Gómez-Hernández, J.J., 1996. Upscaling hydraulic conductivities in heterogeneous media: an overview. *J. Hydrol.*, 183: ix–xxxiii.

Wood, E.F., Lettenmaier, D.P. and Zartarian, V.G., 1992. A land-surface hydrology parameterization with subgrid variability for general circulation models. *J. Geophys. Res.*, 97: 2217–2728.

Zhao, R-J., Zuang, Y-L., Fang, L-R., Liu, X-R. and Zhang, Q-S., 1980. The Xinanjiang model. *Hydrological Forecasting*. Proceedings of the Oxford Symposium, April 1980. IAHS Publ. 129. pp. 351–356.