

Linear System Model of Water Flow and Oxygen-18 Transport on a Steep Hillslope

V J Bidwell¹ and M K Stewart²

¹Lincoln Environmental, P O Box 84, Lincoln University, New Zealand

²Institute of Geological and Nuclear Sciences, P O Box 31312 Lower Hutt, New Zealand

Abstract The purpose of this model was to assist with the determination of the nature of water flow processes on steep ($\approx 35^\circ$) hillslopes in a 3.8 ha forested catchment. The soils are sufficiently permeable that, for most rainstorms, streamflow responds rapidly without significant surface runoff occurring. Scientific debate had focused on whether "old water" held within the soil could be rapidly mobilised by incoming "new water" from storm rainfall. A linear system approach was taken to the analysis of the dynamic response of water flow and concentration of the natural isotope oxygen-18 in the stream to the input series of rainfall and associated oxygen-18 content from one storm. The candidate system components were bounded and unbounded water storages with first-order water flow dynamics, and bounded storages with zero-order dynamics. The upper limits on the bounded storages allow for nonlinearities in flow processes. The dynamic effect on transport of the isotopic tracer was assumed to be due to perfect mixing within each of the water storage components. The model was implemented on spreadsheet software in the form of difference equations and logical expressions. Analysis of the rainfall and streamflow data showed that the hydrometric response could be simulated with one bounded (8.5 mm) zero-order storage to account for initial rainfall loss, followed by a bounded (25.6 mm) and an unbounded first-order storage in parallel. However, this model provided insufficient attenuation of the oxygen-18 signal. Satisfactory simulation of oxygen-18 in the stream was achieved by including a bounded zero-order storage (250 mm) of specified oxygen-18 concentration. The same model structure was fitted to additional data from measurement of subsurface flow collected by troughs at four locations on the hillslopes. The results support the hypothesis that mobilisation of old water is an important component of water flow on the hillslopes. However, the degree of mixing within the old water storage has not been conclusively determined on the basis of the one storm event.

1. INTRODUCTION

The water flow processes contributing to storm-generated streamflow in some small (<4 ha) catchments in the South Island of New Zealand have been the subject of considerable investigation and scientific publication [Stewart and McDonnell, 1991]. The reason for this interest is that most of the quickflow component of runoff comes from subsurface flow on the steep ($\approx 35^\circ$) hillslopes, rather than surface runoff. The role of the thin, highly permeable soils overlying an impermeable substratum is well recognised. However, there has been some debate as to whether the subsurface flow is "new" water from current rainfall, transmitted by macropore flow, or "old" water resident in the soil profile which is displaced or mobilised by current infiltration.

Earlier hydrometric measurements supported the macropore flow hypothesis whereas later research with natural isotopic tracers favoured the involvement of old water in the flow processes. Resolution of hydrometric and isotopic tracer data has been approached with a range of residence time models [Unnikrishna *et al.*, 1995] for the purpose of quantifying the amount and flow paths of new and old water. Most of these models employ the concept of the mixing cell, singly or in series, or formulas which can be shown to be analytical solutions to the mixing cell systems. These analytical solutions assume

steady water flow through the mixing cells, but there are also some variable parameter, or adaptive, models that take account of the more realistic situations of unsteady flow.

The modelling approach described in the present paper involves data-driven identification of a model which simulates the hydrometric response of water flow to rainfall, followed by an assessment of the tracer dispersion dynamics of the model and the requirement for additional dispersive components. The dispersive characteristics of the model implicitly account for unsteady flow by invoking assumptions about the nature of dispersion in porous media, which are commonly applied in soil physics. This approach does not require the concept of residence time, but focuses instead on the water storage needed for dispersive mixing.

2. DATA

The hydrometric data used for the present analysis are the hourly values of: rainfall, flow of the stream draining catchment M8 (3.8 ha), and flow from four 1.7 m long troughs (T6, T10, T11, T24) [Woods and Rowe, 1996] which intercept subsurface flow on the hillslopes, for a rainfall event on 18-19 January 1994 [Stewart and Rowe, 1997]. The associated tracer data are the concentrations

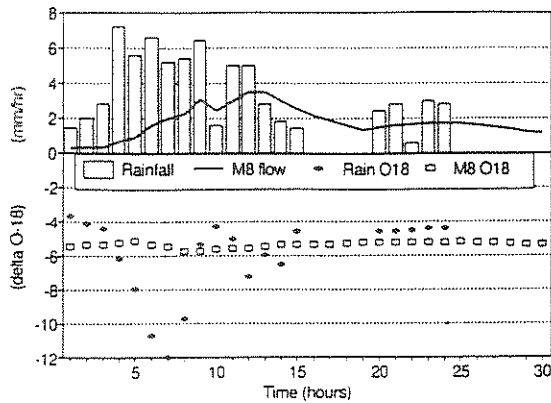


Figure 1: The hydrometric and oxygen-18 tracer data for the stream M8 during the storm of 18-19 January 1994.

of the natural isotope oxygen-18 expressed in units of $\delta^{18}\text{O}$, the deviation from Vienna standard mean ocean water (V-SMOW).

Figure 1 shows the hydrometric data for the rainfall and streamflow, both in unit area scale (mm), and the corresponding oxygen-18 tracer data. The strong oxygen-18 signal in the rainfall is caused by precipitation from air masses with different altitudinal origins. The oxygen-18 signal in the streamflow is highly attenuated, and this behaviour prompted the present examination of dispersive processes. Figure 2 shows how the oxygen-18 concentration of the stream- and trough-flows all converge to a narrow band of values. The trough flow data show a response pattern similar to the stream, but the catchment area of each trough is not well defined and therefore a gain factor was included in the model to achieve mass balance.

3. MODEL

3.1 Initial Modelling Philosophy

The original approach considered for modelling the hydrometric (rainfall-streamflow) data followed that described by Jakeman and Hornberger [1993]. This involves application of time-series analysis to the rainfall (modified for initial losses) and streamflow data to identify a transfer function in the form of a difference equation with minimal parameterisation. A typical candidate model is the second-order difference equation representing two water storage components in parallel:

$$Q_k = a_1 Q_{k-1} + a_2 Q_{k-2} + b_0 P_k + b_1 P_{k-1} \quad (1)$$

where Q_k is streamflow and P_k is precipitation excess for the k th time interval.

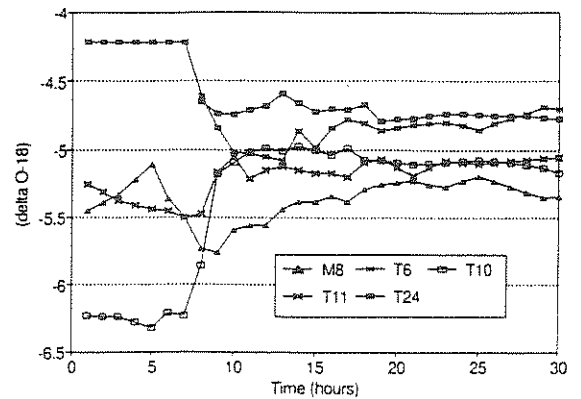


Figure 2: Oxygen-18 tracer data for flow in the stream and troughs.

The analytical techniques available from microCAPTAIN software [Young and Benner, 1991] were applied to the data shown in Figure 1, after allowing for initial losses. The results were inconclusive, in that the “best” model, in terms of minimal parameters was first order, but the fit was unsatisfactory.

3.2 Revised Identification Technique

First- and second-order difference equations were manually fitted to portions of the data, using spreadsheet formulas and graphics. In particular, the “modal” parameters a_1 and a_2 were fitted to the recessional portions of the streamflow record which appeared to be not directly influenced by rainfall. The initial results showed that higher flows could be fitted satisfactorily with a first-order model whereas at lower flows a second order model was required. This suggested the presence of non-linear behaviour which could be simulated with a system of linear components that includes a method of switching between parallel branches in response to the states of the system.

Therefore, the original philosophy was retained of identifying a linear system from the data, which is parsimonious with parameters, but in addition to the fundamental first-order components of candidate systems there was a need to include parameters to indicate switching between flow branches. It was also decided to include a component to simulate the nonlinear effect of accounting for rainfall, in the initial stage of a storm, which does not contribute to streamflow. The candidate structural arrangements were limited to parallel and series combinations of two or three components.

3.3 Hydrometric Model Components

Figure 3 shows the three types of system components, with the relationships between the output water flux q and water storage contents S , with input water flux p , on a continuous time basis. The values of p , q , and S have dimensions of flux [LT^{-1}] and storage [L] for this lumped catchment model.

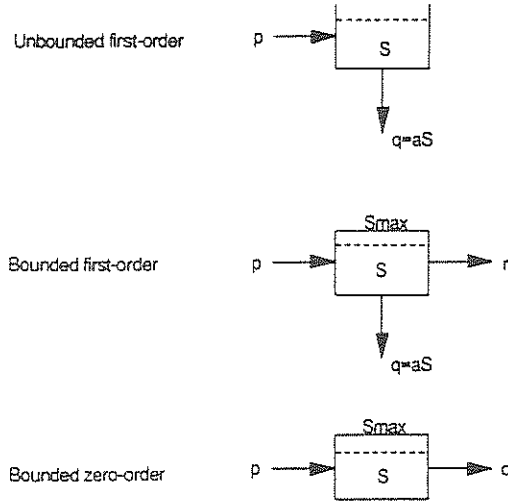


Figure 3: The candidate system components.

For the *unbounded first-order storage*, the differential equations for water balance can be expressed in the (state-space) form:

$$\begin{aligned} \frac{dS}{dt} &= -aS + p \\ q &= aS \end{aligned} \quad (2)$$

and the corresponding difference equations for the k th time interval Δt are:

$$\begin{aligned} S_k &= AS_{k-1} + Bp_k \\ q &= aS_k \end{aligned} \quad (3)$$

in which:

$$A = \exp\{-a\Delta t\} \quad B = \frac{(1-A)}{a} \quad (4)$$

The relationship (4) between the discrete and continuous parameters assumes that q_k and S_k are instantaneous values at the end of the k th interval whereas the input p_k is the average over the interval.

The *bounded first-order storage* has an upper limit on storage capacity, S_{\max} , and an additional output r when it is full. The difference equations for this storage are:

$$\begin{aligned} S_k &= \min\{AS_{k-1} + Bp_k, S_{\max}\} \\ q_k &= aS_k = \max\left\{\frac{AS_{k-1} + Bp_k - S_{\max}}{\Delta t}, 0\right\} \end{aligned} \quad (5)$$

and the effect is to cause diversion of water flow to another component with different dynamic behaviour, as a form of quasi-linearisation of flow processes.

During the time intervals when the threshold value S_{\max} is "switched" on or off, there can be a minor violation of the continuity implied by (4), but this has been ignored in the present model. Except for these intervals, r_k is also the mean value over the time interval as the input to another component.

The *bounded zero-order storage* has a capacity S_{\max} which must be filled before there is any output, after which the output q equals the input p and there is no detectable hydrodynamic behaviour. The discrete-time equations are:

$$\begin{aligned} S_k &= \min\{S_{k-1} + p_k\Delta t, S_{\max}\} \\ q_k &= \frac{\max\{S_{k-1} + p_k\Delta t - S_{\max}, 0\}}{\Delta t} \end{aligned} \quad (6)$$

This component can be used to simulate initial loss from storm rainfall, that does not contribute to streamflow.

3.4 Tracer Dispersion Modelling

Maximum dispersion of a tracer which transits any of the above water storage components is achieved by assuming that the incoming tracer is instantaneously mixed into the whole contents. The outgoing tracer concentration is the same as that in the storage. Lesser degrees of dispersion can be simulated by subdividing the water storage into smaller mixing volumes in series through which the water flows. This concept is the basis of the mixing cell model of advective-dispersive solute transport [e.g., Bidwell, 1997]. For the present model, the maximum dispersion case is considered in order to calculate the minimum soil water required to simulate the attenuation of tracer concentration observed in the streamflow.

Conservation of tracer mass through each system component provides the differential equations relating the concentration c within the storage, and in the output, to the concentration u of the inflow. The relevant differential and difference equations for each type of storage are:

Table 1. Parameter values for the model shown in Figure 4.

Model	S_1 (mm)	S_2 (mm)	a_s	a_r	d	c_0 ($\delta^{18}\text{O}$)	R_w^2	R_r^2
M8	8.5	25.6	0.09	0.42	0	-5.10	0.976	0.967
T6	14.2	25.6	0.04	0.55	2	-4.57	0.862	.0853
T10	13.5	17.0	0.02	0.16	2	-4.65	0.943	0.934
T11	14.1	15.8	0.04	0.32	1	-4.75	0.943	0.939
T24	25.0	16.1	0.06	0.26	2	-4.82	0.962	0.998

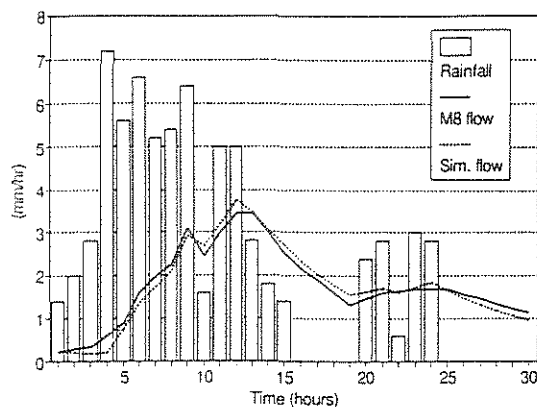


Figure 5: The simulated streamflow for M8.

Old water: a bounded zero-order storage, of capacity S_0 , initially full of water with tracer concentration c_0 .

Slow response: a bounded first-order storage, of capacity S_2 and dynamic coefficient a_s , with initial water content and tracer concentration corresponding to initial stream- or trough-flow.

Fast response: an unbounded first-order storage, with dynamic coefficient a_r , initially empty.

Table 1 shows the values of these model parameters, and the explained variances of water flow R_w^2 and tracer mass flux R_r^2 for the stream and trough data.

Optimisation of the tracer response was found to be sensitive to the initial tracer mass in the old water, $S_0 c_0$, but relatively insensitive to particular combinations of S_0 and c_0 . If c_0 was set, for example, to the initial observed value for the flow record, the value of S_0 was sometimes unrealistically large. The values of c_0 in Table 1 correspond to $S_0=250$ mm. Mass balance of water and tracer in the models was within 1%.

The trough data required a time delay of one or two hours in the output from the model to achieve a good fit, and this is noted in Table 1 as the value for "d".

Figure 5 shows the simulated hydrometric response for the M8 streamflow. The effect on simulation of tracer response by adding "old water" to the hydrometric model is demonstrated in Figure 6. Although the desired attenuation of the oxygen-18 signal was achieved, the model did not satisfactorily simulate the small (relative to

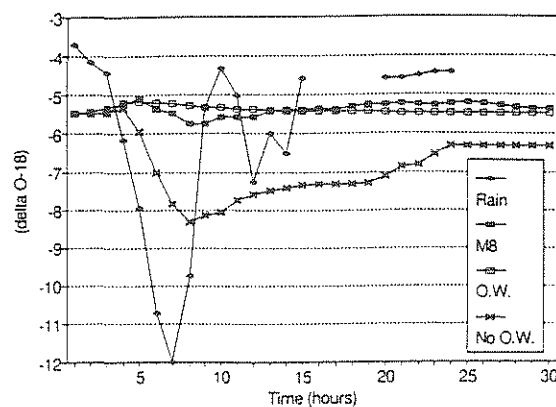


Figure 6: The effect on simulation of tracer response for M8 when the "old water" component is included.

the oxygen-18 in the rainfall) fluctuations in tracer concentration shown in Figure 2.

5. DISCUSSION AND CONCLUSIONS

The parameter values in Table 1 refer to only one storm event, and data from a subsequent event have yet to be analysed. Therefore, discussion will focus on the general pattern of dynamic behaviour for the measured event and the relevance of the model to evaluation of processes.

The model structure can be calibrated to provide very good simulation of water flow and tracer flux at the catchment scale (M8) and for portions of hillslope drained by 1.7 m long troughs (T6 is less satisfactory). The trough models required time delays of one or two hours in the output to achieve a good fit to the data. This suggests the presence of a drained portion of the soil near the troughs which provides the storage for this purely translational flow behaviour. The lack of time delay in the M8 model implies that soil water storage and streamflow are closely coupled.

The results strongly support the involvement of old water in the hillslope flow processes, because it is impossible to achieve mass balance without the presence of this pre-event store of tracer mass. However, there still remains some doubt about the nature of the dispersive processes. Similar levels of tracer signal attenuation could have been obtained by assuming that old water of appropriate initial oxygen-18 concentration was simply displaced by incoming rainfall as a "piston flow" process in which no mixing was involved.

unbounded first-order storage:

$$\frac{d(Sc)}{dt} = -a(Sc) + (pu) \quad (7)$$

$$c_k = \frac{A(S_{k-1}c_{k-1}) + B(p_k u_k)}{S_k}$$

bounded first-order storage:

equation (7) for $S_k < S_{max}$, otherwise:

$$c_k = Dc_{k-1} + (1-D)u_k \quad (8)$$

in which:

$$D = \exp\left\{-\frac{p_k \Delta t}{S_{max}}\right\} \quad (9)$$

bounded zero-order storage:

equation (8).

The relationship (9) is derived as the discrete interval coefficient of a single mixing cell which has linear dynamics on a cumulative-flow basis [Bidwell, 1997]. In the present time-based context the coefficient D is time-varying as it depends on the value of the flow p_k .

The degree of tracer dispersion can be adjusted, independently of water flow dynamics, by inserting additional bounded zero-order storage which is always full of water. The size and initial oxygen-18 concentration of this storage are parameters which allow tracer mass balance and tracer flux simulation to be achieved in the model. As a physical concept, this is "old water" resident in the catchment before the current rain storm, which is hypothesised to be involved in quickflow from the hillslopes.

The above approach to dispersion modelling takes full account of unsteady water flow, and the parameters most relevant to the magnitude of dispersion are the volumes of the storage components, especially the bounded storages. When these storages are full, they behave as linear mixing cells on a cumulative flow basis rather than a time basis. This transformation is commonly used in soil physics [e.g., Bidwell, 1997] to model dispersion in unsteady solute transport. This emphasis contrasts with the methods reviewed by Unnikrishna *et al.* [1995] in which residence time is the measure of dispersion, but becomes a time-varying parameter for unsteady flow.

3.5 Parameter Estimation

An overall "gain" coefficient was applied to the output generated by the linear system model, in order to achieve water balance. This is because the contributing catchment

areas are not known exactly, especially for the trough data.

The candidate models were implemented on a spreadsheet [QUATTRO PRO 5] by use of cell formulas for the difference equations and logic statements. Initial parameter values were estimated by supervised fitting of the models to data in the graphics window, and these values were refined by means of the library optimisation feature. The sequence of parameter optimisation was:

1. Adjust the gain coefficient to achieve preliminary water balance.
2. Optimise the values of "a" and S_{max} of the model components to minimise the mean square error of predicted stream- or trough-flow.
3. Repeat steps 1 and 2 until the fit is satisfactory.
4. Optimise the size and initial $\delta^{18}O$ value of any additional bounded zero-order storage required to minimise the mean square error of predicted oxygen-18 mass flux (flow $\times \delta^{18}O$).

4. RESULTS

Figure 4 shows the structure of the simplest system of candidate components which satisfactorily simulates water flow and tracer response to the storm rainfall for the stream M8, and the troughs T6, T10, T11, and T24.

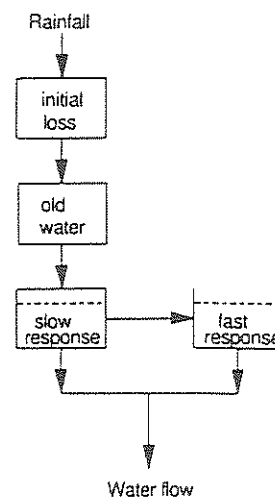


Figure 4: The model structure for testing the "old water" hypothesis

The descriptive names, parameters, and initial states of the four components are:

Initial loss: a bounded zero-order storage, of capacity S_i , initially empty.

The real answer probably lies somewhere between these two extremes of single storage mixing or piston flow without mixing, as would be expected for solute transport through soil. These processes can be simulated by including a series of mixing cells in the model, but the initial resident tracer concentrations of these cells are more difficult to specify as part of model optimisation. Analysis of data from additional storm events and more refined modelling of the output tracer concentration signals may yield a better insight.

6. ACKNOWLEDGEMENTS

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