

Simulation of Solute Transport in a Mountain Pool-and-Riffle Stream: A Transient Storage Model

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The physical characteristics of mountain streams differ from the uniform and conceptually well-defined open channels for which the analysis of solute transport has been oriented in the past and is now well understood. These physical conditions significantly influence solute transport behavior, as demonstrated by a transient storage model simulation of solute transport in a very small ($0.0125 \text{ m}^3 \text{ s}^{-1}$) mountain pool-and-riffle stream. The application is to a carefully controlled and intensively monitored chloride injection experiment. The data from the experiment are not explained by the standard convection-dispersion mechanisms alone. A transient storage model, which couples dead zones with the one-dimensional convection-dispersion equation, simulates the general characteristics of the solute transport behavior and a set of simulation parameters were determined that yield an adequate fit to the data. However, considerable uncertainty remains in determining physically realistic values of these parameters. The values of the simulation parameters used are compared to values used by other authors for other streams. The comparison supports, at least qualitatively, the determined parameter values.

INTRODUCTION

Extensive knowledge exists concerning the mechanisms and simulation of solute transport in streams [Fischer *et al.*, 1979]. From the applications perspective, interest has focused on larger streams located near population centers. As a generalization, these streams are physically low slope, deeper than the roughest bed feature, and relatively uniform (possibly due to flow regulation). Chemically, these streams contain and transport rather high concentrations of diverse constituents. Small mountain pool-and-riffle streams are described by opposing characteristics. Chemically, there are fewer significant constituents present and these are at lower concentrations. These streams cannot be characterized as uniform either in dimension or gradient, and the bed may significantly influence solute transport.

Of late there has been interest in studying the physical [Keller and Tally, 1979; Keller, 1975; Heede, 1972], chemical [Hubbard and Striffler, 1973; Lewis and Grant, 1979], and solute transport [Day, 1975, 1977] characteristics of small mountain pool-and-riffle streams. Certain larger mountain streams maintain the significant pool-and-riffle characteristic. Studies of the overall hydrochemical and transport characteristics of these larger streams are now appearing [Janda, 1977; Kennedy and Malcolm, 1977] and will presumably become more important as society continues to seek new locations to discharge its chemical and thermal pollution.

In this study, application of a transient storage model to a field experiment is presented. The model must reflect the large variability in the physical characteristics of the stream in order to simulate the field experiment. Concurrently, the model is useful in smoothing out this same variability in order to make the simulations tractable.

The importance of differing physical scales becomes evi-

dent, because the short distances and small volumes of water in the system suggest that similarly small-scale physical processes occurring in the stream may have significant consequences. Thus the application of a one-dimensional (or pseudo-two-dimensional) transport analysis remains empirical. The model equations have previously been applied by numerous workers, mostly to improve the shortcomings of the advection-dispersion model, in large streams. After presenting the model and the simulation of the experiment, we will discuss the apparent distinctions between previous applications and the one presented here. This comparison supports the conclusion that the transient storage mechanism is a viable first approximation to the complexity of the physical processes.

MODEL

The typical starting point for the study of solute transport in streams centers on the one-dimensional convection-dispersion analysis. The 'tail' of a solute tracer pulse is often more pronounced than can be accounted for by this analysis. (See Fischer *et al.* [1979] for a complete discussion of solute transport in real streams, the one-dimensional analysis, and alternatives.) A common method for simulating these long tails has been to allow for storage zones or 'dead zones' along the stream channel. These storage zones are assumed to be stagnant relative to the longitudinal flow of the stream and to obey a first-order mass transfer type of exchange relationship. That is, the exchange of solute between the main stream channel and a storage zone is proportional to the difference in concentration between the stream and the storage zone. Implementation of this model requires an estimate of the storage zone cross-sectional area and an empirical exchange coefficient. Under a variety of nomenclatures, various theoretical, laboratory flume, and field aspects of dead zone models have been analyzed [Hays *et al.*, 1966; Thackston and Krenkel, 1967; Thackston and Schnelle, 1970; Pedersen, 1977; Valentine and Wood, 1977; Sabol and Nordin, 1978; Valentine and Wood, 1979a, b; Tsai and Holley, 1979; Nordin and Troutman, 1980].

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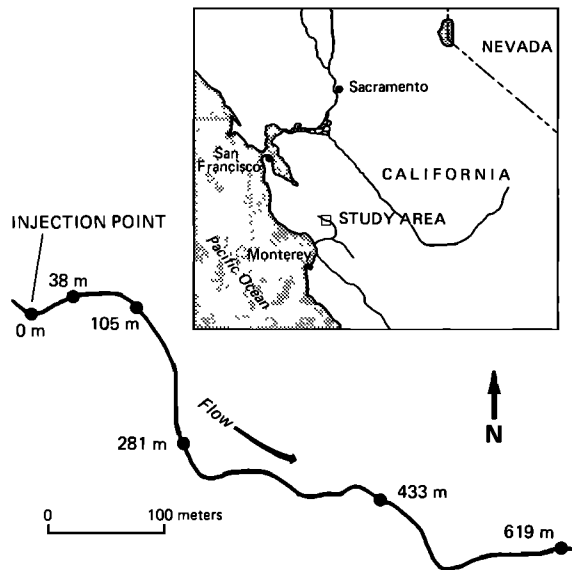


Fig. 1. Experimental reach of Uvas Creek (Santa Clara County, California). Injection point and five monitoring locations are indicated.

The model equations are

$$\frac{\partial C}{\partial t} + \frac{Q}{A} \frac{\partial C}{\partial x} = \frac{1}{A} \frac{\partial}{\partial x} \left(AD \frac{\partial C}{\partial x} \right) + \frac{q_L}{A} (C_L - C) + \alpha (C_S - C) \quad (1)$$

$$\frac{dC_S}{dt} = -\alpha \frac{A}{A_S} (C_S - C) \quad (2)$$

where

- C solute concentration in the stream, mg l^{-1} ;
- Q volumetric flow rate, $\text{m}^3 \text{s}^{-1}$;
- A cross-sectional area of the channel, m^2 ;
- D dispersion coefficient, $\text{m}^2 \text{s}^{-1}$;
- q_L lateral volumetric inflow rate (per length), $\text{m}^3 \text{s}^{-1} \text{m}^{-1}$;
- C_L solute concentration in lateral inflow, mg l^{-1} ;
- C_S solute concentration in the storage zone, mg l^{-1} ;
- A_S cross-sectional area of the storage zone, m^2 ;
- α stream storage exchange coefficient, s^{-1} ;
- t time, s;
- x distance, m.

Equation (2) and the coupling term $\alpha(C_S - C)$ in (1) are deceptively simple, for they embody several physical principles and constraints. They ideally describe a system with the following characteristics.

1. There exists a storage zone that is not moving.
2. Within the storage zone, solute is uniformly and instantaneously distributed.
3. The transport of solute between the storage zone and the channel is determined simply by the difference in concentrations and an exchange coefficient.
4. It is possible to measure the cross-sectional area of the storage zone, the concentration of solute within the storage zone, and the exchange coefficient.

In a mountain pool-and-riffle stream, these characteristics

are observed to varying degrees. It is easy to envision sizable storage zones of stagnant water that are not moving downstream. Such storage zones are located behind protruding logs, boulders, and vegetation in the shallows, along the edges of slowly moving pools, and in the thick gravel and cobble beds of swift riffles. However, it is not easy to envision a linear physical driving mechanism that simultaneously transfers mass between the stream and the storage zone, distributes it uniformly throughout the storage zone and yet prevents the storage zone from moving longitudinally.

In mountain streams, one does, nevertheless, observe significant tails from a solute pulse. Solute mass is removed during the rising phase of a solute pulse, temporarily retained in storage until the pulse passes, and then returned to the stream. From this observation we infer that there is in fact a mechanism that presents itself as transient storage of solute mass along the length of the stream. Hence we do not believe that a strict dead zone model is physically descriptive of the processes occurring in mountain streams, but rather that the observed 'transient storage' can be empirically simulated using the identical equations.

The distinction between describing physical dead zones and simulating observed transient storage is crucial to the determination and interpretation of the model parameters.

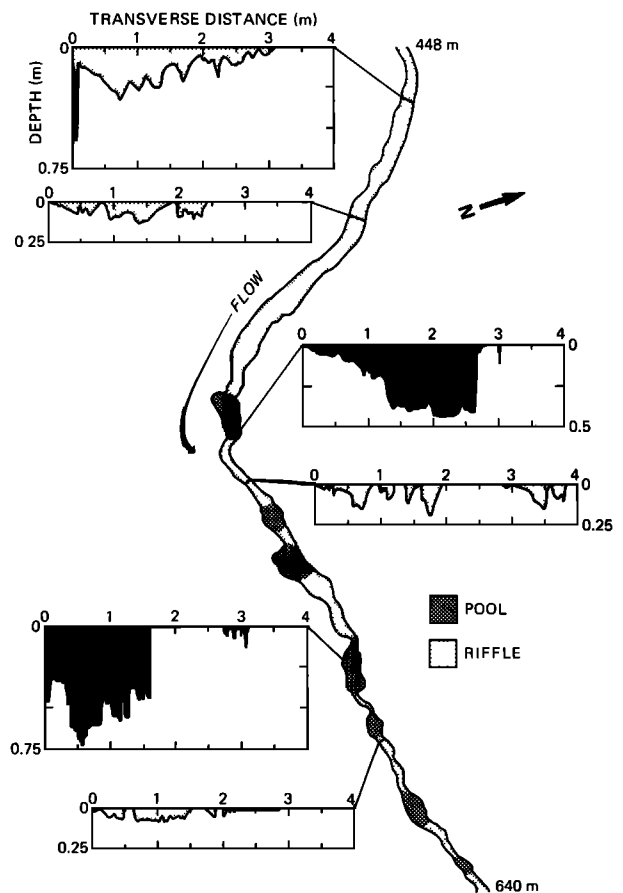


Fig. 2. Detailed mapping and transects (1973) of a reach in Uvas Creek. Note that the downstream distances measured in 1973 (Figures 2, 3, and 4) differ from those measured in 1972 by a few percent. These differences are due to the reworking of the stream channel during the intervening winter's storms and the imprecision of defining the longitudinal distance in a highly irregular channel.

A_S and α become operational parameters, with effective values determined by observing the response of the stream to the injection of a conservative solute.

APPLICATION

Zand *et al.* [1976] describe the steady injection of chloride tracer into Uvas Creek (see Figure 1). The experiment occurred in late summer during a period of low flow ($0.0125 \text{ m}^3 \text{ s}^{-1}$). The chloride was injected at a constant rate for three hours and reached a maximum concentration of 11.9 mg l^{-1} a short distance below the injection point. Background concentration was measured to be 3.7 mg l^{-1} .

An appreciation of the physical characteristics of Uvas Creek is crucial to the interpretation of both the experimental data and the simulations. Approximately one year after the 1972 field experiment a detailed mapping of the study reach was made in which stream elevations and over 100 channel transects were taken. Figures 2, 3, and 4 illustrate several important physical characteristics. The dominant feature is the spatial variability.

Figure 2 shows a detailed top view of a lower reach of Uvas Creek and six representative channel transects. The channel is highly irregular. It is composed of alternating pools and riffles. The transects show the pools to be relatively deep and uniform compared to the riffles. However, even in the pools, the bottom profile is irregular and small zones of water are separated from the main channel. In the riffles, the depth goes to 0.0 m at several locations across the transects in places where cobble and vegetation protrude through the flow. Figure 3 quantifies the image given by Figure 2 and shows the measured channel cross-sectional areas. (The actual values of A are not germane, as there was a higher flow rate in 1973.) The variability is so pronounced as to appear as scatter. Figure 4 shows the water surface elevation decrease over the study reach. The overall slope is steep (0.03 m m^{-1}) as expected for a mountain stream. On a small distance scale of tens of meters there are significant differences in slope ranging from virtually flat to several times the overall value.

These measurements support the picture of the complex water movement one observes in the stream. The water is alternately shooting through riffles with the cross section expanding as the water 'dumps' into the pools and then passing through the pools with the cross section contracting as the water falls into the next riffle. Particularly in riffle sections, the water is in contact with a gravel and cobble bed and can enter easily accessible void spaces.

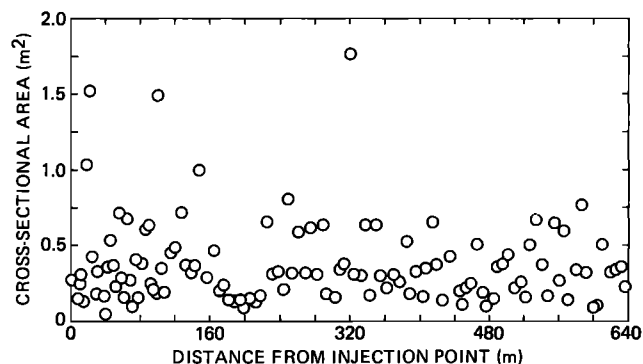


Fig. 3. Measured (1973) channel cross-sectional area in Uvas Creek.

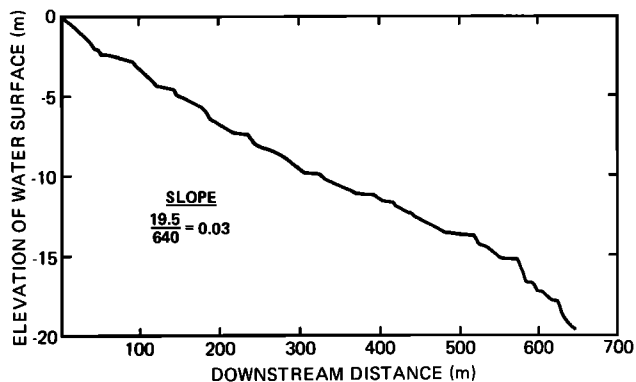


Fig. 4. Measured (1973) elevation of water surface in Uvas Creek.

The transient storage model will be used to simulate the transport of chloride in Uvas Creek resulting from the experimental steady injection. The model equations were solved by standard methods, using both finite difference and finite element (linear bases), spatial discretizations, and a Crank-Nicolson (time-centered) time integration. There were no essential differences between the finite difference and finite element simulations; results from the former are presented herein. The model parameters were selected by visually determining the set of parameters which yielded the 'best fit' to the concentration data. This approach is, of course, highly subjective. However, the spatial variability that exists in the stream makes it highly doubtful that a more complex technique would yield more meaningful results.

Several simulations were run with only the convection-dispersion mechanisms operating, i.e., no exchange with the storage zone ($\alpha = 0.0 \text{ s}^{-1}$). In these simulations, lateral inflow q_L was neglected because simulation experiments showed that physically plausible values of q_L did not alter the overall agreement of the simulations to the data. The model then has two parameters, A and D , with Q fixed by the determination of the chloride injection plateau at the monitoring station at 38 m. (Locations of monitoring stations are shown in Figure 1.) By using spatially uniform values of A and D , values for these parameters were determined by searching for the best fit to the leading edges of the pulses at two monitoring stations. The simulations based on the leading edges observed at 38 m and 619 m are shown in Figures 5a and 5b, respectively. The agreement with data is not good, but more importantly, the characteristics of the data and the simulation are different. The significant features of the concentration data are (1) the decrease in the maximum concentration at the downstream locations, (2) the clipping of the shoulders of the leading edges, (3) the extent of the tails, and (4) an apparent loss of mass at 619 m.

The application of the transient storage model is shown in Figures 6a and 6b. The best fit model parameters were determined in downstream sequence for each of the five reaches between successive monitoring locations (see Table 1). With parameters so determined, the simulation is excellent. Figure 6a compares the improvement of these results over identical parameters with no transient storage. Figure 6b shows the chloride concentration in the storage zones. The persistence of the tails in the storage zone is even more pronounced than in the channel. Elevated levels of chloride can remain in the storage zone long after the pulse has cleared the channel. These simulations exhibit all of the

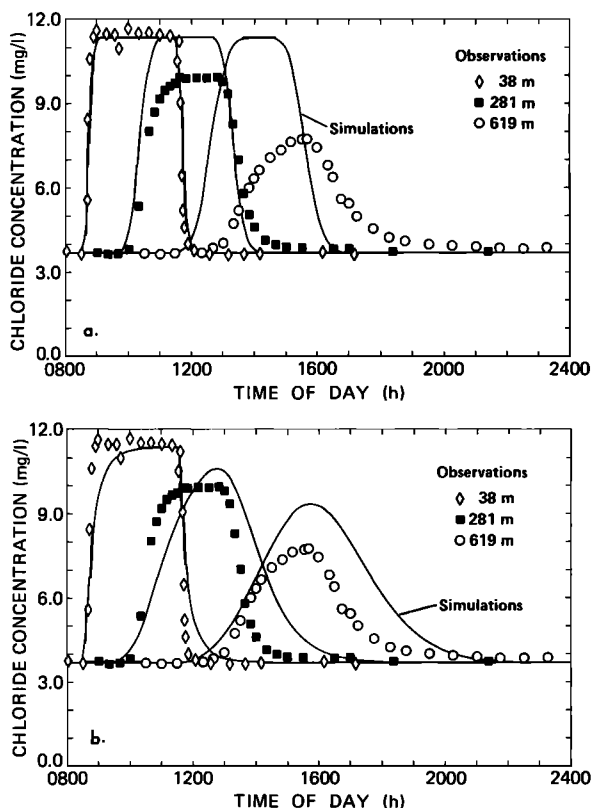


Fig. 5. Observed chloride concentrations and simulations at three locations for steady injection at Uvas Creek. Injection started at 08:30 and ended at 11:30. Data are presented from this period until 23:30 when rain began to fall. (See Table 1 for parameter values). (a) Simulation of convection-dispersion mechanisms; best fit to the leading edge of the pulse at 38 m. (b) Simulation of convection-dispersion mechanisms; best fit to the leading edge of the pulse at 619 m.

significant features of the stream concentration data listed above. In particular, Figure 6b illustrates that the storage zone acts as the needed temporary sink for the apparent loss of mass. In addition to the transient storage mechanism, the decreased maximum concentration at 281 m and 619 m could also be attributed to a chemical loss mechanism or increased discharge. The pH of the stream water was approximately 8; at this pH level the authors are unaware of a chemical loss mechanism for chloride. To simply invoke increased discharge does decrease the maximum concentration but will not account for the clipping of the shoulders of the leading edges and the extent of the tails observed in the data.

Reach-by-reach variation in the physical stream parameters was used in the simulation in Figure 6. The variation is substantial (on a relative basis). As intensive, concurrent monitoring at several locations is often physically or fiscally difficult, we tested the model's response to setting spatially uniform values for the parameters. Figure 7 shows the simulation yielding the best fit at 619 m. The simulation with reach-by-reach variation is, of course, better, but the uniform parameter simulation is also quite good. Uvas Creek, like other mountain streams, is characterized by a high degree of spatial variability and complex hydrology. Figure 7 indicates that although spatial variability in the parameters need not be a major consideration, its effects are, however, evident on scales of only hundreds of meters.

DISCUSSION

The simulations clearly indicate the importance of a transient storage mechanism for solute transport in Uvas Creek (and thus probably other mountain streams). The validity of this result rests heavily on the assertion that the model storage parameters are in fact physically realistic. We will discuss possibilities for the location of storage zones and indicate why the value of $A_S = 0.7 \text{ m}^2$ is not unrealistic. Both A_S and the exchange coefficient α will then be discussed as they relate to parameter values used by other authors for applications to other streams.

That the effective A_S for Uvas Creek is greater than the A is a somewhat curious result of the simulation exercise. There are several possible mechanisms operating in Uvas Creek that allow this to be plausible. Five such mechanisms are listed below. The order is from the most general mechanisms that we would expect to exist in almost any stream to the most specific mechanisms likely to be most important in small mountain streams. Solute may be temporally stored by (1) turbulent eddies generated by large-scale bottom irregularities, (2) large but slowly moving recirculating zones along the sides of pools, particularly located immediately downstream of the entrance to a pool from a riffle section, (3) small but very rapidly mixing recirculating zones located behind flow obstructions, particularly located in riffle sections where cobble, small boulders, and vegetation commonly protrude through the flow, (4) side pockets of water effectively acting as dead ends for solute transport, and (5) flow into, out of, and through a coarse gravel and cobble

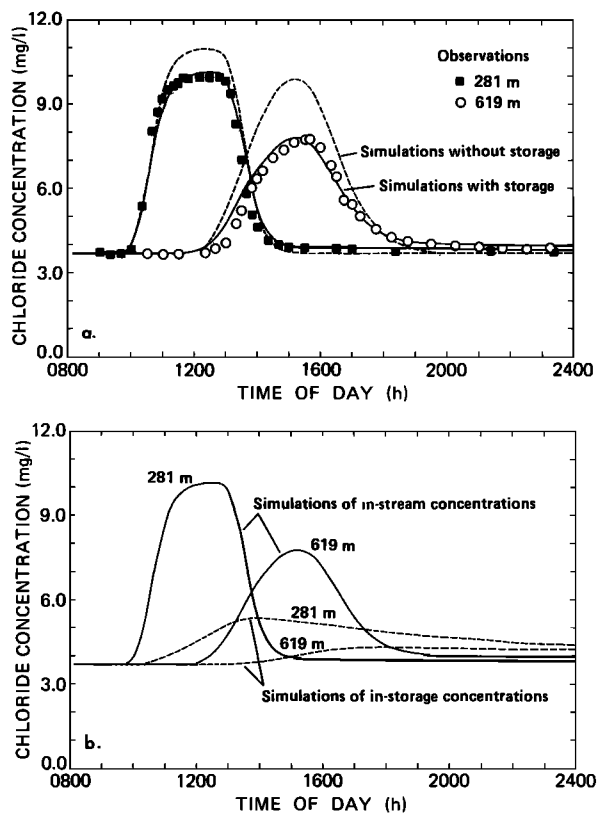


Fig. 6. Observed chloride concentrations and simulations at two locations. (See Table 1 for parameter values). (a) In-stream concentrations for simulations with and without storage mechanisms. (b) In-storage concentrations compared to in-stream concentration for simulation with storage mechanisms.

TABLE 1. Simulation Parameters

Simulation	Figure	Concentration at Injection Location C_{INJ} , mg l^{-1}	Reach, m	Flow Q , $\text{m}^3 \text{s}^{-1}$	Dispersion Coefficient D , $\text{m}^2 \text{s}^{-1}$	Cross-Sectional Areas		Exchange Coefficient α , s^{-1}
						Stream A , m^2	Storage A , m^2	
Convection-dispersion	5a	11.4	0-619	0.0125	0.12	0.30		0.00
	5b	11.4	0-619	0.0125	0.48	0.45		0.00
Storage	6a, 6b	11.4	0-38	0.0125	0.12	0.30	0.00	0.00
			38-105	0.0125	0.15	0.42	0.00	0.00
			105-281	0.0133	0.24	0.36	0.36	0.30×10^{-4}
			281-433	0.0136	0.31	0.41	0.41	0.10×10^{-4}
			433-619	0.0140	0.40	0.52	1.56	0.45×10^{-4}
Convection-dispersion	6a	*	*	*	*	*	*	0.00
Storage:	7							
variable parameters		*	*	*	*	*	*	*
uniform parameters		11.4	0-619	0.013	0.1	0.4	0.7	0.4×10^{-4}

*As above for storage simulation in Figure 6.

bed. All these mechanisms probably operate in Uvas Creek, and it is plausible that acting together they account for 0.7 m^2 of storage cross-sectional area even with a channel cross-sectional area of only 0.4 m^2 .

We are unaware of any a priori physical arguments that would indicate whether or not the value for the exchange coefficient is plausible. The wide variety of spatial and temporal scales present in the above mechanisms require that an effective exchange coefficient will reflect a lumping of many values.

Several other authors have used storage models for a wide variety of stream conditions. Figures 8a and 8b show model parameters determined in three other papers for nearly 40 applications. These figures are revisions of figures appearing in the work of Pedersen [1977] and include additional data points. The individual stream parameters were measured by many different workers, reported in different formats, and attempt to represent variable parameters by only one value. Thus there is considerable uncertainty associated with any individual point on these plots. Trends, not absolute values, are significant.

Figure 8a is a plot of the ratio of storage area to channel area, A_S/A , against $f^{-1/2}$ where

- f friction factor, equal to $8(U_*'/U)^2$;
- U stream velocity, equal to Q/A , m s^{-1} ;
- U' shear velocity, equal to $(gSd)^{1/2}$, m s^{-1} ;
- g acceleration of gravity, m s^{-2} ;
- d channel depth, m;
- S water surface slope,

Taking U_*' as the shear velocity, f is then a measure of friction [Henderson, 1966; Fischer et al., 1979]. Thackston and Schnelle [1970], as well as Pedersen [1977], have found it instructive to relate storage area to various measures of friction. In Figure 8a there is a clear trend between decreased importance of storage area and diminishing 'friction.' The point for Uvas Creek follows this trend.

Henderson [1966] discussed many empirical relationships between measures of surface roughness and $f^{-1/2}$. In pipe flow, and to a lesser extent in open channel flow, there is empirical evidence supporting a linear relationship between $f^{-1/2}$ and the logarithm of the ratio of length scales for surface roughness to flow depth. Figure 8a shows considerable scatter in the data; however, the basic trend observed

for surface roughness also appears with a measure of storage area.

Figure 8b is plot of dimensionless groupings relating a mass transfer grouping, the Nusselt number, to groupings of fluid, channel, and storage zone characteristics. The groupings are defined as follows.

- Nu Nusselt number, equal to $k4d/\epsilon_V$;
- Re Reynolds number; equal to $U4d/\nu$;
- Sc Schmidt number; equal to ν/ϵ_V ;
- d/B channel aspect ratio;
- d_S/B storage zone aspect ratio.

where

- k mass transfer coefficient, equal to αd , m s^{-1} ;
- B channel and storage zone breadth, m;
- d channel depth, equal to A/B , m;
- d_S storage zone depth, equal to A_S/B , m;
- ϵ_V vertical dispersion coefficient, equal to $0.0067 dU_*'$, $\text{m}^2 \text{s}^{-1}$;
- ν kinematic viscosity, $\text{m}^2 \text{s}^{-1}$.

These groupings have been defined to be analogous to those used in chemical engineering operations for mass transfer from a flowing gas or liquid to a flat plat [Bird et al., 1960; McCabe and Smith, 1967; Welty et al., 1969]. In forming the

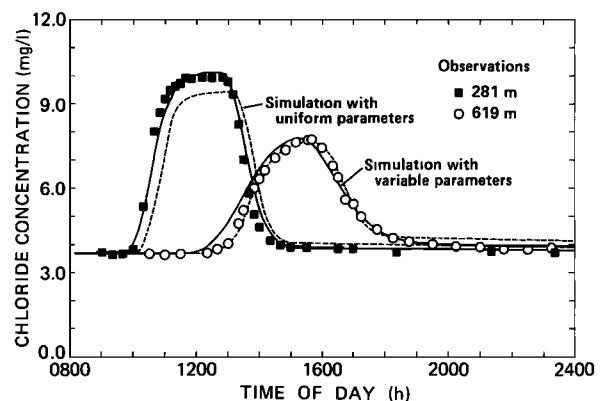


Fig. 7. Observed chloride concentrations and simulations at two locations. In-stream concentrations are compared for simulations with spatially varied and uniform parameter. (See Table 1 for parameter values).

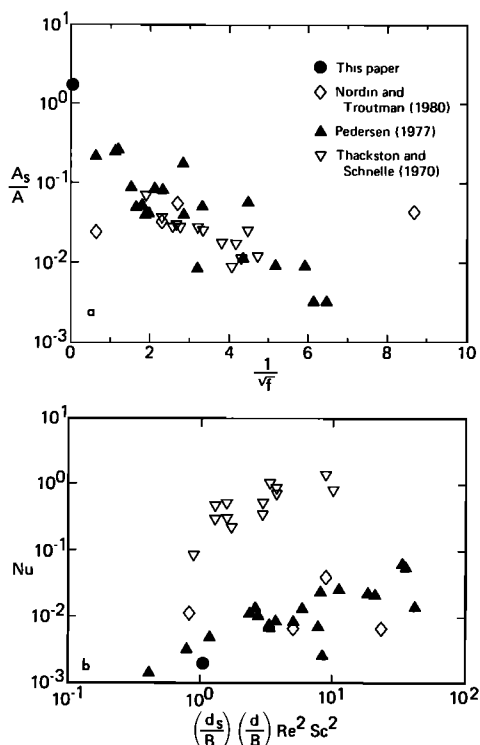


Fig. 8. Dead zone model parameters as determined in several applications. (Different authors define the dead zone model in terms of different parameters. For the cases shown here it was possible to convert to the groups A_s/A and Nu for comparison.) (a) Ratio of storage area to channel area plotted against a 'friction' grouping of channel parameters. (b) Mass transfer Nusselt number plotted against a grouping of fluid, channel, and storage zone parameters.

groupings, the channel and storage zone cross sections were assumed to be rectangular and $d \ll B$. The vertical dispersion coefficient is taken from an empirical relationship for natural channels [Fischer et al., 1979] and a value of $10^{-6} \text{ m}^2 \text{ s}^{-1}$ was used for kinematic viscosity. (The Nusselt number is conventionally defined in terms of k , the mass transfer coefficient. Equations (1) and (2) can be written in terms of k instead of α . The use of the exchange coefficient in the model equations followed the water resources engineering convention for dissolved oxygen models using the reaeration coefficient.)

Figure 8b shows a positive relationship between Nu and the grouping $(d_s/B)(d/B)(Re)^2(Sc)^2$. Similar multiplicative power law relationships have been observed in many mass transfer operations [Bird et al., 1960; McCabe and Smith, 1967; Welty et al., 1969]. For mass transfer to a flat plate it has been shown by dimensional analysis [Welty et al., 1969] that the Nusselt number is a function of the Reynolds and Schmidt numbers. In the storage zone problem two additional parameters, d_s and B , are present. Thus the appearance of the channel and storage zone aspect ratios is consistent with other mass transfer correlations.

In Figure 8b there is a separation of data points between points from Thackston and Schnelle [1970] and those from the papers of Pedersen [1977] and Nordin and Troutman [1980]. Each set follows the same trend. The point for Uvas Creek is closest to the grouping of the Pedersen [1977] and Nordin and Troutman [1980] points and it is located in the range of a very low Nusselt number. We cannot explain the

separation of the data points; however, we can mention a few possibilities. First, there may in fact be fundamental limitations to the storage zone model that preclude any understanding in terms of measurable stream parameters. Second, the differences between authors in the methods by which the model parameters were determined may be so great as to bias or obscure certain physical trends. Finally, Thackston and Schnelle [1970] use data collected 'on relatively short, smooth, and uniform reaches.'

While we do not know the details of the physical characteristics of the other streams studied, we can assume from information given in the reports that the streams are not mountain pool-and-riffle streams and that they have considerably greater volumetric flows and velocities than Uvas Creek. Given the differences in physical conditions, we expect the points for Uvas Creek to be outliers.

Of course, none of this discussion 'proves' the model and, in fact, it shows the model to be a simplification of the physical processes of transport in a mountain stream. The simulation does reproduce the observed transient storage and it can be understood, at least qualitatively, in terms of the storage zone concept. As such, these simulations provide a good empirical transport framework for mountain streams, on which basis the analysis of other solute behavior, for example, solute-sediment interactions, can be pursued with confidence.

Acknowledgments. Most of the chemical data used in this report first appeared in a work by Zand et al. [1976]. Tabular summaries of this and other data on Uvas Creek were made available by G. W. Zellweger and R. J. Avanzino. All the information on Uvas Creek, including the previously unpublished detailed channel cross sections, were obtained under the direction of V. C. Kennedy in cooperation with S. M. Zand. The authors also benefitted from discussions with A. P. Jackman (University of California, Davis) regarding prior applications of storage models and results of his research (supported by the U. S. Geological Survey) on solute transport in Uvas Creek.

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