ESTIMATION OF TRANSIENT STORAGE PARAMETERS FROM A STREAM TRACER STUDY

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ABSTRACT: A stream tracer study was conducted in a 320-m reach of Indian Creek in Philadelphia. The objective was to investigate the role of geomorphology in the transport and exchange of a conservative tracer. The study reach has three geomorphicaly distinct sub-reaches. The experiments were simulated using the transient storage model, whose parameters were estimated by nonlinear optimization. Sub-reach averaged parameters were generally different highlighting the role of geomorphology; parameters estimated from sub-reach 1 provided relatively poor predictions for sub-reaches 2 and 3. Three forms of objective functions were used. The ordinary least square resulted in good fit around the peaks of the breakthrough curves and a relatively poor fit for the tail. The converse occurred when a weighted least square objective function was used.

KEY TERMS: stream tracer study; geomorphology; transient storage

INTRODUCTION

The transport of solutes in streams is affected by mechanisms such as transient storage and dispersion. Transient storage can occur when solute moves laterally into the banks of the stream, flows into the sediment bed or enters areas of the stream surface water that have slow moving or eddying pockets of water (Mullholland *et al* 1997; Fernald *et al*, 2001). The streambed and banks are commonly combined to form a region of the stream known as the hyporheic zone. The physical mechanism influencing the interaction between surface water and surface/subsurface storage zones is geomorphology (Harvey and Bencala 1993; Runkel, 1998). Changes in stream gradient, channel width, sediment composition, streambed topography, and stream curvature are examples of stream geomorphologic characteristics that influence the exchange.

Transient storage of stream water is studied due to the potential of stream water chemistry being altered from the biogeochemical reactions that occur within the active stream channel and hyporheic zone (Mcknight et al, 2002). These reactions occur due to the difference in biochemical properties between the sediments that are rich in microorganisms and the surface water that tends to be rich in dissolved oxygen (DO) and other dissolved nutrients, such as nitrate (Arboretum, 1995). Numerous studies have observed biological activity in the hyporheic zone where oxygen is supplied from the stream. For instance, Dahm *et al* (1987) reported that the average dissolved organic carbon (DOC) concentration increased from 12.5 mg/L in the well-oxygenated zones beneath the channel to 37.7 mg/l in the anaerobic zone at larger depths. Grimm and Fisher (1984) reported high metabolic rates of nitrate disappearance in the hyporheic zone. Mcknight *et al* (2002) examined the modification of DOC's concentration and composition when stream water interacted with chemically reactive streambed sediments.

This research proposed to determine role of stream geomorphology in the transport of conservative solutes in streams. This was evaluated by determining transient storage parameters generated from multiple breakthrough curves. Breakthrough Curves were developed from a tracer injection experiment in Indian Creek. The role of geomorphology was determined by (1) estimating parameters from a reach and using them to quality exchange at different scales (namely larger scales) and (2) relating the estimated parameters to geomorphology.

STUDY AREA

Indian Creek is located outside of the lower Piedmont section of the Wissahickon Watershed in Philadelphia, Pennsylvania. The studied reach consists of three geomorphicaly distinct sub-reaches (Figure 1). The first sub-reach (0-

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85 m) consists of three pool and three riffle sections with moderately sized stream widths, gradual stream slopes, and virtually free of large cobbles and large woody debris within the main channel. The second sub-reach (85-185 m) is more variable than the first section, which has a combination of large and small stream widths and much more large woody debris and large sized cobbles than the first section. The third sub-reach (185-323 m) is much different than the first. Large boulders, sharp stream bends, multiple step-pools, a channel split, steep gradients, and variable stream widths characterize the stream channel and banks. The second sub-reach may be viewed as a geomorphic transition zone between the first and third region. Stream gradients averaged 1.8% for the first sub-reach, 3.0 % for the second sub-reach, and 5.1% for the third sub-reach. Approximation of the stream flow rate was done by measuring cross-sectional area and stream water velocity. A *Global Flow Probe* velocity meter was used to measure stream water velocity. Results indicate that the stream flow rate is about 0.1 m^3/s. The bedrock underlying the region is Wissahickon Shist (National Institute for Environmental Renewal, 2000). Stream and gravel bar sediments are primarily composed of small pebbles (1 mm) to large boulders (0.5 m). The bank sediment is composed of silty clay. Average hydraulic conductivity's for the sediment bed and stream banks are 0.10 cm/s and 6.6×10^{-5} cm/s. Physical measurements of the stream cross-sectional area were made in the first sub-reach. This was done so that the physicality of estimated parameters could be evaluated. The cross-sectional area (m^2) was measured for the following reach lengths: 0-21m; 0.43, 21- 51m; 1.29, 51-58m; 0.50; 58-69m; 0.46, and 69-85m; 0.38.

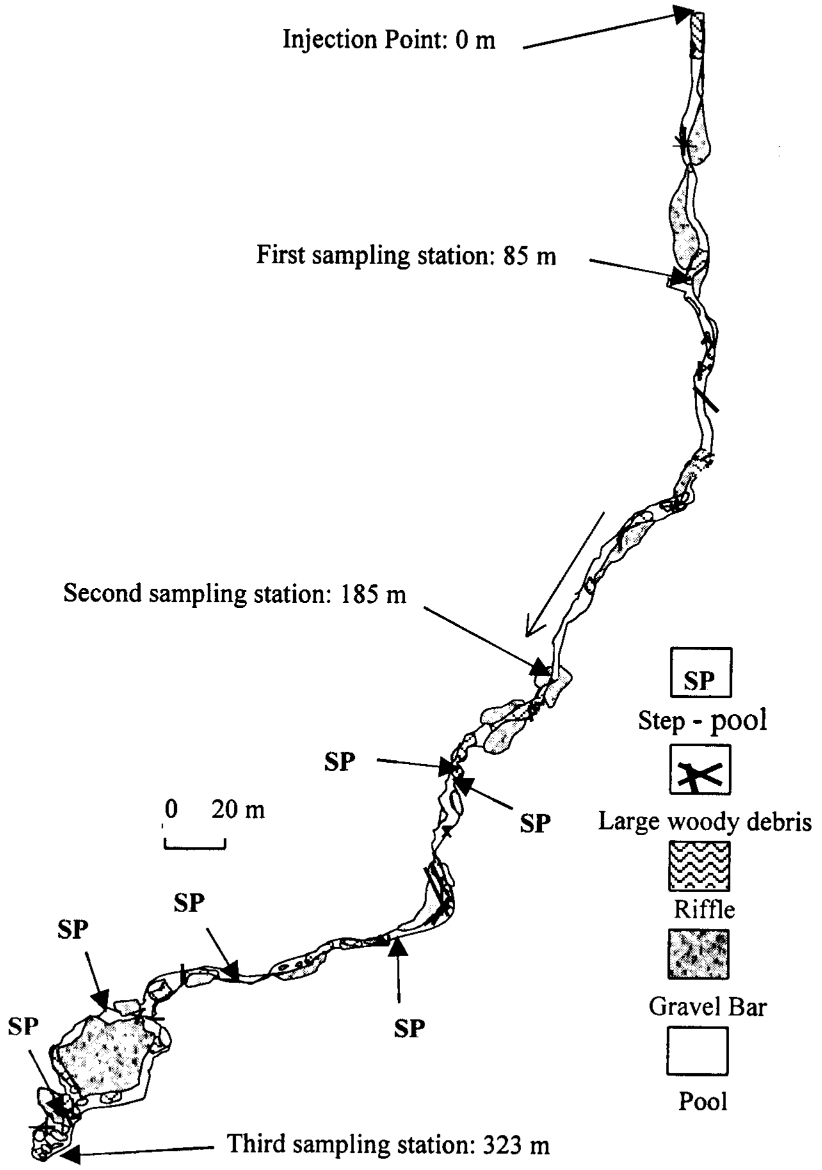

Figure 1. The studied stream reach at Indian Creek

METHODS

The exchange between streamwater and subsurface water is currently quantified using stream tracer studies (Bencala, 1983; Fernald *et al*, 2000). A stream tracer study consists of injecting a tracer into the streamwater at a selected location and monitoring streamwater concentration downstream. A breakthrough curve is obtained and used to determine exchange mechanisms affecting the transport of the tracer. The stream tracer experiment conducted at Indian Creek involved a "short" injection duration, which means that the tracer would not propagate far in the hyporheic zone. As a result, the main storage zones considered were the near surface hyporheic zone or sediment bed and the surface water "dead zones" (Runkel, 1998). The sizes of dead zones are as much of a function of geomorphology as the hyproheic zone, therefore, their dimensions are variable throughout a stream. Changes in stream flow- rate, stream curvature, cobble size, and large woody debris within the channel are major factors controlling these storage areas. Surface water storage zones can result from (1) turbulent eddies generated by large-scale bottom irregularities, (2) large but slowly moving zones along the sides of pools, and (3) well -mixed re-circulating zones located behind flow obstructions, such as cobbles, small boulders, and vegetation (Bencala and Walters, 1983). A decrease in stream flow rate coupled with an increase in cross-sectional area could create large storage areas. The inverse would be true for a larger flow rate with smaller cross-sectional areas.

The following methodology was pursued to obtain multiple breakthrough curves and estimate the stream transient storage parameters; (1) Conducted a stream tracer experiment and measured the streamwater concentration at downstream locations for various times (2) Stream exchange parameters were estimated using O-STREAM (Optimization Stream). This simulation code estimated the parameters using an objective function and equations (1) and (2). The transport parameters were linked to geomorphology by estimating spatially distributed values and using them to quality exchange at larger scales.

This tracer study focused on using a conservative tracer. It was assumed that transport of the tracer (solute) may be simulated using the one-dimensional advection- dispersion equation within the channel with additional terms that account for solute exchange with surface and subsurface storage zones. The governing equations that were used are:

$$\frac{\partial C}{\partial t} = -\frac{Q}{A}\frac{\partial C}{\partial x} + \frac{1}{A}\frac{\partial}{\partial x}\left(AD\frac{\partial C}{\partial x}\right) + \frac{q_{LIN}}{A}(C_L - C) + \alpha(C_s - C) \tag{1}$$

$$\frac{dC_s}{dt} = \alpha\frac{A}{A_s}(C - C_s) \tag{2}$$

where t and x are time and direction along the stream, respectively; C, C_s, and C_L are the concentrations of the stream, storage zones, and regional groundwater [M/L^3], respectively; Q is the in-stream volumetric rate [L^3/T]; D is the longitudinal dispersion coefficient in the stream [L^2/T]; A and A_s are the stream and storage-zone cross-sectional areas [L^2], respectively. The storage zone area, A_s, is the sum of the hyporheic zone area and the surface water storage zones; q_{LIN} is the lateral inflow rate from the banks per unit stream length [L^2/T]; α is the storage exchange coefficient [T^{-1}]. High values of α represent a higher ability for exchange between storage zones and streamwater. These parameters are estimated by fitting a simulated curve to an experimental breakthrough curve. The entire reach was divided into discrete segments. Equations (1) and (2) were applied to each segment to account for the change in the concentration in the main channel and the storage zones. Equations (1) and (2) were simulated using O-STREAM (Optimization Stream), a finite difference code developed in the Department of Civil and Environmental Engineering at Temple University.

Sodium Chloride (NaCl), a conservative tracer, was injected at a concentration of 54 g/l using a step-pulse method. The tracer was held in four 350 gallon high-density polyethylene tanks and released through a 5 cm manifold that was placed across the stream at the injection point. Prior to injection the tracer was well mixed and circulated throughout the tank to create uniform concentration. The tracer was pumped from the tanks through flexible 4 cm PVC hose to the manifold with a self-priming pump at 1 L/s. The entire injection time lasted 81 minutes. Three sampling station were located at 85m, 185, and 323 m as depicted in Figure 1. Samples were retrieved in pre-washed polyethylene bottles. The samples were analyzed for electrical conductivity, which were then converted to total dissolved solids (TDS). To do this, a calibration curve was developed using laboratory standards that had known TDS concentrations and a *Pinpoint* salinity monitor which had a sensitivity rage from 0.0 –200 mS. After analyzing each sample using this process a breakthrough curve was developed. Figures 2 through 5 show plots of observed data for all stations. O-STREAM was used for parameter estimation. O-STREAM consists of two modules: one module is a Fortran Code that solves equations (1) and (2) and the other is the optimization software GRG2 (Lasdon *et al*, 1978). GRG2 requires the user to provide it with an objective function to minimize. The objective function that we used is:

$$F_{obj} = \sum_{i=1}^{N} \left(\frac{C_o(i) - C_m(i)}{C_o(i)^m} \right)^2 \qquad (3)$$

where $C_o(i)$ is the observed concentration, $C_m(i)$ is the simulated concentration at time t, N is the number of samples, and $\frac{1}{(C_o(i))^m}$ is the weight function. The weight function provides an increase or decrease in sensitivity to the higher concentrations along the breakthrough curve. For example, with $m= 0$, termed ordinary least squares (OLS), the fitting algorithm gives more weight to the higher concentrations on the breakthrough curve. With an m value equal to 2, termed weighted least squares (WLS), the fitting algorithm gives more weight to the lower concentrations on the breakthrough curve. When $m=1$ this is an intermediate scenario.

Parameters were estimated for all three sub-reaches of Indian Creek using m = 0, 1, and 2. Upstream observed breakthrough curves were used as input to develop the simulated breakthrough curves. The final estimated parameters are in Table 1. The values presented in this table are the result of a global minimum being found between the simulated and observed data, therefore, these values were the most reliable out of the entire estimation process. Plots of the simulated and observed data for the values are in Figures 2 through 5. For all stations there is little variability between the fits for all three m values. For the third station all three simulations were consistent with one another but all undershot the peak concentration. This is because O-STREAM cannot simulate a splitting stream. But generally, one may consider that the model was able to simulate the major features.

Table 1: Estimated transient storage parameters for Indian Creek

Parameter	0-85m			85-185m			185-323m		
	$m=0$	$m=1$	$m=2$	$m=0$	$m=1$	$m=2$	$m=0$	$m=1$	$m=2$
Stream flow rate, Q (m^3/s)	0.044	0.046	0.048	0.052	0.052	0.052	0.041	0.041	0.041
Dispersion coeff, D (m^2/s)	0.07	0.05	0.05	0.17	0.16	0.16	0.22	0.19	0.18
Cross-sectional area, A (m^2)	0.82	0.89	0.89	0.73	0.73	0.73	0.78	0.77	0.77
Exchange coeff., α (1/s)	5.17×10^{-4}	3.24×10^{-4}	2.60×10^{-4}	1.32×10^{-4}	1.35×10^{-4}	1.33×10^{-4}	6.25×10^{-5}	7.05×10^{-5}	7.45×10^{-5}
Storage area, A_s (m^2)	0.20	0.21	0.22	0.21	0.23	0.26	0.50	0.50	0.50
Lateral infl. rate, q_{LIN} (m^3/s m)	9.87×10^{-5}	5.39×10^{-5}	7.12×10^{-5}	1.40×10^{-4}	1.40×10^{-4}	1.40×10^{-4}	2.31×10^{-5}	2.32×10^{-5}	2.47×10^{-5}

As Table 1 can reveal, all three stream reaches have a similar stream flow rate. If the injection period had been longer, for instance 72 hours, a noticeable change in stream flow rate might have been detected. Stream flow rate mainly shows its sensitivity with the high concentrations or on the overall height of the breakthrough curve. For all three stations the match between the simulated and observed data at the high concentrations is quit close giving further notification of the reliability of the modeled values. Table 6.1 shows that prior physical measurements of 0.1 m^3/s are more than double the value O-STREAM derived. Based on visual observation, the stream stage during the time period when the stream flow rate was physically measured was considerably larger than the stream stage when the tracer experiment took place. Considering this, the model derived values of 0.5 and 0.4 m^3/s therefore appear to be reasonable estimates of the stream flow rate.

The dispersion coefficient, D, increases going down stream. This was unexpected due to the increase in turbulent water going downstream from the increase in stream slope. Turbulent water should have decreased the dispersion coefficient. Although, what could have contributed to the increase in the dispersion coefficient was the small stream cross-sectional areas in the second and third sub-reaches. When stream cross-sectional areas decreased this could have increased the stream velocity therefore increasing longitudinal dispersion. Since the dispersion coefficient represents overall dispersion the pulses of increased longitudinal dispersion could have created an overall larger dispersion coefficient. Also, what could have contributed to dispersion were the increasing storage areas shown from the storage coefficients. When the storage areas increased tracer could have been routed into the storage areas and therefore dispersed the concentration. And as expected, the storage coefficient does show a slight increase going down stream.

The cross-sectional area, A, is consistent throughout the stream. There is a slightly larger area between 0-85 m. From visual observation the cross-sectional areas in the second and third sub-reaches have a large variability. Apparently, this variability had a general cross-sectional area that resembled that of the first sub-reach. On average, the measured cross-sectional areas are 25% smaller than the estimated values. This 25% decrease is probably due to a smaller stream stage during the time period when the cross-sectional area measurements were made in comparison to the stream stage during the tracer experiment. From this it can be initially stated that estimates of *A* are physically based. But determining the overall physicality of estimated values of *A* cannot be determined without duplicate studies.

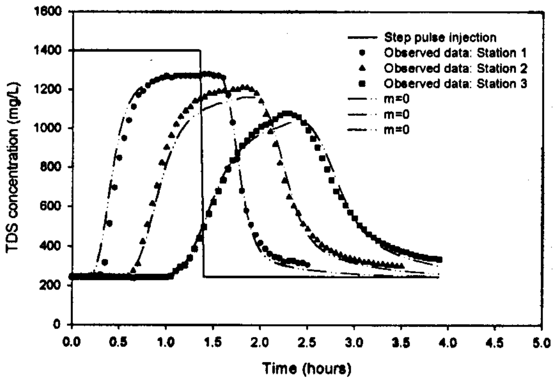

Figure 2. Fit between simulated and observed data using uniform parameters; *m*=0

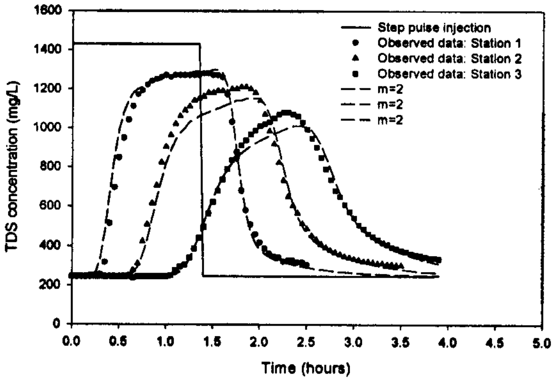

Figure 3. Fit between simulated and observed data using uniform parameters; *m*=2

The exchange coefficient, *α*, shows a gradual decrease from 0 to 185 m and a relatively large decrease from 185 to 323 m. Since stream gradient is a major mechanism for exchange, the opposite was expected to occur due to an increase in stream slope going downstream. Other factors that could contribute to the magnitude of exchange between stream water and the storage areas are flow rate, hydraulic conductivity, and storage area. The flow rate should not have been a factor in this case due to its uniform value through the stream. What could have been a determining factor was a possible slight overall decrease in hydraulic conductivity going down stream. Starting from the second station at 185m there starts an increase in the number of bedrock outcroppings within the streambed. This could have ultimately lessened the exchange with the near-surface hyporheic zone because of solid rock's low permeability. Going downstream the storage area increases. When coupling large stream gradients with increasing storage areas one would expect the magnitude of exchange to increase but as can be seen that was not the case. This finally suggests that *α* was not increased by the increase in stream gradient. Its decrease going downstream was due to other geomorphologic properties such as stream meandering or cross-sectional area.

The storage area, A_s, as previously mentioned shows an increase going down stream, which was expected. The large number of surface water dead zones that begin to increase at the second station from large woody debris, in-stream boulders, and stream bends creates surface storage areas.

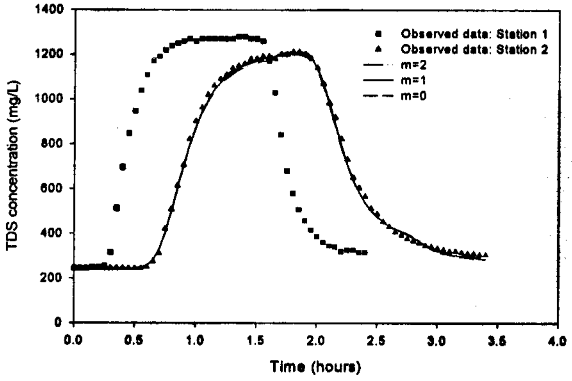

Figure 4. Fit between simulated and observed data at station #2: 185 m

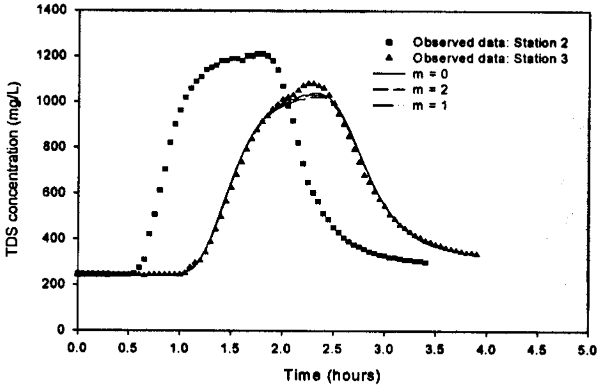

Figure 5. Fit between simulated and observed data at station #3: 323 m

The lateral inflow rate, q_{LIN}, was found to gain in the second reach developing an inflow rate. Therefore this suggests that in this region the groundwater entered the stream channel. From this it can be assumed that 85- 185 m is a gaining sub-reach. This is consistent with the increase in flow rate for the second subreach.

Figures 2 and 3 are plots using uniform parameters for all stations using m=0 and m=2. The estimated parameters were found for the first sub-reach and then used to simulate transient storage for the second and third sub-reaches. The m values equal to 0 and 2 were only used to test both extremes. There is agreement between the parameters with both m values. The fit for all breakthrough curves using one uniform set of parameters is quite poor revealing that estimating the parameters on a uniform basis is not a promising method to quantify exchange. Having close resemblance in parameter values but very different fitting qualities indicates a high sensitivity in these parameters. The spatially estimated parameters shown in Table 1 along with poor fit found with uniform parameters for all reaches ultimately attests that geomorphology has a large effect on the exchange parameters. This finally suggests that using parameters estimated to quantify exchange for one stream reach does not fully quantify the exchange for another downstream reach because significant changes occur even over short distances. This data is consistent with Bencala (1983).

CONCLUSION

Due to the shape of the simulated breakthrough curves for the second and third sub-reaches (Figures 2 and 3) it can be suggested that quantifying exchange for larger reaches dampens the effects of Q, α, and possibly A_s when uniform parameters are used. The reason being, Q effects the maximum concentration of the breakthrough curve, α has a consistent sensitivity in the top left hand corner and tail, and A_s has a somewhat unpredictable sensitivity but many times shows a clear effect in the top left hand corner as well. Based on the variable parameters estimated for all three sub-reaches (Table 1), the poor fit using uniform parameters, and the cumulative effects A_s, Q, and α have on the breakthrough curve it can be concluded that the magnitude of exchange between stream water and storage zones is highly irregular for stream reaches with varying geomorphic characteristics.

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