Integrated Experimental and Computational Hydraulic Science in a Unique Natural Laboratory

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1 Introduction

This chapter is concerned with the initial stage of investigations into stream metabolism, which can be studied by quantifying the fate and transport of dissolved oxygen. In this, for a given stream reach we would perform an oxygen mass balance to determine the rate of endogenous oxygen production (photosynthesis) and consumption (respiration). Before undertaking the oxygen mass balance, however, we need to determine the flow and transport characteristics of the stream, such as discharge, lateral inflow, velocity, surface gas exchange, mixing rates, relative volumes of flowing versus stagnant stream water, etc. Some of these quantities are required in order to perform the oxygen mass balance; others are determined because we hypothesise that they directly influence stream metabolism and therefore will be useful correlates. Most of these characterising parameters may be found through the analysis of tracer experiments. In such experiments, we release a discrete (known) mass of tracer and then measure tracer concentration-time profiles at locations downstream of the tracer release site. In this study, we obtain these parameters by fitting a computational stream transport model to the tracer data. This requires an efficient and accurate numerical solution of the advection–dispersion–transient storage equation and a reliable optimisation approach. The aim of this chapter is to describe our integrated experimental and computational approach and to present the findings for the study site in question. Because we performed these experiments twice (in early spring and in late summer), we are able to discuss

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seasonal changes and seasonal constants in the flow and transport parameters. The emphasis of this chapter is on the transient storage parameters.

2 A Unique Natural Hydraulics Laboratory

The study watershed is situated in south-west Iceland (64°05′ N, 21°30′ W) on the mid-Atlantic ridge between the North American and Eurasian tectonic plates and is characterised by intense volcanic and geothermal activity (Arnason et al. 1969; Franzson et al. 2005). Heating of the stream water is by steam from boiling geothermal water reservoirs, which heats up the upper cold groundwater that feeds the streams (Arnason et al. 1969). The water chemistry is very similar between streams despite large temperature differences. Precipitation, which exceeds 3,000 mm per year, infiltrates the porous volcanic bedrock (Einarsson 1984) and numerous small permanent streams, mostly groundwater fed, emerge from the valley side and discharge into the River Hengladalsá (Friberg et al. 2009).

Before human settlement in Iceland (900 AD), birch woodland and scrub covered the area with unbroken heathland vegetation continuing up to 500–600 m elevation.

The catchment comprises a higher plateau region connected to a lower floodplain by a narrow river gorge. The lower floodplain is surrounded on all sides by steep valley sides. Apart from the moss cover and sparse grassland of the plateau and plain, there are extensive areas stripped of vegetation and soil where rocks of volcanic origin protrude. Allochthonous organic matter input to the streams is therefore considered minimal beyond the dissolved organic carbon coming from the groundwater. Long-term landscape change is the only known anthropogenic pressure on the streams investigated (Simpson et al. 2001).

Sixteen streams in the same watershed were available for experiments with flows ranging from 1 to 16 L/s, typical stream widths varied from 0.25 to 1.25 m and depths were of the order of 0.1–0.4 m.

3 Tracer Experiments

For each experiment, YSI600xlm multi-parameter sondes (YSI, Yellow Spring, USA) were placed at two longitudinal stations (typically 60 m apart) in the study stream and set to record conductivity at fixed 10 s intervals. Pre-weighed NaCl was fully dissolved in 2 L of stream water and then immediately released into the stream at some distance upstream of the upper station. The mixing zone was generally sufficiently long (~11 m) for complete cross-sectional mixing to take place before the upper station. In the shortest streams, additional deflectors and pools were created upstream of the upper station to increase mixing. Any naturally occurring background conductivity signal was subtracted from the observations prior to the modelling. A typical conductivity versus time graph is shown in Fig. 1. Although there were 16 streams in

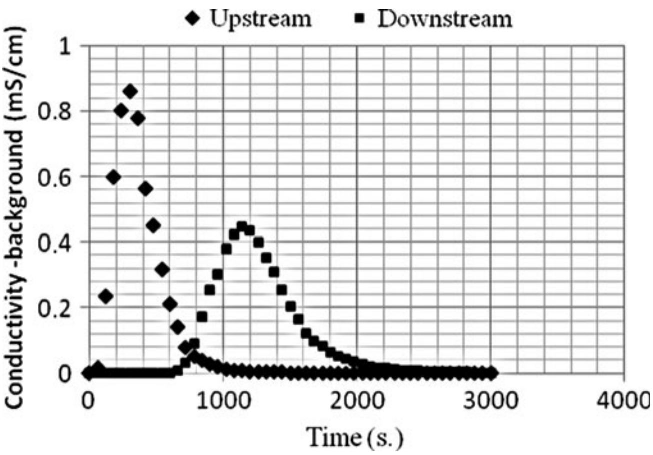

Fig. 1 Typical tracer result showing the spreading of the tracer cloud due to dispersion and transient storage effects

our study site, and we visited the area twice, we do not have 32 experiments to analyse. In our second visit, time and weather conditions prevented us from returning to some of the streams. However, we do have several paired experiments (spring, summer) to present here and a large pool of experimental data for combined analysis.

4 Obtaining Hydraulic Parameters Computationally

The transport of a conservative tracer in a stream with transient storage regions may be described by the following mass conservation equations:

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} + k_1(s - c) - \frac{q}{A}c \quad (1)$$

$$\frac{\partial s}{\partial t} = -k_1\frac{A}{A_s}(s - c) \quad (2)$$

where c is the concentration of tracer in the main channel, s is the concentration of tracer in the transient storage zone, A is the stream channel cross-sectional area, A_s is the transient storage cross-sectional area, D is the longitudinal dispersion coefficient, k_1 is the solute exchange parameter between the main channel and the storage zones, q is the lateral inflow, x is the longitudinal spatial co-ordinate and t is time.

For the experiments described herein, we are concerned with solving these equations over some stream reach length, L, and over some time interval, T, during which the tracer experiment takes place. Thus any parameters derived are recognised as being reach average values. Solutions to these equations are functions of space and time: $c(x, t)$ and $s(x, t)$. The following boundary conditions are appropriate for the scenario in these experiments. At the upstream boundary, the tracer concentration entering the reach is specified for all time, $t = 0$ to T; at the downstream boundary, a zero diffusive flux is assumed which implies that solute is advected out of the domain unhindered. For the initial conditions all concentrations are assumed to be zero at $t = 0$. The data required to furnish the upstream boundary condition is supplied by the observed conductivity data from the upper end of the study reaches.

The model equations are discretised using a control (or finite) volume approach, evaluating the advection term explicitly in time using a semi-Lagrangian method (Manson and Wallis 1995) and by evaluating the dispersion and transient storage terms implicitly in time using the Crank–Nicolson method, which apportions equal weight to both present and future values of c and s (Hoffman 1992). The solution consists of estimates for c and s over some discretised spatial and temporal domain, i.e. (c_i^m, s_i^m) for $i = 1$ to n_x and $m = 1$ to n_t, where n_x is the number of points in the spatial domain and n_t is the number of points in the temporal domain. Note that the spatial domain is divided into $(n_x - 1)$ cells of size Δx and the temporal domain is divided into $(n_t - 1)$ time steps of size Δt. Equation (1) is an advection–diffusion–decay equation and represents a considerable challenge to existing numerical methods. In order to achieve a satisfactory solution, the DISCUS method (Manson and Wallis 1995, 2000) is adopted. This method employs a conservative semi-Lagrangian algorithm that combines a control volume discretisation, the method of characteristics and a flux-based interpolation scheme. The method and its accuracy portrait is explained in detail elsewhere (Manson et al. 2001), but note that in this work, in contrast to earlier applications of this model, the Crank–Nicolson method is adopted for the dispersion and transient storage terms. The discretised form of these equations is a coupled pair of equations linking c_i and s_i to their neighbouring cells for the whole computational domain at the future time level, $n + 1$,

$$\alpha_i c_{i-1}^{n+1} + \beta_i c_i^{n+1} + \gamma_i c_{i+1}^{n+1} + \delta_i s_i^{n+1} = \varepsilon_i \tag{3}$$

$$\beta_i^s c_i^{n+1} + \delta_i^s s_i^{n+1} = \varepsilon_i^s \tag{4}$$

in which $\alpha_i, \beta_i, \gamma_i, \delta_i, \varepsilon_i, \beta_i^s, \delta_i^s, \varepsilon_i^s$ are coefficients related to both physical and numerical parameters. Since there are $(n_x - 1)$ cells, the resulting $2(n_x - 1)$ equations are assembled into a matrix and solved to give c_i^{n+1} and s_i^{n+1} for each computational cell. Note that (4) may be used to eliminate the transient storage term from (3) before it is solved.

The model prediction for concentration versus time at the downstream end of the experimental reach was fitted to the observed data at the lower end of the study reach, which had been collected at n_t points in time. A fitting parameter may be defined as:

$$E = \sum_{m=1}^{n_t} \left(c_{n_x}^m(\text{observed}) - c_{n_x}^m(\text{predicted}) \right)^2 \tag{5}$$

The model fit to the observations was optimised by adjusting the parameters (u, D, k_1, A_s/A) strategically in order to minimise E. Note that lateral inflow (q) was obtained directly from solute dilution calculations and was therefore not adjusted as a fitting parameter. The parameter optimization was undertaken with a direct search method, this being a SIMPLEX method of the Nelder–Mead variety (Lagarias et al. 1998). The numerical solution was coded in FORTRAN and then compiled and linked with the MATLAB mex libraries to create a dynamic linked library, which is a callable function within MATLAB.

5 Results and Discussion

5.1 Pooled Analysis

The model was optimised to several tracer data sets from both the summer and spring conditions to obtain stream transport parameters (u, D, k_1, A_s/A) over a range of flow conditions (flows varied from 1 to 16 L/s in the experiments considered). Figure 2 shows a plot of the transient storage exchange parameter (k_1) versus flow velocity. We might expect that these parameters would correlate with each other; at larger velocities the shear gradient across the boundary layer will be larger with consequently larger mass transport. Admittedly the flow field in these small streams is much more complicated than the simple shear flow for which this exchange mechanism is envisaged and there is considerable scatter; however, we observe a fairly strong correlation ($R = 0.635$, $n = 16$) when a power law model is fitted; we

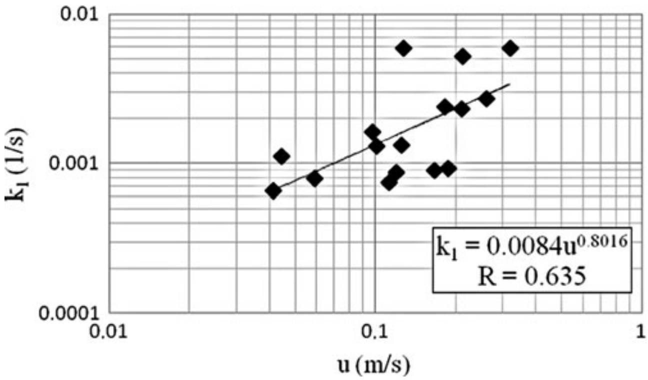

Fig. 2 Plot of transfer coefficient (k_1) versus velocity (u) for all studied streams pooled from summer and spring

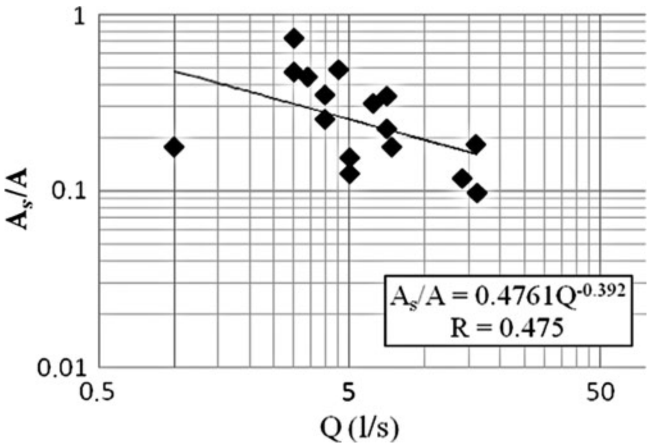

Fig. 3 Plot of fractional storage volume (A_s/A) versus discharge (Q) for all studied streams pooled from summer and spring

find that k_1 scales approximately with $u^{0.8}$. Note that these values of k_1 correspond with a range of transient storage residence times ranging from about 2 to 22 min. These values resonate with field observations.

Figure 3 shows the relationship between the ratio of transient storage volume to main channel volume, expressed as an area ratio on the basis that the reach length is common to both the stream channel and the transient storage zones (A_s/A) and discharge (Q). We observe an inverse power law relationship between A_s/A and discharge ($R = 0.475$, $n = 16$). In this watershed, we find A_s/A scaling approximately with $Q^{-0.4}$. We find for these streams that the transient storage volume varies from about 10% to 70% of the main channel volume. Once again there is some scatter, but these percentages seem reasonable when we consider in situ observations. The value of A_s/A obtained at the lowest flow appears to be an outlier, indeed it may reside in a different flow regime. If it were not included in the regression, the correlation would likely become stronger and the exponential decline steeper.

5.2 *Seasonal Analysis*

We observed several types of potential transient storage zones in these streams: seasonal development of aquatic plants, permanent moss cover, stones and deep pools. Table 1 summarises our expectations and observations. Generally, streams with large swathes of submerged and emergent aquatic vascular plants had less transient storage at the beginning of the spring (April 2009) than in late summer (August 2008), see Table 1 and Fig. 4, reflecting previous findings (Salehin et al. 2003; Ensign and Doyle 2005). The change in predicted transient storage in the

Table 1 Predictions and observations of seasonal changes in transient storage volume according to their nature

Sites	Nature of transient storage	Predictions (late summer to early spring)	Observations
2	Aquatic plants	−−	−
3	Aquatic plants	−−	−−
4	Stony bed	±	−
6	Stony bed	±	+[a]
7	Stony bed with moss	±	−
9	Stony bed (+ hyporheic zone?)	±	−
10	Stony bed with moss	±	+
11	Deep pools ($CaCO_3$ bed)	±	±
14	Stony bed	±	±

± = ±25% change, + or − = 25–50% change, ++ or −− = >50% change
[a]Extensive channel reworking and consequent geomorphological changes during the intervening winter.

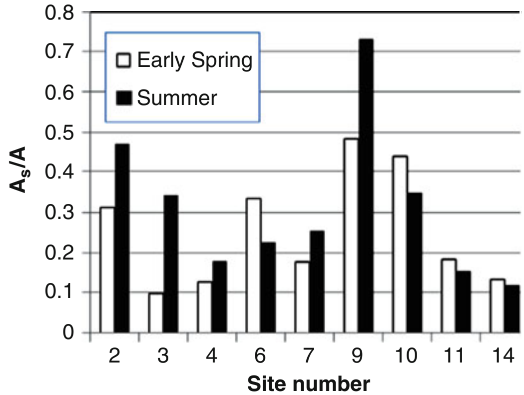

Fig. 4 Bar chart showing A_s/A for all sites for both early spring and summer

streams with more permanent structures such as moss cover and stones was generally slightly more variable than anticipated from the on-site observations of the stream characteristics, with no clear direction of change however.

Figure 5 shows some other interesting seasonal aspects of the system. First, velocities are higher in the early spring than in the previous summer. This is a direct consequence of the higher flows (the spring fed water being augmented by snow melt). We see a consistent increase in velocity (and flow) at virtually all sites and corresponding changes in the exchange coefficient.

We observe decreases in the exchange coefficient from early spring to late summer ranging from 35% up to 100%; these would impact the ecosystem with corresponding increases in the retention time in the transient storage zone. The increase in retention time would allow greater nutrient cycling in the transient storage zone over the growing season.

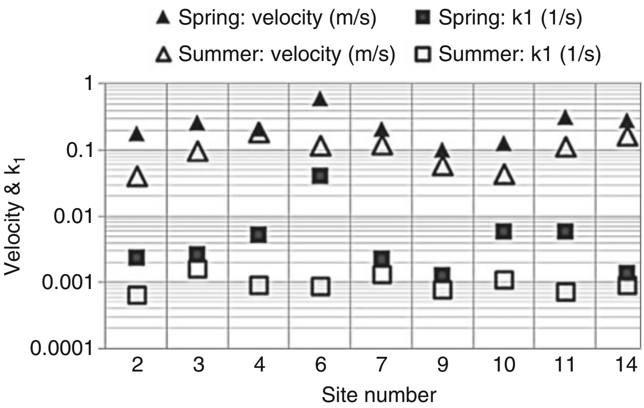

Fig. 5 Velocity and exchange coefficient for each site at both summer and early spring conditions

6 Conclusions

We have performed a stream transport characterisation of several streams within a unique watershed in Iceland as part of a larger stream metabolism study. Results have indicated that: (1) intrinsic exchange rate between main stream and transient storage zones scales with flow velocity; (2) the fractional transient storage volume scales inversely with flow rate; (3) stream transient storage volume can change significantly over the growing season, especially if submerged vascular plants are present and (4) retention time within the transient storage zone can increase by up to 100% over the growing season.

References

Arnason B, Theodorsson P, Björnsson S, Saemundsson K (1969) Hengill, a high temperature thermal area in Iceland. Bull Volcanol 33:245–259

Einarsson MA (1984) World survey of climatology. In: van Loon H (ed) Climate of the oceans, vol 15. Elsevier, Amsterdam, pp 673–697

Ensign SH, Doyle MW (2005) In-channel transient storage and associated nutrient retention: evidence from experimental manipulations. Limnol Oceanogr 50:1740–1751

Franzson H et al (2005) In: Proceedings world geothermal congress, Antalya, Turkey, pp 1–7

Friberg N, Dybkjaer JB, Olafsson JS, Gislason GM, Larsen SE, Lauridsen TL (2009) Relationships between structure and function in streams contrasting in temperature. Freshw Biol 54:2051–2068

Hoffman JD (1992) Numerical methods for engineers and scientists. McGraw-Hill, New York

Lagarias JC, Reeds JA, Wright MH, Wright PE (1998) Convergence properties of the Nelder–Mead simplex method in low dimensions. SIAM J Optim 9(1):112–147

Manson JR, Wallis SG (1995) An accurate numerical algorithm for advective transport. Commun Numer Methods Eng 11:1039–1045

Manson JR, Wallis SG (2000) A conservative, semi-Lagrangian fate and transport model for fluvial systems: Part 1 – theoretical development. Water Res 34(15):3769–3777

Manson JR, Wallis SG, Hope D (2001) Conservative semi-Lagrangian transport model for rivers with transient storage zones. Water Resour Res 37(12):3321–3329

Salehin M, Packman AI, Worman A (2003) Comparison of transient storage in vegetated and unvegetated reaches of a small agricultural stream in Sweden: seasonal variation and anthropogenic manipulation. Adv Water Resour 26:951–964

Simpson IA, Dugmore AJ, Thomson A, Vesteinsson O (2001) Crossing the thresholds: human ecology and historical patterns of landscape degradation. Catena 42:175–192