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An evaluation of analytical streambank flux methods and connections to end-member mixing models: a comparison of a new method and traditional methods

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10419

Abstract

In this paper, a novel method for estimating gross gains and losses between streams and groundwater is developed and evaluated against two traditional approaches. These three streambank flux estimation methods are distinct in their assumptions on the spatial distribution of the inflowing and outflowing fluxes along the stream. The two traditional methods assume that the fluxes are independent and in a specific sequence, while the third and newly derived method assumes that both fluxes occur simultaneously and uniformly throughout the stream. The analytic expressions in connection to the underlying assumptions are investigated to evaluate the individual and mutual dynamics of the streambank flux estimation methods and to understand the causes for the different performances. The results show that the three methods produce significantly different results and that the mean absolute normalized error can have up to an order of magnitude difference between the methods. These differences between the streambank flux methods are entirely due to the assumptions of the streambank flux spatial dynamics of the methods, and the performances for a particular approach strongly decrease if its assumptions are not fulfilled. An assessment of the three methods through numerical simulations, representing a variety of streambank flux dynamics, show that the method introduced, considering simultaneous stream gains and losses, presents overall the highest performance. These streambank flux methods can also be used in conjunction with other end-member mixing models to acquire even more hydrologic information as both require the same type of input data.

1 Introduction

Groundwater and surface water interactions are an important process in hydrologic systems (Winter, 1998). These interactions within and around streams and rivers impact decisions on municipal water supply extractions, water pollution, riverine habitat, and many others. To make better decisions on these impacts, the stream and ground

10420

water interactions (streambank fluxes) need to be accurately quantified as stream losses and gains can account for a substantial proportion of the total flow and chemical load of a stream.

In general, when people consider how to estimate the losses or gains along a stream reach they would take a discharge measurement upstream, a discharge measurement downstream, subtract the two values, and the result would be considered the gain or loss within the stream reach. Although this may be a relatively simple procedure to accomplish, the assumption that all flow within a stream reach must be either flowing into the stream or flowing out of the stream is in many cases an over simplification (Castro and Hornberger, 1991; Harvey and Bencala, 1993). Depending on local topography, geology, and the groundwater table, gains and losses into and out of the stream can be very dynamic even over short distances (Harvey and Bencala, 1993; Anderson et al., 2005; Payn et al., 2009). Consequently, what might have originally been estimated as a small gain to the stream from simply subtracting the upstream and downstream discharges might end up becoming a small loss out of the stream and a large gain into the stream. Without a proper method to estimate streambank fluxes, any attempt at estimating a water or nutrient mass balance would be difficult and laced with errors.

Harvey and Wagner (2000) and many other researchers use a more realistic conceptual model of flow pathways within a stream (Fig. 1). These major flow pathways include initial (or upstream) discharge (Q_{init}), final (or downstream) discharge (Q_{final}), stream gains from groundwater (Q_{in}), stream losses to groundwater (Q_{out}), and hyporheic flow (Q_{hyp}). In this conceptual model, Q_{in} is considered to be pure groundwater entering the stream, and Q_{out} is stream water permanently leaving the stream. Hyporheic flow occurs when stream water temporarily leaves the stream into the surrounding groundwater (or more specifically the hyporheic zone), but returns again to the stream at some downstream location. During this temporary departure from the stream, additional biochemical reactions may occur that would not necessarily have occurred while in the stream itself. The mass is still retained in the stream and not lost (permanently) to the groundwater. Although the hyporheic flow pathways do occur and can be very im-

10421

portant for stream ecosystems (i.e. the movement of oxygen into the hyporheic zone, nitrogen cycling, etc.), hyporheic flow will not be directly addressed in this study as the authors are most interested on fluxes that are permanently adding or removing mass over a significant length of stream. As hyporheic flows only temporarily leave the stream, the mass of the water is still retained over sufficient distances.

There are a number of methods to estimate gross stream gains and losses (Kalbus et al., 2006). The general categories are seepage meters, (heat or chemical) tracer tests, and hydraulic gradients derived from groundwater piezometers. Each has advantages and disadvantages. Seepage meters and groundwater piezometers are point measurements that can be accurate at a specific point, but in a heterogeneous system they may not represent the stream as a whole. On the other hand, chemical tracer tests are an aggregation of all fluxes along a stream reach, but do not represent any particular point along the stream. For this study, the focus is on the total aggregated flows over the stream reaches, so chemical tracer tests were found to be the most appropriate and inexpensive. Kalbus et al. (2006) and Scanlon et al. (2002) have a more thorough qualitative review of the different streambank flux methods.

Using chemical tracer tests for the source of data, the estimation of gross stream gains and losses is most frequently performed through numerical models like those similar to the OTIS model developed by the USGS (Runkel, 1998). While able to estimate fluxes in steady-state conditions, these types of models are primarily designed for non-steady-state conditions and provide many output parameters in addition to the inflow and outflow fluxes, and as a consequence require more input data than in steady-state conditions for estimating only streambank fluxes (i.e. stream cross-sectional area, flow advection, flow dispersion, etc). Additionally, the OTIS type models would require the estimation of parameters through a trial-and-error or an automated nonlinear least squares (NLS) procedure that are not directly measured. Under steady-state conditions, the data and parameter requirements for estimating only streambank fluxes are substantially lower requiring only discharge and tracer concentration measurements

10422

upstream and downstream. If steady-state is appropriate, then analytical methods are sufficient.

There are two traditional analytical methods to estimate streambank fluxes under steady-state conditions ignoring hyporheic flowpaths. These methods use simple mass balance equations to estimate both gains and losses within a stream reach and assume that the fluxes are independent and in a specific sequence. In this paper, a new analytical method has been developed using different assumptions on the spatial distribution of the inflowing and outflowing fluxes along the stream.

The goal of our study is to quantitatively evaluate the accuracy and sensitivity of the new method against the existing steady-state streambank flux tracer methods. This evaluation is performed through a combination of analytical comparisons and numerical stream simulations as described in the following sections.

2 Methods

2.1 Theoretical basis of the streambank flux tracer methods

All tracer based methods designed to estimate streambank fluxes start with the conservation of mass equations under steady-state conditions for both the tracer and the water flux and assume complete mixing of the individual flows:

$$Q_{\text{init}} C_{\text{init}} + Q_{\text{in}} C_{\text{in}} = Q_{\text{final}} C_{\text{final}} + Q_{\text{out}} C_{\text{out}} \quad (1)$$

$$Q_{\text{init}} + Q_{\text{in}} = Q_{\text{final}} + Q_{\text{out}} \quad (2)$$

where Q_{final} is the final discharge (in volume per unit time), C_{final} is the final concentration (in mass per unit volume), Q_{init} is the initial discharge, C_{init} is the initial concentration, Q_{in} is the discharge from the groundwater to the stream, C_{in} is the concentration of Q_{in} , Q_{out} is the discharge from the stream to the groundwater, and C_{out} is the concentration of Q_{out} .

10423

The two traditional streambank flux estimation methods mentioned in the introduction make specific assumptions on the distribution of gains and losses throughout the reach (see Fig. 2). The first method, we call “Loss–Gain”, assumes $C_{\text{out}} = C_{\text{init}}$, while the second method, we call “Gain–Loss”, assumes $C_{\text{out}} = C_{\text{final}}$. In both variants, the methods assume that the mixing of $Q_{\text{in}} C_{\text{in}}$ and $Q_{\text{out}} C_{\text{out}}$ are mixed separately and are mixed in a sequence defined by the above assumptions. The Loss–Gain variant assumes that the mixing sequence begins with Q_{out} followed by Q_{in} , while Gain–Loss is vice-versa.

Combining Eqs. (1) and (2), the solution for Q_{out} for Loss–Gain is:

$$Q_{\text{out,L-G}} = Q_{\text{init}} - Q_{\text{final}} \left(\frac{C_{\text{final}} - C_{\text{in}}}{C_{\text{init}} - C_{\text{in}}} \right) \quad (3)$$

Similarly, the equation for Q_{out} for Gain–Loss is:

$$Q_{\text{out,G-L}} = Q_{\text{init}} \left(\frac{C_{\text{init}} - C_{\text{in}}}{C_{\text{final}} - C_{\text{in}}} \right) - Q_{\text{final}} \quad (4)$$

To get Q_{in} for both methods, we need to include Eq. (2) into Eqs. (3) and (4):

$$Q_{\text{in,L-G}} = Q_{\text{final}} \left(\frac{C_{\text{final}} - C_{\text{init}}}{C_{\text{in}} - C_{\text{init}}} \right) \quad (5)$$

$$Q_{\text{in,G-L}} = Q_{\text{init}} \left(\frac{C_{\text{final}} - C_{\text{init}}}{C_{\text{in}} - C_{\text{final}}} \right) \quad (6)$$

If we use an artificial tracer (i.e. Bromide salt), we can safely assume $C_{\text{in}} \approx 0$ and the resulting equations are as follows:

$$Q_{\text{out,L-G}} = Q_{\text{init}} - Q_{\text{final}} \frac{C_{\text{final}}}{C_{\text{init}}} \quad (7)$$

$$Q_{\text{out,G-L}} = Q_{\text{init}} \frac{C_{\text{init}}}{C_{\text{final}}} - Q_{\text{final}} \quad (8)$$

10424

and Q_{in} becomes:

$$Q_{in,L-G} = Q_{final} \left(1 - \frac{C_{final}}{C_{init}} \right) \quad (9)$$

$$Q_{in,G-L} = Q_{init} \left(\frac{C_{init}}{C_{final}} - 1 \right) \quad (10)$$

5 These methods can be applied conceptually along a stream length as illustrated in the left and central scheme of Fig. 2. Q_{init} is the upstream discharge and Q_{final} represents the downstream discharge. Depending on the equation variant, Q_{in} is added or Q_{out} is removed from Q_{init} at the beginning of the stream and Q_{out} is removed or Q_{in} is added at the end of the stream resulting in a downstream discharge of Q_{final} . As these
10 methods make no assumptions about the exact location along the stream for Q_{in} and Q_{out} , they can occur over any length of the stream as long as they occur in sequence and independently.

From studies that tested multiple stream reaches for streambank fluxes, almost every stream reach had both gains and losses regardless of the method and of the reach
15 length (Anderson et al., 2005; Ruehl et al., 2006; Payn et al., 2009; Covino et al., 2011; Szeftel et al., 2011). Additionally, studies that have tried to identify the spatial distribution of groundwater inflows and outflows to and from the stream have found a wide variety of diffuse flow locations throughout the stream and were not limited to one or two flow locations every several hundred meters (Malard et al., 2002; Wondzell,
20 2005; Schmidt et al., 2006; Lowry et al., 2007; Slater et al., 2010). This indicates that even short stream reaches typically have many instances of gains and losses to and from the stream and that limiting the flux instances to one flux each regardless of the stream length may not be the most accurate assumption.

Following this rationale, this paper presents a novel method based on a different
25 assumption for the spatial distribution of streambank fluxes as compared to the Gain–Loss and Loss–Gain methods, namely that both Q_{in} and Q_{out} occur simultaneously and are constant throughout the entire stream section. This new method is denoted as

10425

“Simultaneous”. Equations requiring the same input data as the Gain–Loss and Loss–Gain methods are derived in Sect. 2.2 and length is integrated into the mass balance equation (Fig. 3).

2.2 Derivation of the method for simultaneous gains and losses

5 In this section, the fundamental equations of mass balance for the tracer and water flows will be applied on a control volume represented in Fig. 3 under the assumption of simultaneous and uniform gains and losses throughout the stream reach and stationarity in time in order to obtain the expressions predicting Q_{in} and Q_{out} as functions of Q_{init} , C_{init} , Q_{final} , C_{final} and C_{in} . First, applying mass balance for discharge:

$$10 \quad Q(x) + q_{in} dx = Q(x) + \frac{\partial Q(x)}{\partial x} dx + q_{out} dx \quad (11)$$

where x is stream length, $Q(x)$ is the discharge at length x , q_{in} is the added discharge per unit length of stream, and q_{out} is the lost discharge per unit of length. Both q_{in} and q_{out} are assumed constant for a given stream reach. In the one-dimensional and stationary case we can write $\frac{\partial Q(x)}{\partial x} dx = dQ$. After rearranging and integrating from the
15 beginning of the reach over an arbitrary length:

$$\int_{Q_{init}}^{Q(x)} dQ = \int_0^x (q_{in} - q_{out}) dx \quad (12)$$

which becomes:

$$Q(x) = Q_{init} + (q_{in} - q_{out})x \quad (13)$$

Then, applying mass balance for the tracer:

$$20 \quad C(x)Q(x) + C_{in} q_{in} dx = \left(C(x) + \frac{\partial C(x)}{\partial x} dx \right) \left(Q(x) + \frac{\partial Q(x)}{\partial x} dx \right) + C(x) q_{out} dx \quad (14)$$

10426

where $C(x)$ is the concentration at length x and C_{in} is the concentration of q_{in} . The inflowing concentration C_{in} is assumed constant for a given stream reach. Again in the one-dimensional and stationary case, we can write $\frac{\partial Q(x)}{\partial x} dx = dQ$ and $\frac{\partial C(x)}{\partial x} dx = dC$. Neglecting second order differentials and rearranging:

$$5 \quad Q(x)dC = C_{in}q_{in}dx - C(x)(dQ + q_{out}dx) \quad (15)$$

Substituting Eqs. (12) and (13) for $Q(x)$ and dQ respectively in Eq. (15), and rearranging:

$$dC = \frac{C_{in}q_{in}dx - C(x)[(q_{in} - q_{out})dx + q_{out}dx]}{Q_{init} + (q_{in} - q_{out})x} \quad (16)$$

Simplifying and integrating from the beginning of the reach over an arbitrary length x :

$$10 \quad \int_{C_{init}}^{C(x)} \frac{dC}{C(x) - C_{in}} = -q_{in} \int_0^x \frac{dx}{Q_{init} + (q_{in} - q_{out})x} \quad (17)$$

which becomes:

$$\ln \frac{C(x) - C_{in}}{C_{init} - C_{in}} = -\frac{q_{in}}{q_{in} - q_{out}} \ln \frac{Q_{init} + (q_{in} - q_{out})x}{Q_{init}} \quad (18)$$

Evaluating Eq. (13) for $x = L$, where L represents the total length of the stream reach:

$$q_{in} - q_{out} = \frac{Q_{final} - Q_{init}}{L} \quad (19)$$

15 Substituting Eq. (19) in Eq. (18) and evaluating for $x = L$:

$$\ln \frac{C_{final} - C_{in}}{C_{init} - C_{in}} = -\frac{q_{in}}{\frac{Q_{final} - Q_{init}}{L}} \ln \frac{Q_{final}}{Q_{init}} \quad (20)$$

10427

Calling $Q_{in} = q_{in} \cdot L$ and rearranging:

$$Q_{in,Sim} = (Q_{init} - Q_{final}) \frac{\ln \left[\frac{C_{final} - C_{in}}{C_{init} - C_{in}} \right]}{\ln \left[\frac{Q_{final}}{Q_{init}} \right]} \quad (21)$$

and the solution for Q_{out} is:

$$Q_{out,Sim} = (Q_{init} - Q_{final}) \frac{\ln \left[\frac{Q_{final} C_{final} - Q_{in} C_{in}}{Q_{init} C_{init} - Q_{in} C_{in}} \right]}{\ln \left[\frac{Q_{final}}{Q_{init}} \right]} \quad (22)$$

5 where $Q_{in,Sim}$ and $Q_{out,Sim}$ are the Simultaneous equations for the streambank fluxes into and out of the stream, respectively.

As with the previous methods, if we use an artificial tracer (i.e. Bromide salt) we can safely assume $C_{in} \approx 0$ and the resulting equations are as follows:

$$Q_{in,Sim} = (Q_{init} - Q_{final}) \frac{\ln \left[\frac{C_{final}}{C_{init}} \right]}{\ln \left[\frac{Q_{final}}{Q_{init}} \right]} \quad (23)$$

10 and

$$Q_{out,Sim} = (Q_{init} - Q_{final}) \frac{\ln \left[\frac{Q_{final} C_{final}}{Q_{init} C_{init}} \right]}{\ln \left[\frac{Q_{final}}{Q_{init}} \right]} \quad (24)$$

Naturally occurring tracers (i.e. Chloride salt) can also be applied to the Simultaneous equations with additional information about C_{in} . As long as a quasi-steady-state condition applies and that $Q_{in} > 0$, the only additional information to be collected would be

10428

the C_{init} and C_{final} prior to the injection of the tracer. The equation to solve C_{in} can be formulated from any of the streambank flux equations by setting itself equal to itself except replacing one side with the C_{init} and C_{final} prior to the injection of the tracer.

$$C_{in} = \frac{C_{init,prior} C_{final} - C_{final,prior} C_{init}}{C_{init,prior} - C_{init} - C_{final,prior} + C_{final}} \quad (25)$$

5 where $C_{init,prior}$ is the upstream concentration prior to the tracer injection, C_{init} is the upstream concentration from the tracer injection, $C_{final,prior}$ is the downstream concentration prior to the tracer injection, and C_{final} is the downstream concentration from the tracer injection. The only main disclaimer to the application of this equation in the field is that the difference between $C_{init,prior}$ and $C_{final,prior}$ must be large enough to be statistically significant when estimated using available laboratory or field measurement techniques. The accuracy of the measurement techniques is a general problem for any chemical tracer test performed to estimate streambank fluxes. If the difference between the Q_{init} and Q_{final} is very small, much tracer may be needed to accurately measure a concentration difference between C_{init} and C_{final} . This issue will become more important with larger rivers as the proportion of the Q_{in} and Q_{out} to the Q_{init} is substantially reduced.

It would also be possible to estimate C_{in} from groundwater piezometers adjacent to the bank of the stream. As the intent of our study was to determine integrated values over a stream reach rather than point values, we preferred to use Eq. (25) as it is an integrated value of C_{in} .

There might also be a need to estimate the groundwater concentration of other chemical compounds entering the stream in addition to the conservative tracer used to estimate the streambank fluxes. If other in-stream gains and losses in the new chemical compound can be neglected (i.e. without biochemical transformations), the only additional information needed would be the concentration of the new compound at the locations of Q_{init} and Q_{final} . The C_{in} of the new chemical compound can be estimated

10429

using the following rearrangement of Eq. (21):

$$C_{in, new} = \frac{\left(\frac{Q_{final}}{Q_{init}}\right) \left(\frac{Q_{in, Sim}}{Q_{init} - Q_{final}}\right) C_{init, new} - C_{final, new}}{\left(\frac{Q_{final}}{Q_{init}}\right) \left(\frac{Q_{in, Sim}}{Q_{init} - Q_{final}}\right) - 1} \quad (26)$$

where $C_{in, new}$ is the concentration of the new compound, $C_{init, new}$ is the upstream concentration of the new compound, and $C_{final, new}$ is the downstream concentration of the new compound. Any of the three streambank flux methods can be rearranged to calculate $C_{in, new}$ and they will all produce the same result.

The application of tracer methods to measure streambank fluxes in the field are typically performed by two different techniques: constant injection and slug injection. These two techniques have been well researched in the scientific community and will not be evaluated in this study (Wagner and Harvey, 1997; Payn et al., 2008). Both techniques can be used with the above streambank flux methods and provide very similar results. For simplicity, we will assume constant injection with steady-state conditions as the slug injection would require C_{final} to be integrated over time.

2.3 Evaluation methods

2.3.1 Analytics

All three streambank flux methods were broken down analytically to better understand the dynamics of the equations of the methods. We wanted to know what caused the differences in the results of the three streambank flux methods and how these differences were related. The relative differences between the methods was accomplished by the ratio of one method's equation to another both analytically and illustratively.

10430

2.3.2 Numerical simulations

Perfect measurements or estimates of streambank fluxes are impossible using any existing method. Arbitrarily comparing results of different methods using field collected data will only indicate that the different methods produce different results, and it will not indicate if one method is more accurate than another. Consequently, we thought that it would be appropriate to simulate an artificial stream with known streambank fluxes for comparisons. With streambank fluxes perfectly known, we could effectively evaluate the accuracy of the different methods.

We simulated the lateral inflows and outflows per unit length throughout a stream using an autoregressive integrated moving average (ARIMA) model performed using the `arima.sim` package in the R statistical computing environment (R Development Core Team, 2011). The routine generates a variety of artificial time series with both a randomness and memory component. In an attempt to create realistic simulations of the streams, we tuned the ARIMA model to have spatial flux dynamics based on studies using distributed temperature sensing (DTS) of groundwater inflows within streams (Lowry et al., 2007; Westhoff et al., 2007; Briggs et al., 2012; Mwakanyamale et al., 2012). The quantitative surrogate we used for the spatial flux dynamics was the average length that the fluxes would switch from inflow to outflow or vice-versa within a stream reach. For example, if we simulate a stream with 1000 m total length and the fluxes in this stream oscillates between inflows and outflows 10 times then the average length per switch would be 100 m. For our simulations, we used two different switch lengths of 100 m and 200 m and total stream lengths of 1000 m and 2000 m. The switch lengths had a strong linear relationship with the correlation lengths and resulted in correlation lengths of 40 m and 70 m for the switch lengths of 100 m and 200 m, respectively. Correlation length is commonly defined as the length at $1/e$ on the autocorrelation distribution (Blöschl and Sivapalan, 1995).

The ARIMA model allowed us to create 5000 simulations of stream fluxes within a hypothetical stream. We ran four series of 5000 simulations. Series A had a 1000 m

10431

stream length and a 100 m average switch length, Series B had a 1000 m and a 200 m average switch length, Series C had a 2000 m and a 100 m average switch length, and Series D had a 2000 m and a 200 m average switch length. The spatial discretization of the model was 1 m for all series and simulations. These four series of simulations were to test the effects of both length and intermittency on the stream flux methods. Without loss of generality, we defined $C_{in} = 0$ for the simulations, which would be equivalent to the use of an artificial tracer (i.e. bromide salt) for the tracer test.

We tested two distinct assumptions when deciding on the appropriate streambank flux ARIMA model. One assumption was that both Q_{in} and Q_{out} can occur simultaneously at one point. For example, if the groundwater table is sloped perpendicular to the stream then water would be flowing into one side of the bank, while water would be flowing out of the other side of the bank. In this assumption, we created two separate and independent vectors of Q_{in} and Q_{out} along the stream. The second assumption was that both Q_{in} and Q_{out} cannot occur simultaneously at one point. In this assumption, only one vector of streambank flux was created that could oscillate between Q_{in} and Q_{out} . We decided to omit the option for simultaneity of Q_{in} and Q_{out} throughout the stream as this assumption coincides with the assumption in the Simultaneous method and consequently the Simultaneous method was vastly superior to the other streambank flux methods. To ensure a more rigorous evaluation against the Simultaneous method, we decided to omit the ARIMA model assumption of simultaneity and only use the non-simultaneity assumption for the simulations.

We attempted to simulate the stream with realistic dynamics of streambank fluxes, but we also tried to keep the model complexity as simple as possible. Although we did attempt to cover a wide range of streambank conditions when creating the many simulations, undoubtedly we did not cover all possible streambank flux conditions that could exist in nature. Realistically, the scientific community does not even know the full range of possibilities for natural streambank fluxes. We have also likely created simulations of streambank fluxes that do not exist in nature. Both issues are unavoidable when creating hydrologic simulations, particularly with the stochastic generation approach used in

10432

this paper. The hope is that the flux distributions of the simulations do closely represent reality for the purpose of our evaluation.

The statistical evaluation consisted of several methods and procedures. First, we took all of the simulated scenarios (5000 in our case) within an individual series and averaged the inflows and outflows for each simulation. This gave us an average inflow to the stream and outflow from the stream over the entire length of the stream for each scenario and served as our “true” values of the fluxes that the other streambank flux methods would be compared to. Next, we calculated the streambank fluxes of each scenario using the three streambank flux methods from the starting and end values of the scenarios. We did not include additional randomness in the input values for the streambank flux methods, which would equate to measurement error. This is due to the large variety of measurement devices and techniques that could be used in a tracer test, and each device and technique would have different measurement errors associated with them. Additionally, we calculated the net flux (we will call “Net”) simply by subtracting Q_{init} from Q_{final} . We considered the Net as the upper error benchmark for the evaluation as the estimation of Net requires less information and should therefore perform worse than the other three streambank flux methods that require more information.

Once the streambank fluxes were calculated for all of the methods to be evaluated, we used as a performance measure the absolute normalized error for method m and for each simulation i , defined as:

$$\varepsilon_i^m = \left| \frac{Q_{\text{est},i}^m - Q_{\text{true},i}}{Q_{\text{true},i}} \right| ; \quad i = 1, \dots, 5000 \quad (27)$$

where $Q_{\text{est},i}^m$ is the estimated gross gain or loss value from the streambank flux method m and simulation i and $Q_{\text{true},i}$ is the average flux from the ARIMA model at simulation i . The results of ε_i^m are two vectors (one for gross gains and one for gross losses) for each of the four methods. Each vector contains 5000 elements, one for each scenario. To make an overall evaluation for each method, we simply took an average of all of the

10433

scenarios in each series for both vectors of gains and losses:

$$\bar{\varepsilon}^m = \frac{1}{n} \sum_{i=1}^n \varepsilon_i^m \quad (28)$$

where $\bar{\varepsilon}^m$ is the mean absolute normalized error for each method m (either flux leaving the stream or entering the stream) and n is the total number of scenarios in each series (5000). This is a compound measure of relative bias and accuracy.

In addition to calculating the $\bar{\varepsilon}^m$ for all of the streambank flux methods, we compared the ε_i^m within each of the streambank flux methods to determine how frequently one method outperformed another:

$$r_{m1,m2} = \frac{1}{n} \sum_{i=1}^n \begin{cases} 1 & \text{if } \varepsilon_i^{m1} < \varepsilon_i^{m2} \\ 0 & \text{if } \varepsilon_i^{m1} \geq \varepsilon_i^{m2} \end{cases} \quad (29)$$

where $r_{m1,m2}$ is the frequency of $m1$ streambank flux method outperforming $m2$ streambank flux method.

Once ε_i^m and $\bar{\varepsilon}^m$ were estimated, we wanted to determine the causes of the errors in the individual methods. This was accomplished through a correlation of the ε_i^m to various combinations of the input parameters.

3 Results

3.1 Analytics

When there is 0 flux of either Q_{in} or Q_{out} all three equations produce the same results. For example, if $Q_{\text{out}} = 0$ then Eq. (2) becomes:

$$Q_{\text{final}} = Q_{\text{init}} + Q_{\text{in}} \quad (30)$$

10434

As Q_{final} and Q_{init} are previously known, there is only one solution for Q_{in} regardless of the other equations. Similarly, as the ratio of Q_{in} to Q_{out} grows to infinity or to 0, the results for the three equations will converge.

Although somewhat obvious, if all of the assumptions are met for any of the streambank flux methods then the method will perfectly reproduce reality. For example, if there is only inflow to the stream from 1–100 m followed by only flow out of the stream from 101–1000 m then the Gain–Loss equation will estimate both fluxes perfectly.

If $Q_{\text{in}} > 0$ then $C_{\text{final}} < C_{\text{init}}$ assuming that $C_{\text{in}} = 0$ from an artificial tracer injection. Subsequently, both C_{final} and C_{init} represent the end points of the concentration profile within the stream. As formulated in Eqs. (7)–(10), the Loss–Gain and Gain–Loss equations are divided by the end point concentrations of the stream and will therefore represent the minimum and maximum values of fluxes within a stream reach. The Loss–Gain equations will always produce the minimum flux values, while the Gain–Loss equations will always produce the maximum flux values. Consequently, as Loss–Gain and Gain–Loss will have the minimum and maximum flux values, the flux values for the Simultaneous equations must be somewhere in between the two.

The Gain–Loss and Loss–Gain methods are very similar, and subsequently can be compared quite easily. Dividing the inflow and outflow equations for the two methods can show the rate of increase of one method over the other:

$$\frac{Q_{\text{out,G-L}}}{Q_{\text{out,L-G}}} = \frac{C_{\text{init}}}{C_{\text{final}}} \quad (31)$$

and

$$\frac{Q_{\text{in,G-L}}}{Q_{\text{in,L-G}}} = \frac{Q_{\text{out}} C_{\text{init}}}{Q_{\text{out}} C_{\text{final}}} \quad (32)$$

For both Q_{out} and Q_{in} , Gain–Loss grows from Loss–Gain at a rate proportional to the concentration ratio, and additionally Q_{in} grows with load ratio. As Q_{out} and Q_{in} increase in a stream reach, Q_{final} will change and C_{final} will decrease. In the case of a lower C_{final}

10435

caused by higher streambank fluxes, the ratio between the results of Gain–Loss and Loss–Gain grows larger (Fig. 4).

Unfortunately, the Simultaneous method does not simplify nearly as well as the others due to the non-linearity of the Simultaneous equations. For a better visual comparison, the three methods were plotted together with axes of concentration and discharge ratios (Fig. 4). As shown analytically in Eqs. (31) and (32), the ratio of Gain–Loss to Loss–Gain is insensitive to discharge for Q_{out} and sensitive to both discharge and concentration for Q_{in} . The ratios of Simultaneous to the other methods illustrate the non-linearity of the method. The methods' ratios for Q_{in} show a surprising similarity in the distribution of the contours even though the magnitudes are different.

3.2 Numerical simulations

Figure 5 presents the major input and output parameter density distributions created by the ARIMA simulations for the inflow and outflow profiles. The parameter distributions for Q_{out} , Q_{in} , and Q_{net} closely follow a normal distribution. As defined in the model, Q_{init} and C_{init} are equally distributed between 1 to 5 L s⁻¹ and 20 to 150 mg L⁻¹, respectively.

The results of the numerical simulations are presented in Tables 1 and 2. Plots of the estimated gains and losses to the actual gains and losses for each of the methods for Series A are illustrated in Fig. 6. The plots for the other scenarios have similar patterns only with a greater or lesser degree of spread. The numerical simulations indicate that the Simultaneous streambank flux equation is on average the best performer when compared to the other two streambank flux methods with a 1 : 1 slope to the true value, the lowest $\bar{\varepsilon}^m$ in every series, and the highest $r_{m1,m2}$ in nearly every series. However, the Loss–Gain method has a slightly higher $r_{m1,m2}$ to Net as compared to Simultaneous. Interestingly, simply using the net discharge between upstream and downstream (Net) results in lower error values for $\bar{\varepsilon}^m$ as compared to Gain–Loss in both 2000 m series. This is attributed to the fact that Net by definition cannot have an error of 1 or greater. Similarly, Loss–Gain also cannot have errors 1 or greater and must have errors less than those of Net. If 0 is used for all the values of Q_{in} and Q_{out} in the error assessment

10436

of $\bar{\varepsilon}^m$ then $\bar{\varepsilon}^m$ would be exactly 1. Gain–Loss and Simultaneous can have errors greater than 1 as they can have values larger than the true value, which is clearly exemplified by the Gain–Loss equation's high $\bar{\varepsilon}^m$ in some series.

Figures 7 and 8 show the six simulations with the smallest ε_i^m for both Loss–Gain and Gain–Loss. Not surprisingly, they performed best when the assumptions of the individual methods were met. Figure 9 shows the six simulations with the smallest ε_i^m for Simultaneous. No obvious conclusion can be drawn from the simulations other than an evenly random spread between Q_{in} and Q_{out} with no clear spatial bias unlike the other methods.

The ratios of C_{init} to C_{final} and $Q_{init}C_{init}$ to $Q_{final}C_{final}$ show a strong correlation to the ε_i^m of the streambank flux methods (Fig. 10). They are the same ratios that were found during the analytical evaluation described by Eqs. (31) and (32). Both Loss–Gain and Gain–Loss have stronger correlations than Simultaneous. Simultaneous appears to have an error bias towards lower values rather than the full range of the correlation.

Loss–Gain and Gain–Loss also have a strong correlation to the midpoint concentrations and loads. Gain–Loss had a strong correlation to the ratios of C_{mid} (the midpoint of the concentration profile of the stream) to C_{final} and $Q_{init}C_{init}$ to $Q_{mid}C_{mid}$ (the midpoint of the load profile of the stream). Loss–Gain had a very strong correlation to the ratios of C_{mid} to C_{init} and $Q_{final}C_{final}$ to $Q_{mid}C_{mid}$.

4 Discussion

4.1 Bank flux methods evaluation

The streambank flux methods followed different patterns through the 4 series of the $\bar{\varepsilon}^m$. Net was only slightly affected by both the switch length and the length of the stream reach. Alternatively, Simultaneous was not significantly affected by the switch length, but was affected by the stream length. Loss–Gain and Gain–Loss were affected by both the switch length and the stream length.

10437

While Simultaneous was the best performer in all categories, Gain–Loss performed substantially worse on the $\bar{\varepsilon}^m$ overall and was only better than Net on the $\bar{\varepsilon}^m$ for Series A and B and for the $r_{m1,m2}$. As described in the previous sections, the Gain–Loss equations can create results that can be many times larger than the other methods and consequently can be many times larger than the true value from the ARIMA model. Although these circumstance may account for a small proportion of the total simulations, they can cause the average error to be very high. Net was clearly superior in Series C and D for the $\bar{\varepsilon}^m$, but Gain–Loss had a solid majority over Net in the $r_{m1,m2}$. In the Series A, Gain–Loss and Net had a similar $\bar{\varepsilon}^m$, but according to $r_{m1,m2}$ Gain–Loss performed better almost 80% of the time. Indeed, if the top 10% of the simulations with the highest errors were removed from Series C then Gain–Loss and Net would have approximately the same $\bar{\varepsilon}^m$. Nevertheless, even with the help of removing 10% or 20% of the simulations with the highest errors, both Loss–Gain and Simultaneous performed substantially better than Gain–Loss.

Most of the ε_i^m errors in Loss–Gain and Gain–Loss could be correlated by the ratio of the upstream and downstream concentrations for Q_{out} and the ratio of the upstream and downstream loads for Q_{in} . $Q_{out,G-L}$ had an especially strong correlation. Loss–Gain on the other hand had an especially strong correlation to the concentration and load midpoints along the stream (not shown in figures). As with much of the previous results, the midpoint correlations follows precisely the assumptions of the methods. Loss–Gain assumes that the Q_{out} occurs at the beginning and if the ratio of C_{mid} to C_{init} does not follow a relationship that the method assumes then it will produce a larger error. At least in Loss–Gain, it appears that if the concentration ratio does not follow the predicted pattern by the time it reaches the midpoint then the method is more likely to create erroneous results. A similar pattern can be seen in Gain–Loss, but not nearly as strong as the upstream and downstream ratios. Unfortunately, Simultaneous did not have such clear correlations. There only appears to have an error trend towards smaller upstream and downstream ratios.

10438

There is much scientific literature on the estimation of streambank fluxes from chemical tracers. Many have preferred to use the well established OTIS numerical model, which effectively solves the differential equations with a finite difference model with similar spatial flux assumptions to our Simultaneous method. We found only one study that took the OTIS model and tested the three different assumptions that we also tested (Szeftel et al., 2011). However, the reasoning behind their test appeared to be precisely the opposite of ours. As they stated in the methods, they assumed that the simultaneous inflow and outflow at a single cell was unrealistic and implemented the Loss–Gain and Gain–Loss type scenarios to provide better alternatives. Although they did not test the accuracy of the three methods, they concluded that the spatial variability of the streambank fluxes had a significant impact on the output and that breakthrough curve (BTC) analysis is not sufficient to determine the spatial variability.

Like us, others have instead preferred to use the more simple analytical equations to estimate streambank fluxes (Harvey and Wagner, 2000; Payn et al., 2009; Covino et al., 2011). One of the earliest to hint at using tracers with analytical equations to determine streambank fluxes was Zellweger et al. (1989). The use of tracers with dilution gauging to estimate streambank fluxes was only mentioned in passing as an explanation for the differences in the estimation of discharge from a current meter and from dilution gauging. Later, Harvey and Wagner (2000) picked up on the idea of using dilution gauging with a current meter to estimate streambank fluxes. Their description for the procedure to estimate streambank fluxes was purely qualitative and did not fully explain the underlying assumptions in the method that they proposed (e.g. the spatial distribution of the fluxes). The dilution gauging method to estimate discharge was referenced back to Kilpatrick and Cobb (1985). Based on the dilution gauging method and the description provided by Harvey and Wagner (2000), they effectively proposed the use of the Gain–Loss method. Interestingly, Covino et al. (2011) also referenced back to Kilpatrick and Cobb, 1985, but they instead used the Loss–Gain method. Payn et al. (2009) and Ward et al. (2013) estimated streambank fluxes using both the Loss–Gain and the Gain–Loss methods. They also found significant differences in the estimations

10439

between the two different methods and correctly identified that the Loss–Gain and the Gain–Loss methods produce the maximum and minimum values for streambank fluxes, respectively.

4.2 Connections with end-member mixing models

End-member mixing models or end-member mixing analysis (EMMA) as they tend to be known is a method to estimate the relative contributions of defined upstream source waters from a downstream discharge measurement point. For example, EMMA can estimate the amount of groundwater contribution within a single hydrograph. EMMA is used extensively for this precise purpose. Similarly to the bank flux methods, EMMA uses the mass balance equations with chemical tracers to formulate the model. The EMMA equations are well known and the equation for two end-members is the following:

$$Q_{\text{gauge},s2} = Q_{\text{gauge}} \left(\frac{C_{\text{gauge}} - C_{s1}}{C_{s2} - C_{s1}} \right) \quad (33)$$

where Q_{gauge} is the discharge at the stream measurement gauge, $Q_{\text{gauge},s1}$ is the part of the discharge of Q_{gauge} from the first source, C_{gauge} is the concentration of the tracer at the stream measurement gauge, C_{s1} is the concentration of the tracer in the first source, and C_{s2} is the concentration of the tracer in the second source.

Equation (33) is strikingly similar to Eq. (5). Additionally, if we consider a bromide tracer test with the first source as upstream discharge and the second source as groundwater with $C_{s2} \approx 0$, then the equation simplifies in the same way as Eq. (9). Although they may look the same, they have different underlining assumptions and derivations.

The derivation of Eq. (33) is usually conceptualized by the conservative mixing of two sources in a large reservoir with only one outflow defined above as Q_{gauge} . What if the equation for EMMA were derived in the context of a stream reach, with both Q_{in}

10440

and Q_{out} included in the derivation? Would Eq. (33) be different? Since these questions have not been directly addressed in the literature, we will provide the derivation setting up a scenario with the two sources similar to the streambank flux scenarios. It will have a first source equal to the upstream discharge with the upstream concentration ($Q_{s1} = Q_{init}$, $C_{s1} = C_{init}$), a second source equal to the the diffuse groundwater entering the stream ($Q_{s2} = Q_{in}$, $C_{s2} = C_{in}$), and the the gauging site equal to the downstream conditions ($Q_{gauge} = Q_{final}$, $C_{gauge} = C_{final}$). First, we write the mass balance equation for the downstream discharge:

$$Q_{gauge} = Q_{gauge,s1} + Q_{gauge,s2} \quad (34)$$

where $Q_{gauge,s1}$ and $Q_{gauge,s2}$ are the respective parts of the discharge Q_{gauge} from the first and second sources, i.e. upstream discharge and groundwater inflow. Separating Q_{out} in their respective components and due to mass balance for the discharges gives us:

$$Q_{gauge,s1} = Q_{s1} - Q_{out,s1} \quad (35)$$

and

$$Q_{gauge,s2} = Q_{s2} - Q_{out,s2} \quad (36)$$

where Q_{s1} is the total discharge of the first source and Q_{s2} is the total discharge of the second source. We then write the mass balance for the tracer flows going out of the stream:

$$Q_{out}C_{out} = Q_{out,s1}C_{s1} + Q_{out,s2}C_{s2} \quad (37)$$

where $Q_{out,s1}$ is loss of water specifically from Q_{s1} and $Q_{out,s2}$ is loss of water specifically from Q_{s2} . Then we apply the mass balance equation for the tracer between the upstream and downstream (similar to Eq. 1):

$$Q_{gauge}C_{gauge} = Q_{s1}C_{s1} + Q_{s2}C_{s2} - Q_{out}C_{out} \quad (38)$$

10441

Combining Eqs. (37) and (38) we get the following equation with some rearrangement.

$$Q_{gauge}C_{gauge} = (Q_{s1} - Q_{out,s1})C_{s1} + (Q_{s2} - Q_{out,s2})C_{s2} \quad (39)$$

Finally, introducing Eqs. (34)–(36) we get the completed derivation solved for $Q_{gauge,s2}$.

$$Q_{gauge,s2} = Q_{gauge} \left(\frac{C_{gauge} - C_{s1}}{C_{s2} - C_{s1}} \right) \quad (40)$$

The outflow components have completely fallen out and Eq. (40) has become Eq. (33). The end-member mixing equations are insensitive to any outflows from the stream system, and subsequently will provide the same result regardless of the streambank flux spatial dynamics occurring within the system upstream of the measurement gauge. Also, if we substitute the parameters in Eq. (40) with the relevant parameters used during the streambank flux derivations (e.g. Q_{init} , Q_{final} , and Q_{in}) then the right hand of the equation becomes identical to the right hand of Eq. (5). The fundamental difference between these two equations is the left hand of the equations: $Q_{gauge,s2}$ and Q_{in} are conceptually different, i.e. the amount of discharge downstream from the groundwater source does not need to be necessarily equal to the gross diffuse inflow throughout the reach. Nevertheless, it is important to realize that the estimation of Q_{in} with the Loss–Gain assumptions leads to the same results as the EMMA estimate for $Q_{gauge,s2}$.

The similarity between Eq. (40) and the Loss–Gain Eq. (5) appears to have led some researchers to inadvertently apply the EMMA Eq. (40) to estimate the gross stream gains and losses (Covino and McGlynn, 2007). Although these streambank flux estimates are correct in terms of the Loss–Gain assumptions, it appears to be more of coincidence than deliberate, as little reasoning and background is given for the implicit Loss–Gain hypothesis on the spatial inflow and outflow dynamics of the EMMA equation when used for estimating streambank fluxes. Similarly, Briggs et al. (2012) referenced the above EMMA model (Kobayashi, 1985) to estimate streambank fluxes, but they instead used the Gain–Loss method without explanation.

Both EMMAs and streambank flux analyses can be performed on a stream reach with the same input data to acquire several important hydrological aspects of surface water and groundwater interactions. They could be applied simultaneously to a given stream reach to estimate both the amount of discharge downstream from the groundwater source and the gross diffuse inflow throughout the reach, which will have different values if assumptions different to those of Loss–Gain are made. The streambank flux equations were derived for steady-state conditions and should be applied as such, while the EMMA derivation has no such critical steady-state requirement and subsequently can also be used in transient conditions (i.e. throughout a flooding event). While the streambank flux equations cannot be used dynamically throughout a flooding event, it would be possible to apply the streambank flux equations lumped over an entire flooding event. For example, the streambank flux equations could be applied by summing the total non-baseflow water in a flood hydrograph and the average concentration of a tracer at an upstream and downstream gauge. This use of the streambank flux equations would not be as accurate as in true steady-state conditions due to the additional assumption of a constant baseflow during the flooding event, which is certainly not going to be true. Nevertheless, as long as the changes in the baseflow water accounts for a small percentage of the total flow during an event, the equations should provide relatively accurate values.

5 Conclusions

A new streambank flux estimation method is presented and derived analytically with the assumptions of constant, uniform, and simultaneous groundwater inflow and outflow throughout a given stream reach. This novel method is confronted against the two traditional methods and presents the smallest error measures when applied to four different sets of generated scenarios. The main control of the model performance for all three cases is the spatial dynamics of the actual streambank fluxes in relationship with the assumptions for each method. Also for the same inputs, the different assumptions

10443

of each method can lead to values of gross stream gains and losses differing up to one order of magnitude between approaches. Estimating streambank fluxes using the proposed simple analytical method over numerical models solving full hydrodynamic sets of partial differential equations has the clear advantages of much less complexity and less parametrization. Although separate from the streambank flux methods, end-member mixing analysis can be used in conjunction with the streambank flux methods to acquire even more hydrologic information as both require the same type of input data. Nevertheless, these two approaches should not be conceptually mixed as they estimate different stream variables and are based on distinct derivations and assumptions.

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10444

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10446

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10447

Table 1. $\bar{\varepsilon}^m$: the average value of ε_i^m for each series and for both Q_{out} and Q_{in} . Sim is abbreviated for Simultaneous.

Series	Stream Length (m)	AVG Switch Length (m)	Corr. Length (m)	Flux Type	Streambank Flux Method			
					Net	Loss–Gain	Gain–Loss	Sim
A	1000	100	40	Q_{out}	0.821	0.243	0.675	0.115
				Q_{in}	0.821	0.264	0.849	0.135
B	1000	200	70	Q_{out}	0.775	0.183	0.421	0.111
				Q_{in}	0.763	0.204	0.591	0.143
C	2000	100	40	Q_{out}	0.852	0.393	2.390	0.170
				Q_{in}	0.855	0.422	2.949	0.194
D	2000	200	70	Q_{out}	0.815	0.306	1.268	0.168
				Q_{in}	0.821	0.339	1.652	0.202

10448

Table 2. $r_{m1,m2}$: the ratios of the frequency that the methods in the rows ($m1$) have a smaller ε_i^m than the methods in the columns ($m2$). In simpler terms, the table shows how often the methods in the rows outperform the methods in the columns. Sim is abbreviated for Simultaneous.

Series	Method	Denominator ($m2$)			
		Net	Loss-Gain	Gain-Loss	Sim
A	Net	0.000	0.000	0.204	0.014
	Loss-Gain	1.000	0.000	0.711	0.149
	Gain-Loss	0.796	0.289	0.000	0.068
	Sim	0.985	0.851	0.931	0.000
B	Net	0.000	0.000	0.143	0.022
	Loss-Gain	1.000	0.000	0.627	0.223
	Gain-Loss	0.857	0.373	0.000	0.163
	Sim	0.978	0.777	0.837	0.000
C	Net	0.000	0.000	0.501	0.029
	Loss-Gain	1.000	0.000	0.869	0.109
	Gain-Loss	0.499	0.131	0.000	0.013
	Sim	0.971	0.891	0.987	0.000
D	Net	0.000	0.000	0.352	0.037
	Loss-Gain	1.000	0.000	0.753	0.177
	Gain-Loss	0.648	0.247	0.000	0.067
	Sim	0.963	0.823	0.933	0.000

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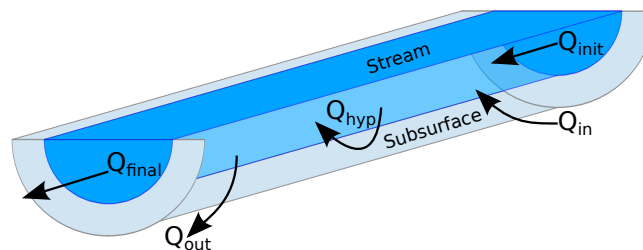


Fig. 1. A conceptual overview of the major inflows and outflows within a stream reach. Q_{init} is the upstream discharge in volume per time, Q_{final} is the downstream discharge, Q_{in} is the groundwater entering the stream, Q_{out} is the stream water leaving the stream to the groundwater, and Q_{hyp} is the hyporheic flow water that is temporarily leaving the stream into the hyporheic zone (reproduced after Harvey and Wagner, 2000).

10450

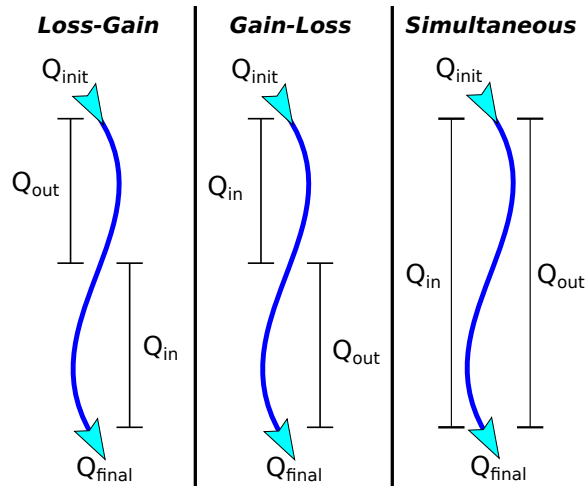


Fig. 2. The conceptualizations of the three streambank flux methods. The Loss–Gain method assumes Q_{in} occurs in the first section followed by Q_{out} in the last section. The Gain–Loss method assumes Q_{out} occurs in the first section followed by Q_{in} in the last section. Both the Loss–Gain and Gain–Loss methods assume that Q_{in} and Q_{out} occur in sequence and independently, although the lengths of the first and last sections are arbitrary and can be of any length that when summed together equal the total length. The Simultaneous method assumes that Q_{in} and Q_{out} are constant and occur simultaneously throughout the entire length of the stream reach.

10451

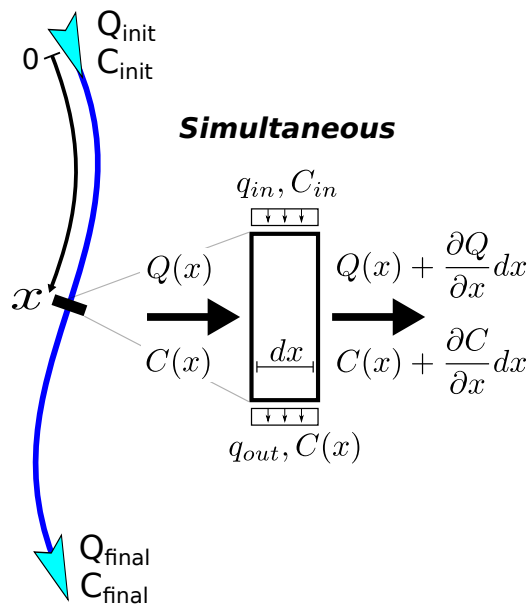


Fig. 3. A conceptual representation of the analytical formulation of the Simultaneous method.

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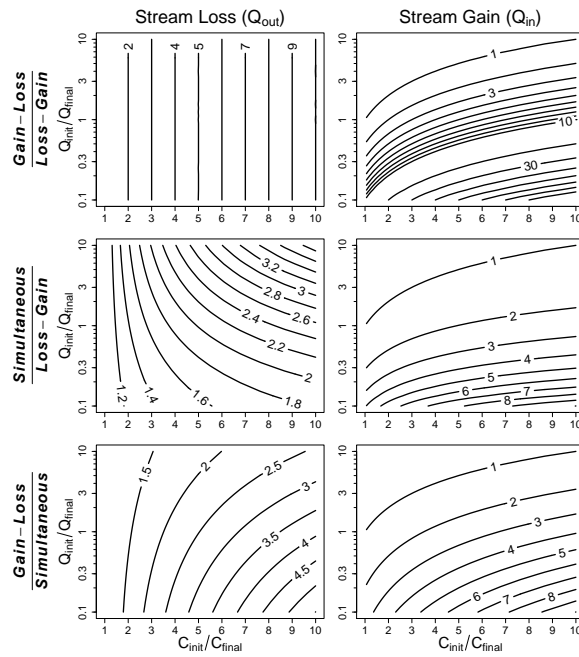


Fig. 4. Relative comparisons between the different methods due to changes in the input ratios. The rows are the ratios of two of the streambank flux methods for both Q_{out} and Q_{in} . For example, if the ratio of the input parameters C_{init} and C_{final} is 5 and the ratio of the input parameters Q_{init} and Q_{final} is 1 then the Simultaneous method will result in a Q_{in} approximately 2 times larger than the Loss-Gain method.

10453

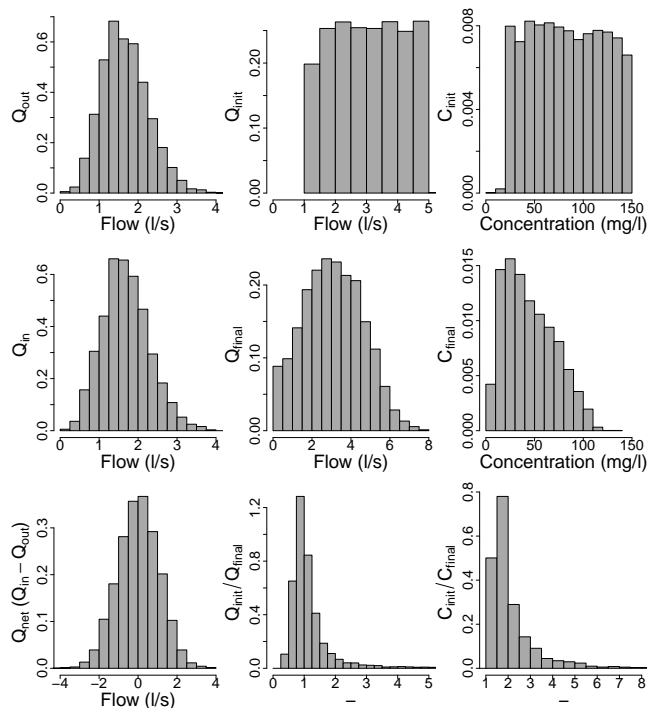


Fig. 5. The major input and output parameter density distributions of the ARIMA numerical model for Series A (1000 m with 100 m AVG switch length).

10454

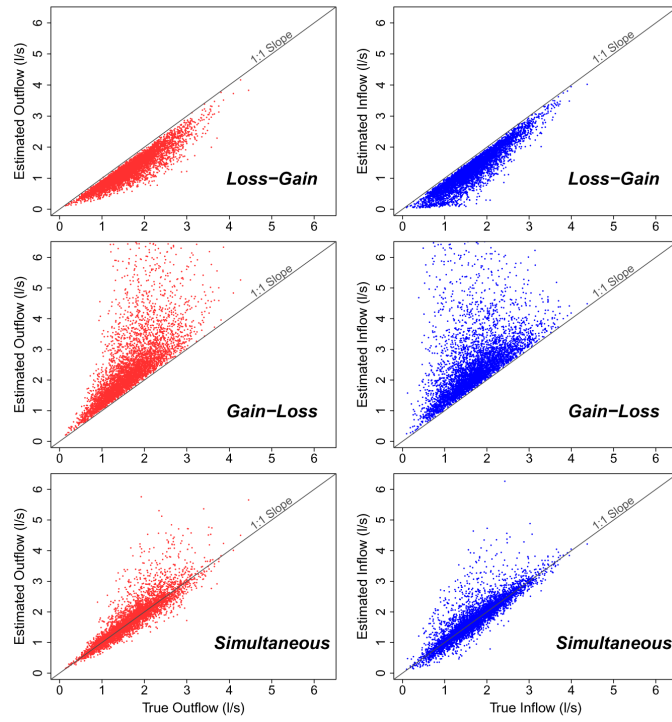


Fig. 6. A plot of true inflow and outflow flux values by the estimated values from the three streambank flux methods for Series A (1000 m with 100 m AVG switch length).

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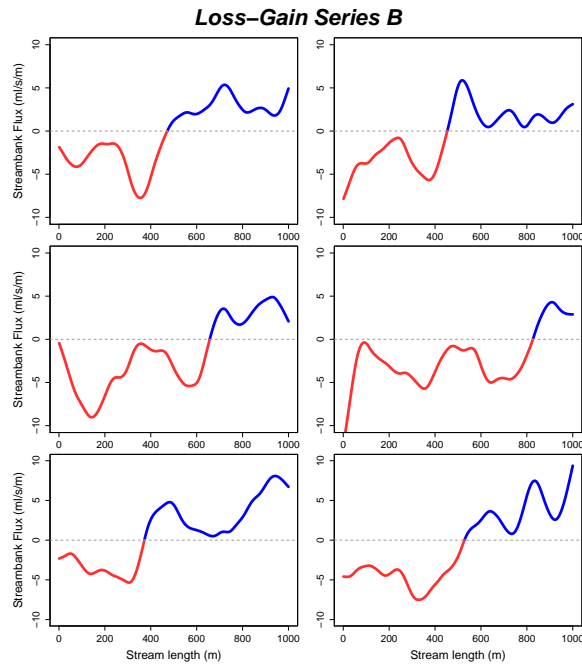


Fig. 7. The simulated streambank flux profiles (Series B, 1000 m with 200 m AVG switch length) of the six scenarios with the smallest normalized error (ϵ_i^m) for Loss-Gain. A clear pattern can be seen according to the spatial assumption of the method. Predominant stream losses are at the beginning, while stream gains are towards the end of the reach. Red indicates losses, while blue indicates gains.

10456

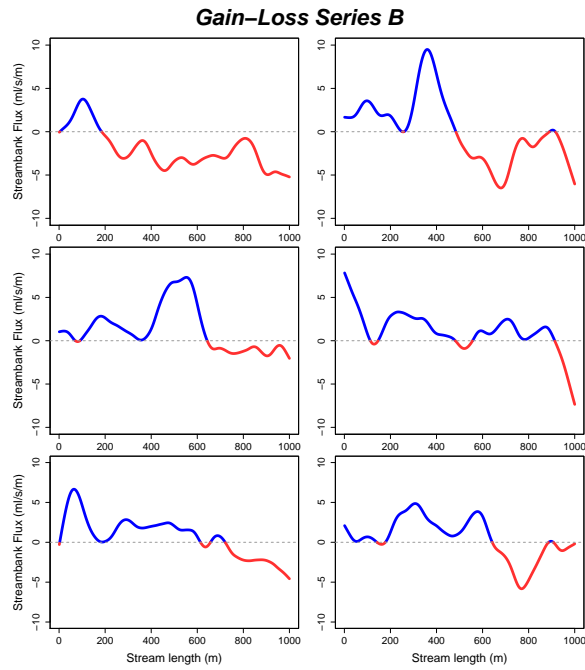


Fig. 8. The simulated streambank flux profiles (Series B, 1000 m with 200 m AVG switch length) of the six scenarios with the smallest normalized error (ε_i^m) for Gain-Loss. A clear pattern can be seen according to the spatial assumption of the method. Predominant stream gains are at the beginning, while stream losses are towards the end of the reach. Red indicates losses, while blue indicates gains.

10457

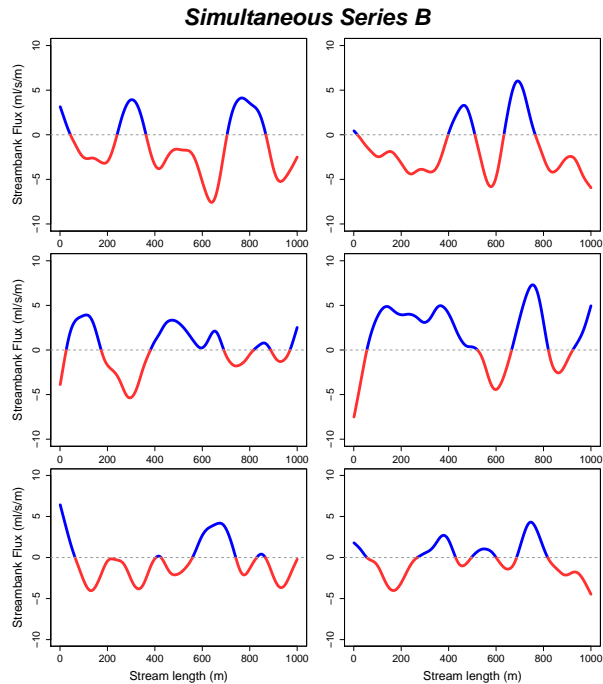


Fig. 9. The simulated streambank flux profiles (Series B, 1000 m with 200 m AVG switch length) of the six scenarios with the smallest normalized error (ε_i^m) for Simultaneous. No consistent or obvious pattern can be seen within the scenarios. Red indicates losses, while blue indicates gains.

10458

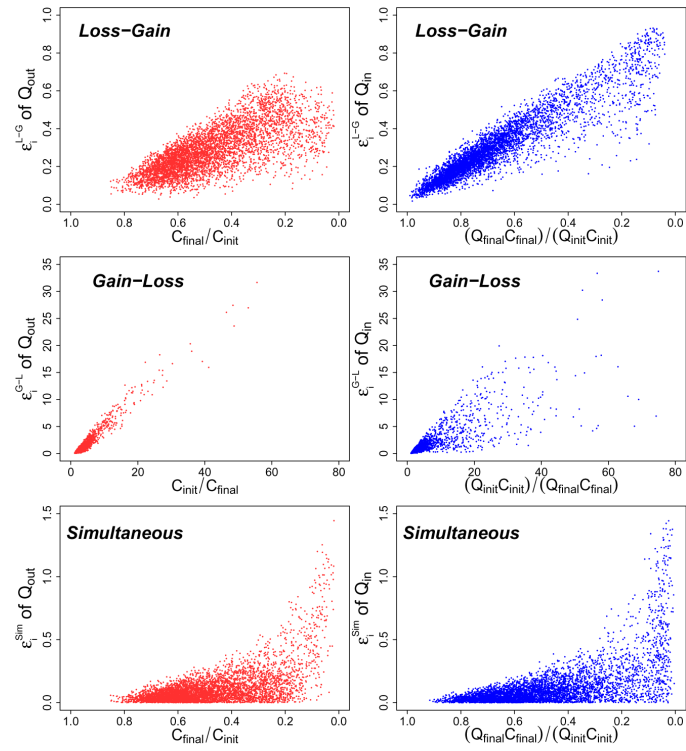


Fig. 10. A correlation of various input parameters to the normalized error (ϵ_i^m) of the stream-bank flux methods for Series A. Both the Loss–Gain and Gain–Loss methods have strong correlations, while Simultaneous only tends to have an error bias at lower ratios.