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TIPT: The Tracer Injection Planning Tool

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ABSTRACT

Despite their frequent use, there are few simple and readily accessible tools to help guide the logistical planning of tracer injections in streams and rivers. We combined the widely used advection-dispersion-reaction equation, peak concentration estimates based on a meta-analysis of hundreds of tracer injections carried out in streams and rivers, and simple mass balances in a dynamic Excel Workbook to 1) help users decide how much tracer mass should be added to achieve a specific dynamic concentration range that reduces known issues associated with breakthrough curve tail truncation, and 2) generate tables and graphs that can be readily used to plan the deployment of resources. Our Tracer Injection Planning Tool, TIPT, handles instantaneous and continuous tracer injections and assumes steady-state and uniform flow conditions, as well as first-order decay or production. While those assumptions do not strictly apply to natural streams and rivers, they help simplify the planning of tracer injections with a predictive ability that is disproportionally favorable with respect to the few inputs required. TIPT is a versatile, user-friendly, and graphical tool that can help design tracer injections and solute transport experiments that are more easily replicated within and across sites. Thus, TIPT contributes directly to advancing Integrated, Coordinated, Open, and Networked (ICON) principles. Similarly, TIPT can help generate datasets that more closely follow Findable, Accessible, Interoperable, and Reusable (FAIR) principles. We demonstrate the use of TIPT through two case studies featuring 1) a continuous injection in a 2nd order stream and 2) an instantaneous injection in a 7th order stream.

1. Introduction

Tracer injections in streams and rivers are commonly used to characterize physical and biochemical processes undergone by solutes and micro-to-nano particles transported in fluvial networks (Covino et al., 2010; Foppen et al., 2011; González-Pinzón et al., 2015; Drummond et al., 2017; Knapp et al., 2018). These techniques help us quantify and visualize a variety of processes controlling the fate and transport of solutes: physical processes, including advection, dispersion, and transient storage; biological processes, including uptake, decay, and production; and chemical processes, including sorption, decay, and production (Stream Solute Workshop 1990; Abbott et al., 2016; Knapp et al., 2017).

Despite their wide use in research and consulting in hydrology, environmental engineering, and earth and aquatic sciences, there are few simple and readily accessible tools to help guide the logistical planning of tracer injections in streams and rivers. Consequently, tracer studies are not easily replicated, i.e., different users might end up choosing considerably different injection and sampling durations, target concentrations, sampling frequencies, and longitudinal extent, even if they have a similar goal (González-Pinzón et al., 2015; Schmadel et al., 2016). Moreover, the lack of optimal sampling frequencies and the anticipation of arrival and passage times may lead to suboptimal decisions about personnel and equipment/supply logistics, which ultimately reduce the quality and quantity of the information retrieved from tracer injections. Paradoxically, the perfect logistical planning of a tracer injection would require carrying it out first and repeating it under the exact same physical and biochemical conditions (Harvey and Gooseff, 2015; Harvey et al., 1996), which is impossible.

Here, we propose to combine 1) the widely used advection-

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dispersion-reaction equation, 2) a meta-analysis of hundreds of tracer injections carried out in streams and rivers spanning four orders of magnitude in discharge and two in size, which was conducted by Jobson (1996), and 3) simple mass balances to more objectively plan the logistics of tracer injections in streams and rivers. We programmed an Excel Workbook to offer a readily accessible product that can be used on multiple operating systems and devices, using basic information about the study site (Supplemental Information 1). The Tracer Injection Planning Tool, TIPT, handles instantaneous and continuous tracer injections to 1) help users decide how much tracer mass should be added to achieve a specific dynamic concentration range (i.e., the ratio between the maximum and minimum tracer concentrations measured) that reduces known issues associated with breakthrough curve tail truncation (Drummond et al., 2012), and 2) generate tables and graphs that can be readily used to plan the deployment of resources.

2. Methods

2.1. The advection-dispersion equation

In TIPT, we use the advection-dispersion equation (ADE) with first-order decay or production to guide the logistical planning of tracer injections because it has analytical solutions for instantaneous and continuous injections of solutes (Chapra 2008). These analytical equations generate exact solutions that are free of numerical dispersion and stability issues (Chapra 2008), and are instantly computed using low memory and power requirements. Moreover, the ADE is the backbone of the most common solute transport models used by ecologists and hydrologists in environmental studies (e.g., González-Pinzón et al., 2013; Runkel, 2007; Stream Solute Workshop, 1990):

$$\frac{dC}{dt} = -u\frac{dC}{dx} + D\frac{d^2C}{dx^2} - \lambda c, \tag{1}$$

where C [M L^{-3}] is the concentration of the reactive solute at a cross-section located downstream of the solute injection site; u [L T^{-1}] is the mean streamflow velocity; D [L T^{-2}] is the dispersion coefficient; λ [T^{-1}] is the first-order rate coefficient (λ =0 for a non-reactive tracer); x [L] is longitudinal distance; and t [T] is time.

2.1.1. Instantaneous vs. continuous tracer injections

An instantaneous (aka pulse, gulp, slug) injection is one in which known tracer masses (conservative and reactive) are dissolved in a volume of water and poured all at once into the stream or river, featuring a duration of the injection, t_{inj} [T], effectively equal to zero. Continuous injections, on the other hand, feature $t_{inj}>0$, i.e., the release of the dissolved tracer masses into the stream occurs over periods typically ranging from hours to weeks. Note, however, that continuous injections do not guarantee reaching steady-state (aka plateau) concentrations downstream. For that to happen, the solute injected must be enough to label and saturate all of the flowpaths upstream of a given observation point, which depends on multiple stream characteristics such as discharge, dispersion, streambed permeability, ambient concentrations, and tracer solubility, as well as variables associated with the design of the tracer injection, such as its duration, the injection rate, and the location of sampling points.

Researchers and practitioners use instantaneous and continuous in-stream tracer injections to answer questions and test hypotheses associated with the fate and transport of solutes that are naturally present or become available through specific events such as storms, spills, leaks, or day-to-day operations of wastewater treatment plants (Hyer 2007; Leibundgut et al., 2009; Williams et al., 2013). Those injections can also be used to estimate river flow (e.g., Kilpatrick and Cobb, 1984), groundwater-surface water interactions (e.g., Bencala and Walters, 1983; González-Pinzón et al., 2015; Triska et al., 1989), stream-atmosphere interactions (e.g., Kilpatrick et al., 1987), and travel and residence times (Kilpatrick and Wilson 1989).

Instantaneous in-stream tracer injections are ideal tools for understanding the fate and transport of solutes instantly added (Kilpatrick and Wilson, 1989) because they represent many real-world situations where a solute becomes suddenly and briefly available (e.g., truck spills and accidental pipe leaks that were quickly resolved), and because they have low costs and simpler logistics. Also, the results from instantaneous injections and principles of superposition could be used with to estimate experimental results for varying injection durations through convolution (i.e., as done in S-curve analyses used in other hydrology applications such as the unit hydrograph).

Recent experimental efforts to discern the main differences in results from using instantaneous vs. continuous injections suggest that longer tracer injections label wider, deeper, and thus longer subsurface flow paths, affecting our in-stream based interpretations of reach-scale residence time distributions, assessment of which compartments contribute more to transient storage, and perhaps more importantly, the existing relationships between physical transport and biochemical reactivity, mainly because of differences in exposure times, the sampling of biomass diversity and functioning, and the concentration ranges and their influence in reaction kinetics (Harvey et al., 1996; Gooseff et al., 2008; Navel et al., 2010; Drummond et al., 2012; Knapp et al., 2017).

2.1.2. ADE solution for instantaneous tracer injections

The analytical solution for instantaneous tracer injections is (Chapra 2008):

$$C(x,t) = \frac{M_{inj}}{2A\sqrt{\pi D t}} e^{-\frac{(x-ut)^2}{4Dt} - \lambda t} \tag{2}$$

where M_{inj} [M] is the mass injected; and A [L^2] is the stream cross-sectional area.

ADE solution for continuous tracer injections: The analytical solution for step or continuous tracer injections is given in two parts (Chapra 2008).

For t< t_{inj}:

$$c(x,t) = \frac{C_{target\ max}}{2}\left[e^{\frac{ux(1-\Gamma)}{2D}} erfc\left(\frac{x-ut\Gamma}{2\sqrt{Dt}}\right) + e^{\frac{ux(1+\Gamma)}{2D}} erfc\left(\frac{x+ut\Gamma}{2\sqrt{Dt}}\right)\right] \tag{3a}$$

For t> t_{inj}:

$$c(x,t) = \frac{C_{target\ max}}{2}\left\{e^{\frac{ux(1-\Gamma)}{2D}}\left[erfc\left(\frac{x-ut\Gamma}{2\sqrt{Dt}}\right) - \mathrm{erfc}\left(\frac{x-u(t-t_{inj})\Gamma}{2\sqrt{D(t-t_{inj})}}\right)\right] + e^{\frac{ux(1+\Gamma)}{2D}}\left[erfc\left(\frac{x+ut\Gamma}{2\sqrt{Dt}}\right) - \mathrm{erfc}\left(\frac{x+u(t-t_{inj})\Gamma}{2\sqrt{D(t-t_{inj})}}\right)\right]\right\}, \tag{3b}$$

$$\Gamma = \sqrt{1+4\eta}, \tag{3c}$$

$$\eta = \frac{\lambda D}{u^2}, \tag{3d}$$

$$C_{target\ max} = \frac{q_{pump}}{Q} C_{target\ injectate}, \tag{3e}$$

where q_{pump} [L^3 T^{-1}] is the continuous injection rate; Q [L^3 T^{-1}] is the mean river discharge; and $C_{target\ injectate}$ [M L^{-3}] is the concentration of the target tracer (i.e., the chemical compound quantified by analytical techniques or sensors) in the injectate.

2.2. Estimation of tracer injection masses

2.2.1. Instantaneous tracer injection

We implemented two methods in TIPT to estimate the mass of a commercially available tracer salt (referred to as *commercial tracer* from here on) that needs to be added to generate a user-specified maximum target tracer concentration at the most downstream sampling location. For example, when NaCl is used as the commercial tracer, Cl^- is the target tracer. For this, we assume that the target tracer is available with 100% purity.

2.2.1.1. Jobson's unit concentration method. We used the unit concentration concept introduced by Jobson (1996) to estimate the tracer mass needed to generate a maximum target concentration from an instantaneous injection. Briefly, the unit concentration, C_u [T^{-1}], standardizes tracer concentrations by the mass of tracer injected, tracer losses due to dilution, and differences in stream discharge:

$$C_u = 1x10^6 \frac{C}{R_r}\frac{Q}{M_{inj}}, \tag{4}$$

where C [M L^{-3}] is an observed tracer concentration; R_r [-] is the ratio of the mass added to the total mass retrieved during the experiment at the sampling location (i.e., $R_r = M_{inj} / \int_0^t C\,Q\,dt$). Note that 1) C_u [T^{-1}] represents the solute mass flow rate (mass per time) per unit of mass injected, 2) the $1x10^6$ factor is used to bring C_u close to a unit value, regardless of the system of units chosen, and 3) discharge must be expressed in units that are consistent with the denominator of the concentration, and the injected mass must be in the same units as the numerator of the concentration.

An analysis of data from 422 experimental observations in 60 different rivers in the United States (Table 1) showed that peak C_u values, C_{u_p}, correlate with increasing times to peak concentrations, t_p. The predicting equation for C_{u_p} [1/s] and t_p [h], is:

$$C_{u_p} = 1105 \ \ t_p^{-0.817} \tag{5}$$

According to Jobson (1996), this equation had a root-mean-square error (RMSE) of 0.502 natural logarithmic units, the coefficient of variation of the regression was 0.112, and the coefficient of determination (R^2) was 0.893. The standard error of estimate of the coefficient was 4.9% and the standard error of estimate for the exponent is 1.7%.

In TIPT, we combined equations (4) and (5) to estimate M_{inj} [M] from user-specified values of Q [L^3 T^{-1}], $C_{target\ max}$ [M L^{-3}], C_o [M L^{-3}], and ADE-derived estimates of t_p values, $t_{p\ ADE}$ [T]. To estimate $t_{p\ ADE}$ [T], we use user-specified values of Q [L^3 T^{-1}], u [L T^{-1}], D [L^2 T^{-1}], λ [T^{-1}], and x [L], and set $\widehat{M}_{inj} = 1$ temporarily, which does not affect the timing of $t_{p\ ADE}$, only the amplitude of the concentrations. Then, we estimate the tracer injection mass using:

$$M_{inj_{Jobson's}} = Q\frac{\left(C_{target\ max} - C_o\right)}{\max\left(a \ \ t_{p\ \ ADE}^{b}\right)}, \tag{6}$$

where a and b represent the unit-consistent coefficient and exponent from equation (5), and $\max\left(a \ \ t_{p\ \ ADE}^{b}\right)$ represents the time to peak at the most distal sampling location, where $C_{target\ max}$ will occur. To help the user select a value for D, TIPT uses a simplified version of the following equation proposed by Fisher et al. (1979):

$$D = 0.011\frac{u^2 w^2}{h\,u_*}, \tag{7}$$

Table 1
Stream characteristics from the USGS experimental database used in TIPT.

Discharge (m^3/s)		Depth (m)		Width (m)		Longitudinal Slope (–)	
min	max	min	max	min	max	min	max
0.1	6824.4	0.1	24.8	2.7	807.7	0.00001	0.0367

where h [L] is the stream depth and is approximated as $h = Q/u\,w$ assuming a rectangular cross-section; $u_* = \sqrt{h\,g\,S}$ [L T^{-1}] is the shear velocity; g [L T^{-2}] is the gravitational acceleration; and S [-] is the longitudinal slope of the stream. However, we note that the estimation of the longitudinal dispersion coefficient is a critical step in the application of the ADE, as recently demonstrated by Peruzzi et al. (2021), and that there are many other empirical equations available (Fischer et al., 1979; Chapra 2008).

Finally, we use the molar masses of the commercial and target tracers, Mm [M mol^{-1}], to estimate the mass of the commercial tracer to be added, $M_{commercial}$ [M], and the commercial tracer solubility, $C_{commercial\ sol.}$ [M L^{-3}], to estimate the volume, $V_{inst.\ inj}$ [L^3], needed to dissolve $M_{commercial}$:

$$M_{commercial_{Jobson's}} = M_{add_{Jobson's}}\frac{Mm_{commercial}}{Mm_{target}}, \tag{8}$$

$$V_{inst.\ inj.} = \frac{M_{commercial_{Jobson's}}}{C_{commercial\ sol.}}. \tag{9}$$

2.2.1.2. ADE-based method. In TIPT, we also propose to estimate the mass needed in an instantaneous tracer injection using the analytical solution of the ADE for the peak concentration, $C_{target\ max}$, and the times to peak concentration at the most distal sampling location, $t_{p\ ADE}$. Like in Jobson's method, we first need to estimate $t_{p\ ADE}$ [T], and then solve for M_{inj} [M] in equation (2) using user-specified values for the most downstream sampling location, x_{distal} [L], and the maximum concentration wanted there at the time to peak, $C_{target\ max}\,(x_{distal}, t_{p\ ADE})$ [M L^{-3}]:

$$M_{inj_{ADE}} = \frac{\left(C_{target\ max}\left(x_{distal},\ t_{p\ ADE}\right) - C_o\right)\,2A\sqrt{\pi D t_{p\ ADE}}}{e^{-\frac{\left(x_{distal} - u\ t_{p\ ADE}\right)^2}{4Dt} - \lambda t_{p\ ADE}}}. \tag{10}$$

$$M_{commercial_{ADE}} = M_{inj_{ADE}}\frac{Mm_{commercial}}{Mm_{target}}, \tag{11}$$

$$V_{inst.\ inj.} = \frac{M_{commercial_{ADE}}}{C_{commercial\ sol.}}. \tag{12}$$

2.2.2. Continuous tracer injection

We used mass balance equations to guide the user through the planning of a continuous tracer injection, i.e., those for which the injection time $t_{inj} > 0$. The mass estimation consists of a trial and verification process, i.e., once the user enters their feasible pump injection rate, q_{pump} [L^3 T^{-1}], and the volume of the injectate, $V_{injectate}$ [L^3], based on equipment and power availability, simple mass balance equations help verify the maximum pump injection rate, $q_{pump\ max}$ [L^3 T^{-1}], the maximum injection time, $t_{inj.max}$ [T], the concentration of the target tracer in the injectate assuming a 100% purity, $C_{target\ injectate}$ [M L^{-3}], the mass of commercial tracer to add to the injectate, $M_{commercial\ injectate}$ [M], and the percent saturation of the commercial tracer in the carboy, $\%sat_{commercial}$ [-].

$$q_{pump\ max} = \frac{V_{injectate}}{t_{inj.}}, \tag{13}$$

$$t_{inj.\ max} = \frac{V_{injectate}}{q_{pump}}, \tag{14}$$

$$C_{target\ injectate} = Q\frac{\left(C_{target\ max} - C_o\right)}{q_{pump}}, \tag{15}$$

$$M_{commercial\ injectate} = C_{target\ injectate}V_{injectate}\frac{Mm_{commercial}}{Mm_{target}}, \tag{16}$$

$$\%sat_{commercial} = \frac{C_{target\ injectate}}{C_{commercial\ sol.}}\frac{Mm_{commercial}}{Mm_{target}}. \tag{17}$$

2.3. Additional considerations

TIPT accounts for uncertainty in the estimation of the velocity of the flow, u, and reports three BTCs at each sampling location using the factors 0.8 u, 1.0 u, and 1.2 u in the analytical solutions of the ADE.

TIPT estimates the length required to attain complete lateral mixing for a tracer injection near the center of the channel. This mixing length, L_{mix}, is (Fischer et al., 1979):

$$L_{mix} = 0.1 \frac{w^2 u}{0.6\, h\, u_*}. \tag{18}$$

Note that if the tracer is released from the side of the channel, the user should quadruple L_{mix} (Chapra 2008).

TIPT provides the option to enter the minimum travel time that the user expects is needed to see significant reactions after releasing a reactive tracer, t_{min}, and uses it to estimate the minimum distance required between the injection and the first sampling location as:

$$L_{min} = 1.2u\, t_{min}. \tag{19}$$

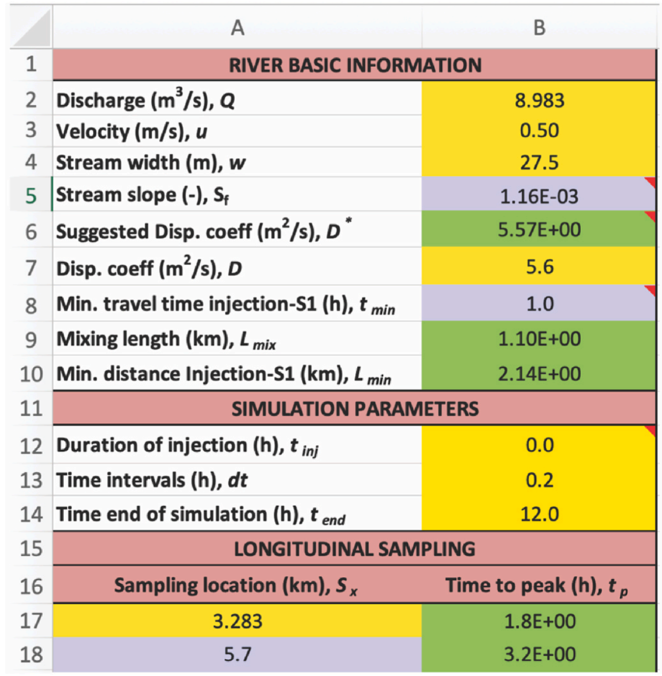
When the user enters a first sampling location at a distance smaller than L_{mix} or L_{min}, TIPT flags that input to alert the user.

2.4. User interaction with TIPT

The Excel Workbook TIPT has multiple sheets, where equations (1)–(17) are used to compute results and generate graphs. However, the user only inputs information in the *Main* sheet (yellow cells in workbook, see Table 2). TIPT requires basic information about the study site, simulation parameters and the distance from the tracer injection site to up to five sampling locations, where breakthrough curve simulations will be computed and graphed (Fig. 1). TIPT also asks for information about the commercial and target tracers to compute stoichiometric relationships and estimate masses to be added and allows the user to select between the Jobson's or ADE-based methods to estimate masses in instantaneous tracer experiments (Fig. 2). For continuous injections, i.e., when $t_{inj} > 0$, TIPT requests information about the pumping rate at which the tracer can be added and the volume of the carboy available to check mass balances, and help the user minimize the masses and injectate volume needed for the experiment (Fig. 3). We set the color convention described in Table 2 to guide the user interaction with TIPT.

To complete the planning of tracer experiments, the users must follow these steps in the *Main* sheet:

- Enter values for all cells in yellow. Cells in light purple are optional but may become yellow when switching between instantaneous and continuous injections.
- Enter values for cells B12 (t_{inj}), B13 (dt), or B14 (t_{end}) to trigger the calculation of new tracer breakthrough curves. Note that $t_{inj} = 0$ triggers results for instantaneous injections, and any positive value triggers results for continuous injections.



	A	B
1	RIVER BASIC INFORMATION	
2	Discharge (m³/s), Q	8.983
3	Velocity (m/s), u	0.50
4	Stream width (m), w	27.5
5	Stream slope (-), S_f	1.16E-03
6	Suggested Disp. coeff (m²/s), D*	5.57E+00
7	Disp. coeff (m²/s), D	5.6
8	Min. travel time injection-S1 (h), t_min	1.0
9	Mixing length (km), L_mix	1.10E+00
10	Min. distance Injection-S1 (km), L_min	2.14E+00
11	SIMULATION PARAMETERS	
12	Duration of injection (h), t_inj	0.0
13	Time intervals (h), dt	0.2
14	Time end of simulation (h), t_end	12.0
15	LONGITUDINAL SAMPLING	
16	Sampling location (km), S_x	Time to peak (h), t_p
17	3.283	1.8E+00
18	5.7	3.2E+00

Fig. 1. TIPT screenshot from the *Main* sheet showing the interface where the user enters river basic information, simulation parameters, and longitudinal sampling information.

- Cells F10:H10 allow the user to enter decay rate coefficients for the tracer that the user wants to graph in the tracer breakthrough curves. If none is entered, the graphs correspond to the conservative tracer.
- For instantaneous injections, select between Jobson's or ADE-based methods to estimate tracer masses. By default, TIPT uses the ADE-based method. Read cells F13:H14 to extract masses and volumes needed, based on the information given in cells F4:H8.
- For continuous injections, make sure that the values entered in cells K10:M11 do not result in red cells or numbers in the range K13:M17. If the results yield red cells or numbers in the range K13:M17, adjust values in K10:M11 until the cells turn green (which indicates mass balance compliance). Keep in mind that the idea is to minimize the mass injected and the volume needed.

The rest of the sheets in TIPT present graphs at different sampling locations and using both arithmetic and semi-log scales, the latter allowing the users to focus more on the timing of the low concentrations so as to avoid sampling truncation errors (Drummond et al., 2012; González-Pinzón et al., 2013), within the known advantages and limitations of using the ADE (Kirchner 2000; Zarnetske et al., 2012; Bardini et al., 2013).

Table 2
Color convention used in TIPT.

Yellow	Required inputs from the user
Light purple	Optional inputs from the user
Green	Result from calculations and validation of constraints
Pink or red	Cells contain input errors or results indicate that a change of inputs is needed to satisfy constraints
Gray	Information or calculations for the conservative (non-reactive) tracer
Light blue	Information or calculations for the reactive tracer

	D	E	F	G	H
1	TRACER INFORMATION				
2			Conservative tracer	Reactive tracer	Reactive tracer
3			NaBr		
4	Background in-stream target tracer concentration (ug/L), C_o		30		
5	Max. conc. target tracer at most downstream site (ug/L), $C_{target\ max}$		1600		
6	Comercial tracer solubility (g/L), $C_{commercial\ sol.}$		940.00		
7	Molar mass comercial tracer (g), $M_{mcommercial}$		102.9		
8	Molar mass target tracer (g), $M_{mtarget}$		79.9		
9	$Mm_{commercial}/Mm_{target}$ (-)		1.3	#DIV/0!	#DIV/0!
10	First-order rate coefficient for decay (1/s), λ				
11					
12	ESTIMATING INJECTION MASSES FOR INSTANTANEOUS INJECTIONS				
13	Mass of commercial tracer to add (kg), $M_{commercial}$		3.30E+01	#DIV/0!	#DIV/0!
14	Water to dissolve commerial tracer (L), $V_{inst.\ inj.}$		3.51E+01	N/A	N/A
15					
16	Mass estimation method	Cu= f(t_p) in (1/s)	M_{inj}=f(C_{max}) in (ug)	M_{inj}=f(C_{max}) in (ug)	M_{inj}=f(C_{max}) in (ug)
17		N/A	1.98E+10	0.00E+00	0.00E+00
18	Jobson (1996) method	N/A	2.56E+10	0.00E+00	0.00E+00
19	0	N/A	N/A	N/A	N/A
20	ADE method	N/A	N/A	N/A	N/A
21	1	N/A	N/A	N/A	N/A

Fig. 2. TIPT screenshot from the *Main* sheet showing the interface where the user enters tracer information and gets the estimated masses for instantaneous injection experiments.

	I	J	K	L	M	N
8	ESTIMATING INJECTION MASSES FOR CONTINOUS INJECTIONS					
9			Conservative tracer, NaCl	Reactive tracer, Raz	Reactive tracer,	Units
10		Pump injection rate (mL/min), q_{pump}		558.000		mL/min
11		Volume of the injectate (L), $V_{injectate}$		135.000		L
12						
13		Max. pump injection rate (mL/min), $q_{pump\ max}$	0.00E+00	5.63E+02	0.00E+00	mL/min
14		Max. injection time (h), $t_{inj.\ max}$	#DIV/0!	4.03E+00	#DIV/0!	h
15		Conc. of target tracer in the injectate (g/L), $C_{target\ injectate}$	#DIV/0!	2.15E-01	#DIV/0!	g/L
16		Mass of commercial tracer to add to injectate (g), $M_{commercial\ injectate}$	#DIV/0!	2.90E+01	#DIV/0!	g
17		% saturation of comercial tracer, % $sat_{commercial}$	#DIV/0!	1.19E-02	#DIV/0!	%

Fig. 3. TIPT screenshot from the *Main* sheet showing the interface where the user enters feasible pump injection rates and the working carboy volume that will be used in a continuous injection experiment.

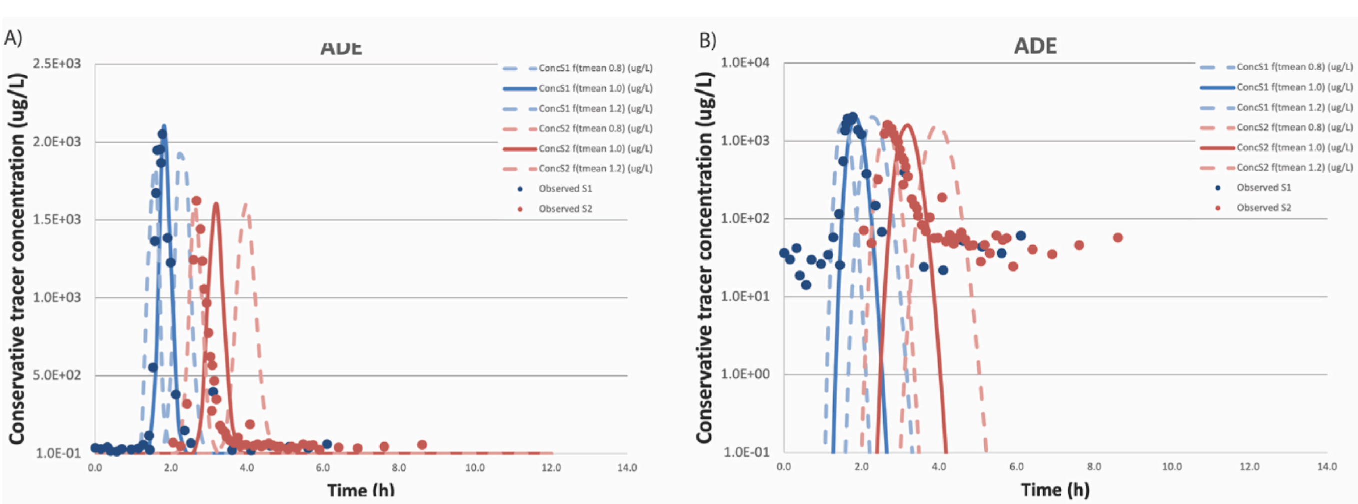


Fig. 4. TIPT was successfully used to plan an instantaneous tracer injection in a 7th order reach in the Rio Grande River, informing tracer mass, team and gear deployment strategies, and sampling time schedules. The figure shows field observations (dots) and TIPT simulations (lines) in A) arithmetic and B) semi-log (bottom) scales.

3. Case studies

3.1. Instantaneous injection

González-Pinzón et al. (2019) conducted an instantaneous tracer injection in the Rio Grande River near Albuquerque, New Mexico (USA), along a 7th order river reach. The team used TIPT to estimate the masses of NaBr and $NaNO_3$ as conservative and reactive tracers, the location of two sampling stations featuring well-mixed conditions, and the time coverage required to sample the tracer breakthrough curves there. On the day of the experiment, the team measured the mean discharge, velocity, and river width using a FlowTracker Handheld-ADV (Sontek, San Diego, USA), and used Google Maps to estimate the longitudinal slope of the reach. That information was entered in TIPT, as shown in Figs. 1 and 2. Using the basic river information collected on site and setting NaBr C_o ~30 μg/L as informed by previous work in the reach, TIPT suggested an injection of 33.3 kg of NaBr to get a desired NaBr $C_{target\ max} = 1600$ μg/L at the station located 5.665 km downstream of the injection site. Fig. 4 shows the predictions from TIPT and the actual concentrations measured from the tracer experiment after adding 31.1 kg of NaBr, 2.2 kg less, due to commercial tracer availability.

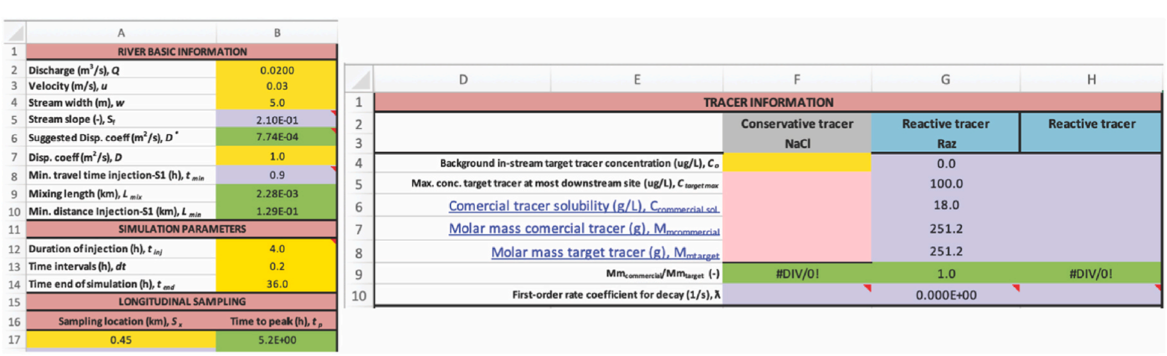
Note that the observed concentrations fell within the time windows predicted by TIPT, set as 0.8x and 1.2x the mean velocity entered to account for uncertainties in the user-specified parameters. Note that we limited the y-axis in the semi-log plot to show the instrument-specific limit of detection for Br samples (i.e., 1.1×10^{-1} μg/L), as any lower concentration would have been undetectable with the Dionex ICS-1000 Ion Chromatograph with AS23/AG23 analytical and guard columns that were used to read the field samples. The day of the experiment, using the results from TIPT, we organized two teams. The first team, with five members and one vehicle, oversaw the mixing and injection of the tracer at the injection site, and then moved to the second station to begin their sampling tasks about 1.7 h after the instantaneous tracer injection. The second team, with four members and a vehicle, was asked to prepare the two sampling stations (i.e., set up working tables and prepare sampling and labeling gear), and be ready to begin sampling at the upstream site from the time of tracer injection the next 6 h, so they could finish their labeling and filtration tasks, work on picking up their gear, and then drive to the second sampling station to support the rest of the crew, and organize the retreat from the field. Both teams returned samples to the laboratory soon after the last field sample was collected 9 h after the instantaneous tracer injection.

Given the size of the reach (which required covering long distances and significant moving times between locations), its proximity to a metropolitan area with ~1 million inhabitants (which limited the use of dyes or other observable tracers due to public concerns), and the low sensitivity that could be achieved with conductivity sensors (which forced us to use NaBr as a conservative tracer), TIPT's predictions of the tracer arrival, peak and passage times simplified the field logistics and allowed us to make objective decisions on *who* was doing *what*, and *where*. TIPT was used to guide our grab sampling in real-time because we could neither see the tracer plume nor measure Br concentrations with a sensor. Finally, TIPT accurately guided us to select the amount of tracer needed to avoid under or overestimations that could result in data (and time) losses, or environmental toxicity, respectively.

3.2. Continuous injections

In the summer of 2018, we conducted a continuous injection of resazurin in Como Creek, Colorado, USA, a steep 2nd order stream surrounded by 20% alpine meadow-tundra and 80% conifer forest (Ries III et al., 2017). The night before the injection, we used pre-verified information from a weir located at the study site to estimate discharge as 0.02 m^3/s for the next experimental day. In TIPT, we entered this and other relevant site and tracer information as shown in Figs. 3 and 5. Note that we set the first-order rate coefficient of resazurin equal to zero, despite knowing that microbial metabolism transforms it to its daughter product resorufin (González-Pinzón et al., 2012, 2014; Knapp et al., 2018) because we did not have a priori, site-specific information about the extent of the transformation of resazurin. With these assumptions, TIPT suggested the addition of 29 g of resazurin dissolved in a volume of 0.135 m^3 (135 L) to guarantee a 4 h injection using a pump injecting the injectate at a rate of 558 mL/min. Out of practicality, we added three pre-weighed 10g bags with resazurin since the saturation level of the tracer was below 12% (Fig. 3). During the experiment, we took 20 ml aliquots from the stream over 36 h and adopted our sampling frequency during the rising and falling limbs to capture the dynamic range of the tracer breakthrough curve following the predictions visualized through TIPT; for this, our injection time of 10:00 a.m. represented the 0h timestamp in TIPT. All samples were filtered immediately after collection using a 0.7 μm GF/F filter (Sigma-Aldrich). Samples were kept frozen at −4 °C to avoid ex-situ transformation. We followed the protocol presented in the Supplementary Information of Knapp et al. (2018) to estimate the resazurin concentrations in the laboratory using a Varian Carry Eclipse spectrofluorometer, with limit of detection of 1.0×10^{-2} μg/L. In Fig. 6, we overlapped the predictions from TIPT that we used to guide our experimental set up and sampling, the resazurin concentrations read in the laboratory, and a post-injection set of simulations from TIPT showing the results that we would have gotten if we had set the transformation rate coefficient of resazurin to $\lambda = 2 \times 10^{-4}\ s^{-1}$. This exercise shows that TIPT's timing was accurate regardless of the assumptions made about λ, and that the experimental λ at the study site was on the high end of values previously reported from tracer injections in stream ecosystems (Haggerty et al., 2008; Knapp et al., 2017), generating experimental concentrations that were one order of magnitude smaller than what was expected under the assumption of negligible transformation (i.e., conservative transport).

From this study case, we emphasize here that any assumption about



	A	B
1	RIVER BASIC INFORMATION	
2	Discharge (m^3/s), *Q*	0.0200
3	Velocity (m/s), *u*	0.03
4	Stream width (m), *w*	5.0
5	Stream slope (-), S_f	2.10E-01
6	Suggested Disp. coeff (m^2/s), D^*	7.74E-04
7	Disp. coeff (m^2/s), *D*	1.0
8	Min. travel time injection-S1 (h), t_{min}	0.9
9	Mixing length (km), L_{mix}	2.28E-03
10	Min. distance Injection-S1 (km), L_{min}	1.29E-01
11	SIMULATION PARAMETERS	
12	Duration of injection (h), t_{inj}	4.0
13	Time intervals (h), *dt*	0.2
14	Time end of simulation (h), t_{end}	36.0
15	LONGITUDINAL SAMPLING	
16	Sampling location (km), S_x	Time to peak (h), t_p
17	0.45	5.2E+00

	D–E	F	G	H
1	TRACER INFORMATION			
2		Conservative tracer	Reactive tracer	Reactive tracer
3		NaCl	Raz	
4	Background in-stream target tracer concentration (ug/L), C_o		0.0	
5	Max. conc. target tracer at most downstream site (ug/L), $C_{target\ max}$		100.0	
6	Comercial tracer solubility (g/L), $C_{commercial\ sol}$		18.0	
7	Molar mass comercial tracer (g), $M_{mcommercial}$		251.2	
8	Molar mass target tracer (g), $M_{mtarget}$		251.2	
9	$Mm_{commercial}/Mm_{target}$ (-)	#DIV/0!	1.0	#DIV/0!
10	First-order rate coefficient for decay (1/s), λ		0.000E+00	

Fig. 5. Site and tracer information entered in TIPT for the continuous tracer injection in Como Creek, Colorado, USA. Fig. 3 shows the information entered for the injectate.

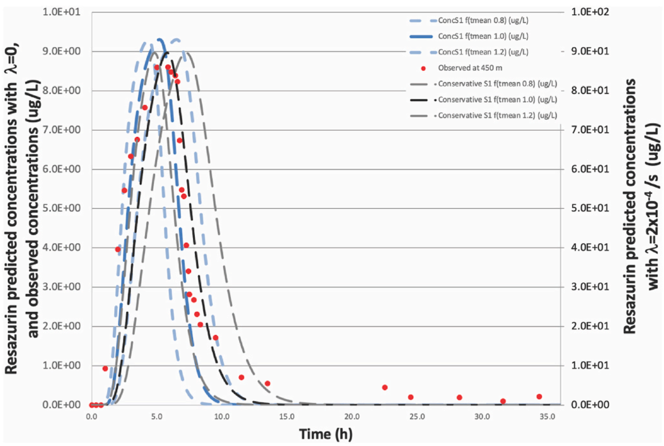


Fig. 6. TIPT was successfully used to plan a continuous tracer injection in a 2nd order reach in Como Creek, informing tracer masses, team and gear deployment strategies, and sampling time schedules. Although the assumption of negligible decay for resazurin did not affect the timing of our sampling, the mass injected generated lower concentrations due to high in-stream transformation. The figure shows field data (dots) and TIPT simulations (lines).

the likely behavior of a reactive solute that undergoes decay must be made judiciously considering that: 1) by assuming conservative transport or negligible decay, the resulting mass injected may generate small or undetectable dynamic concentration ranges due to unanticipated upstream uptake, retention or transformation, and 2) by assuming higher decay or transformation rate coefficients, the resulting concentrations may inadvertently overload the stream and generate maximum concentrations beyond those considered safe for its ecological functioning, and increase the cost of tracer salts unnecessarily.

4. Limitations and advantages of TIPT

4.1. Limitations

TIPT assumes steady-state and uniform flow conditions, i.e., the physical, chemical and biological characteristics of a stream captured by the user inputs are assumed to remain constant over space and time. While these assumptions let us use analytical solutions for the ADE, natural streams and rivers are dynamic and non-uniform. We developed TIPT because we have found that assuming steady-state and uniform conditions for planning the logistics of a tracer injection is practical and useful, i.e., any alternative based on parameterizing dynamic and non-uniform models without formally carrying out a tracer injection can be equally or more uncertain and laborious.

TIPT assumes that the biochemical reactions undergone by a reactive solute can be described using first-order decay or production, λ. Therefore, TIPT cannot anticipate the effects of kinetics-based reactions associated with limitations and co-limitations, among many other possibilities. Also, predicting λ values before a tracer injection may be difficult, so we recommend the use of experimental values reported in studies with similar characteristics. As we noted before, severely overpredicting λ can result in the introduction of too much mass to the stream ecosystem and unnecessary expenses associated with tracer supplies, while severely underpredicting λ can result in low to undetectable concentrations at downstream sites.

The current version of TIPT does not handle transient storage processes, lateral inflows or outflows. Transient storage in the surface or subsurface of the stream increases the residence times of solutes, which is manifested in longer BTC tails (Haggerty et al., 2002; Gomez et al., 2012; Jackson et al., 2013). Accordingly, TIPT would underpredict the time that it takes to recover the tracer mass in streams and rivers with extensive recirculation zones or hyporheic exchange. Also, while lateral outflows do not impact solute concentrations in well-mixed streams and rivers, but do impact mass balances, lateral inflows impact concentrations through dilution, but do not impact mass balances. Therefore, we recommend using TIPT in stream or river segments without significant inflows.

4.2. Advantages

TIPT is a first-approximation tool that can be used to plan tracer injections and design the logistics of experiments involving solute transport processes in streams and rivers. TIPT offers a predictive ability that is disproportionally favorable with respect to the few inputs required and uses Excel, which is readily available software accessible to those without coding experience. TIPT is a versatile, user-friendly, and graphical tool that can help the hydrologic, ecologic, and engineering communities design tracer injections and solute transport experiments that are more easily replicated within and across sites. In doing so, TIPT contributes directly to advancing ICON principles, which call for efforts to become more Integrated across disciplines; Coordinated with consistent protocols; Open across the entire research lifecycle; and Networked whereby a broad range of stakeholders design, implement, and benefit from the work (Goldman et al., 2022). Similarly, TIPT can help generate datasets that more closely follow FAIR principles, i.e., they are Findable, Accessible, Interoperable, and Reusable. Both ICON and FAIR are pillars of the Open Watershed Science by Design approach promoted by the US Department of Energy (Stegen et al., 2019).

Software availability

The Tracer Injection Planning Tool has been uploaded to HydroShare and will be maintained there.

Gonzalez-Pinzon, R., J. Dorley, J. Singley, K. Singha, M. Gooseff, T. Covino (2022). TIPT: The Tracer Injection Planning Tool, HydroShare, http://www.hydroshare.org/resource/6cc58a01c5b7463d97622bb225b73cca.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.envsoft.2022.105504.

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