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Approximation of inverse Laplace transform solution to heat transport in a stream system

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[1] The Laplace transform is a powerful tool used in solving partial differential equations. However, due to considerable difficulty associated with inverting analytical solutions from Laplace space to the original time variable, this final step is often performed by numerical techniques. Unfortunately, this does not deliver a closed form solution to the original model. Here we illustrate a technique for approximating a closed form inversion to the Laplace transformed solution of a heat transport model for a natural river system. We show the approximation method provides good results when compared to the analytical solution that is dependent upon numerical techniques for the inversion of the Laplace transform. Our approximation results in a simple and concise expression in terms of the model parameters without relying on difficult numerical computations. We focus on the contribution to downstream temperatures from upstream boundary conditions, illustrating how boundary condition temperature decays in terms of model parameters.

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1. Introduction

[2] Modeling transport phenomena using partial differential equations (PDE) has been an established paradigm for predicting sediment and heat transport in stream systems for many years. A typical starting point for modeling the various particulars of stream transport is the advection-dispersion equation (ADE) [Fischer, 1979]. Neilson *et al.* [2009, 2010a, 2010b] have developed an ADE heat transport model to predict temperatures in stream systems incorporating transient storage zones and heat flux across the water's surface. Recently Heavilin and Neilson [2012] provided an analytical solution to a simplified version of this heat transport model, focusing just on the main channel temperatures and using a linearized version of the heat flux function. The analytical solution provided is in terms of the transformed variable, and is not a closed form solution in the original state space. Nonetheless, as opposed to numerical simulations, one of the virtues of arriving at an analytical solution to a PDE is the opportunity this solution affords us to understand how the variables and parameters of the model contribute to the overall behavior of the system being modeled. Including the relevant physical processes provide good fits to downstream temperature profiles, and allow closer inspection of the components within the model. Because Neilson *et al.*'s model does a good job of capturing relevant

mechanisms of heat exchange and transport, we can examine more closely the components of the model and how well they individually represent the subsystem they model. For example, we can use the solution from the heat transport model to investigate how upstream temperatures affects downstream temperatures. Numerical approximations accurately simulate the overall behavior but unfortunately seldom shed insight into the relationship between the terms, variables, and parameters of the model.

[3] Some techniques for arriving at analytical solutions include series methods (i.e., Fourier series) and Green's functions. Typically series solutions often require computing several terms to arrive at a reasonable approximation to the solution. A Green's function can yield a tidier expression for a solution, but in the form of an integral where once again we need to resort to a numerical integration to visualize the solution [Weinberger, 1965]. Unfortunately doing so obviates some of the said virtues of the analytical solution, offering little more than numerical approximations. With these solution techniques we lose the expressions articulating the relationships between variables and parameters in the model which we were hoping to discover by solving the problem analytically in the first place. Other common methods for solving PDEs are integral transforms and among these the Laplace transform is one of the most common. This is a highly versatile and relatively easy technique for solving the PDE as long as one remains in the space of the transformed variable (Laplace space). The solution in Laplace space has additional merits stemming from the relationship between the Laplace transform and the moment generating function. For some physical problems the transformed solution conveniently provides the moment generating function of the solution which can be used to further assess the quality of the model [Curtiss, 1942]. Another benefit of the solutions gained via Laplace

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transforms is that the solution is often decomposed in terms of the respective contributions from the boundary condition and the initial conditions. This allows one to explore the dynamics of each component within the model.

[4] The difficulty with Laplace transform solutions often arises when inverting the solution to the original state space (usually time). Typically the transformed solution is too cumbersome to easily invert by means of the associated Bromwich integral, and unless the form of the solution appears in a table of transforms it falls once again to numerical algorithms to return to the time domain. To this end state-of-the-art algorithms like that of *De Hoog et al.* [1982] provide excellent results and are quite easy to implement. Other efforts at inverting the Laplace transform have included the use of rational expressions of infinite series or continued fractions. Regardless of whether one manages to find a closed form inverse to the solution in Laplace space or one resorts to an algorithm like De Hoog, the result is a solution that is far from a transparent appraisal of the interplay between the model terms, parameters, and variables of the system.

[5] Born of an interest to produce an easily interpretable, nice solution to the inverse Laplace transform, we explore the application of rational expressions in a manner akin to *Akin and Counts* [1969], *Luke* [1978], and *Longman and Sharir* [1971]. However, in our case we are not interested in arriving at the solution through an infinite series. Rather we wish to provide a simple, yet accurate tool that can approximate the behavior of the solution over a domain of interest and yield meaningful results that are as simple to calculate as they are easy to interpret.

[6] Moreover, unlike empirical models (which can be very accurate given a good data set) this approximation can convey meaning in terms of the mechanisms of the governing differential equation. We believe that making available simple and powerful tools for analysis strengthens the appeal and utility of a model to a wider range of users and applications. This has motivated us to use rational expressions as approximations to invert the Laplace transform of the solution to a heat transport model with the intent of describing the effects of changes to upstream boundary temperatures on downstream temperature profiles. We will illustrate how this technique can yield a succinct expression in terms of the ADE model parameters. We also show that this approximation compares favorably to the computationally intensive numerical results provided from the De Hoog numerical inversion of Laplace transforms and convolutions using fast Fourier transforms.

2. Rational Expression as Approximations of Inverse Laplace Transforms

[7] The use of continued fractions to approximate numbers otherwise difficult to express dates back at least to John Wallis in the mid 17th century when he published *Arithmetica infinitorum* [Wallis, 1655; *Stedall*, 2000]. Leonard Euler built on the work of Wallis when he published *De fractionibus continuis* illustrating how the method of continued fractions could be used to find approximations for what he termed *transcendentals* and first linked continued fractions to differential equations (e.g., the Riccati equation) [Euler, 1739, 1785; *Sandifer*, 2007]. Later in 1913 Perron published the first comprehensive exposition of the subject of

continued fractions and rational expressions in which he addressed issues of convergence of continued fractions and committed an entire chapter to this idea from Frobenius and Padé [Watson and Perron, 1957]. More recently *Khovanskii* [1963] built on the works of Perron by applying various methods and formulas concerning continued fractions and rational expressions to approximation theory, with which he solved a range of functions and integrals as well as applied rational expressions to solving differential equations.

[8] There are many ways of arriving at a rational expression for a function. As *Akin and Counts* [1969] point out, certain methods are better suited to some problems than others, and there is no generalized method that works in all cases. However, the aspiration of the methods mentioned previously is to find an expression that converges on the true solution for a sufficient numbers of terms. Our motivation here is somewhat different. We want to supply an approximation that captures the behavior of the system in a meaningful and readily interpretable expression. To illustrate how rational expressions can provide just such an approximation, we examine a function that commonly appears in transform tables, but is somewhat difficult to solve by means of the Bromwich integral: $\bar{f}(s) = 1/(s\sqrt{s+1})$.

[9] A table of transforms reveals that $f(t) = \text{erf}(\sqrt{t})$, but whereas one can easily conceptualize an exponentially decaying function in terms of system parameters, the shape of the error function, in terms of its parameters, is a little less transparent. In this illustration we will use the technique illustrated by *Perron* [1913] for deriving a Padé approximant for $\bar{f}(s)$, although it is worth noting that we arrive at the same result using Wallis's continued fraction approach [Wallis, 1655]. We will discover that even low order approximations do a reasonable job of approximating the true inverse, and yield a form that is much easier to associate directly with parameters. We begin with a series expansion for the function in Laplace space,

$$\bar{f}(s) = \frac{1}{s\sqrt{s+1}} = \frac{1}{s} \left(1 - \frac{1}{2}s + \frac{3}{8}s^2 - \frac{5}{16}s^3 + \dots \right). \quad (1)$$

We equate the series in equation (1) to a rational expression of the form

$$\frac{U_p}{V_q} = \frac{\alpha_0 + \alpha_1 s + \dots + \alpha_p s^p}{\beta_0 + \beta_1 s + \dots + \beta_q s^q} \quad (2)$$

with the condition that $N = p + q$, $p < q$ and we normalize the rational expression by setting $\beta_0 = 1$. Thus for an approximation of the form $[\alpha_0/(\beta_0 + \beta_1 s)]$ we have $p = 0$, $q = 1$, and $N = p + q = 1$. Setting equation (1) equal to the expansion in equation (2),

$$1 - \frac{1}{2}s = \frac{\alpha_0}{1 + \beta_1 s}. \quad (3)$$

Multiplying both sides by V_q and arranging like powers of s yields an equation of two polynomials. Equating powers of s on the left- and right-hand sides, we arrive at a system of equations that yield the values of α_0 and β_1 in the rational expression, namely $1 = \alpha_0$ and $-1/2 + \beta_1 = 0$. We now

have a low order approximation for $\bar{f}(s)$ which can be decomposed by partial fractions into a sum of irreducible terms:

$$\bar{f}(s) = \frac{1}{s} \frac{1}{\sqrt{s+1}} \approx \frac{1}{s} \left(\frac{1}{1+\frac{1}{2}s} \right) = \frac{1}{s} - \frac{1}{2+s}. \quad (4)$$

We readily recognize the inverse of the right-hand terms in equation (4) and conclude that $f(t) \approx 1 - e^{-2t}$. Similarly for the next higher order approximation we set $p = 1$ and $q = 2$, and match this to a power series where $N = 3$. Here we use the first four terms of the Taylor series, $(1 - 1/2s + 3/8s^2 - 5/16s^3)(1 + \beta_1s + \beta_2s^2) = \alpha_0 + \alpha_1s$. Again equating powers of s and solving the resulting system of equations we have

$$\begin{aligned} \bar{f}(s) &= \frac{1}{s} \frac{1}{\sqrt{s+1}} \approx \frac{1}{s} \left(\frac{1+\frac{1}{2}s}{1+s+\frac{1}{8}s^2} \right) = \frac{1}{s} - \frac{1}{2} \left(\frac{1}{s+4+2\sqrt{2}} \right) \\ &\quad - \frac{1}{2} \left(\frac{1}{s+4-2\sqrt{2}} \right). \end{aligned} \quad (5)$$

For this approximation we find that $f(t) = 1 - 1/2\{\exp[(-4 - 2\sqrt{2})t] + \exp[(-4 + 2\sqrt{2})t]\}$. Comparing the two low-order approximations found by rational expressions to the error function we find that both do a reasonably good job. Over the domain $(0, 3)$, where the approximation is the worst, we still have a root mean square error of less than 0.06 and 0.02 for the first and second approximations, respectively. In Figure 1 we illustrate how well the two approximations in equations (4) and (5) match $f(t) = \text{erf}(\sqrt{t})$. Encouraged by these results, we turn to the heat transport model and attempt to apply this method to the model's term describing the contribution from boundary conditions to downstream temperature.

3. Mathematical Model

[10] The model that Neilson *et al.* [2010a] have developed for stream temperatures that incorporates surface heat

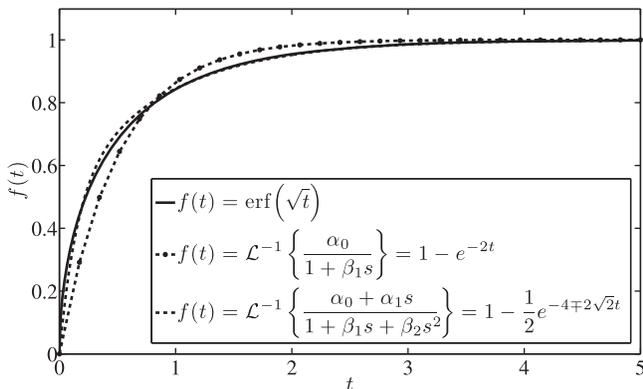


Figure 1. Comparing the two low-order approximations found by rational expressions to the true solution for $\mathcal{L}^{-1}\{1/(s\sqrt{s+1})\}$. We see that even the lowest order approximation does a reasonable job of modeling the error function, and we find that the error function behaves much like the exponentially decaying function $1 - \exp(-2t)$.

fluxes is driven by and calibrated to in situ measurements and applied to the Virgin River in Utah, USA. Neilson *et al.* [2010a, 2010b] have provided numerical approximations demonstrating promising results, providing good predictions of downstream temperatures. Atmospheric exchanges are modeled using Chapra's expressions for various nodes of heat flux: long wave, shortwave, and back radiation, as well as evaporation and conduction [Chapra, 1997]. In a recent work by Heavilin and Neilson [2012] a linearized version of this ADE is solved by means of Laplace transforms. The linearized ADE is given in equation (6) where T_{MC} is the temperature of the main channel ($^{\circ}\text{C}$), U is average velocity in the main channel (km d^{-1}), D is longitudinal dispersion ($\text{km}^2 \text{d}^{-1}$), and where $\bar{\phi}$ and $\bar{\theta}(t)$ constitute the linearization of the heat flux terms:

$$\begin{aligned} \frac{\partial T_{MC}}{\partial t} &= D \frac{\partial^2 T_{MC}}{\partial x^2} - U \frac{\partial T_{MC}}{\partial x} + \bar{\phi} T_{MC} + \bar{\theta}(t), \\ T_{MC}(x, 0) &= T_0, \\ T_{MC}(0, t) &= T_{in}(t). \end{aligned} \quad (6)$$

The solution resulting from Laplace transforms contains three terms, each representing the contribution to downstream temperatures from the boundary condition, the initial condition, and the exchange of heat with the surrounding environment. Equation (7) is the solution to equation (6) in Laplace space, where the Laplace transform of main channel and boundary condition temperatures are \mathcal{T} and \mathcal{T}_{in} , respectively. In both cases we have dropped the explicit dependency on s :

$$\begin{aligned} \mathcal{T} &= \mathcal{T}_{in} e^{\frac{x}{2D}[U - \sqrt{U^2 + 4D(s - \bar{\phi})}]} + \frac{T_0}{s - \bar{\phi}} \left(1 - e^{\frac{x}{2D}[U - \sqrt{U^2 + 4D(s - \bar{\phi})}] \right) \\ &\quad - \frac{\mathcal{L}\{\bar{\theta}(t)\}}{s - \bar{\phi}} \left(1 - e^{\frac{x}{2D}[U - \sqrt{U^2 + 4D(s - \bar{\phi})}] \right). \end{aligned} \quad (7)$$

See Heavilin and Neilson [2012] for details. As we mentioned previously, we would like to get more from the solution to the heat transport model than simply a good fit to downstream temperature profiles. Ultimately, we wish to use this solution to find a simple yet meaningful approximation for the contribution to downstream temperatures resulting from the boundary condition. This means an approximation in the original time domain to the first term in equation (7),

$$\mathcal{A}_1 = \mathcal{T}_{in} e^{\frac{x}{2D}[U - \sqrt{U^2 + 4D(s - \bar{\phi})}]}. \quad (8)$$

We apply the method described in section 2 to the second factor on the right-hand side of equation (8), $\bar{f}(s) = e^{\frac{x}{2D}[U - \sqrt{U^2 + 4D(s - \bar{\phi})}]}$, and solve for a lowest order rational polynomial expression that can be easily inverted. We begin by expanding the transformed function $\bar{f}(s)$ into a low-order Taylor series centered at $s = 0$ and construct

the associated rational expression. The Taylor series is given by

$$\bar{f}(s) = e^{\frac{x}{2D}[U - \sqrt{U^2 + 4D(s - \bar{\phi})}]} \approx e^{\frac{x(U-\eta)}{2D}} \left(1 - \frac{xs}{\eta} + \dots \right), \quad (9)$$

where $\eta = \sqrt{U^2 - 4D\bar{\phi}}$. We set this expansion equal to a rational polynomial. Assuming $N = 1$ and noting the conditions placed on equation (2) from earlier, $N = p + q$, $p < q$, we have $q = 1$ and $p = 0$. Therefore, after normalizing $\beta_0 = 1$, we have the relationship

$$\frac{U_0}{V_1} = \frac{\alpha_0}{1 + \beta_1 s}. \quad (10)$$

Equating the Taylor series to U_0/V_1 ,

$$e^{\frac{x(U-\eta)}{2D}} \left(1 - \frac{xs}{\eta} + \dots \right) = \frac{\alpha_0}{1 + \beta_1 s}. \quad (11)$$

Multiplying by V_1 and collecting terms in s

$$e^{\frac{x(U-\eta)}{2D}} \left[1 + \left(\beta_1 - \frac{x}{\eta} \right) s + \dots \right] = \alpha_0, \quad (12)$$

and equating like powers of s , we see that $\alpha_0 = \exp[x(U - \eta)/2D]$ and $\beta_1 = x/\eta$. From this we construct the low-order rational function described in equation (10) that approximates $\bar{f}(s)$, namely

$$\bar{f}(s) \approx e^{\frac{x(U-\eta)}{2D}} \frac{\eta}{\eta + sx}. \quad (13)$$

Returning once again with this rational expression approximating the exponential factor in equation (8) we write

$$A_1 \approx T_{in} e^{\frac{x(U-\eta)}{2D}} \frac{\eta/x}{\eta/x + s}. \quad (14)$$

At this point we could compute the associated convolution since the term $1/(\eta/x + s)$ has an easily recognizable inverse, $\exp(-\eta t/x)$. Therefore the approximation is

$$A_1 \approx \frac{\eta}{x} e^{\frac{x(U-\eta)}{2D}} \int_0^\infty T_{in}(\tau) e^{-\frac{(t-\tau)\eta}{x}} d\tau. \quad (15)$$

For completeness we apply the same method to the remaining terms in the solution given in equation (7), and find the approximation for the contribution from the initial condition described by the second term in the solution (equation (7)) is

$$A_2 \approx T_0 \left[e^{\bar{\phi}t} - \frac{\eta e^{\frac{x(U-\eta)}{2D}}}{\eta + \bar{\phi}x} (e^{\bar{\phi}t} - e^{-\frac{\eta t}{x}}) \right]. \quad (16)$$

We can see that this term evaluates to the initial condition at $t = 0$, and decays to zero as time increases. The contribution from the term governing heat flux given by the third term in equation (7) is

$$A_3 \approx \int_0^\infty \theta(t) \left[e^{\bar{\phi}(t-\tau)} - \frac{\eta e^{\frac{x(U-\eta)}{2D}}}{\eta + \bar{\phi}x} (e^{\bar{\phi}(t-\tau)} - e^{-\frac{\eta(t-\tau)}{x}}) \right] d\tau. \quad (17)$$

A graph comparing these three approximations to their corresponding model results is given in Figure 2.

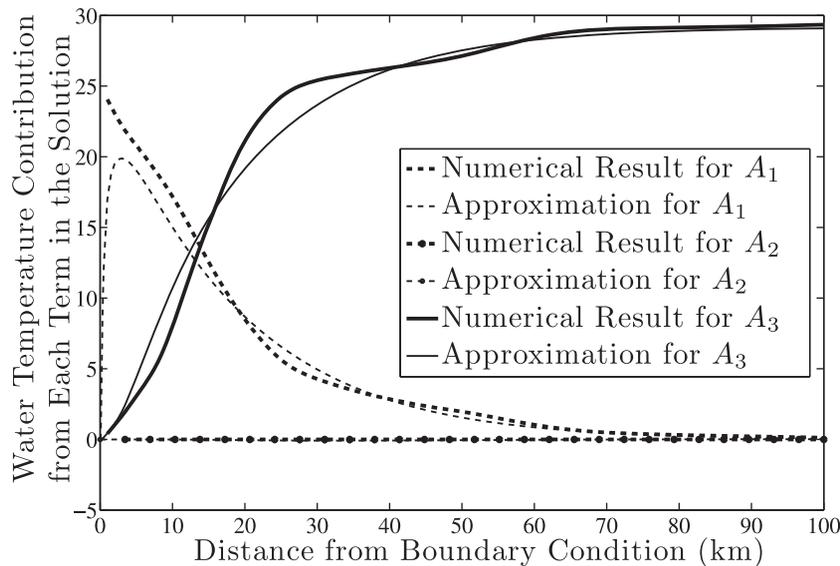


Figure 2. A graph of the three terms in the solution to the heat transport model, A_1 , A_2 , and A_3 at time $t = 3$ days and their corresponding approximations. The convolutions for the approximations were performed by fast Fourier transforms and the inverse Laplace transform needed for the numerical solution was solved using De Hoog’s algorithm. These simulations employ in situ temperature time series recorded at boundary condition in the Virgin River in 2007. The velocity was set to $U = 42 \text{ km d}^{-1}$ and the longitudinal dispersion $D = 3 \text{ km}^2 \text{ d}^{-1}$. The constant term resulting from the linearization of the heat flux function $\bar{\phi}$ is -2.29 day^{-1} . With these parameters η evaluates to 42.3 km d^{-1} .

[11] However, the intent of this approach is to arrive at a nice approximation whose behavior is apparent from a closed form expression and that does not rely on additional computational power to describe the behavior of the system. Rather than wonder what the overall contribution from total boundary condition data is, we can ask what the influence of an additional temperature T_0 at the boundary has on downstream temperatures. We could then assume $T_{in} = \hat{T}_{in} + T_0$ and by the linearity of the integral, investigate the influence of a constant temperature T_0 on the downstream temperatures. Substituting $\mathcal{L}\{T_0\} = T_0/s$ into equation (14) provides an expression for a constant temperature contribution at the upstream boundary. Once again we can decompose the resulting rational expression into a sum of two irreducible terms, and with some simplification

$$A_1 \approx T_0 e^{\frac{s(U-\eta)}{2D}} \left[\frac{1}{s} - \frac{1}{\left(\frac{U}{x} + s\right)} \right]. \quad (18)$$

Again we see that the inverses are simply the exponential function and a constant, meaning our lowest order approximation under the assumption of a constant boundary temperature is $A_1 \approx T_0 \exp[x(U-\eta)/2D][1 - \exp(-\eta t/x)]$. If we examine the approximation for A_1 more closely, we notice that the term $\exp(-\eta t/x)$ decays quickly in time, and since our question concerns downstream temperature (i.e., $x \gg 0$), we let $\exp(-\eta t/x) = 0$. This final simplification results in an expression for the influence of boundary conditions on downstream temperature,

$$A_1 \approx T_0 e^{\frac{s(U-\eta)}{2D}}. \quad (19)$$

It tells us that the boundary condition is decaying at a rate proportional to the distance from the boundary condition and at a rate approximately equal to $(U-\eta)/2D$. In Figure 3 we plot this approximation against the numerical

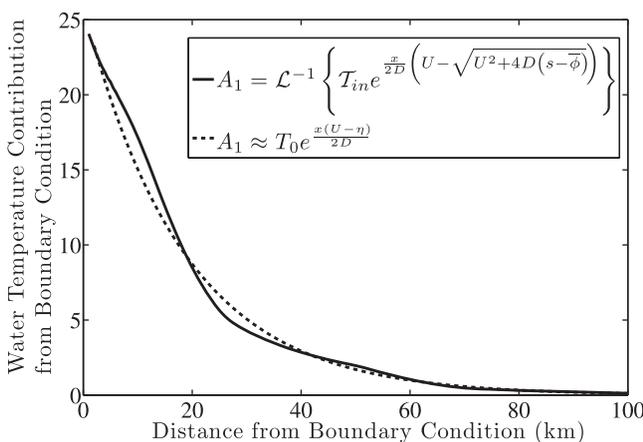


Figure 3. A graph of the contribution from the boundary to the main channel temperature. We compare the numerically inverted solution for term A_1 at time $t = 3$ days to the low order, time independent approximation for A_1 under the simplifying assumption of equation (18). The calculations used the same parameter values as in Figure 2.

inverse of the boundary condition term from the model in equation (12) using actual time series recorded at the most upstream site in the Virgin River by *Bandaragoda and Neilson* [2011]. For the purpose of illustration we will simply use the initial condition to represent a constant boundary condition temperature $T_0 = 25.9^\circ\text{C}$. For the convolution we use fast Fourier transforms and the Laplace inverse employs De Hoog's algorithm [*De Hoog et al.*, 1982]. The result of this approximation effort is a very simple and concise expression that describes the decay of influence from the boundary condition on downstream temperatures. Moreover, the expression is very intuitive and clearly reveals the relationship between velocity dispersion, and those components from the surface heat flux function that contribute to exchange of energy from boundary heat.

4. Conclusion

[12] Although techniques exist for very accurate numerical approximations for ADE models, the results can lack the transparency of a clear mathematical expression to illustrate the relationship between the movement of heat and the parameters in the model. To make management decisions regarding stream systems it is important to have predictive tools that are easy to parameterize and inform how proposed changes may impact the ecology. Here we provide a simple tool that predicts the downstream temperature contributions from a change in upstream temperature. We have established and quantified the interactions between instream velocities, dispersion, and surface heat fluxes on the transport of heat, and provided a prediction based on a parameterized ADE transport model of heat in the Virgin River, Utah, USA.

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