Stream heat budget modeling with HFLUX: model development, evaluation, and applications
across contrasting sites and seasons

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Abstract

Process-based models of fluid flow and heat transport in fluvial systems can be used to quantify unknown spatial and temporal patterns of hydrologic fluxes and to predict system response to change. In this study, a deterministic stream heat budget model, the HFLUX Stream Temperature Solver (HFLUX), is developed and evaluated using field studies. Field studies are conducted across two sites with different streamflow rates (0.07 vs $1.4 \text{ m}^3/\text{s}$), and point sources versus diffuse sources of groundwater discharge, to demonstrate model transferability. A winter versus summer comparison at one site suggests latent heat flux should be derived using energy-based methods in summer and mass balance approaches during winter. For each field study, HFLUX successfully modeled stream temperatures through space and time with normalized root mean square errors of 3.0 to 6.2%. Model calibration to observed temperature data in order to quantify groundwater contributions and a sensitivity analysis are demonstrated using HFLUX.

Keywords: stream temperature, Matlab, sensitivity analysis, distributed temperature sensing

Software and Data Availability: The HFLUX Stream Temperature Solver (HFLUX) is written by AnneMarie Glose, Laura Lautz, and Emily Baker in the Matlab computing language. The program files, documentation, and sample data are available as a 0.2 GB ZIP file. HFLUX was initially released online in 2014. The program can be downloaded at no cost from <http://hydrology.syr.edu/hflux>. The program comes with a sample dataset, which is available as an Excel file.

1. Introduction

Stream temperature is an essential water quality variable for the healthy functioning of fluvial systems (Caissie, 2006). The ecological health of streams is often dependent on water temperature, which also has an impact on economic interests, such as drinking water resources, aquaculture, and recreation (Webb *et al.*, 2008). Deterministic stream temperature models are useful for assessing water temperature dynamics. In contrast to statistical models, which use stochastic relationships to determine stream temperature, deterministic models use mathematical representations of physical processes to model stream temperature based on heat exchange with the environment (Benyahya *et al.*, 2010). Some of these processes include channel flow, the interaction of surface water with groundwater (SW-GW interaction), and fluxes of energy to and from the stream. While statistical models are useful for regional predictions of stream temperature, deterministic models allow for more detailed studies of systems because the underlying physical processes controlling temperature change are represented.

Recently, scientists have used deterministic stream heat budget models to address a broad spectrum of research topics, including determining dominant heat fluxes to streams (Caissie *et al.*, 2007; Evans *et al.*, 1998; Webb and Zhang, 1997), quantifying stream-groundwater interactions (Becker *et al.*, 2004; Loheide and Gorelick, 2006; Magnusson *et al.*, 2012; Westhoff *et al.*, 2011; Westhoff *et al.*, 2007), assessing stream temperature sensitivity to changing climate (Diabat *et al.*, 2012; Gooseff *et al.*, 2005; Yearsley, 2009) and land use (Roth *et al.*, 2010; Sun *et al.*, 2015), inferring channel geometry (Magnusson *et al.*, 2012), and determining in-stream versus near-stream transient storage (Neilson *et al.*, 2010). In the context of these studies, a variety of heat budget models exist, with different mathematical bases, computer interfaces, and intended uses (Becker *et al.*, 2004; Benyahya *et al.*, 2010; Boyd and Kasper, 2003; Carrivick *et*

al., 2012; Cox and Bolte, 2007; Evans *et al.*, 1998; Magnusson *et al.*, 2012; Neilson *et al.*, 2010; Webb and Zhang, 1997; Westhoff *et al.*, 2007). Many of the stream heat budget models featured in the literature were developed for specific field sites and studies (Becker *et al.*, 2004; Carrivick *et al.*, 2012; Magnusson *et al.*, 2012; Neilson *et al.*, 2010) and therefore may not translate easily to other uses, are not readily available to the public, or are not easily adapted to different systems, input data, or modeling objectives. Heat budget models often quantify changes in stream temperature through time at a specific location along a stream (e.g. Magnusson *et al.*, 2012) or through space at a specific point in time (e.g. Becker *et al.*, 2004), but few models are continuous in both space and time. Meteorological energy inputs have been modeled as a lump sum derived through model calibration, rather than through actual meteorological data and process-based understanding of energy fluxes (Becker *et al.*, 2004). Boyd and Kasper (2003) created an open-source heat budget computer code called HeatSource that has been used by government agencies (i.e. Oregon State Department of Environmental Quality) and in other studies (Diabat *et al.*, 2012; Loheide and Gorelick, 2006). While this is a comprehensive model with detailed documentation, the HeatSource program is coded using Visual Basic macros in Microsoft Excel and is therefore not readily adapted to routines that require many repetitive model runs, such as model calibration, sensitivity analysis, or Monte Carlo error analysis. Other stream temperature codes written in FORTRAN or C/C++ (e.g. Cox and Bolte, 2007) require significant experience and knowledge of the program language itself to make code modifications, which may not be readily made by the typical model user (Kourakos and Harter, 2014).

This study presents a new heat budget modeling program, the HFLUX Stream Temperature Solver (HFLUX), which provides a tool for predicting stream temperatures through space and time. HFLUX returns modeled stream temperatures as well as energy fluxes to and

from the stream (shortwave and longwave radiation, latent heat flux, sensible heat flux, and bed conduction). HFLUX is run using a line of code in Matlab, one of the most commonly used and computationally powerful programming languages. Matlab is a high-level scripting language that provides a computing environment where code is visible and may be annotated in detail for easy user modification (Kourakos and Harter, 2014). The Matlab environment lends itself to running a program repeatedly, making it ideal for performing sensitivity or error analyses. The HFLUX subroutines are provided online at <http://hydrology.syr.edu/hflux/> as a package of open-source m-files, which are clearly annotated for the user such that the model can be readily modified. The program produces graphical displays of calculated stream temperatures and heat fluxes, and it includes a separate function for calculating and visualizing error between modeled and measured stream temperatures, and has a program for conducting a simple model sensitivity analysis. These additional programs offer applications complimentary to, but different from, what is commonly provided by other publicly available models. Quantifying energy fluxes to a stream requires a large quantity of data and computation that can make this approach difficult and overwhelming for practitioners; a simple one-dimensional stream heat budget model with a user-friendly interface that uses readily available data would be a beneficial addition to currently available hydrologic models.

The aims of this study are threefold: to introduce the HFLUX Stream Temperature Solver, to evaluate its ability to accurately simulate stream temperatures through space and time across a variety of field sites during multiple seasons, and to explore its utility. Data from two streams in upstate New York are used to evaluate the capacity of this new heat budget tool to correctly model heat exchange between a stream channel and its environment. Applications of

this tool, including inverse modeling of streamflow rates and a sensitivity analysis of temporally constant variables, are proposed and demonstrated.

2. Methods

2.1. Development of the HFLUX Stream Temperature Solver

Using hydrological, meteorological, and other information about the surrounding environment, HFLUX calculates stream temperature with respect to space and time. The model uses a Eulerian approach, simulating the stream as a series of longitudinal nodes, and the temperature of each node is a function of the temperature of the stream flow into and out of the node, the lateral inflow of groundwater, and heat fluxes to and from the node that are controlled by meteorological inputs. Using the necessary input data (Table 1), the model solves the mass and energy equations for heat transport using finite difference methods, and applies the heat fluxes along the stream profile at each time step. The output is a matrix of stream temperatures along the length of the stream and with respect to time. Input data sampled at uniform temporal and spatial scales are not required to run HFLUX; the program uses linear interpolation to resample the data to the spatial and temporal scale specified by the user. The HFLUX program files may be downloaded from the following web site: <http://hydrology.syr.edu/hflux>. A simple model run can be executed using these two lines of Matlab code:

```
[input_data] = hflux_format ('example_data.xlsx');
[temp matrix node flux] = hflux (input_data);
```

The first line of code formats all input data provided in the Excel worksheet template into the required Matlab structured array format, which is then used as input to the HFLUX model. In this way, minimal experience manipulating data in Matlab is required. The HFLUX program files and documentation for the program, which includes a detailed discussion of how to operate the HFLUX Stream Temperature Solver, are available at <http://hydrology.syr.edu/hflux/>.

The HFLUX Stream Temperature Solver is a one-dimensional (longitudinal) transient model that was developed based on common energy balance formulations presented in the literature (e.g. Boyd and Kasper, 2003; Caissie *et al.*, 2007; Cox and Bolte, 2007; Kim and Chapra, 1997; Westhoff *et al.*, 2007), with additional modification. The model solves the mass and energy balance equations for energy transport:

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = q_L \quad [1]$$

$$\frac{\partial (AT_w)}{\partial t} + \frac{\partial (QT_w)}{\partial x} = q_L T_L + R \quad [2]$$

where Q is the discharge of the stream (m^3/s), A is the cross-sectional area of the stream (m^2), T_w is the stream temperature ($^{\circ}\text{C}$), x is stream distance (m), t is time (s), q_L is the groundwater inflow per unit stream length (m^2/s), and T_L is the temperature of the groundwater ($^{\circ}\text{C}$). Note that this formulation is based on a thermal datum of 0°C , which impacts the absolute value of the advective heat flux term (Kurylyk *et al.*, 2016). In the event that q_L is negative, as would occur in a losing stream, the first term on the right hand side of equation [2] is $q_L T_w$. R is the energy flux (source or sink) per unit stream length:

$$R = \frac{B\Phi_{total}}{\rho_w c_w} \quad [3]$$

where Φ_{total} is the total energy flux to the stream per surface area (W/m^2), B is the width of the stream (m), and ρ_w and c_w are the density (kg/m^3) and specific heat ($\text{J}/\text{kg}^{\circ}\text{C}$) of water, respectively. Dispersion is considered negligible in streams with fairly uniform water temperature, where longitudinal changes in temperature are generally small compared to temporal changes (Caissie *et al.*, 2007), and is thus ignored. Changes in discharge between

consecutive model nodes are used to derive groundwater inflows (q_L) to each node, similar to Cox and Bolte (2007).

Discharge rates in streams can vary through both space and time, although limited direct observations of such temporal and spatial variability may limit the available input data for a given model user. With this in mind, HFLUX has the option to input a constant discharge rate, or discharge rates that vary through space and/or time. When discharge rates vary through time, the model adjusts channel dimensions through time as a function of that varying discharge. Such adjustments are important to estimate: (1) increases in channel width with discharge, which increase the magnitude of heat fluxes to the stream (equation [3]); and (2) increases in water mass per node at higher discharges, which reduce the change in temperature associated with a given heat flux. HFLUX uses Manning's equation to estimate changes in stream width and depth as a function of discharge. The channel geometry is adjusted assuming a triangular channel shape, as well as a constant stream angle (θ), channel slope, and roughness at a given location through time.

Because Q , A , and T_w are all changing with respect to time and/or space, a finite difference method is used to approximate the solutions to the differential equations. HFLUX includes the option to use either a Crank-Nicolson scheme or a second-order Runge-Kutta scheme to solve the energy and mass balance equations. The Crank-Nicolson scheme is central in both time and space, and it is numerically stable, meaning that the method for approximating solutions from node to node does not introduce spurious mathematical oscillations (Zheng and Bennett, 1995). However, the Crank-Nicolson scheme has the potential to quantify changes in stream temperature incorrectly if the heat fluxes are changing rapidly through time. The second-order Runge-Kutta method is conditionally stable and requires the use of a Courant time step to

eliminate instability. The Runge-Kutta method can be more computationally expensive, but this method is more adept at capturing quickly changing heat fluxes and their impact on the stream temperature.

Four meteorologically driven heat fluxes are considered in this model: shortwave radiation, longwave radiation, latent heat flux, and sensible heat flux. Streambed conduction and heat exchange due to groundwater inflow are also included. In HFLUX, the sign convention is such that heat fluxes to the stream are positive and heat fluxes from the stream are negative.

2.1.1. Shortwave radiation

The total shortwave radiation reaching the stream ($F_{shortwave}$) is the difference between the incoming shortwave radiation (S_{in} , W/m²), which is measured, and the reflected shortwave radiation (S_{refl} ; 0 to 1, or no shortwave radiation reflected to all shortwave radiation reflected, respectively):

$$F_{shortwave} = (1 - SF)(S_{in}) - (S_{refl})(1 - SF)(S_{in}) \quad [4]$$

(Caissie *et al.*, 2007; Neumann and Pierson, 1966; Ouellet *et al.*, 2014).

For this study, incoming shortwave radiation from the sun is measured with a pyranometer and then corrected in the model, as needed, for an estimated percentage of shading (SF ; 0 to 1, or no shade to complete shading, respectively). SF was estimated for each study site based on observed vegetation conditions along the stream reach at the time of each study (e.g. higher value of SF during the summer, when foliage is thicker, as compared to the winter, when trees have dropped their leaves). Complete shading (an SF value of 1) is considered unrealistic for real-world stream systems, as diffuse shortwave radiation that penetrates the canopy contributes to this flux even in highly shaded systems (Boyd and Kasper, 2003). The percent of incoming shortwave radiation

that is reflected is calculated by the model using solar position throughout the day and Fresnel's reflectivity (Boyd and Kasper, 2003; Neumann and Pierson, 1966).

Because calculating shortwave radiation is described in a variety of ways in the literature, the HFLUX Stream Temperature Solver has two options for calculating this flux: correct the measured shortwave radiation for shading and the reflected shortwave radiation, as described above [4], or correct the measured shortwave radiation for shading and use an assumed value for albedo at the stream surface [5].

$$F_{shortwave} = (1 - albedo)(1 - SF)(S_{in}) \quad [5]$$

(Magnusson *et al.*, 2012; Maidment, 1993).

2.1.2. Longwave radiation

The net longwave radiation ($F_{longwave}$) to or from the stream is the sum of atmospheric longwave radiation ($F_{atmospheric}$), back radiation off the surface of the stream ($F_{back_radiation}$), and landcover longwave radiation ($F_{landcover}$). Although longwave radiation can be measured directly in the field (e.g. using a pyrgeometer), such direct observations are rare in stream temperature studies. As a result, HFLUX predicts incident longwave radiation using the Stefan-Boltzman Law and observations of water and air temperatures.

Atmospheric longwave radiation is calculated using air temperature (T_{air} , °C), cloud cover (C_L , 0 to 1, or clear skies to overcast skies, respectively), the Stefan-Boltzmann constant (S_{sb} , W/m²°C⁴), the view-to-sky coefficient (vts ; 0 to 1, or no view to sky to clear view to sky, respectively) and relative humidity (H , %) (Benyahya *et al.*, 2010; Boyd and Kasper, 2003; Westhoff *et al.*, 2011; Westhoff *et al.*, 2007)

$$F_{atmospheric} = 0.96e_{atm}vtsS_{sb}(T_{air} + 273.2)^4 \quad [6]$$

where emissivity of the atmosphere (e_{atm} , dimensionless) is computed from (Kustas *et al.*, 1994):

$$e_{atm} = 1.72 \left(\frac{e_a}{T_{air} + 273.2} \right)^{\frac{1}{7}} (1 + 0.22 C_L^2) \quad [7]$$

where e_a is the actual vapor pressure (kPa). Actual vapor pressure (e_s , kPa) (Dingman, 1994;

Maidment, 1993), is computed as:

$$e_a = \frac{H}{100\%} e_s \quad [8]$$

Saturation vapor pressure is computed as (Dingman, 1994; Evans *et al.*, 1998; Maidment, 1993;

Westhoff *et al.*, 2007):

$$e_s = 0.611 e^{\frac{17.27 T_{air}}{237.3 + T_{air}}} \quad [9]$$

Back radiation, the longwave radiation from the stream surface, is calculated using water temperature (Boyd and Kasper, 2003; Evans *et al.*, 1998; Kim and Chapra, 1997; Ouellet *et al.*, 2014; Westhoff *et al.*, 2007):

$$F_{back_radiation} = -0.96 S_{sb} (T_w + 273.2)^4 \quad [10]$$

The emissivity of water in equation [10] is set at 0.96, which is consistent with other stream energy balance models (Boyd and Kasper, 2003; Westhoff *et al.*, 2007). Elsewhere, estimates of water emissivity are higher (e.g. 0.97 in Ouellet *et al.*, 2014; Caissie *et al.*, 2007). Similar to other constants set in HFLUX, this value can be readily adjusted by the user in the Matlab code.

Landcover radiation, or the radiation to or from surrounding vegetation, is calculated using water temperature and the view-to-sky coefficient (Boyd and Kasper, 2003; Westhoff *et al.*, 2007):

$$F_{landcover} = 0.96(1 - vts)0.96 S_{sb} (T_a + 273.2)^4 \quad [11]$$

Atmospheric, back, and landcover longwave radiation are all calculated according to the Stefan-Boltzmann law under the assumption that the water surface, surrounding vegetation, and the atmosphere act similarly to blackbody radiators. The net longwave radiation to or from the stream is the sum of these three fluxes:

$$F_{longwave} = F_{atmospheric} + F_{back_radiation} + F_{landcover} \quad [12]$$

2.1.3. Latent heat flux

Latent heat flux ($F_{evaporation}$), which is the energy used for either evaporation from or condensation to a body of water, is calculated using the rate of evaporation (E , m/s), the density of water (ρ_w , kg/m³), and the latent heat of vaporization (L_e , J/kg) (Evans *et al.*, 1998; Webb and Zhang, 1997; Westhoff *et al.*, 2007):

$$F_{evaporation} = -\rho_w L_e E \quad [13]$$

A negative value for the latent heat flux indicates that heat is being lost from the water body through evaporation, while a positive value indicates that condensation is adding energy to the water body (Dingman, 1994).

The rate of evaporation is often calculated in the literature using one of two methods: the Penman combination method for evaporation from open water (e.g. Westhoff *et al.*, 2007), the mass transfer methods (Webb and Zhang, 1997; Caissie *et al.*, 2007; Leach *et al.*, 2014; Magnusson *et al.*, 2012; Evans *et al.*, 1998), or both (Boyd and Kasper, 2003; Ouellet *et al.*, 2014).

The Penman combination method was developed to combine the energy from net radiation and mass transfer in order to calculate evaporation. The meteorological variables used in the Penman method include air temperature, water temperature, relative humidity, wind speed (v_{wind} , m/s), and net radiation, which is the sum of shortwave and longwave radiation (F_r ,

W/m²) (Maidment, 1993). Latent heat of evaporation is a function of water temperature and can be estimated as (Maidment, 1993):

$$L_e = 10^6 (2.501 - 0.002361T_w) \quad [14]$$

Penman open water evaporation is computed as (Maidment, 1993; Westhoff *et al.*, 2007):

$$E = \frac{sF_r}{r_w L_e (s + g)} + \frac{c_{air} r_{air} g (e_s - e_a)}{r_w L_e r_a (s + g)} \quad [15]$$

where r_w is the density of water (kg/m³), c_{air} is the specific heat of air (J/kg°C), r_{air} is the density of air (kg/m³), g is the psychrometric constant (J/kg°C), and F_r is the sum of short and longwave radiation.

Slope of the saturation vapor pressure curve (s , kPa/°C) is calculated as (Maidment, 1993):

$$s = \frac{4100e_s}{(237 + T_{air})^2} \quad [16]$$

Aerodynamic resistance (r_a , s/m) is calculated as (Westhoff *et al.*, 2007):

$$r_a = \frac{245}{0.54v_{wind} + 0.5} \quad [17]$$

Ideally, the exact form of equation [17] would be specific to a given site, given the difficulty in accurately estimating r_a . For a comprehensive evaluation of different equations for the evaporative heat flux, and specifically empirical coefficients in these formulations, the reader is referred to Ouellet *et al.* (2014). An individual user can modify the form of equation [17] (and any other empirical constants in HFLUX) within the Matlab script to customize coefficients and equation forms for their individual site.

The mass transfer method does not take into account net radiation and instead is driven by wind speed and vapor pressure differences. Equations of this form take into account two empirical constants, b_0 and b_1 , that are dependent on the heights at which wind speed and vapor

pressure are measured (Dingman, 1994). Using a mass transfer method, E is calculated as (Dingman, 1994):

$$E = (b_0 + b_1 v_{wind}) (e_s^w - e_a) \quad [18]$$

where the saturation vapor pressure of the evaporating surface (e_s^w , kPa) is (Dingman, 1994; Maidment, 1993):

$$e_s^w = 0.61 \exp \left(\frac{17.27 T_w}{237.3 + T_w} \right) \quad [19]$$

Because b_0 and b_1 are dependent on site-specific parameters, these values vary in the literature from study to study. Boyd and Kasper (2003) give a selection of values from different studies and Cox and Bolte (2007) have these constants as user-specified model input parameters. Using the values developed by Dunne and Leopold (1978) and correcting for units, the evaporation rate is computed in HFLUX as:

$$E = (1.505 \times 10^{-8} + 1.6 \times 10^{-8} v_{wind}) (e_s^w - e_a) \quad [20]$$

The user can adjust the empirical constants, b_0 and b_1 , within the Matlab code for their specific site. For a detailed assessment of how field measurements can be used to develop site-specific empirical constants for latent heat flux calculations, the reader is referred to Maheu *et al.* (2013).

2.1.4. Sensible heat flux

Sensible heat flux ($F_{sensible_heat}$) is the exchange of heat between the surface of the stream and the air. This flux is often calculated in the literature using the Bowen ratio (B_r), which relates latent and sensible heat (Benyahya *et al.*, 2012; Boyd and Kasper, 2003; Cox and Bolte, 2007; Evans *et al.*, 1998; Leach *et al.*, 2014; Webb and Zhang, 1997; Westhoff *et al.*, 2007).

$$F_{sensible_heat} = B_r F_{evaporation} \quad [21]$$

where the Bowen ratio is (Evans *et al.*, 1998; Magnusson *et al.*, 2012; Webb and Zhang, 1997; Westhoff *et al.*, 2007):

$$B_r = 6.1 \cdot 10^{-4} P_A \frac{T_w - T_{air}}{e_s^w - e_a^w} \quad [22]$$

and the actual vapor pressure of the evaporation surface (e_s^w , kPa) is:

$$e_a^w = \frac{H}{100\%} e_s^w \quad [23]$$

Adiabatic atmospheric pressure adjusted for elevation above sea level, z (m), is computed as (Westhoff *et al.*, 2007):

$$P_A = 101.3 \exp\left(\frac{293 - 0.0065z}{293}\right)^{5.256} \quad [24]$$

Because B_r goes to infinity when humidity approaches 100%, sensible heat can also be calculated separately from the latent heat flux (Dingman, 1994). This method relies on the temperature difference between the water surface and the air and the wind speed:

$$F_{sensible_heat} = -K_H v_{wind} (T_w - T_{air}) \quad [25]$$

where the exchange coefficient for sensible heat (K_H , J/°Cm³) is calculated as:

$$K_H = \frac{D_H}{D_M} c_{air} r_{air} \frac{k^2}{\left| \ln\left(\frac{z_m - z_d}{z_0}\right) \right|^2} \quad [26]$$

where $\frac{D_H}{D_M}$ is the ratio between the diffusivity of heat and the diffusivity of momentum (1 under stable atmospheric conditions), z_m is the height at which wind speed measurements were taken (m), z_d is the zero-plane displacement (m), z_0 is the roughness height (m), and k is a dimensionless constant equal to 0.4 (Dingman, 1994). The zero-plane displacement and the

roughness height are calculated based on the height of vegetation (z_{veg} , m) using the following relationships (Dingman, 1994):

$$z_d = 0.7z_{veg} \quad [27]$$

$$z_0 = 0.1z_{veg} \quad [28]$$

This method of calculating sensible heat is valid when $z_m > z_d + z_0$, or when the measurements for wind speed are taken at a height that is greater than the canopy. In order to make this equation applicable to a specific location, the user can change the value of z_{veg} within the Matlab code to a value that is representative for their site.

2.1.5. Streambed heat fluxes

Streambed conduction (F_{sed}) is a function of the gradient between stream temperature and the bed temperature (T_{sed} , °C) over distance, d (m), and the thermal properties of the sediment (K_{sed} , W/m°C) (Lapham, 1989):

$$F_{sed} = \frac{WP}{B} - K_{sed} \frac{T_w - T_{sed}}{d} \quad [29]$$

The ratio of the wetted perimeter (WP , m) to the stream width accounts for the fact that energy exchange with the riverbed occurs over the wetted perimeter, whereas energy exchange with the atmosphere occurs only over the stream width. For simplicity, wetted perimeter is computed from stream width and depth data. The thermal properties of the sediment are designated based on the type of sediment that makes up the streambed (clay, sand, gravel, or cobbles).

Streambed heat advection is a function of the rate of groundwater flux to (positive) or from (negative) the stream (q_L). Groundwater flux to or from the stream is computed directly in HFLUX from the input discharge data; any changes in discharge with distance are attributed to

gains or losses of groundwater. When the stream is gaining groundwater and q_L is positive, the advective heat flux is $q_L T_L$. In the event that q_L is negative, as would occur in a losing stream, the advective heat flux is computed as $q_L T_w$.

2.2. Field Sites

To evaluate the accuracy of the HFLUX Stream Temperature Solver across contrasting field sites and seasons, field data were collected from two streams in Syracuse, New York, during three separate field campaigns. The two streams represent unique fluvial systems in terms of size and dominant processes and different methods of data collection were used during each study. Field data from multiple seasons were also used in order to test the applicability of the model to different meteorological conditions with different dominant heat exchange mechanisms.

2.2.1. Meadowbrook Creek: Syracuse, NY

Meadowbrook Creek is a first order stream in the city of Syracuse, New York (Figure 1a.). The stream is highly urbanized for about 4 kilometers as it flows through armored channels between city streets. Downstream, Meadowbrook Creek meanders through a broad flood plain with riparian vegetation (Ledford and Lautz, 2015). Input data for HFLUX were collected in both June of 2012 and December 2012 to January 2013 using a 460 to 475-meter reach in the most downstream section of Meadowbrook Creek (Figures 1b. and 1c.).

During both field studies, the stream channel was outfitted with iButtons (model DS1922L, accuracy of $\pm 0.5^\circ\text{C}$, resolution of 0.0625°C) about every 20 meters along the reach (Figures 1b. and 1c.). The iButtons recorded temperature every five minutes for the summer field study and every ten minutes for the winter field study. The iButtons were deployed in the stream channel, between 5 and 20 cm above the streambed. Meteorological data, including solar

radiation, air temperature, relative humidity, and wind speed, were recorded at the field site using a VantagePro2 weather station using the same time intervals as the iButtons (Figures 1b. and 1c.). Bed temperatures through time were not observed in the June study. To estimate bed conduction, the subsurface temperature was assumed to be equal to the groundwater temperature at a depth of 2 m. In order to improve the quantification of this flux, iButtons were installed 20 cm into the bed at three locations to measure bed temperature every 10 minutes during the entire study for the winter fieldwork (Figure 1c.).

A constant rate tracer injection of Rhodamine Water Tracer (RWT) was conducted during each study to determine a spatially distributed stream discharge profile using dilution gauging. Samples were collected approximately every 15 m along the stream (Figures 1b. and 1c.) when the concentration of RWT in the channel plateaued at the reach outlet. The concentration of RWT in these samples was measured using a benchtop fluorometer, and a longitudinal profile of discharge was calculated based on the dilution of the dye as it moved down the stream during the test. Differential gauging with a Sontek Acoustic Doppler Velocimeter (ADV) at five locations along the reach on subsequent days following the injection experiments confirm the rate of streamflow increase with distance and that the creek is uniformly gaining water over its length. ADV measurements were also used to measure the width, depth, and cross-sectional area of the stream (Figure 1b. and 1c.).

Shade and the view to sky coefficient were not directly measured during these field campaigns; therefore, qualitative observations of riparian vegetation, aerial photos of the site, and model calibration were used to estimate the shade and view to sky coefficient. Groundwater temperatures were assumed to vary somewhat seasonally, being slightly cooler than the average air temperature of 10 °C in the winter (7 °C) and warmer in the summer (13 °C). The assumption

that the temperature of advecting groundwater is a function of the annual average air temperature can be problematic (e.g. Kurylyk et al., 2016). More sophisticated estimates of T_L can be incorporated into HFLUX by simply modifying the input T_L values. Measurements of cloudiness during the summer and winter field studies were measured at Syracuse Hancock International Airport, approximately 16 kilometers from the site. Table 1 summarizes the field data for Meadowbrook Creek.

2.2.2. *Ninemile Creek: Syracuse, NY*

Ninemile Creek is a second order stream in Syracuse, New York, that flows into Onondaga Lake (Figure 2a.). During a 2009 study (Briggs *et al.*, 2012), a fiber optic distributed temperature sensing (DTS) cable was deployed over a 900 m reach for 24 hours (9 September 2009 to 10 September 2009) to record stream temperature (Figure 2b.). Details on field data collection and analysis are presented in Briggs *et al.* (2012) and briefly summarized here. Temperature measurements were averaged over 4.5 minutes at 1.5 m intervals along the stream. The cable was laid out on the streambed in the middle of the channel, and the stream was assumed to be well mixed laterally and vertically. Ninemile Creek is larger than Meadowbrook Creek, with a baseflow discharge of $1.4 \text{ m}^3/\text{s}$ at the time of data collection. It has a substantial point source input from a groundwater spring (58.6 to 72.8 L/s) that cooled the stream during the study period. Differential and dilution gauging methods were used to measure stream discharge; for this study specifically, the discharge values longitudinally along the stream were calculated using concentrations of calcium ions in an end-member mixing analysis (Figure 2b.). Meteorological data were recorded approximately 10 kilometers from the site during the study period at the Syracuse Hancock International Airport. These data were compared with less comprehensive meteorological data from weather stations at the site owned by an engineering

company working in the area (O'Brien and Gere, Syracuse, New York) in order to verify that they were representative of the site. Stream dimensions (width, cross-sectional area) were measured using ADV measurements in the channel (Figure 2b.). The groundwater temperature was assumed to be equal to the annual average air temperature of 10 °C. Assuming a groundwater temperature equal to the average annual air temperature may be over simplistic in some modeling scenarios, but along this study reach groundwater is strongly upwelling at one discrete location, thereby minimizing error of this particular assumption. The shade was assumed to be minimal (0.1), due to observations of no overhanging riparian vegetation, and view to sky coefficient was assumed to be high (0.7) based on field observations and aerial photography. Because no bed temperature data were collected during the original field campaign, bed conduction was estimated by assuming a subsurface temperature equal to the groundwater temperature at a depth of 2 m (Table 1). In both instances where bed temperatures were not measured directly (Ninemile Creek and Meadowbrook Creek in the summer), the bed conduction heat flux was an order of magnitude smaller than all other heat fluxes, suggesting minimal error is introduced by the simplifying assumption that bed temperatures are equal to the groundwater temperature at a depth of 2 m. For more information about data collection at Ninemile Creek, see Briggs *et al.* (2012).

3. Results and Discussion

3.1. Model evaluation across contrasting field sites

In many previous studies, deterministic models for predicting stream temperature have been developed solely for the purposes of the individual studies (Becker *et al.*, 2004; Benyahya *et al.*, 2010; Evans *et al.*, 1998; Magnusson *et al.*, 2012; Westhoff *et al.*, 2007). Because of this, the ability of these models to translate from one site to another has not been tested. Ninemile

Creek and Meadowbrook Creek offer an opportunity to test the HFLUX Stream Temperature Solver's ability to accurately model stream temperature at sites with contrasting physical and hydrological characteristics. Ninemile Creek is larger than Meadowbrook Creek, with a streamflow rate that is more than 15 times higher. It also has a distinct point source input of groundwater that contributes about 5% of the overall discharge in the stream (Briggs *et al.*, 2012), while Meadowbrook Creek has more uniform, diffuse groundwater inputs along the reach. The successful simulation of the longitudinal pattern of temperature in Ninemile Creek in comparison to that of Meadowbrook Creek is demonstrative of the applicability of HFLUX at contrasting sites.

Figure 3 and Dynamic Content (DC) 1 and DC 2 show the results for Meadowbrook Creek from the HFLUX Stream Temperature Solver in summer (a., DC 1) and winter (b., DC 2). The summer and winter modeled temperatures have RMSEs of 0.40 and 0.18 °C, respectively (Table 2). The plots compare the average measured longitudinal stream temperature to the average simulated stream temperature (i.e. the average of observations collected/temperatures simulated at one location through time). During the summer, Meadowbrook Creek cools by 0.2 to 0.3 °C along the 475 m reach, while in winter, the stream warms by 0.3 to 0.5 °C downstream. These longitudinal changes in stream temperature are driven by the linear increase in discharge along the stream, and reflect the input of colder groundwater in summer and heat gain from warmer groundwater in winter. In the winter, the model results are slightly warmer than the actual stream along the reach. This discrepancy between simulated and observed longitudinal temperature is due to the assumption that discharge does not vary with time; intermittent snowmelt was likely causing modest changes in streamflow during the study period that were not accounted for in the winter model. The difference between the measured and modeled

temperature for the winter study, however, is minimal (root mean square error (RMSE) of 0.18 °C) despite the potential for variation in discharge from day to day. Accurately simulating longitudinal stream temperature under both summer and winter conditions demonstrates HFLUX's ability to account for groundwater's role in heat exchange in streams when there is relatively uniform, diffuse groundwater discharge.

The summer and winter Meadowbrook studies also show how HFLUX simulates diurnal temperature changes resulting from heat exchange with the environment. The comparison between the average modeled and measured stream temperature (i.e. the average of observations collected/temperatures simulated at one time across all locations) with respect to time is shown in Figure 4. In the summer, stream temperature has distinct daily minima and maxima that occur in the early morning and late afternoon, respectively. With respect to time, the heat fluxes to and from the surrounding environment exert a greater control on fluctuations in stream temperature than groundwater inputs. DC 1 and 2 show the measured longitudinal stream temperature compared to the modeled longitudinal stream temperature as they change through time. Figure 5 shows the total heat flux as well as the five individual heat fluxes for the summer (a.) and the winter (b.), and Table 3 summarizes the average contributions of the heat fluxes over the study period for each site. In the summer, solar radiation is the dominant heat flux for heat gain while evaporation results in the greatest heat loss. Patterns in water temperature lag behind those of solar radiation and correspond to the air temperature. In the winter, the timing of the daily peak in stream temperature is less predictable because although shortwave radiation has a diurnal signal, the magnitude of this flux is smaller and spans a shorter time than in summer. As a result, other heat fluxes (such as longwave radiation) that do not have a clear diurnal signal exert a greater relative influence on the total heat flux during the day in winter. The normalized root

mean square error (nRMSE) between the measured and simulated temperatures is 5.8% for the summer study and 3.0% during the winter study.

The stream temperature along the study reach of Ninemile Creek is generally uniform from the top of the reach to about 335 meters downstream, where a spring discharges to the creek (Figure 6b.). The water temperature drops by 0.24 °C on average after this input, and then the stream rewarms to the pre-spring temperature by the end of the reach (Briggs *et al.*, 2012). The cooling and rewarming of the stream are controlled by separate processes: the cooling is a function of the magnitude of the groundwater input and the temperature of the water being discharged to the stream, and the rewarming is accomplished by heat exchange with the environment as the water moves downstream from the spring. In order for HFLUX to accurately model the stream temperature in Ninemile Creek, it must accurately model both the timing and magnitude of the contribution of heat from these processes.

Groundwater inputs as determined using end-member mixing analysis are small and relatively constant along the stream with the exception of the spring at 335 meters along the reach (Briggs *et al.*, 2012). Figure 6b. shows the average modeled and measured stream temperature along the study reach over the 24-hour measurement period. DC 3 shows the measured longitudinal stream temperature compared to the modeled longitudinal stream temperature as they change through time. The HFLUX Stream Temperature Solver accurately simulates the cooling at about 335 m and the rewarming after this groundwater input. The RMSE between measured and modeled stream temperature is 0.19°C and the normalized RMSE is 6.2%. The meteorological data for this study were collected off-site, which could explain these discrepancies between the measured stream temperature and the temperature simulated by the heat budget model; differences in microclimate have been shown to have a significant impact

on stream temperature generated by deterministic models (Benyahya *et al.*, 2010). This example suggests that while good results can be obtained with remote weather stations, in-situ measurements may provide better results. Another likely explanation for the error in the modeled stream temperatures at Ninemile Creek is the systematic, high frequency noise that is inherent to fiber optic DTS data collected over short integration times and distances (DC3; Briggs *et al.*, 2012; Voigt *et al.*, 2011). Discrepancies exist between the measured temperatures, which include this high frequency noise, and the modeled temperatures. The result is an RMSE that reflects differences between actual stream temperatures and stream temperatures measured with DTS through space and time (measurement error), as well as actual differences between the true stream temperature and the modeled stream temperature (model error).

The heat fluxes and the water temperature calculated by HFLUX using the field data support the idea that groundwater is controlling changes in longitudinal temperature at the spring while heat exchange with the environment serves to return the water temperature to its upstream value by the end of the reach. The location and magnitude of the temperature change at the spring in the modeled results is comparable to the actual temperature drop, and the modeled stream rewarms along with the measured data (Figure 6b.). Recreating the cooling and subsequent rewarming of the stream after the groundwater input demonstrates how HFLUX can be used to identify and quantify the impacts of point source contributions of groundwater.

3.2 Sensitivity analysis of steady-state variables

Assessing the sensitivity of model results to changes in input data provides useful information about the results of model simulations as well as the fluvial system being studied (Wagener and Kollat, 2007). For example, it gives the user an idea of how much uncertainty there will be in the model results if there is uncertainty in input data, it can help the user make

decisions during data collection, and it can inform the user about how a system is likely to change if the environment changes (Hanby, 1994).

The HFLUX Stream Temperature Solver includes a function for performing a sensitivity analysis for model parameters, including discharge, groundwater temperature, shade, and the view to sky coefficient. This tool can be used to assess the sensitivity of modeled stream temperatures to increasing or decreasing the value of any of these variables by varying each individually and holding the others at their base case values. This relatively simple approach to sensitivity analysis is provided with the HFLUX program for exploratory purposes, but other approaches to sensitivity analysis (e.g. Monte Carlo routines) could readily be programmed as wrapper codes around the basic HFLUX program (e.g. Wagener and Kollat, 2007).

Output from the sensitivity analysis function includes a plot of average stream temperature with distance for the base case for each variable compared to the results with the adjusted values. Figure 7a is an example of this plot for the summer study from Meadowbrook Creek. In this case, the uncertainty in groundwater temperature was taken to be $\pm 15\%$ ($1.95\text{ }^{\circ}\text{C}$) and the shade and view to sky coefficient had an uncertainty of $\pm 20\%$ (0.155 and 0.045 , respectively). The uncertainty in ADV measurements is typically $\pm 10\%$, so the discharge measurements were increased and decreased by this amount ($0.0067\text{ m}^3/\text{s}$). The sensitivity analysis reveals that longitudinal stream temperature in Meadowbrook Creek during the summer is most sensitive to groundwater temperature; changing this variable by $1.95\text{ }^{\circ}\text{C}$ results in a $\pm 0.2\text{ }^{\circ}\text{C}$ change in average stream temperature.

The sensitivity of stream temperature in Meadowbrook Creek during the winter was also explored (Figure 7b). The uncertainty of groundwater temperature and the discharge measurements (15% and 10% , respectively) are considered the same in the winter as in the

summer. Shading and the view to sky coefficient, however, are at the boundaries of the possible range for these values in the winter (0.95 to 1 for vts and 0 to 0.05 for shade). Because neither of these values can exceed one or be less than zero, for the winter sensitivity analysis shading was increased by 0.10 and 0.20 and the view to sky coefficient was decreased by 0.10 and 0.20. These adjustments are similar in absolute magnitude to those used in the summer sensitivity analysis. In the winter, stream temperature remains most sensitive to groundwater temperature; a 1.05 °C change results in a ± 0.1 °C change in average stream temperature. Sensitivity to shade becomes minimal, even with an increase of 0.40, as solar radiation is not a primary driver of stream temperature change in the winter. Based on the results of the sensitivity analysis for Meadowbrook Creek, future studies on this stream should focus on constraining the groundwater temperature as well as possible, as uncertainty in this variable is likely to be a source of error in model results.

3.3. Seasonal considerations for heat flux calculations

In many studies, the use of deterministic heat budget models has been limited to spring, summer, and fall months (Benyahya *et al.*, 2010; Diabat *et al.*, 2012; Magnusson *et al.*, 2012; Neilson *et al.*, 2010; Westhoff *et al.*, 2007), with some exceptions (e.g. Leach and Moore, 2014; Garner *et al.*, 2015). Webb and Zhang (1997) discuss seasonality in heat fluxes for several streams in Great Britain, but they used the same methodology to calculate turbulent heat fluxes regardless of season. Based on the summer and winter field studies at Meadowbrook Creek, the physical basis for choosing equations for calculating latent and sensible heat flux changes from season to season. A combination approach for calculating latent heat flux produced reasonable results for the June dataset, with evaporation rates reaching a maximum at the sunniest time of day (Figure 5a.). As radiation is a major driver of evaporation, the use of this method during

very sunny periods was logical, especially since wind, the main driver in the mass-transfer method, was negligible during this period (average wind speed of 0.07 m/s with a standard deviation of 0.18 m/s; Linsley *et al.*, 1975). The Bowen ratio method for sensible heat transfer also produced realistic results during the summer study; the stream gained sensible heat from the air when it was warmer than the water and lost sensible heat when the opposite conditions were true.

During the winter, the combination method for calculating latent heat flux ceases to produce physically logical results. Solar radiation is minimal in Syracuse, New York, during the winter, so this is no longer a dominant flux either on its own or as a driver for evaporation (Figure 5b.). Longwave radiation, which is also used in the calculation for latent heat when using the combination method, changes sign and becomes negative as the warm stream radiates heat to the environment and the lack of foliage allows more heat loss than in the summer (Figure 5b., Table 3). As longwave radiation becomes increasingly negative in winter, the net radiative energy term becomes negative in the latent heat flux equation, and the combination method predicts condensation (i.e. negative evaporation) to the stream surface over the study period. These results are not physically sound, as loss of heat through longwave radiation does not generally have a physical basis for causing condensation; longwave radiation normally does not cause the temperature of the water to drop enough to change the vapor pressure gradient, in which case differences in vapor pressure have more control over evaporation (Linsley *et al.*, 1975). Because solar radiation is no longer a major driver for latent heat flux and because wind speeds increase during the winter at this site, it is more reasonable to use a mass transfer method to calculate the latent heat flux.

The use of the Bowen ratio method for calculating sensible heat flux requires accurate calculations for the latent heat flux. In order to separate the potentially compounding error that arises from tying these two fluxes together, the HFLUX Stream Temperature Solver includes a method for calculating sensible heat directly rather than as a function of the latent heat flux. Seasonal considerations regarding heat flux calculations allow the user to produce better simulations of stream temperatures, as the physical processes controlling heat exchange are modeled more correctly. The ability to switch the methodology used by HFLUX to calculate heat fluxes to and from the stream makes the model flexible and applicable to multiple sites and seasons.

3.4. Model application: calibration to determine discharge profile

Stream heat budget models have been used to quantify groundwater discharge to streams by calibrating models of the spatial and temporal distribution of groundwater discharge to observed temperature records in streams (Becker *et al.*, 2004; Loheide and Gorelick, 2006; Westhoff *et al.*, 2007). Identifying and measuring groundwater inflows allows for a more thorough understanding of fluvial systems as a whole; the location and quantity of groundwater entering a stream impacts the overall health of streams, as groundwater can help moderate stream temperature, provide thermal refugia for organisms, be a source of contaminants, and alter stream chemistry (Briggs *et al.*, 2012; Loheide and Gorelick, 2006; Torgersen *et al.*, 1999; Winter *et al.*, 1998). Despite advances in methodology, obtaining spatially distributed estimates of groundwater inputs to streams remains difficult (Briggs *et al.*, 2012); through calibration, HFLUX provides a means by which to quantify longitudinal contributions from groundwater.

In order to demonstrate the use of a calibration routine to back out streamflow rates using HFLUX, the data from the summer study at Meadowbrook Creek were used. The spatially

distributed profile of discharge measured using a constant-rate tracer injection of RWT provided a means by which to evaluate the results of the calibration to stream discharge. During the summer, Meadowbrook Creek cools slightly from the top of the study reach to the bottom (a decrease in temperature of about 0.2 °C). This decrease in temperature is generally linear along the reach and was attributed to groundwater inputs. The cooling pattern shows a steeper gradient (slope) for the upstream section of the stream and a slightly shallower slope for the downstream section (Figure 3a.).

Assuming linear increases in streamflow along the upper 250 m and lower 200 m of Meadowbrook Creek, the calibration routine used to quantify longitudinal changes in streamflow was built around a known upstream value for discharge (obtained with an ADV). The gradients of the linear increases in discharge for the upstream and downstream sections of the stream were varied during calibration. For each optimization, the initial discharge was set at 0.06 m³/s and the discharge gradient of the upstream section (0 m to 252 m) and downstream section (252 m to 475 m) were varied through a range of slope values. The initial discharge value and the slopes of the two linear trends were used to generate input values of streamflow for the HFLUX model run along the stream reach using the following equations:

$$Q_{upstream_i} = m_{upstream} (x_{upstream_i} - x_0) + Q_0 \quad [30]$$

$$Q_{downstream_i} = m_{downstream} (x_{downstream_i} - x_u) + Q_u \quad [31]$$

where $Q_{upstream_i}$ and $Q_{downstream_i}$ are the calculated discharge values at points, i , along the stream reach, $m_{upstream}$ and $m_{downstream}$ are the slope values (ΔQ with distance, in m²/s) that are varied to generate the different discharge profiles, x_0 is the most upstream point (0 meters), and Q_0 is the initial discharge at the most upstream point (0.06 m³/s). x_u is the point along the reach where

the slope of the discharge profile changes (252 meters) and Q_u is the discharge calculated at x_u by equation [30].

The new discharge profiles calculated using $m_{upstream}$ and $m_{downstream}$ were used in HFLUX until the pair of m -values that minimized the error in the modeled stream temperature was found. Figure 8 shows the error in simulated stream temperature for each combination of m values for the June dataset. This plot shows that a unique minimum error in simulated stream temperatures was found in this set of m values. Figure 9a. shows the modeled stream temperature using the optimized discharge profile compared to the measured stream temperature and Figure 9b. shows the comparison between the optimized discharge profile and the measured discharge from the constant rate tracer injection.

3.5. Model limitations

In an effort to maintain model simplicity and ease of use, some simplifying assumptions were made in development of HFLUX that present some model limitations. Despite these simplifications, the model still requires a fair amount of input data to run (Table 1), which is a limitation of HFLUX and most other deterministic stream temperature models. Additionally, the model is one-dimensional, making it appropriate for simulating longitudinal thermal diversity in streams, but not vertical or transverse thermal diversity.

HFLUX does not have a function for estimating heat exchange due to hyporheic exchange of water between the stream and the streambed. Also, changes in streamflow with distance are assumed to be due to discharge of groundwater, rather than other potential sources of additional streamflow, such as tributaries or storm runoff, a model assumption common in the literature (Cox and Botle, 2007; Westhoff et al., 2007). The advantage of this assumption is that groundwater discharge rates to individual model nodes are computed automatically by the

HFLUX program as the difference between streamflow rates in neighboring nodes, thereby simplifying the number of inputs that need to be set directly by the user. Additionally, adding a tributary or storm runoff component necessitates specification of the temperature of that additional water input, which is another model input that would be required of the user. The disadvantage of omitting tributaries as an option in the model is that individual reaches of streams, between tributaries, must be modeled separately, or the contributions of tributaries must be lumped with groundwater discharge (e.g. Somers et al., 2016). The disadvantage of omission of storm runoff is that HFLUX is not appropriate for modeling stream temperatures during storm events.

Currently, HFLUX does not include modules to generate sophisticated estimates of shading due to vegetation and topography (e.g. Boyd and Kasper, 2003; Cox and Bolte, 2007); rather, shade estimates are set manually in the input files. Although this is a potential limitation, output from external models that generate shade estimates based on geospatial data (e.g. TTools, Boyd and Kasper, 2003) can be input to HFLUX, as has been done in other energy balance models (e.g. Westhoff *et al.*, 2007).

4. Conclusions

Deterministic heat budget models have proved useful in many studies of temperature dynamics in fluvial systems (e.g. Becker *et al.*, 2004; Carrivick *et al.*, 2012; Diabat *et al.*, 2012; Gooseff *et al.*, 2005; Loheide and Gorelick, 2006; Westhoff *et al.*, 2007). Fundamentally, these models are developed based on the same framework: the physical processes that control heat exchange between a stream and the environment as water moves along a stream reach. However, heat budget models are often difficult to use, overwhelming in terms of data requirements, not transferable from site to site, and not easily modified for use by others. The HFLUX Stream

Temperature Solver is a new program for simulating stream temperature along a reach through time that builds upon previous advancements in stream temperature modeling and seeks to improve on some prior shortcomings. HFLUX requires little programming knowledge to operate and interfaces with Microsoft Excel for data management in order to simplify its use. The program is also flexible, including two finite difference methods for solving the governing equations of the model and options for equations to calculate shortwave radiation, latent heat flux, and sensible heat flux. Because HFLUX is a publicly available model that is annotated with the intention of modification by users, a user with some familiarity with Matlab could change the code to suit their specific study, if necessary.

This study has shown that HFLUX is effective for simulating stream temperature spatially and temporally at sites with distinct flow regimes, geomorphology, and meteorological variables. The utility of this tool extends beyond temperature modeling: it can be used to explore surface water-groundwater interactions through calibration to a discharge profile, and to assess the controls on temperature in a fluvial system. As a publicly available, user-friendly program, the HFLUX Stream Temperature Solver is a beneficial addition to currently available methodology for simulating stream temperature that can help further the use of deterministic models to investigate temperature dynamics in fluvial systems.

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Notation

- 706 A cross-sectional area of the stream, m^2
- 707 B width of the stream, m
- 708 B_r Bowen ratio, dimensionless
- 709 b_0 empirical constant, kPa m/s
- 710 b_1 empirical constant, 1/kPa
- 711 c_{air} specific heat of air, J/kg°C
- 712 C_L cloud cover, dimensionless
- 713 c_w specific heat of water, J/kg°C
- 714 d vertical distance in streambed, m
- 715 $\frac{D_H}{D_M}$ ratio between the diffusivity of heat and the diffusivity of momentum, dimensionless
- 716 E rate of evaporation, m/s
- 717 e_a^w actual vapor pressure of the evaporation surface, kPa
- 718 e_s^w saturation vapor pressure of the evaporation surface, kPa
- 719 e_a actual vapor pressure, kPa
- 720 e_s saturation vapor pressure, kPa
- 721 H relative humidity, %
- 722 k constant equal to 0.4, dimensionless
- 723 K_H exchange coefficient for sensible heat, J/°Cm³
- 724 K_{sed} thermal conductivity of sediment, W/m°C
- 725 L_e latent heat of vaporization, J/kg
- 726 $m_{upstream}$ upstream slope values that are varied to generate the different discharge profiles, m²/s

- 727 $m_{downstream}$ downstream slope values that are varied to generate the different discharge profiles,
- 728 m^2/s
- 729 P_A adiabatic atmospheric pressure, kPa
- 730 Q discharge of the stream, m^3/s
- 731 Q_0 initial discharge at the most upstream point, m^3/s
- 732 $Q_{upstream_i}$ calculated discharge values at points, i , along the upstream reach, m^3/s
- 733 $Q_{downstream_i}$ calculated discharge values at points, i , along the downstream reach, m^3/s
- 734 Q_u discharge calculated at x_u by equation, m^3/s
- 735 q_L groundwater inflow per unit stream length, m^2/s
- 736 R energy flux (source or sink) per unit stream length, $m^2\ ^\circ C/s$
- 737 r_a aerodynamic resistance, s/m
- 738 s slope of the saturation vapor pressure curve, $kPa/^\circ C$
- 739 S_{in} incoming shortwave radiation, W/m^2
- 740 S_{refl} percentage of incoming shortwave radiation reflected, dimensionless
- 741 SF percent shade, dimensionless
- 742 t time, s
- 743 T_{air} air temperature, $^\circ C$
- 744 T_L temperature of the groundwater, $^\circ C$
- 745 T_{sed} sediment temperature, $^\circ C$
- 746 T_w stream temperature, $^\circ C$
- 747 v_{wind} wind speed, m/s
- 748 vt_s view to sky coefficient, dimensionless
- 749 WP wetted perimeter, m

1	
2	
3	
4	750 x stream distance, m
5	
6	
7	751 x_0 is the most upstream point, m
8	
9	752 x_u point along the reach where the slope of the discharge profile changes, m
10	
11	
12	753 z elevation above sea level, m
13	
14	754 z_m height at which wind speed measurements were taken, m
15	
16	
17	755 z_d zero-plane displacement, m
18	
19	756 z_0 roughness height, m
20	
21	
22	757 z_{veg} height of vegetation, m
23	
24	758 e_{atm} emissivity of the atmosphere, dimensionless
25	
26	
27	759 ρ_{air} density of air, kg/m ³
28	
29	
30	760 ρ_w density of water, kg/m ³
31	
32	761 g psychrometric constant, J/kg°C
33	
34	762 Φ_{total} total energy flux to the stream per surface area, W/m ²
35	
36	
37	763 $F_{shortwave}$ shortwave radiation, W/m ²
38	
39	764 F_{latent} latent heat flux, W/m ²
40	
41	
42	765 $F_{longwave}$ longwave radiation, W/m ²
43	
44	
45	766 $F_{atmospheric}$ atmospheric longwave radiation, W/m ²
46	
47	
48	767 $F_{back_radiation}$ back radiation off the surface of the stream, W/m ²
49	
50	
51	768 F_{land_cover} landcover longwave radiation, W/m ²
52	
53	769 F_r sum of short and longwave radiation, W/m ²
54	
55	
56	770 $F_{sensible_heat}$ sensible heat flux, W/m ²
57	
58	
59	771 S_{sb} Stefan-Boltzmann constant, W/m ² °C ⁴
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Tables

Table 1. Summary of required model input data and sources of observations used in models of the field sites, as discussed in the text.

Input Data Required^a		Meadowbrook Creek		Ninemile Creek
Excel worksheet	Description	Summer: June 2012	Winter: Dec – Jan 2013	September 2009
time_mod	Times (min) at which temperatures are computed	Every minute for 7040 min	Every minute for 23490 min	Every minute for 1449 min
dist_mod	Distances (m) on reach at which temperatures are computed	Every meter for 475 m	Every meter for 460 m	Every meter for 900 m
temp_x0_data	Temperatures (°C) through time (min) at the upstream boundary	Measured: discrete temperature sensor	Measured: discrete temperature sensor	Measured: continuous fiber optic distributed temperature sensor
temp_t0_data	Temperatures (°C) with distance (m) at the initial time step (t=0)	Measured: discrete temperature sensor	Measured: discrete temperature sensor	Measured: continuous fiber optic distributed temperature sensor
dim_data	Stream cross-sectional area (m ²), width (m), and depth (m) at specified locations along the stream reach (m)	Measured	Measured	Measured
dis_data	Stream discharge rates (m ³ /s) at given distances (m)	Measured: dilution gauging	Measured: dilution gauging	Measured: end-member mixing
time_dis	Times at which stream discharge rates are given in dis_data (min)	-	-	-
T_L	Groundwater temperatures (°C) at given distances (m)	Estimated from annual air temperature	Estimated from annual air temperature	Estimated from annual air temperature
met_data	Solar radiation (W/m ²), air temperature (°C), relative humidity (%), and wind speed (m/s), as observed at specified times	Measured: On-site weather station	Measured: On-site weather station	Measured: Regional weather station
bed_data1	Distances (m) and depths (m) at which streambed temperatures were observed	-	Measured	-
bed_data2	Temperatures (°C) through time (min) at locations specified in bed_data1	-	Measured: discrete temperature sensors	-
sed_type	Bed sediment type (clay, silt, sand, or gravel) at locations specified in bed_data1	-	Observed in the field	-
shade_data	Percent shade (0-1) and view to the sky (0-1) with distance (m) along the reach	Observed in the field and from aerial photographs	Observed in the field and from aerial photographs	Observed in the field and from aerial photographs
cloud_data	Cloud cover (0-1) through time (min)	Measured: Regional weather station	Measured: Regional weather station	Measured: Regional weather station
site_info	Site latitude, longitude, time zone, and elevation	Obtained from public data	Obtained from public data	Obtained from public data
settings	Specification of the finite difference solution scheme and methods selected for computing shortwave radiation, latent heat,	Crank-Nicolson; Shortwave - Eq [4]; Latent Heat - Eq [15]; Sensible Heat - Eq [21]	Crank-Nicolson; Shortwave - Eq [4]; Latent Heat - Eq [18]; Sensible Heat - Eq [25]	Crank-Nicolson; Shortwave - Eq [4]; Latent Heat - Eq [15]; Sensible Heat - Eq [21]

	and sensible heat fluxes			
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^a Each set of input data is entered by the user as an individual worksheet within one Excel spreadsheet. A sample input Excel file is provided in the supplementary material and titled “input_data.xlsx”. Additional descriptions of input data can be found in the computer program documentation provided with the program files.

Table 2. Summary of error

Site	RMSE (°C)	nRMSE (%)
Meadowbrook Creek (summer)	0.40	5.8%
Meadowbrook Creek (winter)	0.18	3.0%
Ninemile Creek	0.19	6.2%

Table 3. Summary of average heat flux contributions for each study period

Flux	Site		
	Meadowbrook Creek (summer) (W/m ²)	Meadowbrook Creek (winter) (W/m ²)	Ninemile Creek (W/m ²)
Shortwave radiation	188.7	16.6	170.0
Longwave radiation	-27.6	-95.8	-31.9
Latent heat flux	-122.6	-22.3	-99.2
Sensible heat flux	62.8	-5.3	39.4
Bed conduction	-3.3	2.2	-4.5

Figure captions

Figure 1. Location and topography of the Meadowbrook Creek watershed within New York State (inset) (a.) with study sites outlined by black box. Instrumentation at the summer study site is shown in b. and instrumentation at the winter study site is shown in c.

Figure 2. Location of Ninemile Creek study site within New York State (inset) in a. with instrumentation shown in b.

Figure 3. Measured and modeled temperature in Meadowbrook Creek during the summer (a.) and winter (b.). Plots show the average stream temperature along the reach with modeled temperatures in red and measured temperatures in blue. The gray shaded areas show uncertainty about the means due to uncertainty in each individual temperature sensor measurement.

Figure 4. Measured and modeled stream temperature in Meadowbrook Creek during the summer (a.) and winter (b.). Plots shows average stream temperature through time across all modeled nodes, with modeled temperatures in red and measured temperatures in blue.

Figure 5. Average modeled heat fluxes for Meadowbrook Creek with respect to time. a. shows summer fluxes and b. shows winter fluxes.

Figure 6. Discharge profile (a.) and modeled and measured stream temperatures (b. and c.) for Ninemile Creek. For b., red line indicates average modeled stream temperature along the reach and blue dots indicate average measured stream temperature along the reach. For c., red line indicates average modeled stream temperature over the study period and blue line indicates average measured stream temperature over the study period.

Figure 7. Average temperature along Meadowbrook Creek for the base case (field data) and decreasing and increasing temporally constant variables by the estimated uncertainty of their measured value. The summer study period is shown in a. and the winter study period is shown in

b. Note that in winter (b.), shading is increased by 0.1 and 0.2 and the view to sky (vts) is decreased by 0.1 and 0.2 for the “low” and “high” cases, respectively, due to the parameter values being at the boundaries of their possible ranges (e.g. 1 for vts and 0 for shade).

Figure 8. Normalized root mean square error in stream temperature in June at Meadowbrook Creek for combinations of slopes of the calculated discharge profile for the upstream and downstream sections. Minimum error was found for an upstream slope of $3.5 \times 10^{-5} \text{ m}^2/\text{s}$ and a downstream slope of $2.1 \times 10^{-5} \text{ m}^2/\text{s}$.

Figure 9. Measured and simulated average stream temperature along Meadowbrook Creek using optimized discharge profile (a.) and comparison between the measured discharge and the optimized discharge profile that minimized error in stream temperature (b.) for Meadowbrook Creek in June 2012.

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Calibrated Stream Temperature: Meadowbrook Creek, June 2012

Streamflow: Meadowbrook Creek, June 2012