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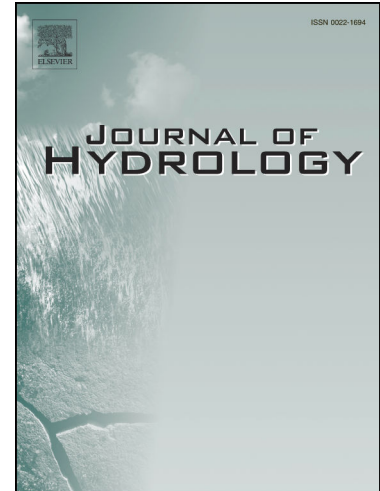
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1 **BDFLUX: A new bounded domain model for quantifying vertical streambed**
2 **fluxes in streambeds using heat as a tracer**

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29 **Highlights**

- 30 ● Heat-based bounded domain analytical model for vertical streambed flux presented.
- 31 ● Particle swarm optimization and Markov Chain Monte Carlo methods used.
- 32 ● Model is evaluated using synthetic, laboratory experimental, and field data.
- 33 ● Method to estimate nonvertical flow components presented.
- 34

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35 **Abstract**

36 The use of heat as a tracer has become a widely used approach to estimate vertical streambed
37 fluxes (VSFs). We present BDFLUX, a new bounded domain model that can be used as a rapid-
38 screening tool to quantify VSFs and thermal properties of streambed sediments by analyzing on-
39 site temperature-time series. BDFLUX uses a closed-form analytical solution that takes thermal
40 advection and thermal conduction into account. BDFLUX, unlike other one-dimensional closed-
41 form analytical solutions, does not assume an infinitely extending semi-infinite half-space. The
42 initial and boundary conditions are described by arbitrary functions that can be directly
43 determined by fitting the measured temperature-time series in the streambed at various depths.
44 The particle swarm optimization (PSO) method and Markov Chain Monte Carlo (MCMC)
45 method are used to estimate VSFs using temperature-time series observed at three depths.
46 BDFLUX is validated using synthetic temperature-time series, demonstrating that it can perform
47 well when the top and bottom boundary conditions are determined directly by the measured data.
48 The capabilities of BDFLUX are further evaluated using laboratory and field data. The
49 simulation results show that BDFLUX performed well in terms of interpreting laboratory
50 experiments and field data, with a root mean square error as low as 0.059. The simulation of
51 laboratory experiments shows that the MCMC method has a lower computational efficiency than
52 PSO method. The magnitude of nonvertical flow components at a field site were quantified by
53 analyzing the results of estimated VSFs in different vertical subdomains. Overall, BDFLUX
54 improves one-dimensional heat analytical models in terms of assessing the magnitude of the
55 nonvertical flow component in heterogeneous streambed sediments.

56 **Keywords:** Heat tracer method, Vertical streambed fluxes, Thermal conduction, Parameter
57 estimation, Groundwater-surface water interaction.

58 1. Introduction

59 Vertical streambed fluxes (VSFs) are critical for understanding surface water-groundwater
60 interactions and impact biogeochemical processes in riparian zones (Chen et al., 2022a; Irvine et
61 al., 2020; Rau et al., 2014). However, accurately determining VSFs is challenging due to their
62 dynamic nature over time and space (Irvine et al., 2016; Irvine et al., 2015a; Keery et al., 2007),
63 as well as the intricate three-dimensional flow fields involved (Banks et al., 2017; Irvine and
64 Lautz, 2015; Reeves and Hatch, 2016). As evidenced by reviews of Anderson (2005), Constantz
65 (2008), Rau et al. (2014), Abbott et al. (2016), and Tripathi et al. (2021), using heat as a natural
66 tracer represents a powerful tool for determining VSFs and has many advantages over alternative
67 methods such as geochemical tracer and hydraulic methods (Ren et al., 2018; Saar, 2011). For
68 instance, compared to geochemical tracers, heat is inexpensive, ubiquitous, and easily measured
69 *in situ* with a large number of loggers and probes available (Ghysels et al., 2021; van Kampen et
70 al., 2022). VSFs and effective thermal diffusivity of streambed sediments can be estimated by
71 fitting a heat transport model to temperature data collected from streambed sediments
72 (Bredehoeft and Papaopulos, 1965; Hatch et al., 2006; Irvine et al., 2017; Stallman, 1965). The
73 accuracy and robustness of parameter estimation from the abovementioned methods are heavily
74 dependent on the reliability and performance of the chosen conceptual model, which must
75 effectively represent to the physical processes of flow and heat transport.

76 A variety of analytical models in a semi-infinite domain have been developed to determine
77 VSFs using temperature-time series collected within the stream and at different depths in the
78 sediments of the streambed. Suzuki (1960) pioneered the use of streambed temperature
79 measurements to estimate VSFs by developing an analytical solution to the one-dimensional
80 (1D) vertical heat transport equation, where the upper boundary is represented by a sinusoidal
81 temperature function, and the lower boundary is maintained at a constant temperature. Following
82 the work of Suzuki (1960), three types of models were developed based on temperature
83 measurements. The first type of models estimate VSFs using time-invariant temperature-depth
84 profiles, such as Bredehoeft and Papaopulos (1965), Kurylyk et al. (2017), and Lin et al. (2022).
85 The main limitation of these models is related to the challenges in estimating VSFs in the
86 presence of varying surface temperatures. Irvine et al. (2020) showed that these limitations can
87 be overcome using daily averaged temperatures, but that the approach can only be applied for
88 groundwater discharge (upwards flow) conditions. The second type of models were developed to
89 determine VSFs using temperature-time series measured at different depths within the streambed
90 (Chen et al., 2018; Kurylyk and Irvine, 2016; Luce et al., 2017; . For example, by assuming heat
91 transport in a semi-infinite domain streambed system, Shi and Wang (2023) recently developed a
92 multi-layered heat transport model. However, as demonstrated by van Kampen et al. (2022)
93 using synthetic and field data, this assumption can result in erroneous estimations of streambed
94 fluxes. The use of MATLAB routines facilitates the application of the analytical models such as
95 Hatch et al. (2006), Keery et al. (2007), McCallum et al. (2012) and Luce et al. (2013) in
96 estimating VSFs in the streambed by using temperature signal characteristics like amplitude ratio
97 and phase shift, such as VFLUX (Gordon et al., 2012) and VFLUX 2 (Irvine et al., 2015b).
98 When using VFLUX 2, the shallow sensor pair outperforms the deep sensor pair due to the fast
99 attenuation of temperature signals at streambed depths (Chen et al., 2018). All the above-
100 mentioned analytical solutions are semi-infinite domain models. In comparison to these models,
101 finite (bounded) domain models can offer significant advantages in terms of straightforward
102 calculation and boundary conditions that more appropriately reflect real-world field conditions.

103 For example, the top and bottom boundary conditions can be directly determined from observed
104 temperature-time series from different locations using a spline interpolation method, which is
105 reliable, and it has been used to fit the top boundary condition and initial temperature
106 distributions at various streambed depths in some semi-infinite domain models (Kurylyk and
107 Irvine, 2016; Lin et al., 2022).

108 Unlike the analytical solutions mentioned above, models that use third type boundary
109 conditions can apply frequency domain methods, which use spectral scaling factors of
110 temperature-time series data in frequency domain to quantify VSFs (van Kampen et al., 2022;
111 Schneidewind et al., 2016; Vandersteen et al., 2015). These models can divide the input
112 temperature-time series data into noise, transient, and periodic components, as well as determine
113 uncertainties of VSFs and streambed effective thermal diffusivity. These methods employ the
114 local polynomial (LP) technique and maximum likelihood estimator (MLE) to address noise in
115 input temperature-time series in the frequency domain, facilitating the estimation of VSFs and
116 streambed effective thermal diffusivity. For example, the LPMLE model, which is coupled with
117 LP and MLE, (Vandersteen et al., 2015) assumes heat transfer in a semi-infinite half-space, and
118 requires two observations from different depths to estimate VSFs and streambed effective
119 thermal diffusivity. Like the two types of methods mentioned above (i.e., Bredehoeft and
120 Papaopulos (1965), and Hatch et al. (2006)), one important assumption contained in the LPMLE
121 model is that heat transfer occurs in a semi-infinite half-space, where the lower boundary
122 condition extends infinitely and is fixed at a constant temperature. Schneidewind et al. (2016)
123 used local upper and lower boundary conditions to extend the LPMLE model to the LPMLE3
124 model to quantify VSFs and streambed thermal diffusivity. The LPMLE3 model is a bounded
125 domain model, and it requires three observed points (at different depths) for each streambed
126 subdomain of interest, where the observed points at the top and bottom of the streambed
127 subdomain are worked as the boundary conditions, and the observed point inside the streambed
128 subdomain is used for the estimation of VSFs and streambed effective thermal diffusivity.
129 Recently, van Kampen et al. (2022) developed the LPMLE_n model, which extends the
130 capabilities of the LPMLE and LPMLE3 methods. This model facilitates the estimation of VSFs
131 and streambed effective thermal diffusivity in bounded and infinite streambed domains,
132 incorporating temperature measurements from n sensors in the parameter estimation process. The
133 availability of advanced temperature sensors like fiber-optic distributed temperature sensing
134 (DTS) (Selker et al., 2006; Vogt et al., 2010) or multilevel temperature lances (Munz et al.,
135 2016) has made it straightforward to collect high spatial resolution temperature measurements.

136 The purpose of this study is to introduce BDFLUX, a new bounded domain model, that can
137 be coupled with various inverse algorithms, like the particle swarm optimization (PSO) method
138 or Markov Chain Monte Carlo (MCMC) methods, applied in the present study. BDFLUX is
139 designed to solve an inverse problem by analyzing on-site temperature-time series, to extend the
140 semi-infinite domain analytical models (Chen et al., 2018; Lin et al., 2022; Luce et al., 2013) to
141 describe heat transport in a bounded (finite) streambed of interest (or streambed with layers).
142 BDFLUX has three primary advantages over existing analytical methods: first, the BDFLUX can
143 describe arbitrary initial conditions, arbitrary top and bottom boundary conditions based on
144 temperature measurements in the finite streambed at various depths. Second, BDFLUX is simple
145 to implement, and the VSFs, streambed effective thermal diffusivity and their uncertainties can
146 be estimated simultaneously using a broad range of solver methods. BDFLUX is easily coupled
147 with other parameter estimation methods such as the trial-and-error method (Chen et al., 2022b)

148 and iterative Levenberg-Marquardt method (Lin et al., 2022). Finally, it is more representative to
149 quantify the VSFs for a bounded streambed or a layered streambed than to assume the streambed
150 is homogeneous (van Kampen et al., 2022; Schneidewind et al., 2016; Vandersteen et al., 2015).
151 Meanwhile, estimated VSFs in different vertical subdomains can be used to delineate the
152 magnitude of nonvertical flow components. Compared to other 1D closed-form analytical
153 models, BDFLUX does not assume an infinitely extending semi-infinite half-space with the
154 lower boundary condition tending towards infinity. In contrast to LPMLE, LPMLE3 and
155 LPMLEn methods, BDFLUX can handle arbitrary initial conditions based on temperature
156 measurements at different depths within the finite streambed. The new analytical solution is
157 specifically designed to solve an inverse problem by analyzing on-site temperature-time series.
158 The capabilities of BDFLUX are tested using synthetic data, laboratory experimental data from
159 Zhang et al. (2021), and field data from Ferencz et al. (2021).

160 **2. Methodology**

161 *2.1 Mathematical model*

162 The flow chart in Figure 1 depicts the process of estimating the VSFs and effective thermal
163 diffusivity of a streambed using our newly developed analytical solution for heat transport in
164 streambed materials. The workflow consists of three steps. First, developing a mathematical
165 model of heat transport in a finite streambed with arbitrary initial and boundary conditions,
166 which can be solved analytically using Green's function. The conceptual model is shown in
167 Figure 1a. A cartesian coordinate system is used to develop the mathematical model, and the
168 origin is located at the interface between the streambed and stream with the z -axis downward.
169 The boundary conditions are described by arbitrary functions that can be directly determined by
170 fitting the measured temperature-time series in the streambed at different depths. Second, the
171 temperature-time series data collected from different depths of the streambed, as shown in Figure
172 1b, are used to estimate VSFs and thermal properties of streambed. BDFLUX, like the LPMLE3
173 and LPMLEn models, requires at least three observed points for a streambed subdomain of
174 interest. For example, the four observation data sets in Figure 1a could be divided into two
175 subdomains: subdomain 1 (SD1) for OBS1, OBS2, and OBS3, and subdomain 2 (SD2) for
176 OBS2, OBS3, and OBS4. In the SD1, OBS1 and OBS3 are served as boundary conditions,
177 whereas OBS2 is used for parameter estimation. Similarly, OBS2 and OBS4 are used as
178 boundary conditions in the SD2, while OBS3 is used for parameter estimation. All four
179 observations can also form a subdomain, where the middle two observations are used
180 simultaneously for parameter estimation. Third, BDFLUX model, when combined with a broad
181 range of solver methods like the PSO method, allows for the simultaneous estimation of VSFs
182 and the effective thermal diffusivity for each streambed subdomain. Theoretically, if there is no
183 nonvertical flow component in the streambed, the estimated VSFs are the same in SD1 and SD2.
184 Otherwise, there will be a difference of the estimated VSFs between SD1 and SD2, where the
185 differences in VSFs among distinct streambed subdomains indicates alterations in the magnitude
186 of the nonvertical flow component.

187 The 1D advection-dispersion equation has been commonly used to describe heat transport
188 processes in the streambed (e.g., Hatch et al., 2006; Luce et al., 2013; McCallum et al., 2012).
189 The mathematical model of 1D vertical heat transport in a bounded domain with an arbitrary
190 boundary and initial conditions is:

$$191 \quad \frac{\partial T}{\partial t} = D \frac{\partial^2 T}{\partial z^2} - v \frac{\partial T}{\partial z}, \quad 0 \leq z \leq L, t > 0, \quad (1)$$

$$192 \quad T(z, t = 0) = h(z), \quad 0 \leq z \leq L, t > 0, \quad (2)$$

$$193 \quad T(z = 0, t) = f(t), \quad t > 0, \quad (3)$$

$$194 \quad T(z = L, t) = g(t), \quad t > 0, \quad (4)$$

195 where T is temperature [°C]; v is the thermal front velocity [m/d]; $h(z)$ is initial temperature
 196 distribution [°C]; $f(t)$ and $g(t)$ are arbitrary functions that describe the temperature [°C] at the
 197 top and bottom boundaries, respectively; t is time [d]; z is space [m]; L is the thicknesses [m] of
 198 streambed of interest; D is effective thermal diffusivity [m²/d].

199 For a saturated streambed, D and v can be described as (Chen et al., 2022b; Chen et al.,
 200 2018; Schneidewind et al., 2016):

$$201 \quad D = \frac{k}{\rho c}, \quad (5)$$

$$202 \quad k = k_s(1 - \theta) + \theta k_w, \quad (6)$$

$$203 \quad v = \frac{\rho_w c_w}{\rho c} q, \quad (7)$$

$$204 \quad \rho c = \theta \rho_w c_w + (1 - \theta) \rho_s c_s, \quad (8)$$

205 where k is thermal conductivity [W/(m · K)] of saturated streambed sediment; k_s and k_w are
 206 thermal conductivities [W/(m · K)] of solid and fluid phases, respectively, θ is porosity [-]; q is
 207 VSF [m/d], where a positive q indicates downwelling, and a negative q indicates upwelling; $\rho_w c_w$
 208 and ρc are volumetric heat capacities [J/(m³ · K)] of water and saturated streambed,
 209 respectively; $\rho_s c_s$ is specific volumetric heat capacity of the solids [J/(m³ · K)]. ρ , ρ_w and ρ_s are
 210 densities [kg/m³] of the saturated streambed, water and solid, respectively; c , c_w and c_s are
 211 specific heat capacities [J/(kg · K)] of saturated streambed, water and solid, respectively. To
 212 account for thermal dispersion caused by flow velocity, some researchers include an additional
 213 thermal dispersivity term in Eq. (5) (Gossler et al., 2020; McCallum et al., 2012; Rau et al.,
 214 2012). However, thermal dispersivity will not be considered in this study because it becomes
 215 relatively minor and can be negligible when fluxes are small and over short spatial scales (Hatch
 216 et al., 2006; Luce et al., 2017; Schneidewind et al., 2016), especially when VSFs are slower than
 217 10 m/d (Rau et al., 2012).

218 **2.2 Closed-form solution**

219 Eqs. (1) - (8) compose the 1D heat transport accounting for both conduction and advection
 220 in a bounded domain with an arbitrary boundary and initial conditions. The analytical solution
 221 for this model could be derived by applying Green's function method, which is easy to handle
 222 when arbitrary boundary and initial conditions are involved (Chen et al., 2018; Leij et al., 2000).
 223 This approach allows the top and bottom boundary conditions to be directly determined by
 224 interpolation (e.g., spline interpolation) from temperature-time series observed at different

225 locations. This method is reliable and has been successfully applied to simulate heat transport
 226 behavior in streambed sediments (Shi et al., 2023a; Shi et al., 2023b). Also, this method is unlike
 227 the models solved using the Laplace transform method, which requires a specific mathematical
 228 equation for the fitted function to be specified, for example, the models of Kurylyk and
 229 MacQuarrie (2014), Kurylyk and Irvine (2016), and Lin et al. (2022). The detailed solution
 230 derivation is provided in the supporting information, and the analytical solution is given as
 231 follows:

$$232 \quad T = A(z,t) \left\{ \int_0^L B(\lambda) G(z,t;\lambda,\tau = 0) d\lambda + D \int_0^t [E(\tau)C(\tau) - H(\tau)F(\tau)] d\tau \right\}, \quad (9)$$

$$233 \quad A(z,t) = \exp \left[-\frac{v(vt-2z)}{4D} \right], \quad (10a)$$

$$234 \quad B(\lambda) = h(\lambda) \exp \left[-\frac{v\lambda}{2D} \right], \quad (10b)$$

$$235 \quad C(\tau) = \sum_{n=1}^{\infty} \frac{2n\pi}{L^2} \sin\left(\frac{n\pi z}{L}\right) \exp \left[-D \left(\frac{n\pi}{L}\right)^2 (t - \tau) \right], \quad (10c)$$

$$236 \quad E(\tau) = f(\tau) \exp \left[\frac{v^2\tau}{4D} \right], \quad (10d)$$

$$237 \quad F(\tau) = \sum_{n=1}^{\infty} \frac{2n\pi}{L^2} (-1)^n \sin\left(\frac{n\pi z}{L}\right) \exp \left[-D \left(\frac{n\pi}{L}\right)^2 (t - \tau) \right], \quad (10e)$$

$$238 \quad G = \sum_{n=1}^{\infty} \frac{2}{L} \sin\left(\frac{n\pi\lambda}{L}\right) \sin\left(\frac{n\pi z}{L}\right) \exp \left[-D \left(\frac{n\pi}{L}\right)^2 (t - \tau) \right], \quad (10f)$$

$$239 \quad H(\tau) = g(\tau) \exp \left[\frac{v(v\tau-2L)}{4D} \right], \quad (10g)$$

240 where λ and τ refer to dummy variables, in which λ varies between 0 and L , τ varies between 0
 241 and t , corresponding to the independent variables z and t , respectively.

242 Our model is an extension of previous 1D analytical models (Luce et al., 2013; McCallum
 243 et al., 2012; Stallman, 1965). For instance, if $L \rightarrow \infty$, $h(z) = T_0 + a_1 z + \delta \exp(dz)$, $g(t) = T_0$,
 244 and $f(t)$ is a step functions of time, in which a_1 , δ and d are coefficients, T_0 is subsurface
 245 temperature [°C] that is unaffected by surface temperature variation, the new model can be
 246 reduced to the model of Kurylyk and Irvine (2016). When $L \rightarrow \infty$, $g(t) = T_0$, $f(t)$ is described by
 247 a cosine function with an arbitrary amplitude, period, and phase shift, the present model can be
 248 reduced to the model of Chen et al. (2018).

249 **2.3 Inverse modeling for VSFs estimation**

250 We couple the present BDFLUX with the PSO method in order to search the optimal VSFs
 251 and D . Shi and Wang (2023) took a similar approach, using the PSO algorithm to estimate VSFs
 252 and streambed thermal characteristics in a multi-layered streambed system. The main advantages
 253 of PSO algorithm with respect to other inverse algorithms are: (1) PSO provides flexibility in
 254 estimating multiple parameters and enables efficient modification of the parameter count by

255 simply adjusting the initial settings without expanding the computations (Dya et al., 2021; Shi
 256 and Wang, 2023). (2) The PSO method converges rapidly by iteratively comparing the local and
 257 global extremum values, leading to a reduction in the number of iterations required. (3) It is
 258 simple to implement because it has been packaged into MATLAB (Ebbesen et al., 2012).
 259 Moreover, for comparison purposes, despite the high computational resources required for
 260 conducting MCMC simulations (Zhang et al., 2017), this study incorporates the application of
 261 the MCMC method in one of the laboratory experiments of Zhang et al. (2021). We used the
 262 method developed by Goodman and Weare (2010) as compared to traditional MCMC method, it
 263 can achieve much faster convergence, meanwhile, it is very simple to implement through using
 264 MATLAB code package “gwmcmc” (<https://github.com/grinsted/gwmcmc>).

265 **2.4 Validation with numerical modelling**

266 Two numerical models were developed in the COMSOL Multiphysics platform (COMSOL
 267 Inc., Burlington, MA, USA) to verify BDFLUX and to investigate the potential influence of
 268 bottom boundary condition on parameter estimation. The first numerical model, a 1D bounded
 269 domain model, was developed using the mathematical model of Eqs. (1) - (4) to verify
 270 BDFLUX. The model domain was 0.40 m long and was linearly discretized with a uniform
 271 spatial increment of 0.005 m ($dz = 0.005$ m), and a uniform time step of 0.01 d was used for
 272 simulation. The value of grid Péclet Number is less than 2 for the numerical simulations in this
 273 study, ensuring no numerical dispersion occurs. As observed temperature-depth profiles are not
 274 available and the temperature at a depth of 0.5 m is fluctuating around 28 °C (Figure 1b), the
 275 temperature at 0.5 m was taken as an initial temperature distribution $h(z)$. The top and bottom
 276 boundary conditions were taken from the measured data of Ferencz et al. (2021), namely, the
 277 measured temperature-time series at “OBS1” and “OBS3”, as shown in Figure 1b, serve as top
 278 and bottom boundary conditions, respectively. More specifically, $f(t)$ and $g(t)$ were directly
 279 determined from observed temperature-time series at “OBS1” and “OBS3” using a spline
 280 interpolation method. The other model parameters are as follows: $k_s = 1.4$ W/(m · K), $k_w = 0.6$
 281 W/(m · K), $c_s = 700$ J/(kg · K), $\rho_s = 2600$ kg/m³, $\rho_w c_w = 4.20 \times 10^6$ J/(m³ · K), $q = 0.1$
 282 m/d, $L = 0.40$ m, and $\theta = 0.3$. These parameters, except q , were from the investigation of
 283 Ferencz et al. (2021). To access the simulation results, the root mean square error (RMSE) was
 284 employed, which can be calculated by:

$$285 \quad RMSE = \sqrt{\frac{\sum_i^N (Y_i^{obs} - Y_i^{sim})^2}{N}}, \quad (11)$$

286 where N is total number of the observations, Y_i^{obs} is true value (synthetic truth or observations)
 287 at time i , Y_i^{sim} is simulated value of the i^{th} realization at time i .

288 In many previous studies, the bottom boundary condition extended infinitely and was fixed
 289 at a constant temperature (Chen et al., 2022b; Lin et al., 2022; Rau et al., 2012). For the sake of
 290 comparison, a semi-infinite domain model was developed as the second numerical model to
 291 investigate the potential effects of bottom on parameter estimation. The semi-infinite domain
 292 ($0 \leq z < \infty$) was replaced by a finite domain ($0 \leq z < 10$ m). This assumption was validated
 293 through additional numerical testing on two different model domains ($0 \leq z < 10$ m and
 294 $0 \leq z < 500$ m) and the results shows a good agreement between both finite domains (see Figure

295 S1 in section S2 of supporting information for further information). This setup is reasonable
 296 because the diurnal temperature signals attenuate considerably in the streambed sediments
 297 approximately 0.5 meters below the surface (Kurylyk et al., 2019). In addition, like the treatment
 298 of Liang et al. (2019), a component within COMSOL known as an infinite element domain was
 299 used at $z = 10$ m to effectively represent the infinite boundary, this component employed
 300 rational coordinate scaling within a series of virtual domains that envelop the physical region.
 301 The model domain was linearly discretized with a uniform spatial step of 0.005 m. The initial
 302 and top boundary conditions, as well as the parameters used in the second numerical model, were
 303 the same as those used in the first numerical model, whereas the bottom boundary condition was
 304 set to 28 °C.

305 To further validate the accuracy of BDFLUX in estimating q and D , the semi-infinite
 306 domain model with pre-defined input parameters was employed to produce temperature-time
 307 series at depths of 0.10, 0.20 and 0.30 m. The pre-defined parameter values are listed in Table 1.
 308 The BDFLUX model, coupled with PSO was then used to best-fit the synthetic temperature-time
 309 series to estimate the values of q and D simultaneously, in which the temperature-time series
 310 generated at depths of 0.1 and 0.3 m were worked as upper and lower boundary conditions,
 311 respectively, and the temperature-time series generated at depth of 0.2 m was used to parameter
 312 estimation. The accuracy of parameter estimation is evaluated using a relative error.

313 ***2.5 Validation with laboratory thermal tracer test data***

314 The temperature-time series recorded from a laboratory column experiment reported by
 315 Zhang et al. (2021) were used to test the capabilities of BDFLUX. The sand column was
 316 constructed of Perspex pipe with a length of 0.45 m and an inner diameter of 0.075 m. The
 317 schematic representation of the laboratory experimental setup is shown in Figure 2 or in Figure 2
 318 of Zhang et al. (2021). The sand column was uniformly filled with quartz sand with particle sizes
 319 ranging from 0.40 to 0.60 mm, with a measured total porosity of 0.45. Water in the supply tank
 320 is periodically heated and injected from the top of the sand column to produce a sinusoidal-like
 321 temperature input. Temperature-time series were measured at depths of 0.00, 0.10 and 0.20 m
 322 from the top of the filled media, and the filled media from the top to a depth of 0.20 m was
 323 considered a subdomain, as shown in Figure 2. Temperature-time series collected at depths of
 324 0.00 and 0.20 m served as upper and lower boundary conditions, respectively, and temperature
 325 measurements recorded at depth of 0.10 m were used for estimating VSFs and effective thermal
 326 diffusivity. Downwelling flows were produced using two different q values (0.351 m/h and
 327 0.199 m/h), which are denoted by Run1 and Run2 hereinafter. To simulate these data, we used a
 328 subordinated heat transport model (called Sub-HTE model) developed by Zhang et al. (2021).
 329 The Sub-HTE model extended the classical 1D heat transport equation (HTE) by incorporating a
 330 time factor (α) to account for thermal retardation or storage resulting from hydro-biogeochemical
 331 processes. Although Zhang et al. (2021) developed the analytical solutions for the Sub-HTE
 332 model in the finite and semi-infinite domain scenarios, the lower boundary condition of the Sub-
 333 HTE model is assumed to be a constant. In addition, the Sub-THE model with a semi-infinite
 334 domain reduces to the HTE model when $\alpha = 1$. Note that the Sub-HTE model of Zhang et al.
 335 (2021) for simulation of the experiments of Run1 and Run2 is a bounded domain model. A more
 336 detailed information about these laboratory experiments can be found in Zhang et al. (2021). The
 337 best-fit values of thermal front velocity and effective thermal diffusivity for Run1 were 0.54

338 m/h and 1×10^{-4} m²/h, respectively; and the corresponding best-fit values for thermal front
 339 velocity and effective thermal diffusivity in Run2 were 0.26 m/h and 1×10^{-4} m²/h,
 340 respectively.

341 **2.6 Application of BDFLUX using temperature-time series measured in Lower Colorado River**

342 To test the field application of BDFLUX, temperature-time series data collected during 20-
 343 27 July 2017 at the Lower Colorado River, a dam-controlled fourth order river, as reported by
 344 Ferencz et al. (2021), are used in this study. The temperature-time series data were collected
 345 using purpose-built vertical temperature profilers. In each vertical temperature profiler, four
 346 thermistors were installed on an aluminum rod at 0.10, 0.20, 0.30, and 0.50 m intervals from the
 347 streambed. Most of the vertical flow is likely to occur at shallow depths beneath the center of the
 348 stream. In addition, using a 2D numerical simulation, Ferencz et al. (2021) found that the
 349 temperature distribution close to the river banks were dependent on advective heat transfer
 350 caused by hydrostatic fluctuations in river level, whereas the temperatures in the remaining part
 351 of the channel were primarily influenced by thermal conduction. Thus, two observations near the
 352 center of the river, denoted by VA1 and VA2 hereinafter, were chosen to reduce the effects of
 353 hydropeaking in this study. The majority of the streambed sediments in VA1 and VA2 are sand.
 354 Unlike the numerical model and sand column data, the Ferencz et al. (2021) dataset allows the
 355 application of BDFLUX to estimate the influence of non-vertical flows. To achieve this purpose,
 356 the four observed temperature-time series in each vertical temperature profiler could be divided
 357 into three subdomains: SDI for $z = 0.10, 0.20$ and 0.30 m, SDII for $z = 0.20, 0.30$ and 0.50 m,
 358 and SDIII for $z = 0.10, 0.30$ and 0.50 m. The SDIII is used to investigate the impact of the
 359 selected domain in BDFLUX on the estimation of VSFs by comparing it to the SDII results. The
 360 thermal properties of streambed sediment are the same as those used in Section 2.4.

361 **3. Results and Discussions**

362 **3.1 Comparison of the present and numerical models in simulating temperature-time series**

363 To verify the approaches used in BDFLUX, we used the numerical solution developed in
 364 Section 2.4 to produce temperature-time series at $z = 0.10, 0.20$ and 0.30 m to compare with
 365 those generated by BDFLUX (Eqs. (6) - (7)). Figures 3a-3c show the comparison of temperature-
 366 time series between BDFLUX (green circle symbols) and the numerical solution (black solid
 367 curves) at $z = 0.10, 0.20$ and 0.30 m, respectively. Figure 3 shows that the temperature-time
 368 series produced by the numerical solution are almost in agreement with those predicted by
 369 BDFLUX at given depths. All the *RMSE* values between the BDFLUX and numerical solution
 370 are less than 0.0056. Figure 3 demonstrates that BDFLUX performs well when the top and
 371 bottom boundary conditions are determined directly by the measured data.

372 **3.2 Comparison of the semi-infinite domain model with BDFLUX**

373 The semi-infinite domain model developed in Section 2.4 is used to test the potential effects
 374 of bottom on heat transport in streambed. The temperature-time series are generated using the
 375 semi-infinite domain model and BDFLUX at depths of 0.10, 0.20 and 0.30 m. Figures 4a-4c
 376 show the comparison of BDFLUX and the semi-infinite domain model in terms of temperature-
 377 time series for $q = 0.01, 0.10$ and 0.50 m/d, respectively. Two interesting observations can be

378 made from these results. First, the differences between these two models decrease as the VSFs
 379 increase, implying that the use of semi-infinite domain model may result in errors at low q .
 380 Second, although the top boundary condition is the same in these two models, the RSME values
 381 of temperature-time series increase as the depth of the observed locations increases (i.e., RSME
 382 values increase from 0.0193 to 0.3216 when $q = 0.10$ m/d), which is consistent with the
 383 findings of Zhang et al. (2021), who compared the capability of 1D bounded domain model
 384 (Sub-THE model with a finite domain) and semi-infinite domain model (THE model). Table 1
 385 shows the estimated D and v values by BDFLUX with negligible error (i.e., all relative error
 386 levels less than 5%), indicating that BDFLUX can accurately estimate the D and v in a finite
 387 streambed domain. Further comparison of the BDFLUX with other bounded and semi-infinite
 388 domain models is shown in the Section 3.3.

389 *3.3 Simulation results of laboratory experiments*

390 In this section, the PSO method and MCMC method are employed to estimate v and D
 391 using the experimental data of Zhang et al. (2021) described in the section 2.5. The temperature-
 392 time series observed in the laboratory experiments at $z = 0.10$ m for Run1 ($q = 0.351$ m/h) and
 393 Run2 ($q = 0.199$ m/h) are displayed by green circle symbols in Figures 5a and 5b, respectively.
 394 The red solid curves and their corresponding 95 % confidence intervals are generated by
 395 BDFLUX using the estimated parameters obtained from the PSO method, in which the estimated
 396 parameters are listed in Table 2. For the sake of comparison, the simulation results of Zhang et
 397 al. (2021) are also included, where the “HTE model” and “Sub-HTE model” in the legend refer
 398 to the semi-infinite domain heat transport model and bounded domain heat transport model,
 399 respectively. Figure 5 shows that BDFLUX fits temperature-time series for both Run1 and Run2
 400 slightly better than the two models of Zhang et al. (2021) mentioned above (i.e., RMSE of 0.059
 401 compared to 0.354 and 0.366). As evidenced in Table 2, the thermal front velocities estimated by
 402 BDFLUX for both Run1 and Run2 are slightly lower than the models proposed by Zhang et al.
 403 (2021), whereas the estimated D by BDFLUX are close to three orders of magnitude higher than
 404 the values used in Zhang et al. (2021). It is worth noting that the effective D values for quartz
 405 sand estimated by the models of Zhang et al. (2021) may be lower than the true value. For
 406 example, Stonestrom and Constantz (2003) listed the thermal properties of various materials,
 407 including quartz, which has a thermal diffusivity of 0.0155 m²/h, a thermal conductivity of 8.4
 408 W/(m · K) and a specific volumetric heat capacity of 1.9×10^6 J/(m³ · K). Based on the
 409 estimated thermal front velocities and effective thermal diffusivities by Zhang et al. (2021), we
 410 can further determine the thermal conductivity and volumetric heat capacity of quartz sand based
 411 on Eqs. (5) - (7), the estimated ρc , $\rho_s c_s$, k and k_s values by Sub-HTE and HTE models are listed
 412 in Table 3, where the values of θ and k_w used here for calculation are 0.45 and 0.60 W/(m · K),
 413 respectively. As mentioned above, the estimated thermal conductivity values using the both Sub-
 414 HTE and HTE models of Zhang et al. (2021) are lower than those of organic matter (Stonestrom
 415 and Constantz (2003) reported the thermal conductivity of organic matter is 0.25 W/(m · K)),
 416 and the estimated thermal conductivity values using the Sub-HTE model are negative, which is
 417 physically unreasonable. According to Zhang et al. (2021), decreasing the best-fit fractional
 418 order (α) in the Sub-HTE model enhances thermal energy storage in the medium, that might
 419 explain the lower thermal conductivities estimated by the Sub-HTE model than the HTE model.
 420 Also, unlike BDFLUX, although the Sub-HTE model is a bounded domain model (the model

421 domain length is set to the length of the sand column), the lower boundary condition of the Sub-
 422 HTE model is treated as a constant like the HTE model.

423 As mentioned above, the D values estimated by BDFLUX are almost three orders of
 424 magnitude higher than the values used in Zhang et al. (2021), the likely reason is that the thermal
 425 dispersion processes occur due to the very high velocities q used during the two experiments
 426 (8.424 m/d for Run1 and 4.776 m/d for Run2). In order to calculate the potential thermal
 427 dispersion, we separated the D estimated by BDFLUX into two parts, the first one is thermal
 428 diffusivity and the second one is thermal dispersion, which can be described as (De Marsily,
 429 1986; Rau et al., 2014):

$$430 \quad D = \frac{k}{\rho c} + \beta \frac{\rho_w c_w}{\rho c} q, \quad (12)$$

431 where β is thermal dispersivity [m]. In this section, BDFLUX coupled with the PSO method was
 432 used to search the optimal parameters of k_s , $\rho_s c_s$, θ , and β . Porosity is also used as an objective
 433 parameter for optimization because the Run1 and Run2 were carried out in two different sand
 434 columns with potentially different porosities. For comparison, we also searched for parameter
 435 values of k_s , $\rho_s c_s$, and θ without β . The estimated results are listed in Table 3, in which D and v
 436 are also calculated based on the estimated results. When the optimal parameters are k_s , $\rho_s c_s$, and
 437 θ , the estimated thermal conductivity values for Run1 and Run2 using BDFLUX are 22.071 and
 438 12.439 W/(m · °C), which are obviously physically unreasonable. In addition, the porosity
 439 values also seem to be underestimated. In contrast, when the optimal parameters are k_s , $\rho_s c_s$, θ
 440 and β , the estimated thermal conductivity values for Run 1 and Run 2 are close to the reference
 441 value in the literature of Stonestrom and Constantz (2003), and the estimated porosities for Run1
 442 and Run2 are 0.4514 and 0.3856, respectively, in which the estimated porosity for Run1 closely
 443 matching the measured value. Although the same medium was used in both Runs 1 and 2, the
 444 estimated thermal property parameters (k_s and $\rho_s c_s$) are different. One probable explanation is
 445 that when the number of optimization parameters increases, the PSO method falls into a local
 446 optimum due to the inclusion of stochastic processes (Pallero et al., 2018). Comparing Table 2,
 447 however, we can find that using BDFLUX-optimized search parameters k_s , $\rho_s c_s$, θ , and β yields
 448 estimated D and v values that are remarkably close to the results obtained by only optimizing for
 449 D and v , especially for Run1. Finally, the estimated thermal dispersivity values of Run1 and
 450 Run2 are 0.0291 and 0.0181 m, respectively, as shown in Table 3. The estimated thermal
 451 dispersivity values are physically reasonable and are consistent with previous field studies
 452 (Keery et al., 2007; Rau et al., 2010; Ronan et al., 1998). As a result, we can infer that the
 453 thermal dispersion occurs in these two experiments.

454 Figures 6a and 6b show the frequency histograms of the v and D estimated by the MCMC
 455 method using temperature-time series collected from experiment of Run1, respectively. The
 456 simulation results of PSO method (red solid curve) and the model of Zhang et al. (2021)
 457 (magenta solid curve) are also included for comparison. The posterior distributions of v and D
 458 are close to normal while exhibiting fluctuations, and the posterior distribution of D fluctuates
 459 more significantly, suggesting that the uncertainty of D is larger, potentially due to thermal
 460 dispersivity. Figure 6c displays the comparison between the measured data and predicted
 461 temperature-time series generated by BDFLUX using the parameter samples from MCMC. The
 462 simulation results of PSO method (Figure 5a) are also included for comparison. It is important to

463 note that, although only a portion of the observations presented in Figure 6c were chosen for
 464 parameter estimation, the MCMC method took over 24 hours to yield the results presented (We
 465 used a standard desktop PC with a 6-core 2.60 GHz processor and 16.0 GB RAM). However, the
 466 PSO utilized all the observations and took only 36 minutes. Considering that MCMC has a low
 467 computational efficiency, it is not used for parameter estimation in the following sections.
 468 Similarly, the same observations can be found in Run2, as shown in Figure 7.

469 **3.4 Simulation results of field tests in the Lower Colorado River**

470 Quantification of VSFs across streambeds has become essential in the investigation of the
 471 transport and fate of contaminants and nutrients, ecological habitat, the management of water
 472 resources, and biochemical processes (Ghysels et al., 2021; Rau et al., 2014; Tripathi et al.,
 473 2021). Here, BDFLUX coupled with the PSO method was employed to estimate VSFs and D of
 474 streambed profile VA1 and streambed profile VA2 at two different depths based on the observed
 475 temperature-time series in the Lower Colorado River, which were divided into two subdomains
 476 as detailed in Section 2.6. The differences in VSFs between subdomains SDI and SDII were used
 477 to analyze the magnitude of potential nonvertical flow components, and the differences in VSFs
 478 between subdomains SDII and SDIII were employed to evaluate the impact of the selected
 479 domain in BDFLUX on the estimation of VSFs. Figures 8a to 8c show that the fitting of the
 480 temperature-time series (green circle symbols) observed in streambed profile VA1 by the
 481 proposed BDFLUX (red solid curves) for SDI, SDII, and SDIII, respectively. The estimated D of
 482 SDI, SDII and SDIII in streambed profile VA1 are 0.0798, 0.0790 and 0.0792 m²/d,
 483 respectively, and the estimated VSFs are 0.0347 m/d for SDI, 0.0333 m/d for SDII, and 0.0341
 484 m/d for SDIII. Similarly, Figures 9a to 9c show that the fitting of the temperature-time series
 485 observed at streambed profile VA2 by BDFLUX for SDI, SDII and SDIII, respectively. The
 486 estimated D of SDI, SDII, and SDIII in streambed VA2 are 0.1034, 0.1018 and 0.1022 m²/d,
 487 respectively, and the estimated VSFs are -0.0090 m/d for SDI, -0.0769 m/d for SDII, and -
 488 0.0738 m/d for SDIII. The estimated D of SDI and SDII differs slightly for each streambed
 489 profile (VA1 and VA2). This is reasonable because the distance between SDI and SDII is
 490 relatively short, inferring that the streambed sediments are more likely to be of similar materials. As
 491 for the estimated VSFs, those in streambed profile VA1 are downwelling and the magnitude of
 492 nonvertical flow components in streambed profile VA1 is 0.0014 m/d, as shown in Figure 10a.
 493 The estimated VSFs in streambed profile VA2 are upwelling and the magnitude of nonvertical
 494 flow components in streambed profile VA2 is 0.0679 m/d, as shown in Figure 10b. Note that the
 495 direction of the nonvertical flow component cannot be determined. The VSF estimated in SDIII
 496 is less than that estimated in SDII for both VA1 and VA2, which is most likely due to the
 497 presence of nonvertical flow between the depths of 0.1 and 0.2 m. In theory, the estimated VSF
 498 in SDII should be consistent with that of SDIII when there is no nonvertical flow component.

499 Moreover, by selecting shorter intervals of interest from the collected temperature-time
 500 series, BDFLUX coupled with the PSO method also allows for the estimation of time-variant
 501 VSFs and D . For example, the 5.75-day temperature-time series of SDI collected at VA1 (Figure
 502 8a) was divided into 79 segments (the time interval is ~100 min), BDFLUX then estimated VSF
 503 and D within each time interval (the results are shown in Figure S2 of supporting information).
 504 The estimated VSF and D values using the entire dataset (5.75 days) are slightly higher than
 505 those estimated using the shorter time intervals. For comparison, the river stage observed by
 506 Ferencz et al. (2021) is also included, and the result shows that, although variations in estimated

507 VSF appear to be associated with river stage, the estimations have different degrees of
508 fluctuation. This phenomenon is consistent with the findings of Shi et al. (2023a).

509 **3.5 Limitations of BDFLUX**

510 Compared to existing analytical solutions to the 1D heat transport models, BDFLUX can
511 handle arbitrary initial and boundary conditions based on temperature measurements at different
512 depths within the finite streambed, and BDFLUX does not assume an infinitely extending semi-
513 infinite half-space with the lower boundary condition tending towards infinity. BDFLUX, like
514 previous heat tracer approaches, has the following limitations.

515 (1) The BDFLUX approach considers the subsurface to be a homogeneous, finite domain
516 with hydraulic and thermal characteristics that are assumed constant within the model domain.
517 However, these assumptions can be violated in natural settings, particularly with the existence of
518 significant heterogeneity (Irvine et al., 2016; Irvine et al., 2015a; Klepikova et al., 2016). Also,
519 the BDFLUX approach can not consider the temperature dependency of viscosity and density.
520 To date, these effects can only be investigated using numerical models, such as Lautz (2010) and
521 Klepikova et al. (2016).

522 (2) As demonstrated in Section 3.4, although BDFLUX can infer the magnitude of
523 nonvertical flow components, the direction of the nonvertical flow component cannot be
524 predicted accurately. In addition, the estimation of VSF is subject to uncertainties associated
525 with sensor precision, sensor actual depth, and surface temperature variations due to weather
526 change (Irvine et al., 2016).

527 (3) BDFLUX approach cannot consider the temperature difference between the fluid and
528 adjacent solid phases in saturated streambed sediment, i.e., the local thermal nonequilibrium
529 effects. Previous investigations have highlighted that local thermal nonequilibrium effects are
530 expected to be strong in fast flowing gravel media (Baek et al., 2022; Gossler et al., 2020;
531 Gossler et al., 2019; Roshan et al., 2014). Furthermore, due to the lag of temperature change
532 compared to water level (or hydraulic gradient) change, heat may not be an efficient tracer for
533 rapid changes in hydraulic gradient (Constantz, 2008; Lapham, 1989).

534 (4) There are no constraints on applying BDFLUX to estimate sub-daily VSFs provided the
535 temperature dataset has a sufficiently high resolution, as demonstrated by Shi et al. (2023a) and
536 van Kampen et al. (2022). It would be a straightforward modification in the code to change the
537 grouping of data and units for VSF estimation (e.g., from m/d to m/hour). Similar to other
538 approaches of this type, BDFLUX obtains point estimates for a specific time, which are not
539 necessarily representative of the surroundings or for another moment due to flux
540 heterogeneity/temporal variability. In addition, the use of BDFLUX for estimating VSFs through
541 temperature-time data is only feasible in the shallow subsurface or environment with
542 concentrated groundwater fluxes (Kurylyk et al., 2019).

543 **4. Summary and Concluding Remarks**

544 This study presents BDFLUX, a new bounded domain model and associated MATLAB
545 code to solve an inverse problem by analyzing on-site temperature-time series, which can be

546 used as a rapid- tool to quantify VSFs and thermal properties of streambed sediments. This
 547 method is based on a closed-form analytical solution that considers thermal advection and
 548 thermal conduction in a bounded (finite) streambed of interest (or streambed with layers). The
 549 VSFs, thermal properties of the streambed, and their uncertainties can be estimated
 550 simultaneously using the PSO-based parameter estimation technique and the MCMC-based
 551 parameter estimation technique. In contrast to other 1D closed-form analytical solutions,
 552 BDFLUX can handle arbitrary initial and boundary conditions based on temperature
 553 measurements at different depths within the finite streambed, and it does not assume an infinitely
 554 extending semi-infinite half space with the lower boundary condition tending towards infinity.
 555 Instead, it incorporates local top and bottom boundary conditions. Using synthetic temperature-
 556 time series, we validated the newly presented BDFLUX and demonstrated that it performs well
 557 when the top and bottom boundary conditions are determined directly by the measured data.
 558 BDFLUX also performed well in terms of interpreting laboratory experiments and field data, and
 559 the magnitude of nonvertical flow components in field of Ferencz et al. (2021) were estimated by
 560 analyzing the results of estimated VSFs in different vertical subdomains. The simulation of
 561 laboratory experiments demonstrated that the MCMC method has a lower computational
 562 efficiency than PSO method. BDFLUX can be used for assessing the magnitude of the
 563 nonvertical flow component in heterogeneous streambed sediments and is an insightful addition
 564 to current 1D closed-form analytical models.

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813

814 **Figure Captions:**

815 **Figure 1.** Flow chart of proposed conceptual model with the three steps for parameter
 816 estimation: (a). Conceptual model and its analytical solution; (b). Collected temperature-time
 817 series in the streambed at different depths, data from Ferencz et al. (2021); (c). Parameter
 818 estimation using particle swarm optimization (PSO) and Markov Chain Monte Carlo (MCMC)
 819 techniques.

820 **Figure 2.** (a) Schematic diagram for the laboratory experimental system; (b) - (d) are
 821 temperature-time series observed at $z = 0.0, 0.1$ and 0.2 m, respectively, where (b) and (d) serve
 822 as top and bottom boundary conditions of the BDFLUX model, and (c) is used for parameter
 823 estimation. These observed data are from the experiment Run1 of Zhang et al. (2021).

824 **Figure 3.** Comparison of temperature-time series between BDFLUX (black solid curves) and
 825 numerical solution (green circle symbols) at $z = 0.1, 0.2$ and 0.3 m, respectively. The top and
 826 bottom boundary conditions are from Ferencz et al. (2021), as shown in Figure 1b, where “BS1”
 827 and “OBS3” serve as top and bottom boundary conditions, respectively.

828 **Figure 4.** Comparison of temperature-time series predicted by the BDFLUX (solid curves) and
 829 semi-infinite domain model (dashed curves) at $z = 0.1, 0.2$ and 0.3 m. (a) $q = 0.01$ m/d, (b)
 830 $q = 0.10$ m/d, (c) $q = 0.50$ m/d. “BC” in the legend represents boundary condition, “BDM”
 831 and “SIM” refer to bounded domain model and semi-infinite domain model, respectively.

832 **Figure 5.** Simulation results of the laboratory experiments of Run1 (a) and Run2 (b) at $z = 0.1$
 833 m: The observed data (green circle symbols) versus the BDFLUX (red solid curves) and the
 834 models of Zhang et al. (2021).

835 **Figure 6.** Simulation results of the laboratory experiment of Run1 using MCMC method. The
 836 results of PSO method (Red solid curve) and the Sub-HTE model of Zhang et al. (2021)
 837 (Magenta solid curve) are also included for comparison. The frequency histograms of the
 838 thermal front velocity (a) and the effective thermal diffusivity (b) estimated by the MCMC
 839 method. (c) Comparison between the measured data and predicted temperature-time series,
 840 where the blue solid curve generated by BDFLUX based on the parameter samples from MCMC.

841 **Figure 7.** Simulation results of the laboratory experiment of Run2 using MCMC method. The
 842 results of PSO method (Red solid curve) and the Sub-HTE model of Zhang et al. (2021)

843 (Magenta solid curve) are also included for comparison. The frequency histograms of the thermal
 844 front velocity (a) and the effective thermal diffusivity (b) estimated by the MCMC method. (c)
 845 Comparison between the measured data and predicted temperature-time series, where the blue
 846 solid curve generated by BDFLUX based on the parameter samples from MCMC.

847 **Figure 8.** Fitting of the temperature-time series (green circle symbols) observed at VA1 by the
 848 BDFLUX (red solid curves) using the estimated parameters obtained from the PSO method for
 849 (a) SDI, (b) SDII, and (c) SDIII. The top and bottom boundary conditions of the BDFLUX are
 850 represented by the blue and black solid curves. Data from Ferencz et al. (2021).

851 **Figure 9.** Fitting of the temperature-time series (green circle symbols) observed at VA2 by
 852 BDFLUX (red solid curves) using the estimated parameters obtained from the PSO method for
 853 (a) SDI, (b) SDII, and (c) SDIII. The top and bottom boundary conditions of BDFLUX are
 854 represented by the blue and black solid curves. Data from Ferencz et al. (2021).

855 **Figure 10.** The estimated VSFs and the inferred magnitude of nonvertical flow components in
 856 streambed profile VA1 (a) and streambed profile VA2 (b). Differences in VSFs between SDI and
 857 SDII imply a change in the magnitude of the nonvertical flow component (magenta arrow). The
 858 unit of VSFs are in m/d.

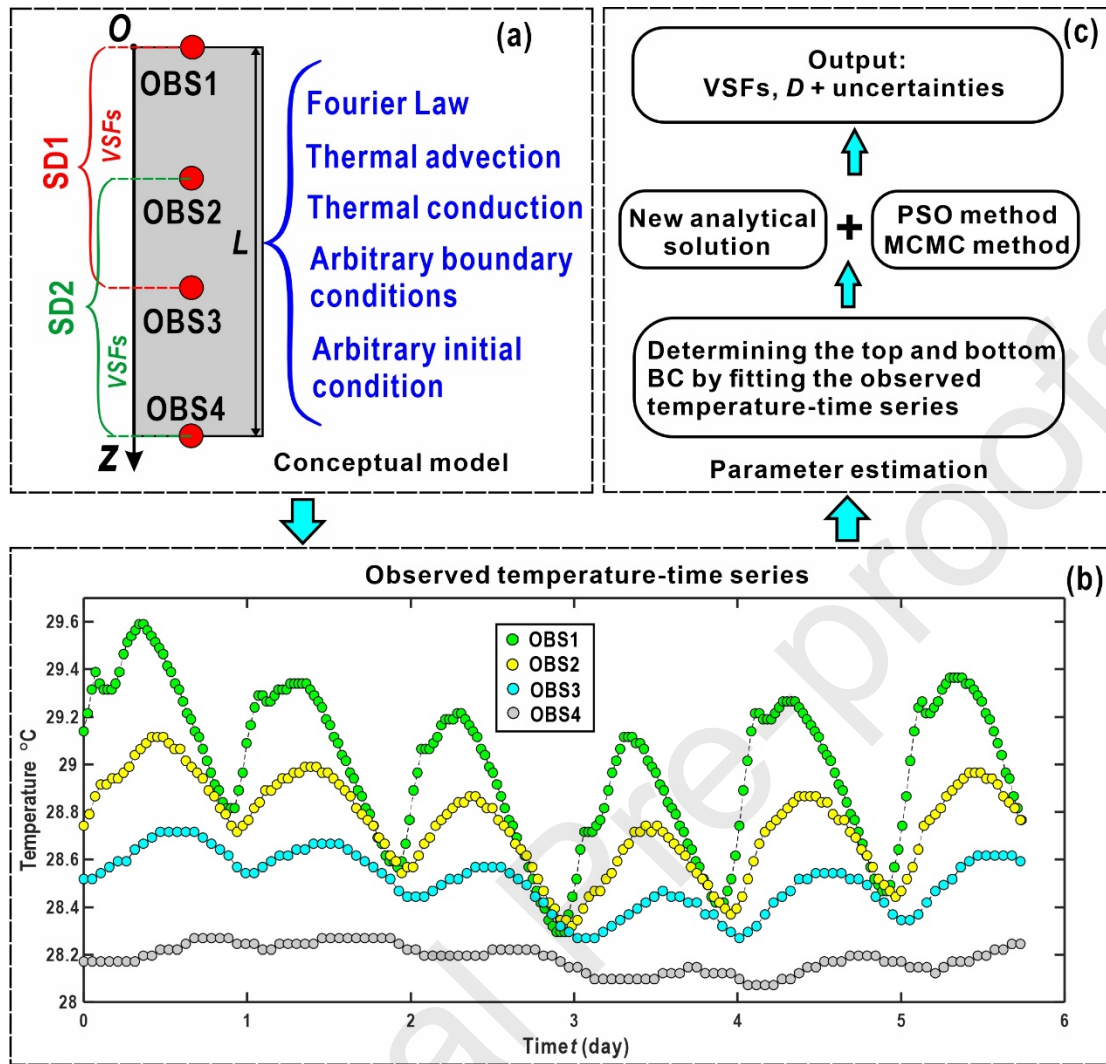
859

860 Table Captions

861 **Table 1.** The values of D and v are used as true values in the numerical model (NUM) and are
 862 estimated by BDFLUX, and the relative error between true and estimated values are calculated.
 863 The generated temperature-time series at the depths of 0.1, 0.2 and 0.3 m are used to estimate D
 864 and v by BDFLUX.

865 **Table 2.** Parameters estimated by different models using laboratory experimental data

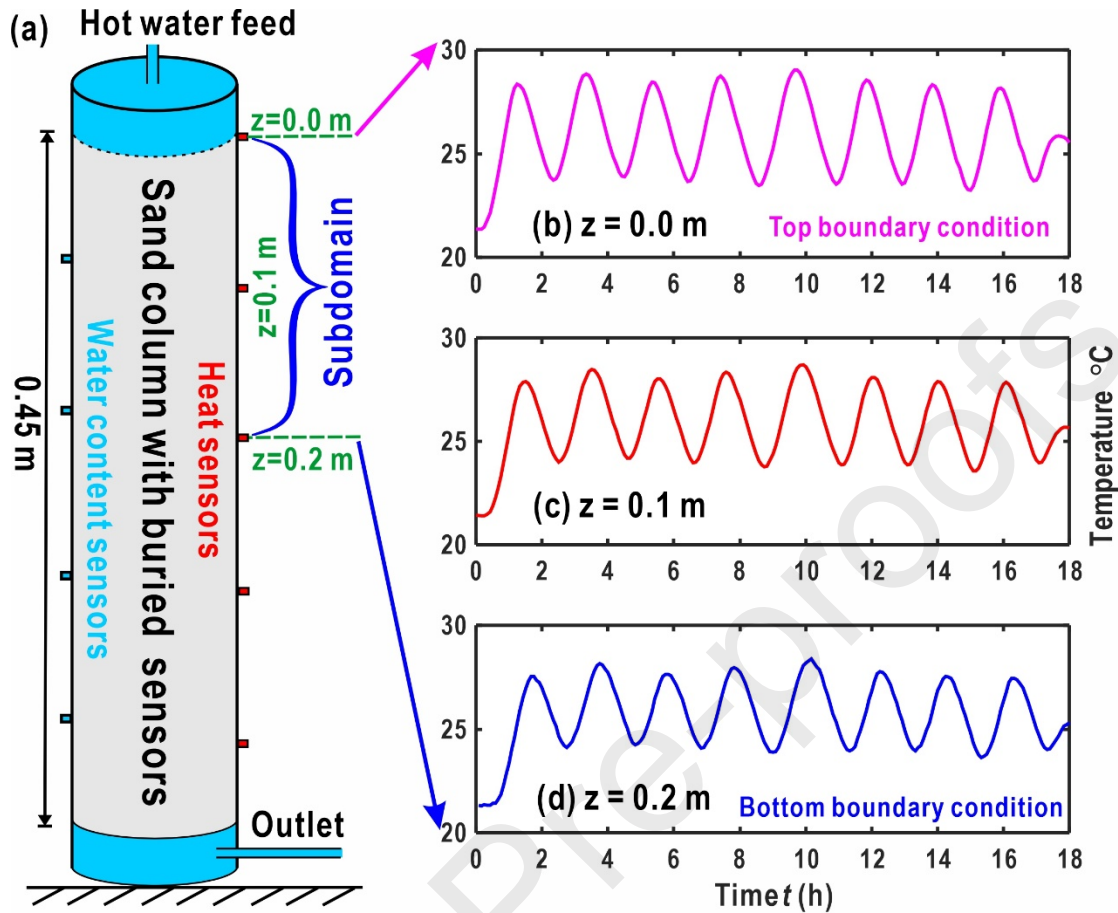
866 **Table 3.** Estimated thermal conductivity and volumetric heat capacity using different models.



867

868 **Figure 1.** Flow chart of proposed conceptual model with the three steps for parameter
 869 estimation: (a). Conceptual model and its analytical solution; (b). Collected temperature-time
 870 series in the streambed at different depths, data from Ferencz et al. (2021); (c). Parameter
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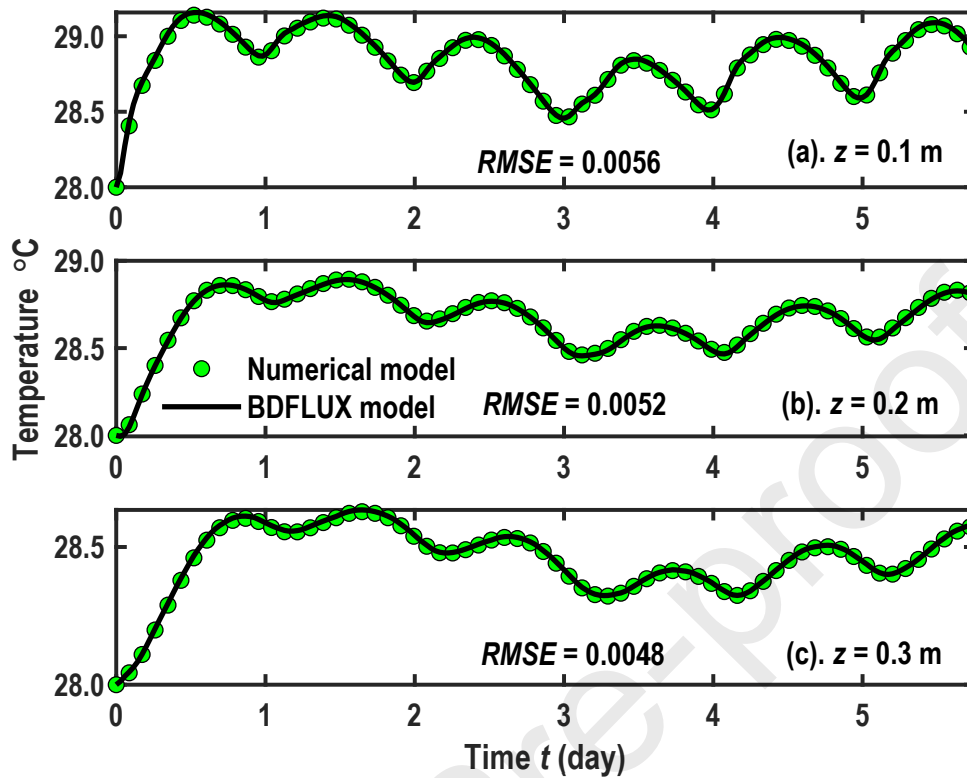
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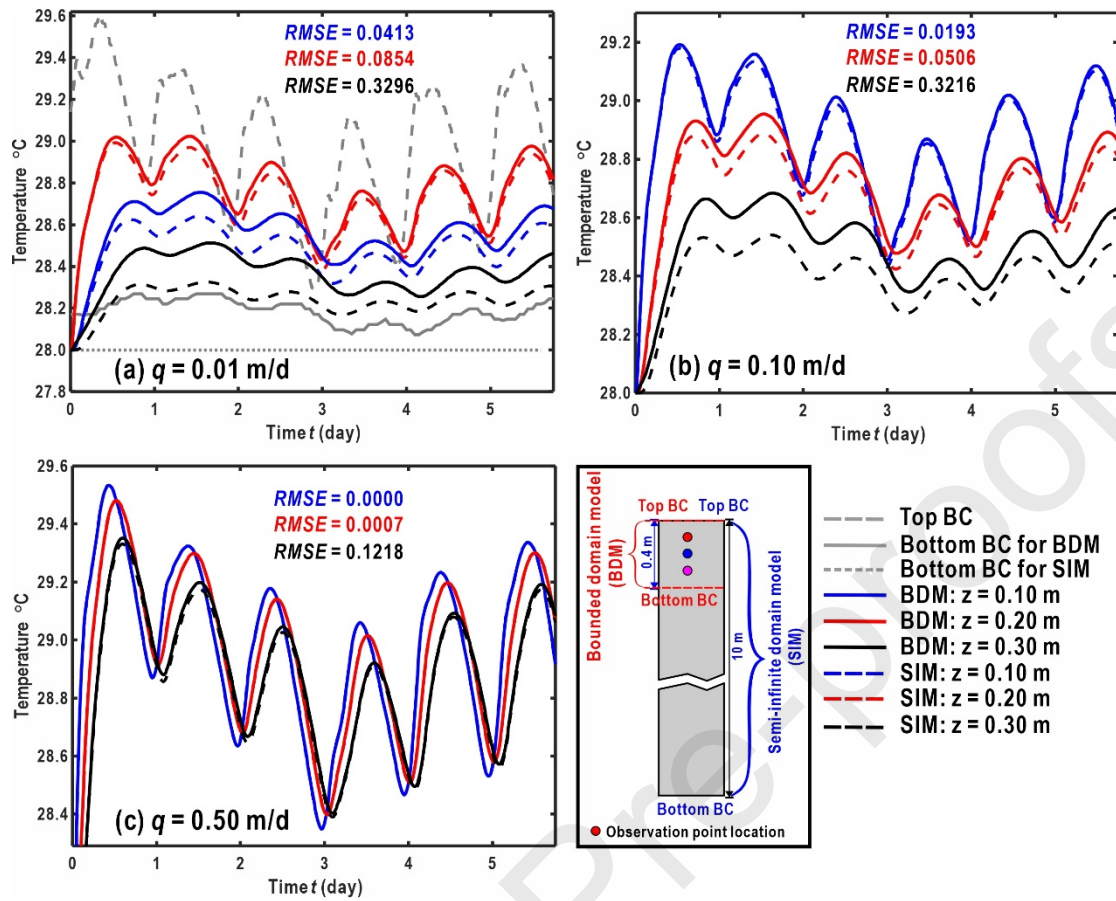
875 **Figure 2.** (a) Schematic diagram for the laboratory experimental system; (b) - (d) are
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 878 estimation. These observed data are from the experiment Run1 of Zhang et al. (2021).

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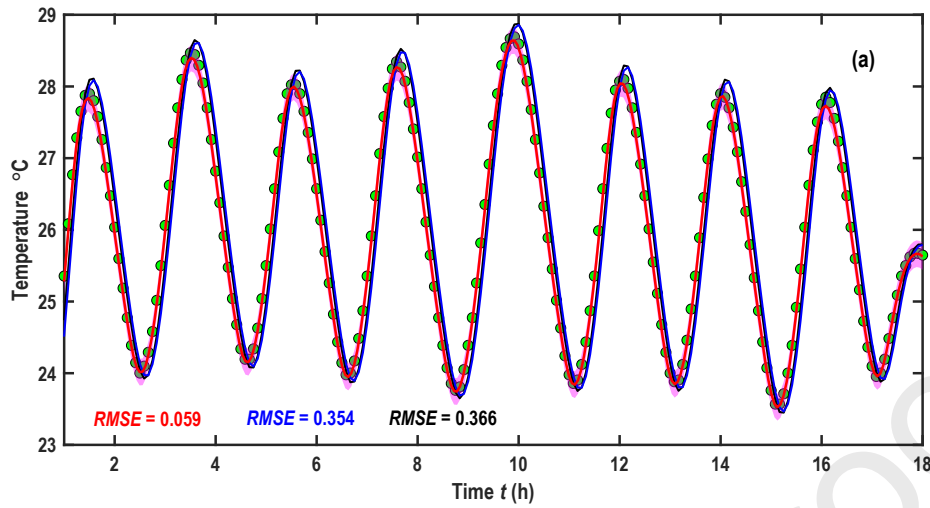
881 **Figure 3.** Comparison of temperature-time series between BDFLUX (black solid curves) and
 882 numerical solution (green circle symbols) at $z = 0.1, 0.2$ and 0.3 m, respectively. The top and
 883 bottom boundary conditions are from Ferencz et al. (2021), as shown in Figure 1b, where “BS1”
 884 and “OBS3” serve as top and bottom boundary conditions, respectively.



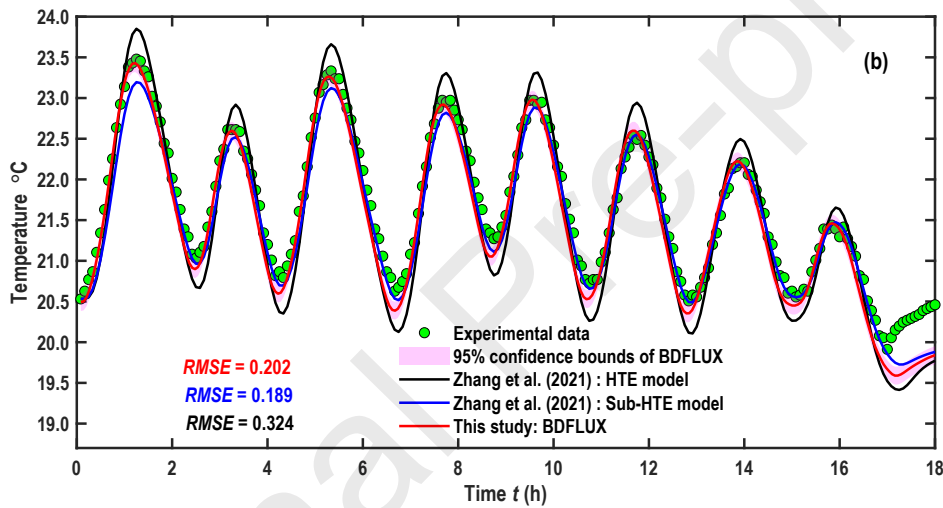
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886 **Figure 4.** Comparison of temperature-time series predicted by the BDFLUX (solid curves) and
 887 semi-infinite domain model (dashed curves) at $z = 0.1, 0.2$ and 0.3 m. (a) $q = 0.01$ m/d, (b)
 888 $q = 0.10$ m/d, (c) $q = 0.50$ m/d. “BC” in the legend represents boundary condition, “BDM”
 889 and “SIM” refer to bounded domain model and semi-infinite domain model, respectively.

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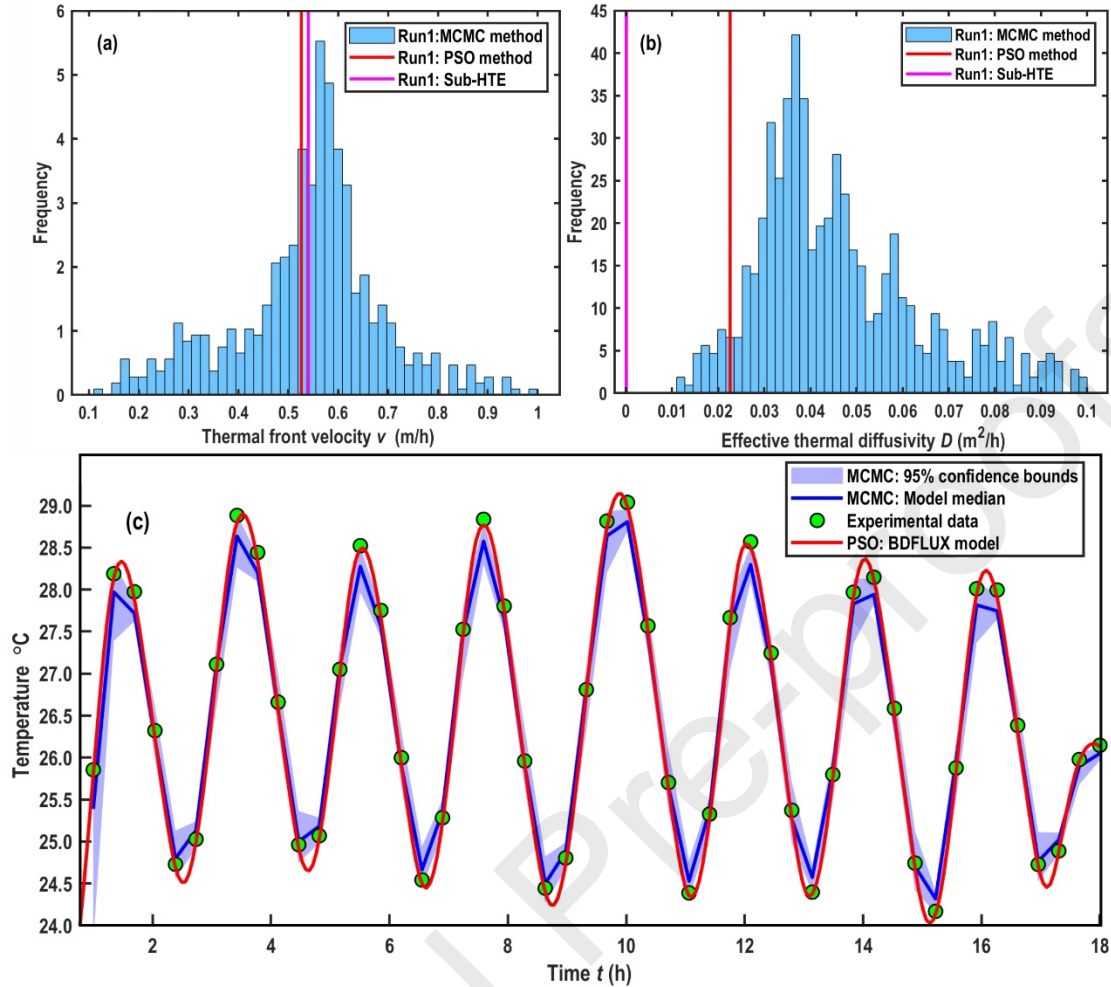
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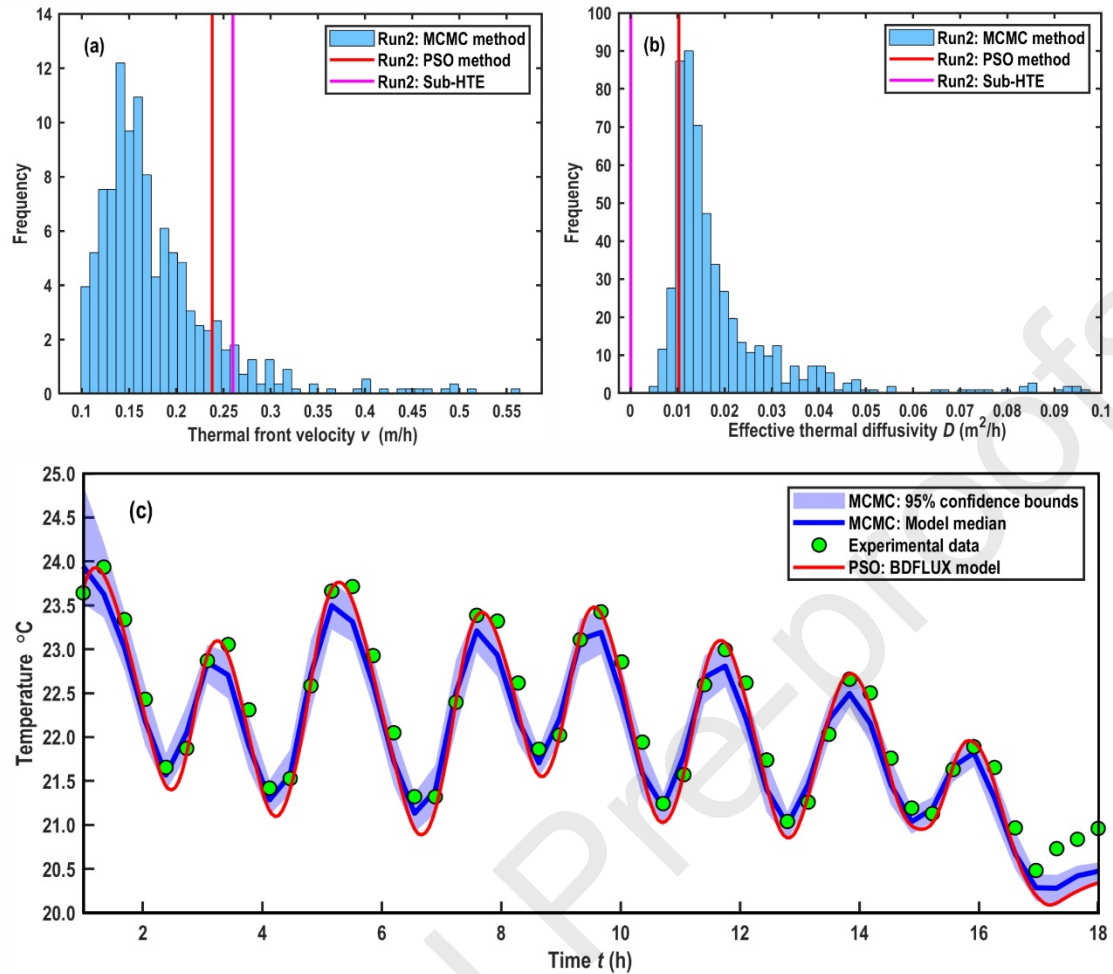
Simulation results of the laboratory experiments of Run1 (a) and Run2 (b) at $z = 0.1$ m: The observed data (green circle symbols) versus the BDFLUX (red solid curves) and the models of Zhang et al. (2021).

Figure 5.



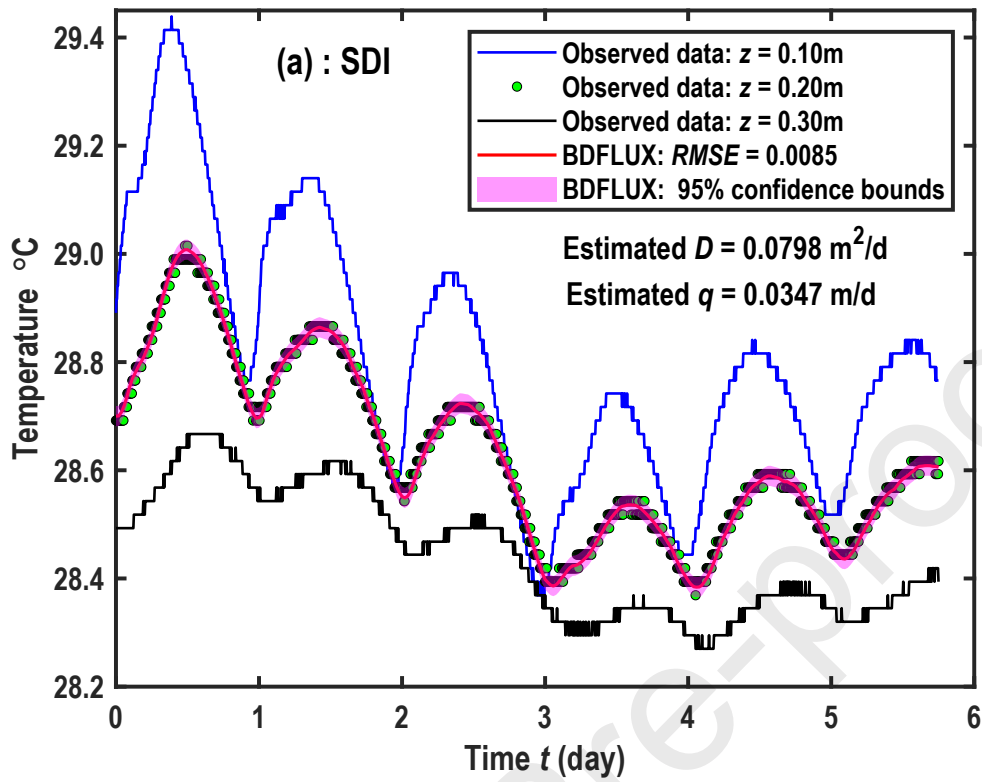
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897 **Figure 6.** Simulation results of the laboratory experiment of Run1 using MCMC method. The
 898 results of PSO method (Red solid curve) and the Sub-HTE model of Zhang et al. (2021)
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 900 thermal front velocity (a) and the effective thermal diffusivity (b) estimated by the MCMC
 901 method. (c) Comparison between the measured data and predicted temperature-time series,
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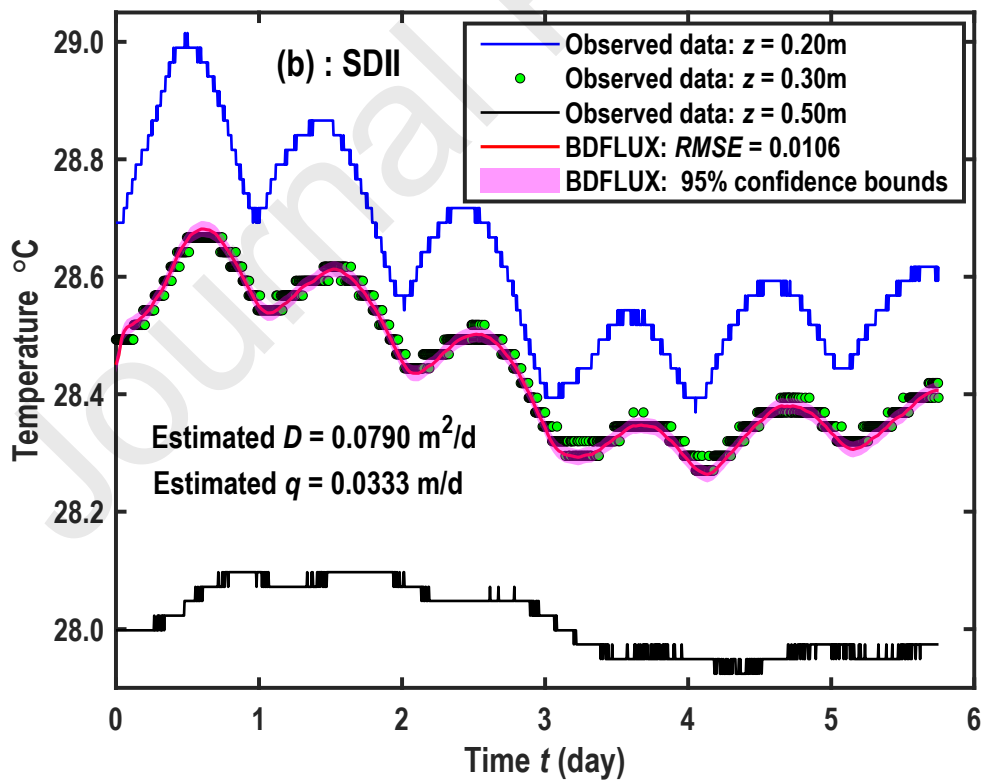


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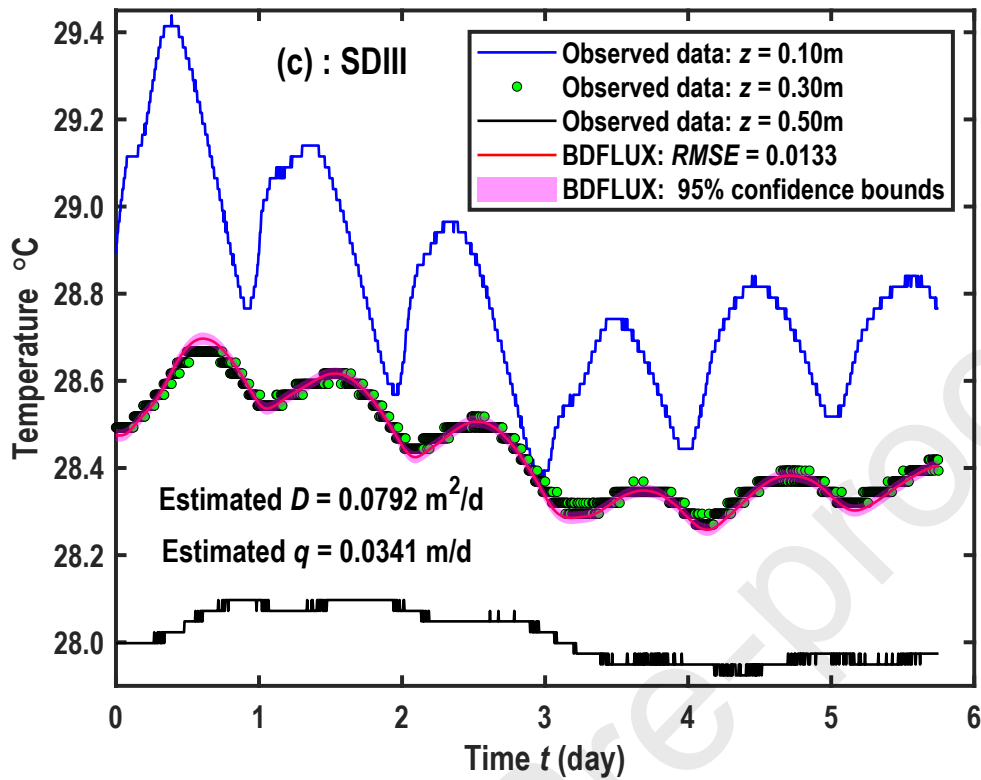
904 **Figure 7.** Simulation results of the laboratory experiment of Run2 using MCMC method. The
 905 results of PSO method (Red solid curve) and the Sub-HTE model of Zhang et al. (2021)
 906 (Magenta solid curve) are also included for comparison. The frequency histograms of the thermal
 907 front velocity (a) and the effective thermal diffusivity (b) estimated by the MCMC method. (c)
 908 Comparison between the measured data and predicted temperature-time series, where the blue
 909 solid curve generated by BDFLUX based on the parameter samples from MCMC.



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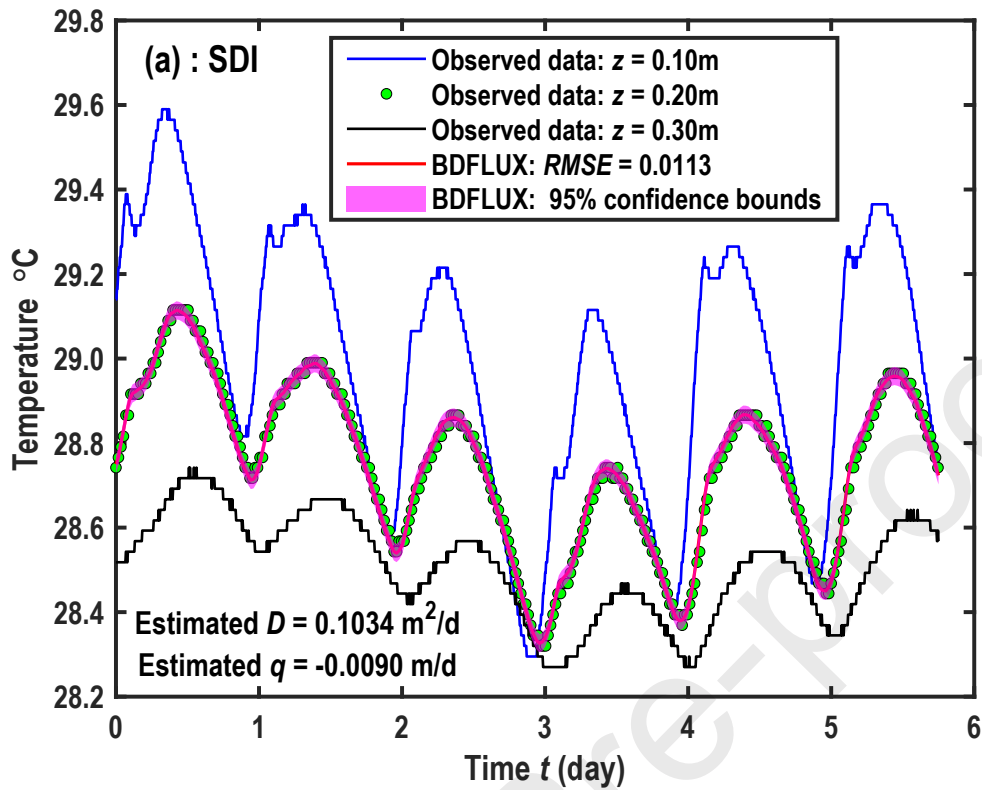
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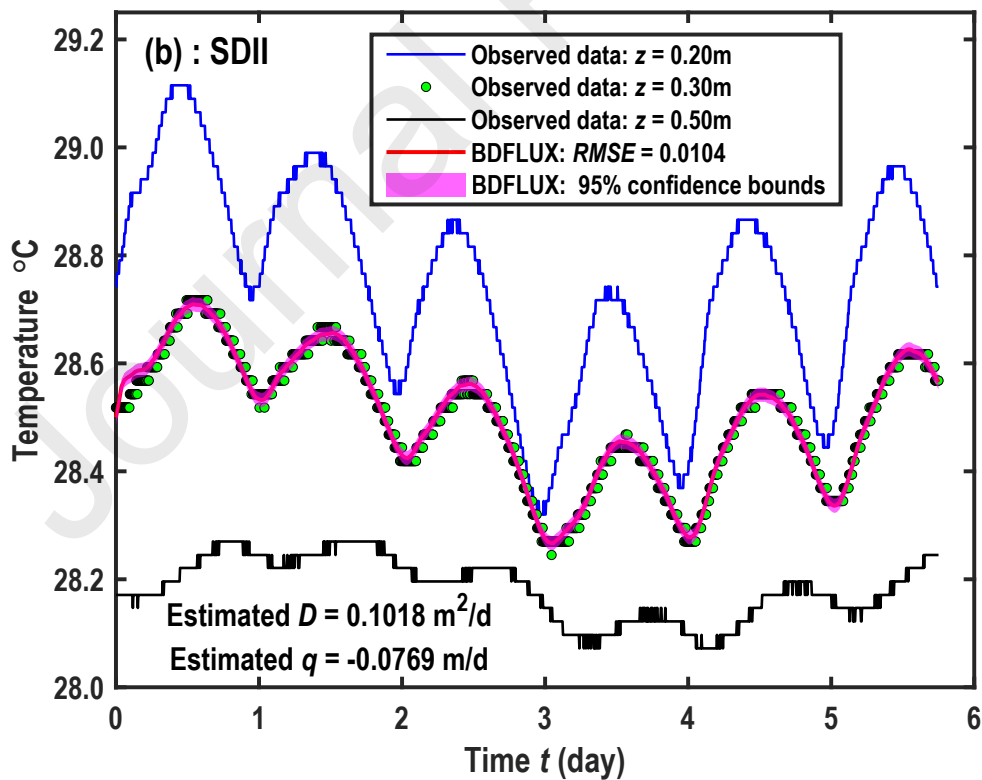
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913 **Figure 8.** Fitting of the temperature-time series (green circle symbols) observed at VA1 by the
 914 BDFLUX (red solid curves) using the estimated parameters obtained from the PSO method for
 915 (a) SDI, (b) SDII and (c) SDIII. The top and bottom boundary conditions of the BDFLUX are
 916 represented by the blue and black solid curves. Data are from Ferencz et al. (2021).

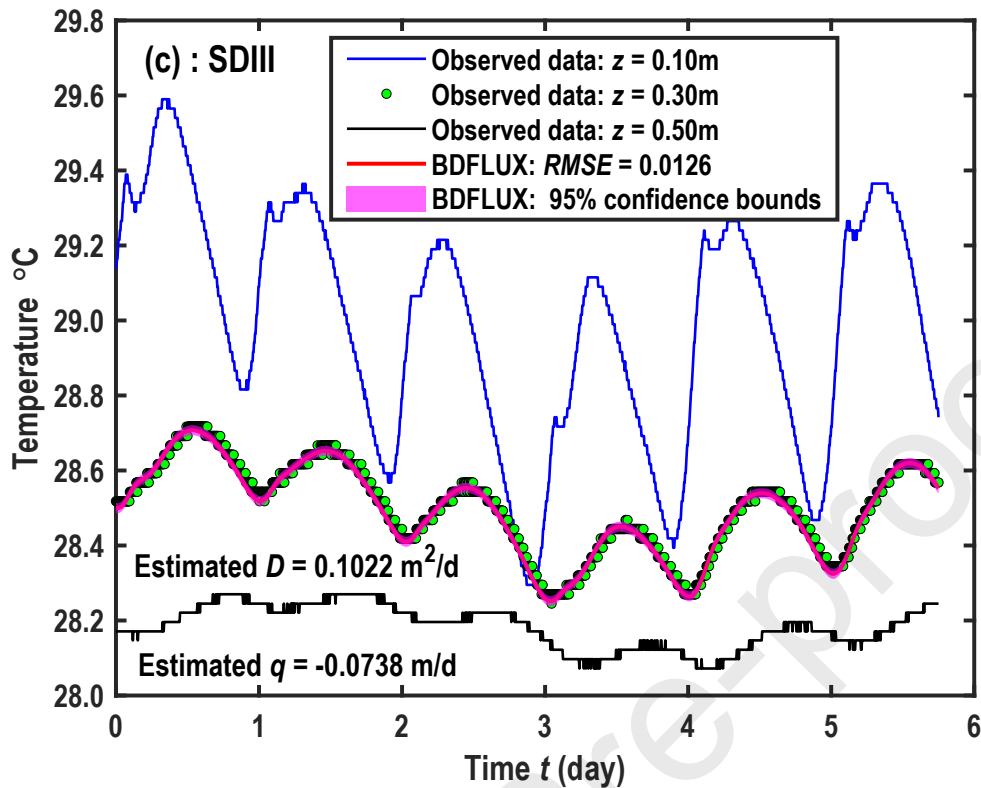
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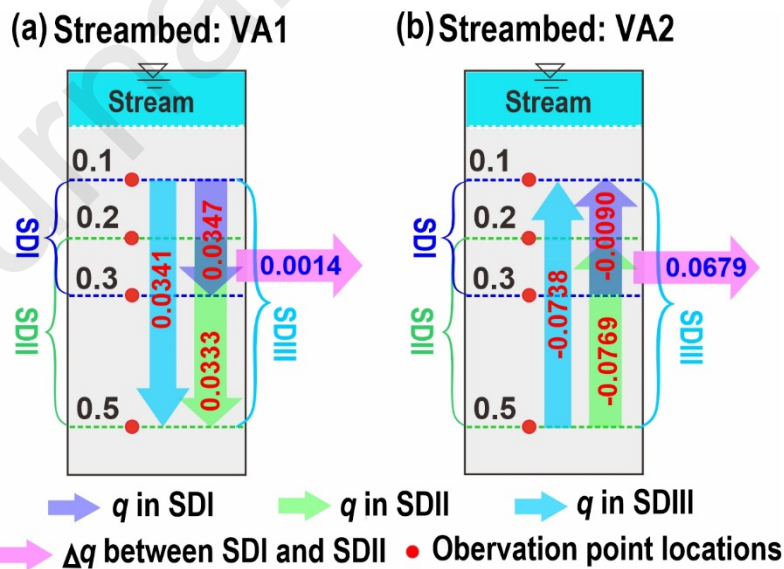


919



920

921 **Figure 9.** Fitting of the temperature-time series (green circle symbols) observed at VA2 by
 922 BDFLUX (red solid curves) using the estimated parameters obtained from the PSO method for
 923 (a) SDI, (b) SDII and (c) SDIII. The top and bottom boundary conditions of BDFLUX are
 924 represented by the blue and black solid curves. Data are from Ferencz et al. (2021).



925

926 **Figure 10.** The estimated VSCs and the inferred magnitude of nonvertical flow components in
 927 streambed profile VA1 (a) and streambed profile VA2 (b). Differences in VSCs between SDI and

928 SDII imply a change in the magnitude of the nonvertical flow component (magenta arrow). The
 929 unit of VSFs are in m/d.

930

931 **Table 1.** The values of D and v are used as true values in the numerical model (NUM) and are
 932 estimated by BDFLUX, and the relative error between true and estimated values are calculated. The
 933 generated temperature-time series at the depths of 0.1, 0.2 and 0.3 m are used to estimate D and v by
 934 BDFLUX.

Scenarios	Parameters	True values	Estimated value by BDFLUX	Relative error (%)
$q = 0.01$ [m/d]	D [m ² /d]	0.0491	0.0479	2.44
	v [m/d]	0.0231	0.0238	3.03
$q = 0.10$ [m/d]	D [m ² /d]	0.0491	0.0475	3.25
	v [m/d]	0.2308	0.2340	1.39
$q = 0.50$ [m/d]	D [m ² /d]	0.0491	0.0469	4.07
	v [m/d]	1.1538	1.1781	2.11

935 The other parameters used to calculate D and v are: $k = 1.44$ W/(m · K), $\rho c = 2.534 \times 10^6$ J/
 936 (m³ · K), and $\rho_w c_w = 4.20 \times 10^6$ J/(m³ · K).

937

938 **Table 2.** Parameters estimated by different models using laboratory experimental data

Tests	Parameters	Symbols	Models		
			BDFLUX	Sub-HTE ^[a]	HTE ^[a]
Run1	Best-fit effective thermal diffusivity	D [m ² /h]	0.0226	0.0001	0.0004

	Best-fit thermal front velocity	v [m/h]	0.5261	0.5400	0.5800
	Best-fit fractional order ^[a]	α [-]	N/A	0.90	N/A
	Root mean square error	$RMSE$ [-]	0.0590	0.3540	0.3660
	Best-fit effective thermal diffusivity	D [m ² /h]	0.0103	0.0001	0.0004
Run2	Best-fit thermal front velocity	v [m/h]	0.2380	0.2600	0.3200
	Best-fit fractional order ^[a]	α [-]	N/A	0.78	N/A
	Root mean square error	$RMSE$ [-]	0.202	0.189	0.324

939 [a]. The models and parameter values are from Zhang et al. (2021).

940

941 **Table 3.** Estimated thermal conductivity and volumetric heat capacity using different models.

Tests	Models	Estimated parameters					
		θ [-]	k_s [W/(m · K)]	$\rho_s c_s$ [J/(m ³ · K)]	β [m]	D [m ² /h]	v [m/h]
	Sub-THE model	0.45	-0.357	1.527×10^6	N/A	0.0001	0.5400
Run1	HTE model	0.45	0.022	1.182×10^6	N/A	0.0004	0.5800
	BDFLUX with β	0.4514	9.820	1.652×10^6	0.0291	0.0226	0.5261

BDFLUX without β	0.2093	22.071	2.432×10^6	N/A	0.0226	0.5261
<hr/>						
Sub-THE model	0.45	-0.329	2.400×10^6	N/A	0.0001	0.2600
HTE model	0.45	0.036	1.291×10^6	N/A	0.0004	0.3200
Run2						
BDFLUX with β	0.3856	9.069	3.192×10^6	0.0181	0.0101	0.2334
BDFLUX without β	0.1898	12.439	3.386×10^6	N/A	0.0104	0.2361

942

943

944 **Highlights**

- 945 ● Heat-based bounded domain analytical model for vertical streambed flux presented.
- 946 ● Particle swarm optimization and Markov Chain Monte Carlo methods used.
- 947 ● Model is evaluated using synthetic, laboratory experimental, and field data.
- 948 ● Method to estimate nonvertical flow components presented.

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950 **Declaration of interests**

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

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