The Stream Temperature Model Component

Caleb A. Buahin
caleb.buahin@gmail.com
Utah Water Research Laboratory

This document describes the Stream Temperature model component (STMComponent) that solves the one-dimensional advection dispersion equation using the explicit finite volume approximation for heat and solute transport. The STMComponent was developed to be primarily used within the HydroCouple component-based modeling framework (Buahin and Horsburgh, 2016). However, it can be compiled and executed as a standalone executable.

1. Formulations

The 1D advection dispersion heat transport equation that is solved by the STMComponent model is shown in Equation 1.

$$\rho_w c_p \frac{\partial T}{\partial t} = -\rho_w c_p \frac{\partial (vT)}{\partial x} + \rho_w c_p \frac{\partial}{\partial x}\left(D \frac{\partial T}{\partial x}\right) + \sum \frac{\Phi}{\mathrm{Y}} + \sum S \tag{1}$$

where T is the water temperature (K), t is the time (s), v is the velocity of the water in the channel $\left(\frac{\mathrm{m}}{\mathrm{s}}\right)$, x is the distance along the channel (m), D longitudinal dispersion $\left(\frac{\mathrm{m}^2}{\mathrm{s}}\right)$, ρ_w is the water density $\left(\frac{\mathrm{kg}}{\mathrm{m}^3}\right)$, c_p is the specific heat capacity of water $\left(\frac{\mathrm{J}}{\mathrm{kg.K}}\right)$, T is the temperature of the water (K), Φ are external radiant heat fluxes $\left(\frac{\mathrm{J}}{\mathrm{m}^2\mathrm{s}}\ or\ \frac{\mathrm{W}}{\mathrm{m}^2}\right)$ incident on the water surface, S are heat supplied by other external sources $\left(\frac{\mathrm{J}}{\mathrm{m}^3\mathrm{s}}\right)$, Y is the depth of water in the channel (m). Equation 1 is approximated numerically using the finite volume method as shown subsequently. The integral version of Equation 1 over a time step from t to Δt over the control volume i (i.e., CV_i in Figure 1) is shown in Equation 2.

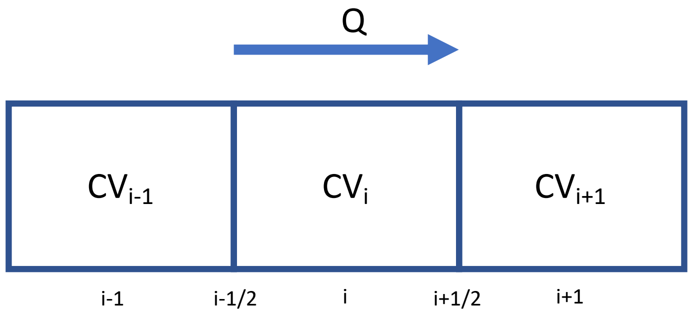

Figure 1. 1D control volume

$$\rho_w c_w \int_t^{t+\Delta t} \int_{CV} \frac{\partial T}{\partial t} dV dt = \rho_w c_w \int_t^{t+\Delta t} \int_{CV} \left(-\frac{\partial (vT)}{\partial x}\right) dV dt + \rho_w c_w \int_t^{t+\Delta t} \int_{CV} \frac{\partial}{\partial x}\left(D \frac{\partial T}{\partial x}\right) dV dt + \int_t^{t+\Delta t} \int_{CV} \sum \frac{\Phi}{\mathrm{Y}} dV dt + \int_t^{t+\Delta t} \int_{CV} \sum S \, dV dt \quad (2)$$

where V is the volume of the CV (m^3), t represents the current time step (s), and $t + \Delta t$ represents the next time step where we seek a solution. Using Gauss's divergence theorem and expanding the terms for Equation 3 yields:

$$\int_t^{t+\Delta t} \rho_w c_w \frac{\partial T}{\partial t} V \, dt = \int_t^{t+\Delta t} \rho_w c_w \sum_{k=1}^{NB} (-vTA) \, dt + \int_t^{t+\Delta t} \rho_w c_w \sum_{k=1}^{NB} \left(D \frac{\partial T}{\partial x} A\right) dt + \int_t^{t+\Delta t} \sum \frac{\Phi}{\mathrm{Y}} V dt + \int_t^{t+\Delta t} \sum S \, V dt \quad (3)$$

where NB represents the number of inlet and outlet boundaries for the CV, $\sum_{k=1}^{NB}(-vTA)$ represents summation of the advective heat fluxes across the inlet and outlet boundaries of the CV, $\sum_{k=1}^{NB}\left(D \frac{\partial T}{\partial x} A\right)$ represents the sum of the dispersive heat fluxes across the inlet and outlet boundaries of the CV, and A is the cross sectional (m^2) of flow. Using an explicit time marching approximation for the CV depicted in Figure 1 yields Equation 4, which is expands to Equation 5.

$$\rho_w c_w \frac{T_i^{t+\Delta t} - T_i^t}{\Delta t} V_i = \rho_w c_w \sum_{k=1}^{NI} (-QT)_i^t + \rho_w c_w \sum_{k=1}^{NI} \left(D \frac{\partial T}{\partial x} A\right)_i^t + \rho_w c_w \left(\sum \frac{\Phi}{\mathrm{Y}} V\right)_i^t + \left(\sum S \, V\right)_i^t \quad (4)$$

$$\rho_w c_w \frac{T_i^{t+\Delta t} - T_i^t}{\Delta t} V_i = \overbrace{\rho_w c_w (QT)_{i-\frac{1}{2}}^t - \rho_w c_w (QT)_{i+\frac{1}{2}}^t}^{Advection} + \overbrace{\rho_w c_w \left(D \frac{\partial T}{\partial x} A\right)_{i+\frac{1}{2}}^t - \rho_w c_w \left(D \frac{\partial T}{\partial x} A\right)_{i-\frac{1}{2}}^t}^{Dispersion} + \overbrace{\left(\sum \frac{\Phi}{\mathrm{Y}} V\right)_i^t + \left(\sum S \, V\right)_i^t}^{External\ Sources} \quad (5)$$

where fluxes out of the CV take on positive values, fluxes into the CV take on negative values, values with the superscripts t and $t+\Delta t$ represent values at the current time step and next time step respectively, values with the subscripts i, $i-\frac{1}{2}$, and $i+\frac{1}{2}$ represent values at the current CV, its left boundary, and right boundary respectively, Δt is the time step (s), and Q is the flow for the CV $\left(\frac{\mathrm{m}^3}{\mathrm{s}}\right)$.

External sources of heat fluxes, including latent heat from evaporation and condensation as well as sensible heat exchanges from conduction and convection with the atmosphere can be specified in the input file or retrieved from other models that are coupled to the STMComponent.

1.1 Advection

Several methods are available for discretizing the advection terms in Equation 5. These include the upwind, central and hybrid differencing methods. Additionally, several total variation diminishing (TVD; Harten, 1983) schemes are also available for problems that have sharp discontinuities in their solution domain. An exhaustive treatment of TVD schemes is provided by Versteeg and Malalasekera (2007) and are not described here.

For the first-order accurate upwind differencing scheme, the assumptions made for inlet and outlet advective heat fluxes for boundaries of the control volume are prescribed as follows:

$$\rho_w c_w (QT)_{i-\frac{1}{2}} = \rho_w c_w Q_{i-\frac{1}{2}} T_{i-1} \tag{6}$$

$$\rho_w c_w (QT)_{i+\frac{1}{2}} = \rho_w c_w Q_{i+\frac{1}{2}} T_{i} \tag{7}$$

For the second-order accurate central differencing scheme, the inlet and outlet advective heat fluxes at the boundaries of the control volume are interpolated using the inverse distance weighting (IDW) interpolation scheme as shown in equations 8 and 9.

$$\rho_w c_w (QT)_{i-\frac{1}{2}} = \rho_w c_w Q_{i-\frac{1}{2}} \frac{\left(T_{i-1}\left(x_{i-\frac{1}{2}} - x_{i-1}\right) + T_i\left(x_i - x_{i-\frac{1}{2}}\right)\right)}{x_i - x_{i-1}} \tag{8}$$

$$\rho_w c_w (QT)_{i+\frac{1}{2}} = \rho_w c_w Q_{i+\frac{1}{2}} \frac{\left(T_{i}\left(x_{i+\frac{1}{2}} - x_{i}\right) + T_{i+1}\left(x_{i+1} - x_{i+\frac{1}{2}}\right)\right)}{x_{i+1} - x_{i}} \tag{9}$$

While the upwind differencing scheme is stable, it is only first order accurate, which gives rise to false diffusion. This contrasts with the central differencing scheme, which although second-order accurate, does not possess the transportiveness property (i.e., ability to account for flow direction as well as the upwind scheme especially for highly advective flows) (Versteeg and Malalasekera, 2007). The hybrid differencing scheme proposed by Spalding (1972) attempts to split these tradeoffs be assessing whether advection or dispersion is the dominant transport mechanism. The hybrid differencing scheme proceeds by first estimating the Peclet number (Pe) at the face of the control volume of interest as follows:

$$Pe_{i-\frac{1}{2}} = \frac{v_{i-\frac{1}{2}}}{\left(\frac{D_{i-\frac{1}{2}}}{x_i - x_{i-1}}\right)} \tag{10}$$

The flux through that face of the control volume is then estimated as follows:

$$\rho_w c_w (QT)_{i-\frac{1}{2}} = \rho_w c_w Q_{i-\frac{1}{2}} \left[f_{i-1}\, T_{i-1} \left(1 + \frac{1}{f_{i-1} Pe_{i-\frac{1}{2}}}\right) + f_i T_i \left(1 - \frac{1}{f_i Pe_{i-\frac{1}{2}}}\right)\right] \text{ for } -2 < Pe_{i-\frac{1}{2}} < 2 \tag{11}$$

$$\rho_w c_w (QT)_{i-\frac{1}{2}} = \rho_w c_w Q_{i-\frac{1}{2}} T_{i-1} \text{ for } Pe_{i-\frac{1}{2}} \geq 2 \tag{12}$$

$$\rho_w c_w (QT)_{i-\frac{1}{2}} = \rho_w c_w Q_{i-\frac{1}{2}} T_i \text{ for } Pe_{i-\frac{1}{2}} \leq -2 \tag{13}$$

where f_{i-1} and f_i are the IDW interpolation factors for the current and left control volumes that surround the boundary under consideration respectively.

1.2 Dispersion

The spatial gradients of temperature at inlet and outlet of the CV used for computing dispersion in Equation 5 is discretized numerically as follows:

$$\left.\frac{\partial T}{\partial x}\right|_{i-\frac{1}{2}} = \frac{T_i - T_{i-1}}{x_i - x_{i-1}} \tag{14}$$

$$\left.\frac{\partial T}{\partial x}\right|_{i+\frac{1}{2}} = \frac{T_{i+1} - T_i}{x_{i+1} - x_i} \tag{15}$$

Following the QUAL2K model, the STMComponent adopts the formulations by Fischer *et al.* (1979) to calculate longitudinal dispersion when it is not explicitly provided as follows:

$$D_i = 0.11\frac{v_i^2 B_i^2}{Y_i U_i^*} \tag{16}$$

where B_i is the channel width (m), Y_i is the mean flow depth (m), and U_i^* is shear velocity $\left(\frac{m}{s}\right)$ of the CV. The shear velocity is calculated as:

$$U_i^* = \sqrt{gY_iS_i} \tag{17}$$

where S_i is the channel slope. The computed dispersion coefficient is compared with the numerical dispersion estimated using Equation 18.

$$E_i = \frac{v_i(x_{i+1} - x_{i-1})}{2} \tag{18}$$

If the computed numerical dispersion is less than the computed dispersion in Equation 8, $D_i - E_i$ is used as the dispersion coefficient used in Equation 5 otherwise the dispersion coefficient is set to zero.

1.3 Solvers

The STMComponent solves Equation 5 using several ordinary differential equation (ODE) solvers including the classical fourth order Runge-Kutta method (i.e., RK4) or the adaptive step size controlled fifth order Runge-Kutta-Cash-Carp (RKQS, Cash and Karp, 1990) method. Alternatively, users can select variable multistep methods including the Adams-Moulton (i.e., ADAMS) formulas or the Backward Differentiation Formulas (i.e., BDF) that are provided through the CVODE (Hindmarsh *et al.*, 2017) external ODE solver library.

2. Input File Formats

The STMComponent input file format is illustrated below.

```
[OPTIONS]
START_DATETIME month/day/year hour/minute/second
END_DATETIME month/day/year hour/minute/second
REPORT_INTERVAL seconds
MAX_TIME_STEP seconds
MIN_TIME_STEP seconds
NUM_INITIAL_FIXED_STEPS value
USE_ADAPTIVE_TIME_STEP YES/NO
TIME_STEP_RELAXATION_FACTOR value
ADVECTION_MODE UPWIND/CENTRAL/HYBRID/etc
COMPUTE_DISPERSION YES/NO
TEMP_SOLVER RK4/RKQS/ADAMS/BDF
TEMP_SOLVER_ABS_TOL value
TEMP_SOLVER_REL_TOL value
WATER_DENSITY value
```

```
WATER_SPECIFIC_HEAT_CAPACITY value
NUM_SOLUTES value
VERBOSE YES/NO
NUM_STEPS_PER_PRINT value

[OUTPUTS]
CSV "CSV output file path"
netCDF "NetCDF output file path"

[SOLUTES]
;;SOLUTE_NAME  SOLVER  SOLVER_ABS_TOL  SOLVER_REL_TOL
;;=====================================================

[JUNCTIONS]
;;JUNCTION  X  Y  Z
;;=================

[ELEMENTS]
;;CONDUIT  FROMJUNCTION  TOJUNCTION  LENGTH  DEPTH  XSECTION_AREA  WIDTH  SLOPE  DISPERSION_COEFF  TEMPERATURE  SOLUTE1
;;=================================================================================================================

[BOUNDARY_CONDITIONS]
;;JUNCTION  VARIABLE  TYPE  VALUE/FILEPATH
;;=========================================

[POINT_SOURCES]
;;CONDUIT  VARIABLE  TYPE  VALUE/FILEPATH
;;=======================================

[NON_POINT_SOURCES]
;;START_CONDUIT  END_CONDUIT  VARIABLE  TYPE   VALUE/FILEPATH
;;==========================================================

[TIME_VARYING_HYDRAULICS]
;;VARIABLE  FILEPATH
;;==================
```

Section: [Options]

Purpose: Used to set the general parameters for the model

Formats:

START_DATETIME	month/day/year hour/minute/second
END_DATETIME	month/day/year hour/minute/second
REPORT_INTERVAL	seconds
MAX_TIME_STEP	seconds
MIN_TIME_STEP	seconds
NUM_INITIAL_FIXED_STEPS	value
USE_ADAPTIVE_TIME_STEP	YES/NO
TIME_STEP_RELAXATION_FACTOR	Value

START_DATETIME

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