Channel and Sub-Surface Solute and Heat Transport Modeling Using the HydroCouple Component-Based Modeling Framework

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1 Introduction

This document describes a set of model components developed to simulate channel and sub-surface flow, solute, and heat transport within the HydroCouple component-based modeling framework (Buahin and Horsburgh, 2016; Buahin and Horsburgh, 2018). The component-based model development paradigm involves encapsulating a process formulation or a group of related process formulations into independently developed and deployed units (i.e., components) that can be readily stitched together to simulate a more complex system. The foundation for this model development approach is the provision of a set of standard interfaces that when implemented by a model developer, allows a model to exchange information with other models develop using the same interfaces at runtime.

The benefits of this approach to model development are numerous. On the software development front, the component-based approach leads to faster development times and more flexible and maintainable code bases. On the science front, since modelers are able switch one component with another with a different structure that simulates the same process, modelers can more efficiently evaluate the appropriateness of different model structures for a particular study. Additionally, since components are independently developed and deployed, different research disciples can focus on developing components within their domains of specialty with the goal of coupling them to reconstitute a larger system from more holistic evaluations.

The HydroCouple framework adopts the Open Geospatial Consortium's Open Modeling Interface (OpenMI 2.0) standard (Vanecek and Moore, 2014) but provides new interfaces to support parallel and distributed simulations on high performance computing cyberinfrastructure, standard geospatial data formats, and more customizable data exchange workflows. The HydroCouple framework provides a graphical user interface (GUI) called HydroCouple Composer, which doubles as a command line interface (CLI) for setting up and executing coupled model compositions. This software is briefly described in Section 2.0 and can be downloaded from the HydroCouple Github repository.

The core components available for channel solute and heat transport modeling include the following components:

1) SWMMComponent: A hydraulic routing component developed from the Environmental Protection Agency's Stormwater Management Modeling (SWMM) hydraulic routing engine.
2) CSHComponent: A channel solute and heat advection and dispersion component. This component also computes latent heat from evaporation and condensation as well as sensible heat from conduction and convection.
3) HTSComponent: A two-layer sediment conduction and hyporheic exchange component.
4) RHEComponent: A radiative heat exchange component that computes the radiative heat fluxes at the water surface.
5) GWComponent: A two-dimensional groundwater component that solves the vertically averaged saturated groundwater equations to compute water, heat, and solute fluxes that are exchanged between the channel and groundwater.

In addition to the four core components, three other components are available for calibrating and optimizing the coupled models. These components include:

1) TimeSeriesProviderComponent: A component for providing spatio-temporal forcing data to various components.

2) CalibrationComponent: A calibration component for calibrating the coupled solute and heat transport model.

3) TSObjectiveFunctionComponent: A component for computing various time series comparison efficiency indexes and constraints for optimization/calibration applications.

2 HydroCoupleComposer

Figure 2.1 shows the HydroCoupleComposer GUI. The left panel shows the list of available components that can be used in a model composition. The central panel is a display area that shows the components involved in a coupled model composition and the connections between them. Blue dots represent inputs a component can retrieve in for its computations. Red dots represent outputs one component can provide to another. The lines connecting red dots to blue dots represent the coupling between outputs and inputs of components over which information are exchanged. On the right is a panel that shows a list of data modifiers that can be used mediate the data exchange between components by performing the necessary data transformations needed to supply data (e.g., time series interpolation, data aggregation, spatial interpolation, etc.). The panels at the bottom show the simulation progress and message logs for debugging errors. The collapsed panels on the right are the properties panel and workflow components panel that can be used to direct the data exchange workflow between components. The properties panel provides a dialog for modifying the properties of objects that are selected in display area. The workflow components provide a list of a type of component that controls the order of data exchange during simulation. These workflow components can be used as an alternative to the default “pull driven” data exchange workflow used in the HydroCoupleComposer GUI.

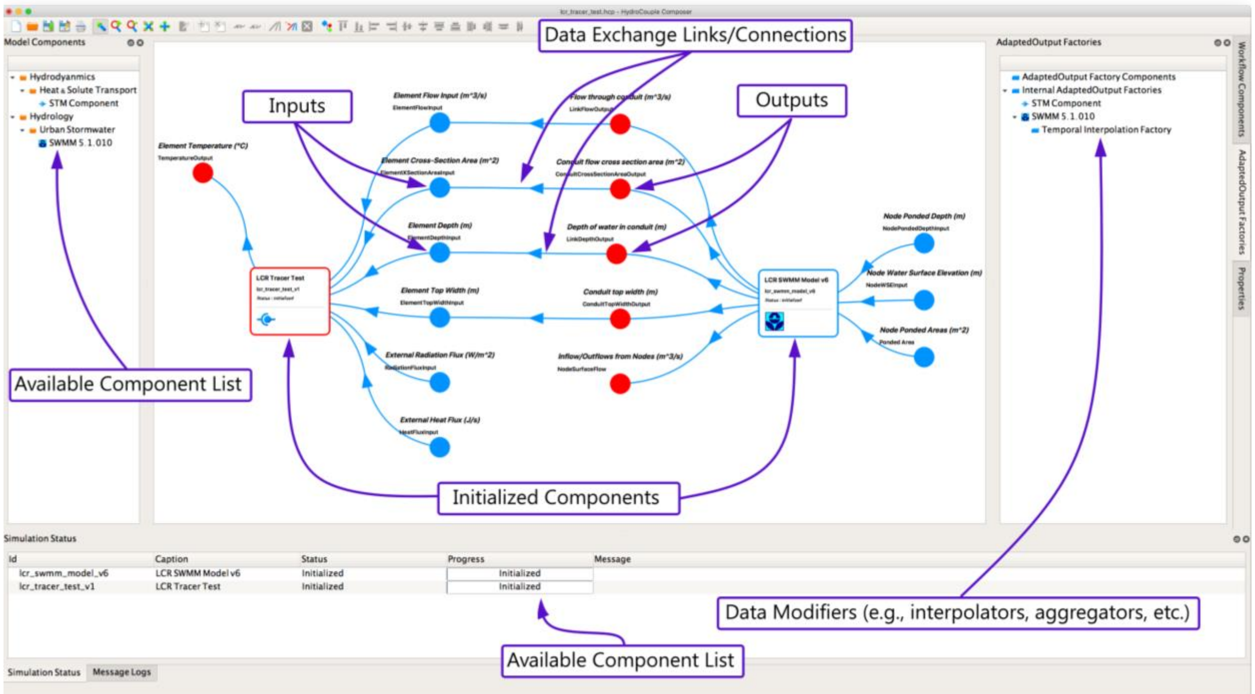

Figure 2.1 HydroCoupleComposer GUI

2.1 User Instructions

The following subsections provide step-by-step instructions on how to add a component to a coupled model composition, supply input arguments, initialize components, couple components together so that they can exchange data, execute coupled model compositions, and save compositions.

2.1.1 Creating a Component Instance

To create an instance of a component:

1. First, locate the component that you want to use in the list of available components. If the component is not in the list, locate the shared library for the component in its folder

on disk and open it using the ***File*** ->***Open*** button on the menu bar. Shared libraries are files with extensions *.dll, *.so, and *.dylib for Window, Linux, and Mac operating systems respectively.

2. Once the component has been added and selected, right click the component and click ***Add Component*** to add a new instance of a component. Alternatively, you can double click the component or click and drag the component into the display area to create a component instance.

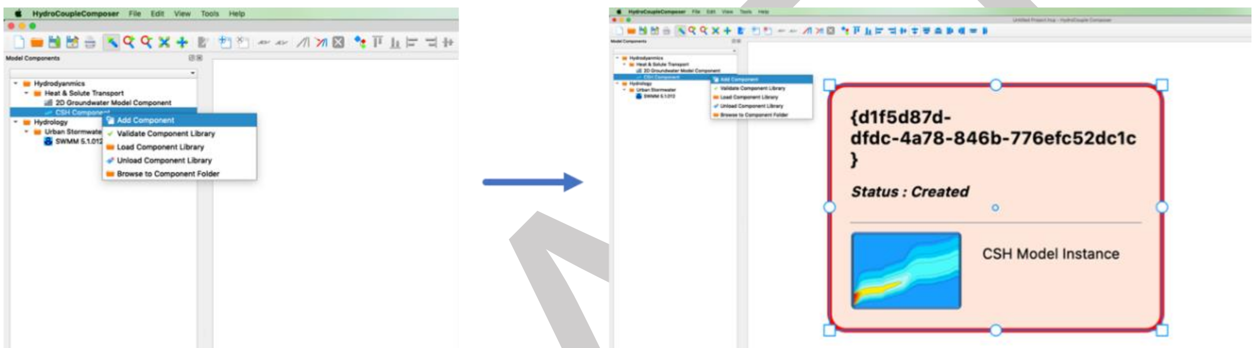

Figure 2.2 Adding a component instance

2.1.2 Specifying Component Arguments

Component instances are initialized using one or more arguments. Arguments may represent component identifiers/descriptors, input and output file paths, model parameters, etc. Arguments are specified using the extensible markup language (xml) format. To specify a component instance's arguments:

1. Select the component instance in the display area and click ***Edit Selected Item*** button on the toolbar to show the argument editor. Alternatively, double clicking a component instance will show the argument editor.

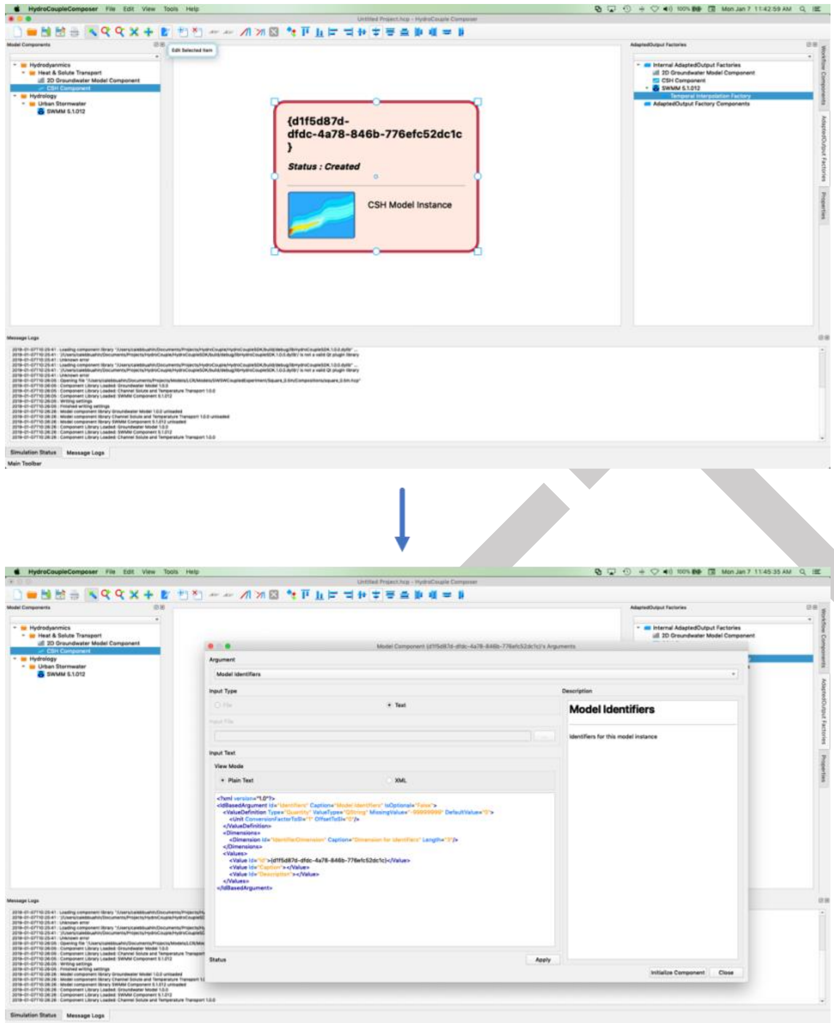

Figure 2.3 Component argument dialog

2. To specify an argument, select the argument from the list of arguments in the dropdown list in the argument dialog. Specify the argument values in the plain text viewer by modifying the contents within the ***Value*** tags. Argument values representing file paths may be provided using the relative file path convention. Relative file path values can be specified relative to the composition project file (*.hcp) or if a component instance file (*.hcc) is being used, relative to the component file path.

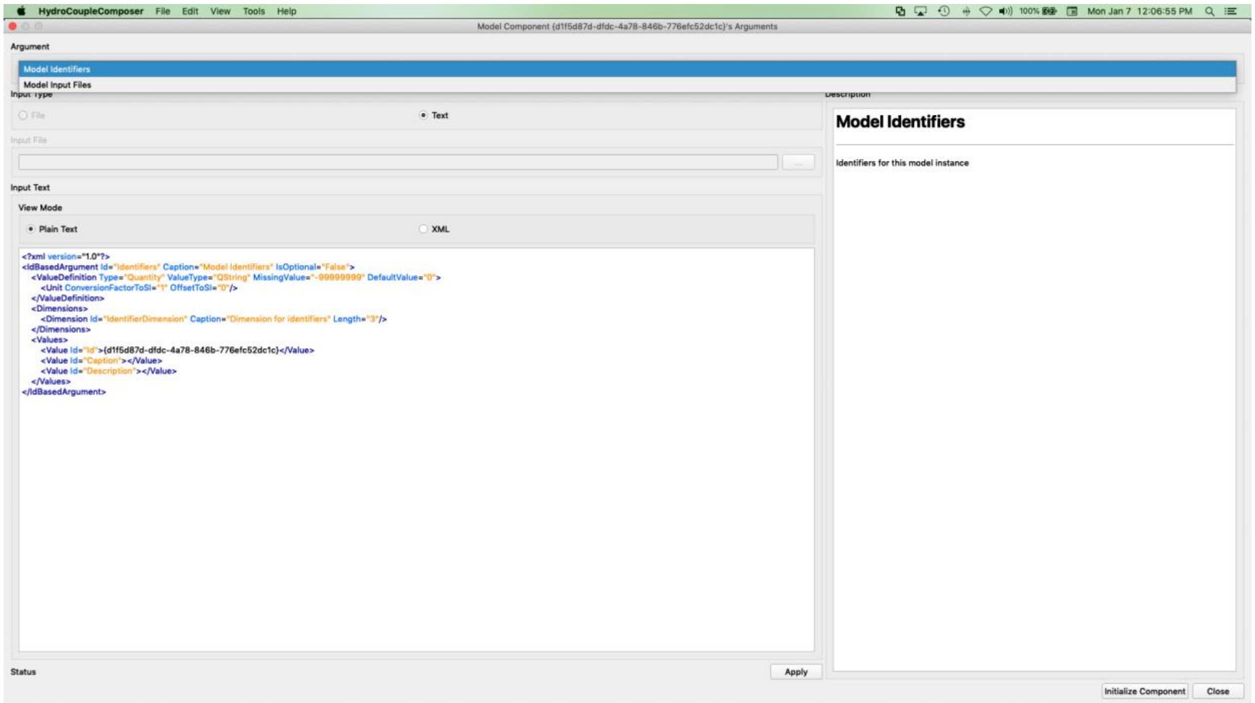

Figure 2.4 Component argument dialog editor

3. Once the argument values have been specified, a component instance can be initialized be selecting component instance in the display area, right clicking, and clicking initialize in the shortcut menu. If initialization is successful, the component instance will show the inputs it can consume and the outputs it can provide to other components (Figure 2.5). If initialization fails, check the message logs window at the bottom of the GUI to see if the output messages can help debug the source of the initialization failure.

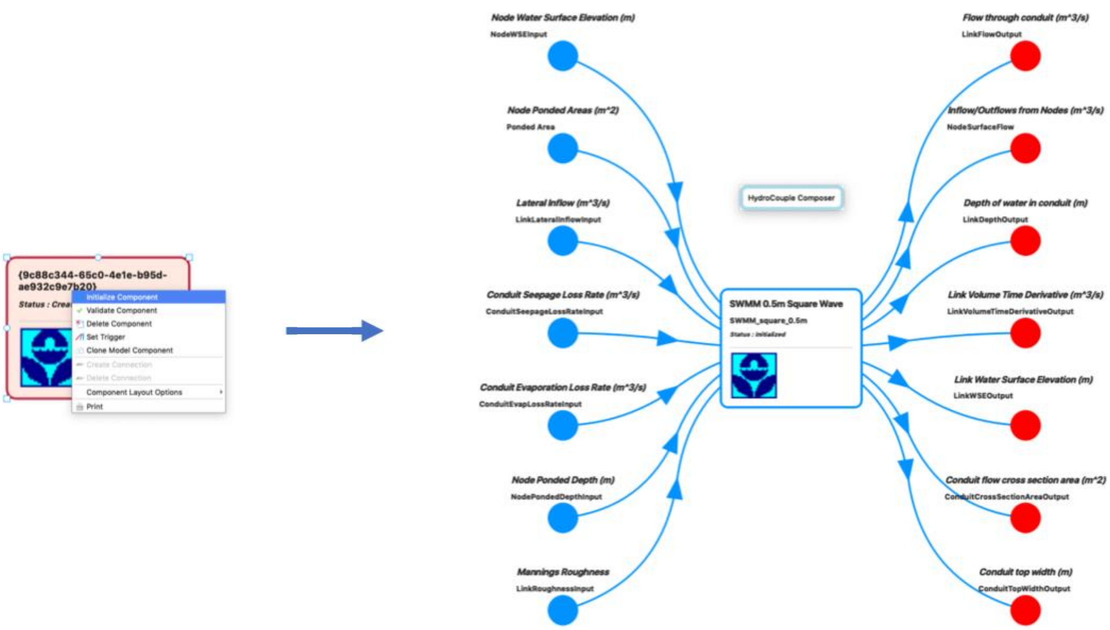

Figure 2.5 Initialized component instance

2.1.3 *Connecting Inputs and Outputs*

To connect an output from one component to an input of another component:

1. Toggle the create connection button on the toolbar.

Figure 2.6 Create connection button on toolbar

2. Click the output you want to provide to another component and the input that will use this data. If the output is compatible with the input selected, a connection will be established. Otherwise look in the message logs for a reason for the incompatibility.

Figure 2.7 Creating a connection between components

2.1.4 Saving Compositions

A coupled model composition involving multiple component instances can be saved to disk and reopened several times for execution. HydroCouple projects are saved to files with the extension *.hcp. Projects may contain references to component instances directly or to component instance files that have the file extension *.hcc. To save a project:

1. Click ***File -> Save*** on the menu bar and browse to file location where you want to save the project. Make sure to select the file filter for a HydroCouple project (i.e., *.hcp).
2. To save a component instance, select the component instance in the display area and click ***File -> Save As*** and browse to the path where you want to save the component instance file. Make sure to select the *.hcc file extension.

2.1.5 Running Compositions

The default data exchange workflow for HydroCouple is based on a pull-based approach, where one component, usually the component at lowest end of a component chain, acts as a trigger that propagates queries for data to upstream components in a cascading manner depicted in Figure 2.8.

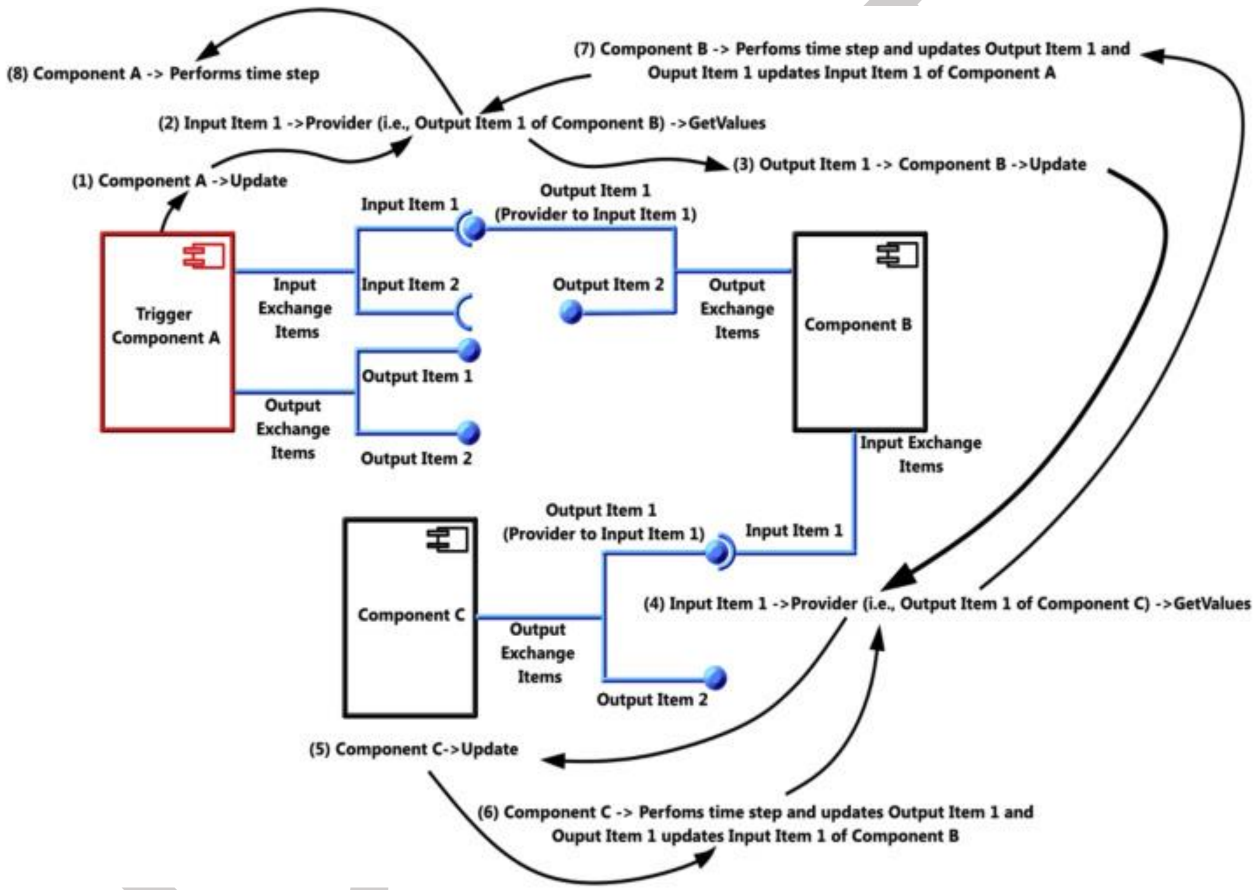

Figure 2.8 Pull driven data exchange workflow

To specify the trigger component and execute a coupled model composition:

1. Select the component you want to set as the trigger and click the ***Set Component as Trigger*** button on the toolbar. Alternatively, you can right click the component and click the ***Set Component as Trigger*** in the shortcut menu.

2. Click the ***Execute Composition*** button on the toolbar to run the coupled model. The simulation status window will show the progress of each component.
3. Composition files can also be executed using the command line interface using the command below:

```
HydroCoupleComposer.exe -r inputprojectfile.hcp –n
```

4. For simulations that utilize MPI use the command below to specify the number of nodes to use:

```
mpiexec -n 20 HydroCoupleComposer.exe -r inputprojectfile.hcp –n
```

2.2 Parallel Multi-Scenario Execution

3 Hydraulic Routing Component (SWMMComponent)

The SWMMComponent was developed from the United States Environmental Protection Agency's (EPA's) Stormwater Management Model (SWMM), which calculates runoff from sub-catchments and routes the resulting runoff through a network of open channels and closed conduits with regular and irregular cross-sections connected together by nodes representing inlets, junctions, outfalls and other nodes types (Rossman, 2010). The routing component of the SWMM model can solve the full dynamic wave equations or the reduced physics diffusive and kinematic wave approximations. It is, therefore, able to handle flows in non-dendritic networks, pressurized flows, flow reversals, and backwater effects. In addition to these features, SWMM is open source and has been well validated over the years by an engaging community of users.

Instructions for setting up SWMM input files have not been provided here and can be found in the SWMM user manual. It is however important to note that for open channel hydraulics simulations, storage associated with nodes that connect conduits together must be set to zero. This can be done by setting the MIN_SURFAREA option in SWWM to a very small number like 1e-8 m^2.

4 Channel Solute and Heat Transport Component (CSHComponent)

The 1D advection dispersion heat transport equation solved by the CSHComponent is:

$$\rho_w c_p \frac{\partial T}{\partial t} = -\rho_w c_p \frac{\partial (vT)}{\partial x} + \rho_w c_p \frac{\partial}{\partial x}\left(D \frac{\partial T}{\partial x}\right) + \sum \frac{J}{Y} - \frac{J_e + J_c}{Y} + \sum S \qquad (4.1)$$

where T is the water temperature $(℃)$, 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 is 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 $\left(\frac{\mathrm{J}}{\mathrm{kg℃}}\right)$, J 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, J_e is the evaporation and condensation from the water surface $\left(\frac{\mathrm{J}}{\mathrm{m}^2\mathrm{s}}\ or\ \frac{\mathrm{W}}{\mathrm{m}^2}\right)$, J_c is the convection and conduction from the water surface $\left(\frac{\mathrm{J}}{\mathrm{m}^2\mathrm{s}}\ or\ \frac{\mathrm{W}}{\mathrm{m}^2}\right)$, S is the heat supplied by other external sources $\left(\frac{\mathrm{J}}{\mathrm{m}^3\mathrm{s}}\right)$, and Y is the depth of water in the channel (m). Equation 1 is approximated numerically using the finite volume method.

The integral version of the heat advection and dispersion equation over a time step from t to Δt over computational element (i.e., CV_i) is:

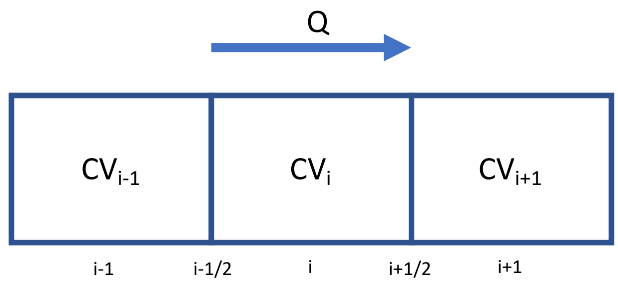

Figure 4.1 1D control volume element

$$\rho_w c_w \int_t^{t+\Delta t} \left(\int_{CV} \frac{\partial T}{\partial t} dV \right) dt = \rho_w c_w \int_t^{t+\Delta t} \int_{CV} \left(-\frac{\partial (vT)}{\partial x} \right) dV dt + \rho_w c_w \int_t^{t+\Delta t} \int_{CV} \frac{\partial}{\partial x} \left(D \frac{\partial T}{\partial x} \right) dV dt + \int_t^{t+\Delta t} \int_{CV} \sum \frac{J}{Y} dV dt - \int_t^{t+\Delta t} \int_{CV} \frac{J_e + J_c}{Y} dV dt + \int_t^{t+\Delta t} \int_{CV} \sum S \, dV dt \tag{4.2}$$

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 yields:

$$\int_t^{t+\Delta t} \rho_w c_w \frac{\partial TV}{\partial t} dt = \int_t^{t+\Delta t} \rho_w c_w \sum_{k=1}^{NB} (-vTA) \, dt + \int_t^{t+\Delta t} \rho_w c_w \sum_{k=1}^{NB} \left(D \frac{\partial T}{\partial x} A \right) dt - \int_t^{t+\Delta t} \sum \frac{\mathrm{J}}{\mathrm{Y}} V dt \int_t^{t+\Delta t} \frac{J_e + J_c}{Y} V dt + \int_t^{t+\Delta t} \sum S \, V dt \tag{4.3}$$

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 area (m^2) of flow. Using an explicit time marching scheme for the CV depicted in Figure 4.1 yields Equation 4.4, which expands to Equation 4.5:

$$\rho_w c_w \left(\frac{T_i^{t+\Delta t} - T_i^t}{\Delta t} V_i + T_i^t \frac{V_i^{t+\Delta t} - V_i^t}{\Delta t} \right) = \rho_w c_w \sum_{k=1}^{NI} (-QT)_i^t + \rho_w c_w \sum_{k=1}^{NI} \left(D \frac{\partial T}{\partial x} A \right)_i^t + \left(\sum \frac{\mathrm{J}}{\mathrm{Y}} V \right)_i^t - \left(\frac{J_e + J_c}{Y} V \right)_i^t + \left(\sum S \, V \right)_i^t \tag{4.4}$$

$$\rho_w c_w \left(\frac{T_i^{t+\Delta t} - T_i^t}{\Delta t} V_i + T_i^t \frac{V_i^{t+\Delta t} - V_i^t}{\Delta t} \right) = \overbrace{\rho_w c_w (QT)_{i-\frac{1}{2}}^t - \rho_w c_w (QT)_{i+\frac{1}{2}}^t}^{Advection} +$$

$$\overbrace{\rho_w c_w \left(D \frac{\partial T}{\partial x} A \right)_{i+\frac{1}{2}}^t - \rho_w c_w \left(D \frac{\partial T}{\partial x} A \right)_{i-\frac{1}{2}}^t}^{Dispersion} + \overbrace{\left(\sum \frac{\mathrm{J}}{\mathrm{Y}} V \right)_i^t + \left(\sum S\, V \right)_i^t}^{External\ Heat\ Sources} + \overbrace{\left(\frac{J_e + J_c}{Y} V \right)_i^t}^{Sensible\ and\ Latent\ Heat} \tag{4.5}$$

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 $\left(\frac{\mathrm{m}^3}{\mathrm{s}} \right)$.

4.1 Advection Discretization

Several methods are available for discretizing the advection terms in Equation 4.5. 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. 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 inlet and outlet advective heat fluxes for boundaries of the control volume are prescribed as follows:

$$\rho_w c_w (QT)_{i-\frac{1}{2}} = \rho_w c_w Q_{i-\frac{1}{2}} T_{i-1} \tag{4.6}$$

$$\rho_w c_w (QT)_{i+\frac{1}{2}} = \rho_w c_w Q_{i+\frac{1}{2}} T_i \tag{4.7}$$

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 4.8 and 4.9.

$$\rho_w c_w (QT)_{i-\frac{1}{2}} = \rho_w c_w Q_{i-\frac{1}{2}} \frac{\left(T_{i-1}\left(x_{i-\frac{1}{2}}-x_{i-1}\right)+T_i\left(x_i-x_{i-\frac{1}{2}}\right)\right)}{x_i-x_{i-1}} \tag{4.8}$$

$$\rho_w c_w (QT)_{i+\frac{1}{2}} = \rho_w c_w Q_{i+\frac{1}{2}} \frac{\left(T_i\left(x_{i+\frac{1}{2}}- x_i\right)+T_{i+1}\left(x_{i+1}-x_{i+\frac{1}{2}}\right)\right)}{x_{i+1}-x_i} \tag{4.9}$$

While the upwind differencing scheme is stable, it is only first order accurate. This contrasts with the central differencing scheme, which while 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 by 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:

$$Pe_{i-\frac{1}{2}} = \frac{v_{i-\frac{1}{2}}}{\left(\frac{D_{i-\frac{1}{2}}}{x_i-x_{i-1}}\right)} \tag{4.10}$$

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

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

for $-2 < Pe_{i-\frac{1}{2}} < 2$ (4.11)

$\rho_w c_w (QT)_{i-\frac{1}{2}} = \rho_w c_w Q_{i-\frac{1}{2}} T_{i-1}$ for $Pe_{i-\frac{1}{2}} \geq 2$ (4.12)

$\rho_w c_w (QT)_{i-\frac{1}{2}} = \rho_w c_w Q_{i-\frac{1}{2}} T_i$ for $Pe_{i-\frac{1}{2}} \leq -2$ (4.13) where f_{i-1} and f_i are inverse distance weighted interpolation factors for the current and left control volumes that surround the boundary under consideration, respectively.

4.2 Dispersion Discretization

The spatial derivatives of temperature at inlet and outlet of the CV used for computing dispersion terms in Equation 4.5 are discretized numerically as follows:

$$\left.\frac{\partial T}{\partial x}\right|_{i-\frac{1}{2}} = \frac{T_i - T_{i-1}}{x_i - x_{i-1}} \tag{4.15}$$

$$\left.\frac{\partial T}{\partial x}\right|_{i+\frac{1}{2}} = \frac{T_{i+1} - T_i}{x_{i+1} - x_i} \tag{4.16}$$

Following the QUAL2K model (Pelletier and Chapra, 2008), the CSHComponent adopts the formulations by (Fischer et al., 1979) to calculate longitudinal dispersion when it is not explicitly provided as follows:

$$D_i = 0.11 \frac{v_i^2 B_i^2}{Y_i U_i^*} \tag{4.17}$$

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:

$$U_i^* = \sqrt{g Y_i S_i} \tag{4.18}$$

where S_i is the channel bottom slope. The computed dispersion coefficient (D_i) is compared with the numerical dispersion estimated using Equation 4.19.

$$E_i = \frac{v_i(x_{i+1} - x_{i-1})}{2} \tag{4.19}$$

If the computed numerical dispersion is less than the computed dispersion in Equation 4.19, $D_i - E_i$ is used as the dispersion coefficient used in Equation 4.19. Otherwise, the dispersion coefficient is set to zero.

4.3 Continuity at Junctions

Following Islam and Chaudhry (1998), internal junctions where 3 or more elements meet are treated as internal boundary conditions, where temperatures are estimated using the simple mass balance equation (Equation 4.20). This equation assumes complete mixing at the junction:

$$T_j = \frac{\sum_{i=1}^{M} Q_i T_i}{\sum_{i=1}^{M} Q_i} \tag{4.20}$$

where T_j is the temperature at the junction of interest $\left(°C, \frac{kg}{m^3}\right)$, M is the number of elements with flows entering the junction, Q_i is the flow from incoming element i $\left(\frac{kg}{m^3}\right)$, and T_i is the temperature/constituent concentration in the incoming element i $\left(°C, \frac{kg}{m^3}\right)$.

4.4 Evaporation and Condensation

Evaporation/condensation is a function of the sensible heat carried with the evaporated water, the latent heat of evaporation, density of water, and the evaporative rate as expressed in Equation 4.21 (Webb and Zhang, 1997; Evans et al., 1998; Boyd and Kasper, 2003).

$$J_e = \rho_w L_e E \tag{4.21}$$

where L_e is the latent heat of vaporization $\left(\frac{J}{kg}\right)$ and E is the evaporative rate $\left(\frac{m}{s}\right)$. The latent heat of vaporization is estimated as a weak function of water temperature using Equation 4.22 (Martin and McCutcheon, 1998):

$$L_e = 1000(2499 - 2.36T) \tag{4.22}$$

where T is the water temperature in the channel (℃). Several approaches are available for estimating the evaporative rate, including mass transfer methods, explicit energy balance methods, and combination methods that combine both mass and energy balance methods. In the CSHComponent, a mass balance method was implemented. Following Dingman (2008), the evaporative rate is estimated using Equation 4.23:

$$E = f(\vec{w})(e_s^w - e_a) \tag{4.23}$$

where e_s^w is the saturation vapor pressure of the evaporating surface (kPa), e_a is the actual vapor pressure (kPa), and $f(\vec{w})$ is a wind function used to estimate the adiabatic portion of evaporation (Boyd and Kasper, 2003). e_s^w is computed using Equation 4.24 (Raudkivi, 1979; Chapra, 2008):

$$e_s^w = 0.61275e^{\left(\frac{17.27T}{237.3+T}\right)} \tag{4.24}$$

where T is the temperature of the water in the channel. The actual vapor pressure (e_a) is calculated as a function of relative humidity (H) and saturation vapor pressure (e_s) using Equation 4.25:

$$e_a = \frac{H}{100\%}e_s \tag{4.25}$$

where e_s is computed using Equation 4.26:

$$e_s = 0.61275e^{\left(\frac{17.27T_a}{237.3+T_a}\right)} \tag{4.26}$$

where T_a is air temperature in $(°C)$.

Extensive observations have yielded Equation 4.27 as the general form of the wind function (Shanahan et al. 1984):

$$f(\vec{w}) = a + b\vec{w} \tag{4.27}$$

where a and b are empirical coefficients with units $kPa^{-1}ms^{-1}$ and kPa^{-1}, respectively, and $\vec{w}$ is the wind speed measured 2 meters above the water surface $\left(\frac{m}{s}\right)$. Several authors have proposed values for these coefficients, including Dunne and Leopold

(1978), who proposed the values $1.505 \cdot 10^{-8}$ and $1.6 \cdot 10^{-8}$ for the coefficients a and b, respectively. These values are used as the defaults in the CSHComponent but can be overridden by user specified coefficients.

4.5 Convection and Conduction

Estimating sensible heat lost or gained through conduction/convection with air in the atmosphere is typically performed using the Bowen ratio (B_r), which relates latent heat to sensible heat (Equation 4.28) (Bowen, 1926; Webb and Zhang, 1997; Evans *et al.*, 1998; Westhoff *et al.*, 2007; Glose *et al.*, 2017).

$$B_r = \frac{J_c}{J_e} \tag{4.28}$$

Martin and McCutcheon (1998) prescribed Equation 4.29 for estimating the Bowen ratio:

$$B_r = \frac{J_c}{J_e} = C_B \frac{P_a}{P} \left(\frac{T - T_a}{e_s^w - e_a} \right) \tag{4.29}$$

where C_B is a Bowen's coefficient usually equal to 0.0651 $\left(\frac{kPa}{°C}\right)$, P_a is atmospheric pressure (kPa), and P is a reference pressure at sea level (kPa). While the ratio $\frac{P_a}{P}$ is often assumed to be unity, the pressure difference cannot be neglected in higher elevations (Martin and McCutcheon, 1998).

4.6 CSHComponent ODE Solvers

The CSHComponent can solve transport equations using several ordinary differential equation (ODE) solvers provided, including the classical fourth order Runge-Kutta method (i.e., RK4) or the adaptive step size controlled fifth order Runge-Kutta-Cash-Carp (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. Readers are referred to the CSHComponent code in the GitHub repository (https://github.com/HydroCouple/CSHComponent) for implementation details.

4.7 CSHComponent Validation

4.8 CSHComponent Input File Format

Input file specification for the CSHComponent is based on the *inp plain file format used by the EPA SWMM model, where attributes are organized into sections that are demarcated using headers provided in brackets (i.e., []) and rows of attribute value below that are space/tab delimited. Comments may be added to input file at any location in the file by placing ";;" before each comment line.

4.8.1 OPTIONS Section

The [OPTIONS] section allows a user to prescribe the global options associated with a simulation including start and end times, solution methods, solvers etc. They are specified by providing an attribute tag followed by its value. These attributes and their acceptable values are provided in Table 4.1.

Table 4.1 [Options] section attributes

Tag	Description	Required	Default Value
START_DATETIME	Starting date and time for the simulation specified using the format MM/DD/YYYY hh:mm:ss	Yes	N/A

END_DATETIME	End date and time for the simulation specified using the format MM/DD/YYYY hh:mm:ss	Yes	N/A
REPORT_INTERVAL	Numeric value specifying how often to report outputs in seconds	Yes	N/A
USE_ADAPTIVE_TIME_STEP	Specified as either YES/NO indicating whether to use an adaptive time stepping option	No	YES
MAX_TIME_STEP	The maximum timestep value in seconds that cannot be exceeded when using the adaptive time stepping option	No	0.5
MIN_TIME_STEP	The minimum timestep value in seconds that cannot be exceeded when using the adaptive time stepping option. This is the default timestep when the adaptive timestep option is turned off	No	0.001
TIME_STEP_RELAXATION_FACTOR	A value typically > 0.5 and < 1 that is multiplied with the computed adaptive timestep	No	0.8
NUM_INITIAL_FIXED_STEPS	It is sometime advisable to run the model at the smaller minimum timestep a few times at the beginning of a simulation before applying the adaptive timestep to give the model time to stabilize. This option specifies the number of times to perform the minimum time step at the begging of a simulation	No	2
ADVECTION_MODE	The advection discretization approach to use. Options include: UPWIND CENTRAL HYBRID TVD	No	UPWIND

TVD_FLUX_LIMITER	If the TVD advection mode is selected various flux limiters are available including: 0 – Min-Mod 1 – Superbee 2 – Van Leer 3 – MUSCL 4 – Sweby 5 – Van Albada 6 – QUICK 7 – UMIST	No	0
COMPUTE_DISPERSION	YES/NO indicating whether to compute dispersion using the Fischer formulation or user provided dispersion values	No	NO
SOLVER	ODE solver to use to solve the transport equations include: EULER RK4 RKQS ADAMS BDF	No	ADAMS
SOLVER_ABS_TOL	Temperature solver absolute tolerance	No	1e-8
SOLVER_REL_TOL	Temperature solver relative tolerance	No	1e-6
LINEAR_SOLVER	Linear Solver to use when using the function newton iteration method for BDF. Options include: 1 – GMRES 2 – FGMRES 3 – BI CGStab 4 – TFQMR 5 – PCG	No	1
WATER_DENSITY	Water density (kg/m^3)	No	1000
WATER_SPECIFIC_HEAT_CAPACITY	Water specific heat capacity (J/kg/C)	No	4184
NUM_SOLUTES	Number of conservative solutes to simulate	Yes	N/A
EVAPORATION	YES/NO to indicate whether to compute	No	NO

	evaporation and condensation.		
CONVECTION	YES/NO to indicate whether to compute convection and conduction	No	NO
WIND_FUNC_COEFF_A	Wind function coefficient A $(kPa^{-1}ms^{-1})$	No	1.505e-8
WIND_FUNC_COEFF_B	Wind function coefficient B (kPa)	No	1.600e-8
BOWENS_COEFF	Bowens Coefficient $\left(\frac{kPa}{°C}\right)$	No	0.061
PRESSURE_RATIO	Ration between atmospheric pressure and pressure at sea level	No	1.0
VERBOSE	YES/NO to indicate whether to print detailed data to the console during a simulation	No	No
PRINT_FREQ	Number of timesteps to skip before printing to console	No	10
FLUSH_TO_DISK_FREQ	Number of output timesteps to cache in memory before flushing to disk	No	10

An example snippet of the options section for the CSHComponent is provided below:

```
[OPTIONS]
START_DATETIME 01/01/2018 12:00:00
END_DATETIME   01/06/2018 00:00:00
REPORT_INTERVAL 600.0
MAX_TIME_STEP 30.0
MIN_TIME_STEP 0.005
NUM_INITIAL_FIXED_STEPS 100
USE_ADAPTIVE_TIME_STEP YES
TIME_STEP_RELAXATION_FACTOR 0.65
ADVECTION_MODE TVD
TVD_FLUX_LIMITER 0
COMPUTE_DISPERSION NO
TEMP_SOLVER ADAMS
TEMP_SOLVER_ABS_TOL 1e-10
TEMP_SOLVER_REL_TOL 1e-10
WATER_DENSITY 1000.0
WATER_SPECIFIC_HEAT_CAPACITY 4184
NUM_SOLUTES 1
VERBOSE YES
FLUSH_TO_DISK_FREQ 10
PRINT_FREQ 20
EVAPORATION NO
CONDENSATION YES
EVAP_WIND_FUNC_COEFF_A 1.505e-8
```

```
EVAP_WIND_FUNC_COEFF_B 1.600e-8
BOWENS_COEFF 0.061
```

4.8.2 OUTPUTS Section

The [OUTPUTS] section is used to specify the file path for the output NetCDF file. File paths may be specified relative to the model input file (.inp) as shown in the section below.

```
[OUTPUTS]
NETCDF ./outputs/outputfile.nc
```

4.8.3 SOLUTES Section

The [SOLUTES] section is used to specify attributes of the conservative solutes that are to be simulated. Table 4.2 provides details for this section.

Table 4.2 [SOLUTES] section attributes

Column	**Value**	**Required**	**Default Value**
SOLUTE_NAME	Name of solute. Cannot have spaces.	Yes	N/A
FIRST_ORDER_REACTION_RATE	Reaction rate (1/s)	Yes	N/A

An example of the [SOLUTES] section is provided below:

```
[SOLUTES]
;;SOLUTE_NAME  FIRST_ORDER_RATE
;;=============================
Tracer_1       0.0250
Tracer_2       0.0125
```

4.8.4 ELEMENTJUNCTIONS Section

The [ELEMENTJUNCTIONS] section is used to specify the coordinates of the downstream and upstream nodes of each computational element. Table 4.3. details how to specify the coordinates. While the coordinates are not used in computations, they must match the coordinates of computational elements of other components that are to be coupled to the CSHComponent so that correct spatial matching can be accomplished.

Table 4.3 [ELEMENTJUNCTIONS] section attributes

Column	Value	Required	Default Value
JUNCTION	Unique identifier for element junction	Yes	N/A
X	X coordinate (m). Must match coordinates of computational elements in other components to be coupled.	Yes	N/A
Y	Y coordinate (m). Must match coordinates of computational elements in other components to be coupled.	Yes	N/A
Z	Z coordinate (m)	Yes	N/A

An example snippet of the [ELEMENTJUNCTIONS] section is provided below:

```
[ELEMENTJUNCTIONS]
;;JUNCTION  X      Y   Z
;;===========================
J_0        0.000  0.0 100.0
J_1        100.0  0.0 99.95
J_2        200.0  0.0 99.90
J_3        300.0  0.0 99.85
J_4        400.0  0.0 99.80
```

4.8.5 ELEMENTS Section

The [ELEMENTS] section is used to provide attributes of the computational elements as illustrated in Table 4.4.

Table 4.4 [ELEMENTS] section attributes

Column	Value	Required	Default Value
ELEMENT	Unique identifier for element	Yes	N/A
FROM_J	Identifier for upstream element junction	Yes	N/A
TO_	Identifier for downstream element junction	Yes	N/A

LENGTH	Length of the computational element (m)	Yes	N/A
DEPTH	Flow depth (m). This value is overridden when time varying depth data is supplied from a hydraulic model that is coupled to the CSHComponent.	Yes	N/A
XSECTION_AREA	Flow cross section area (m^2). This value is overridden when time varying depth data is supplied from a hydraulic model that is coupled to the CSHComponent.	Yes	N/A
WIDTH	Flow width (m). This value is overridden when time varying depth data is supplied from a hydraulic model that is coupled to the CSHComponent.	Yes	N/A
SLOPE	Slope used for computing Fischer dispersion	Yes	N/A
FLOW	Flow (m^3/s). This value is overridden when time varying depth data is supplied from a hydraulic model that is coupled to the CSHComponent.	Yes	N/A
DISPERSION_COEFFICIENT	Dispersion coefficient (m/s^2). This value is overridden if the compute dispersion flag is turned on.	Yes	N/A
TEMPERATURE	Initial temperature of water in the computation element	Yes	N/A

Tracer_1	Initial concentration of first solute (kg/m^3)	Yes	N/A
Tracer_2	Initial concentration of second solute (kg/m^3). Specified as many times as needed.	Yes	N/A

A snippet of the [ELEMENTS] section is provided below:

```
[ELEMENTS]
;;ELEMENT FROMJ TOJ LENGTH DEPTH XSECTION_AREA WIDTH SLOPE FLOW DISPERSION_COEFF TEMPERATURE TRACER
;;==================================================================================================
L_1       J_0   J_1 100.00 1.00  0.00          80.00 0.00  0.00 0.00             25.00       100.00
L_2       J_1   J_2 100.00 1.00  0.00          80.00 0.00  0.00 0.00             25.00       100.00
L_3       J_2   J_3 100.00 1.00  0.00          80.00 0.00  0.00 0.00             25.00       100.00
L_4       J_3   J_4 100.00 1.00  0.00          80.00 0.00  0.00 0.00             25.00       100.00
L_5       J_4   J_5 100.00 1.00  0.00          80.00 0.00  0.00 0.00             25.00       100.00
```

4.8.6 TIMESERIES Section

The [TIMESERIES] section is used to provide time series file that are used to prescribe boundary condition and forcing data to the component. A snippet of a timeseries entry is shown below:

```
[TIMESERIES]
;;NAME                    FILE
;;=========================================================
peak_0.5m_temp           ./peak_0.5m_temp.csv
peak_1.0m_temp           ./peak_1.0m_temp.csv
```

Time series files are provided using comma-separated values files, where the first column is date and time and the remaining columns numeric values. Date time must be provided using the format MM/DD/YYYY hh:mm:ss.

4.8.7 BOUNDARY_CONDITIONS Section

The [BOUNDARY_CONDITIONS] section is used to prescribe boundary conditions at element junctions. Table 4.4 provides details about this section.

Table 4.4 [BOUNDARY_CONDITIONS] section attributes

Column	Value	Required	Default Value
JUNCTION	Identifier for junction where boundary conditions are to be applied	Yes	N/A
VARIABLE	TEMPERATURE or name of solute associated with the boundary condition	Yes	N/A
TYPE	VALUE/TIMESERIES indicating whether a constant value is to be applied or a timeseries	Yes	N/A
VALUE/TIMESERIES	Constant value or name of time series file to be applied	Yes	N/A

4.8.8 SOURCES Section

The sources section is used to prescribe solute and heat fluxes to computational elements. Table 4.5 provides details about this section.

Table 4.5 [SOURCES] section attributes

Column	Value	Required	Default Value
START_ELEMENT	Identifier for beginning element of the reach where the source it to be applied	Yes	N/A
START_ELEMENT_LFACTOR	The fraction of the length of the beginning element where source is to be applied	Yes	N/A
END_ELEMENT	Identifier for the end element of the reach where the source is to be applied	Yes	N/A
END_ELEMENT_LFACTOR	The fraction of the length of the end element where source is to be applied	Yes	N/A

VARIABLE	Options include HEAT FLOW Solute Identifier If HEAT is specified, the flux must be provided in J/s/m (i.e., energy per unit time per unit length of the reach) If FLOW is specified, a value of flow per unit length must be provided (m3/s/m). Heat and solute fluxes are removed or added to the element cell based on the element's temperature or solute concentration If the name of a Solute is provided, a value representing solute mass per unit time per unit length of the reach (kg/s/m).	Yes	N/A
TYPE	VALUE/TIMESERIES indicating whether a constant value is to be applied or a timeseries	Yes	N/A
VALUE/TIMESERIES	Constant value or name for time series file to be applied. If the number of columns in the time series matches the number of computational elements in the reach, each column is matched to an element. Otherwise, the first column is	Yes	N/A

	applied to all elements.		

4.8.9 HYDRAULICS Section

The hydraulic section is used to provide external constant or time varying hydraulic information to be used in the transport equations. Values provided in the section may be overridden using hydraulics supplied from another component. Details for this section are provided in Table 4.6.

Table 4.6 [HYDRAULICS] section attributes

Column	Value	Required	Default Value
START_ELEMENT	Identifier for beginning element of the reach where the hydraulic data it to be applied	Yes	N/A
END_ELEMENT	Identifier for the end element of the reach where the hydraulic data is to be applied	Yes	N/A
VARIABLE	Options include: DEPTH WIDTH XSECTION_AREA FLOW	Yes	N/A
TYPE	VALUE/TIMESERIES indicating whether a constant value is to be applied or a timeseries	Yes	N/A
VALUE/TIMESERIES	Constant value or name for time series file to be applied. In units of m for depth and width, m^2 for cross sectional area, and m^3/s for flow.	Yes	N/A

	If the number of columns in the time series matches the number of computational elements in the reach, each column is matched to an element. Otherwise, the first column is applied to all elements.		

A snippet of the [HYDRAULICS] section is provided below:

```
[HYDRAULICS]
;;START_ELEMENT    END_ELEMENT    VARIABLE    TYPE        VALUE/TIMESERIES
;;==========================================================================
L1                 L1             FLOW        VALUE       20.0
L2                 L100           DEPTH       TIMESERIES  flow_depth
```

4.8.10 RADIATIVE_FLUXES Section

The [RADIATIVE_FLUXES] section is used to provide external radiative heat fluxes to the model. Table 4.7 provides details for how this section is prescribed.

Table 4.7 [SOURCES] section attributes

Column	**Value**	**Required**	**Default Value**
START_ELEMENT	Identifier for beginning element of the reach where the radiation flux data it to be applied	Yes	N/A
END_ELEMENT	Identifier for the end element of the reach where the radiation flux is to be applied	Yes	N/A
TYPE	VALUE/TIMESERIES indicating whether a constant value is to be applied or a timeseries	Yes	N/A
VALUE/TIMESERIES	Constant value or name for time series	Yes	N/A

	file to be applied. Data must be provided in units of W/m^2. If the number of columns in the time series matches the number of computational elements in the reach, each column is matched to an element. Otherwise, the first column is applied to all elements.		

```
[RADIATIVE_FLUXES]
;;START_ELEMENT    END_ELEMENT    TYPE        VALUE/TIMESERIES
;;============================================================================
L1                 L1          VALUE       800.0
L2                 L100        TIMESERIES  attn_shortwave_radiation
```

4.8.11 METEOROLOGY Section

The [METEOROLOGY] section is used to provide the meteorology forcing data used to compute evaporation and convection. Table 4.8 provides details about how this section is prescribed.

Table 4.8 [METEOROLOGY] section attributes

Column	**Value**	**Required**	**Default Value**
START_ELEMENT	Identifier for beginning element of the reach where the met data it to be applied	Yes	N/A
END_ELEMENT	Identifier for the end element of the reach where the met data is to be applied	Yes	N/A
VARIABLE	Options include: RELATIVE_HUMIDITY AIR_TEMPERATURE	Yes	N/A

	WIND_SPEED.		
TYPE	VALUE/TIMESERIES indicating whether a constant value is to be applied or a timeseries	Yes	N/A
VALUE/TIMESERIES	Constant value or name for time series file to be applied. Values must be in units of % for relative humidity, °C for temperature, and m/s for wind speed. If the number of columns in the time series matches the number of computational elements in the reach, each column is matched to an element. Otherwise, the first column is applied to all elements.	Yes	N/A

5 Hyporheic Transient Storage Component (HTSComponent)

The HTSComponent was developed based on formulations presented within Neilson et al. (2010a and 2010b) which extend transient storage model formulations originally developed for solute transport (e.g., Bencala and Walters, 1983) to heat. Heat and solute exchange between the hyporheic transient storage zone and the river channel uses a first-order heat transfer relation for each computational element (Equation 5.1):

$$\rho_{sed} c_{p,sed} \frac{\mathrm{dT}_{HTS}}{\mathrm{dt}} V_{HTS} = \rho_{sed} c_{p,sed} \frac{\alpha_{sed} B_{HTS} \Delta x (T_{CSHComponent} - T_{HTS})}{Y_{HTS}} +$$

$$\rho_{sed} c_{p,sed} \frac{\alpha_{sed} B_{HTS} \Delta x (T_{gr} - T_{HTS})}{Y_{gr}} + \rho_w c_p Q_{HTS} (T_{STM} - T_{HTS}) + \sum SV_{STS} \quad (5.1)$$

where ρ_{sed} is the density of the sediment in the hyporheic transient storage (HTS) zone $\left(\frac{\mathrm{kg}}{\mathrm{m}^3}\right)$, $c_{p,sed}$ is the specific heat capacity of sediment in the HTS zone $\left(\frac{\mathrm{J}}{\mathrm{kg}°C}\right)$, T_{HTS} is the temperature of the HTS zone $(°C)$, V_{HTS} is the volume of the HTS zone (m^3), α_{sed} is the coefficient of thermal diffusivity for the sediment in the HTS computational element, B_{HTS} is the width of the HTS zone (m), Δx is the length of the HTS CV (m), $\mathrm{T}_{CSHComponent}$ is the temperature of water in the main channel overlying the HTS zone $(°\mathrm{C})$, Y_{HTS} and Y_{gr} represent the depths of the HTS and ground conducting zones, respectively (m), T_{gr} is the ground temperature $(°\mathrm{C})$, Q_{HTS} is the coefficient of advective transport $(\frac{m^3}{s})$, and S are heat fluxes supplied by other external sources $\left(\frac{\mathrm{J}}{\mathrm{m}^3\mathrm{s}}\right)$ (e.g., groundwater).

Equation 2 can be solved using various ordinary differential equation (ODE) solvers provided within the HTSComponent, including the classical fourth order Runge-Kutta method or the adaptive step size controlled fifth order Runge-Kutta-Cash-Carp (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 that are provided through the CVODE (Hindmarsh *et al.*, 2017) external ODE solver library.

5.1 HTSComponent Input File Format

As with the CSHComponent, the HTSComponent input file is also specified using the *.inp file format. The sections that must/can be prescribed are enumerated in the following sections.

5.1.1 OPTIONS Section

The [OPTIONS] section allows a user to prescribe the global options associated with a simulation including start and end times, solution methods, solvers etc. They are specified by providing an attribute tag followed by its value. These attributes and their acceptable values are provided in Table 5.1.

Table 5.1 [Options] section attributes

Tag	Description	Required	Default Value
START_DATETIME	Starting date and time for the simulation specified using the format MM/DD/YYYY hh:mm:ss	Yes	N/A
END_DATETIME	End date and time for the simulation specified using the format MM/DD/YYYY hh:mm:ss	Yes	N/A
REPORT_INTERVAL	Numeric value specifying how often to report outputs in seconds	Yes	N/A
USE_ADAPTIVE_TIME_STEP	Specified as either YES/NO indicating whether to use an adaptive time stepping option	No	YES
MAX_TIME_STEP	The maximum timestep value in seconds that cannot be exceeded when using the adaptive time stepping option	No	0.5
MIN_TIME_STEP	The minimum timestep value in seconds that cannot be exceeded when using the adaptive time stepping option. This is the default timestep when the adaptive timestep option is turned off	No	0.001
TIME_STEP_RELAXATION_FACTOR	A value typically > 0.5 and < 1 that is multiplied with the computed adaptive timestep	No	0.8
NUM_INITIAL_FIXED_STEPS	It is sometime advisable to run the model at the	No	2

	smaller minimum timestep a few times at the beginning of a simulation before applying the adaptive timestep to give the model time to stabilize. This option specifies the number of times to perform the minimum time step at the begging of a simulation		
TEMP_SOLVER	ODE solver to use to solve the transport equations include: EULER RK4 RKQS ADAMS BDF	No	ADAMS
TEMP_SOLVER_ABS_TOL	Temperature solver absolute tolerance	No	1e-8
TEMP_SOLVER_REL_TOL	Temperature solver relative tolerance	No	1e-6
WATER_DENSITY	Water density (kg/m^3)	No	1000
WATER_SPECIFIC_HEAT_CAPACITY	Water specific heat capacity (J/kg/C)	No	4184
NUM_SOLUTES	Number of conservative solutes to simulate	Yes	N/A
VERBOSE	YES/NO to indicate whether to print detailed data to the console during a simulation	No	No
PRINT_FREQ	Number of timesteps to skip before printing to console	No	10
FLUSH_TO_DISK_FREQ	Number of output timesteps to cache in memory before flushing to disk	No	10

An example snippet of the options section for the HTSComponent is provided below:

```
[OPTIONS]
START_DATETIME 01/01/2018 12:00:00
END_DATETIME   01/06/2018 00:00:00
REPORT_INTERVAL 600.0
MAX_TIME_STEP 30.0
MIN_TIME_STEP 0.005
NUM_INITIAL_FIXED_STEPS 100
USE_ADAPTIVE_TIME_STEP YES
```

```
TIME_STEP_RELAXATION_FACTOR 0.65
TEMP_SOLVER ADAMS
TEMP_SOLVER_ABS_TOL 1e-10
TEMP_SOLVER_REL_TOL 1e-10
WATER_DENSITY 1000.0
WATER_SPECIFIC_HEAT_CAPACITY 4184
NUM_SOLUTES 1
VERBOSE YES
FLUSH_TO_DISK_FREQ 10
PRINT_FREQ 20
```

5.1.2 OUTPUTS Section

The [OUTPUTS] section is used to specify the file path for the output NetCDF file. File paths may be specified relative to the model input file (.inp) as shown in the section below.

```
[OUTPUTS]
NETCDF ./outputs/outputfile.nc
```

5.1.3 SOLUTES Section

The [SOLUTES] section is used to specify attributes of the conservative solutes that are to be simulated. Table 452 provides details for this section.

Table 5.2 [SOLUTES] section attributes

Column	**Value**	**Required**	**Default Value**
SOLUTE_NAME	Name of solute. Cannot have spaces.	Yes	N/A
FIRST_ORDER_REACTION_RATE	Reaction rate (1/s)	Yes	N/A
SOLVER_TYPE	ODE Solver to use for solute transport. Options include: EULER RK4 RKQS ADAMS BDF	Yes	N/A
SOLVER_ABS_TOL	Solute solver absolute tolerance	Yes	N/A
SOLVER_REL_TOL	Solute solver relative tolerance	Yes	N/A

An example of the [SOLUTES] section is provided below:

```
[SOLUTES]
;;SOLUTE_NAME  FIRST_ORDER_RATE  SOLVER_TYPE  SOLVER_ABS_TOL  SOLVER_REL_TOL
;;===========================================================================
Tracer_1      0.0250            BDF          1e-10           1e-10
Tracer_2      0.0125            BDF          1e-10           1e-10
```

5.1.4 ELEMENTJUNCTIONS Section

The [ELEMENTJUNCTIONS] section is used to specify the coordinates of the downstream and upstream nodes of each computational element. Table 5.3. details how to specify the coordinates. While the coordinates are not used in computations, they must match the coordinates of computational elements of other components that are to be coupled to the CSHComponent so that correct spatial matching can be accomplished.

Table 4.3 [ELEMENTJUNCTIONS] section attributes

Column	Value	Required	Default Value
JUNCTION	Unique identifier for element junction	Yes	N/A
X	X coordinate (m). Must match coordinates of computational elements in other components to be coupled.	Yes	N/A
Y	Y coordinate (m). Must match coordinates of computational elements in other components to be coupled.	Yes	N/A
Z	Z coordinate (m)	Yes	N/A

An example snippet of the [ELEMENTJUNCTIONS] section is provided below:

```
[ELEMENTJUNCTIONS]
;;JUNCTION  X      Y   Z
;;=========================
J_0         0.000  0.0 100.0
J_1         100.0  0.0 99.95
J_2         200.0  0.0 99.90
J_3         300.0  0.0 99.85
```

```
J_4        400.0  0.0 99.80
```

5.1.5 ELEMENTS Section

The [ELEMENTS] section is used to provide attributes of the computational elements as illustrated in Table 5.4.

Table 4.4 [ELEMENTS] section attributes

Column	Value	Required	Default Value
ELEMENT	Unique identifier for element	Yes	N/A
FROM_J	Identifier for upstream element junction	Yes	N/A
TO_J	Identifier for downstream element junction	Yes	N/A
LENGTH	Length of the computational element (m)	Yes	N/A
DEPTH	Depth (m) of HTS Zone. This value is overridden when time varying depth data is supplied from a hydraulic model that is coupled to the CSHComponent.	Yes	N/A
TEMPERATURE	HTS zone temperature (°C)	Yes	N/A
ADVECTION_COEFFICIENT	Advection coefficient between main channel and HTS zone (m^3/s)	Yes	N/A
MC_TEMPERATURE	Main channel temperature (°C)	Yes	N/A
GROUND_DEPTH	Ground conduction zone depth (m)	Yes	N/A
GROUND_TEMP	Ground conduction zone temperature (°C)	Yes	N/A
SED_THERM_DIFF_COEFF	Sediment thermal diffusivity coefficient	Yes	N/A
Tracer_1	Concentration for first solute in HTS zone (kg/m^3)		

Main Channel Tracer_1	Main channel concentration for first solute (kg/m^3)	Yes	N/A
SOLUTE_DIFF_COEFF Tracer_1	Diffusivity coefficient for first solute (m^2/s). The last 3 columns must be repeat for each solute.	Yes	N/A

5.1.6 TIMESERIES Section

The [TIMESERIES] section is used to provide time series file that are used to prescribe boundary condition and forcing data to the component. A snippet of a timeseries entry is shown below:

```
[TIMESERIES]
;;NAME                    FILE
;;===========================================================
peak_0.5m_temp          ./peak_0.5m_temp.csv
peak_1.0m_temp          ./peak_1.0m_temp.csv
```

Time series files are provided using comma-separated values files, where the first column is date and time and the remaining columns numeric values. Date time must be provided using the format MM/DD/YYYY hh:mm:ss.

5.1.7 SOURCES Section

The sources section is used to prescribe solute and heat fluxes to computational elements. Table 5.5 provides details about this section.

Table 5.5 [SOURCES] section attributes

Column	**Value**	**Required**	**Default Value**
START_ELEMENT	Identifier for beginning element of the reach where the source it to be applied	Yes	N/A

START_ELEMENT_LFACTOR	The fraction of the length of the beginning element where source is to be applied	Yes	N/A
END_ELEMENT	Identifier for the end element of the reach where the source is to be applied	Yes	N/A
END_ELEMENT_LFACTOR	The fraction of the length of the end element where source is to be applied	Yes	N/A
VARIABLE	Options include HEAT FLOW Solute Identifier If HEAT is specified, the flux must be provided in J/s/m (i.e., energy per unit time per unit length of the reach) If FLOW is specified, a value of flow per unit length must be provided (m3/s/m). Heat and solute fluxes are removed or added to the element cell based on the element's temperature or solute concentration If the name of a Solute is provided, a value representing solute mass per unit time per unit length of the reach (kg/s/m).	Yes	N/A
TYPE	VALUE/TIMESERIES indicating whether a constant value is to	Yes	N/A

	be applied or a timeseries		
VALUE/TIMESERIES	Constant value or name for time series file to be applied. If the number of columns in the time series matches the number of computational elements in the reach, each column is matched to an element. Otherwise, the first column is applied to all elements.	Yes	N/A

5.1.8 HYDRAULICS Section

The hydraulic section is used to provide external constant or time varying hydraulic information to be used in the transport equations. Values provided in the section may be overridden using hydraulics supplied from another component. Details for this section are provided in Table 5.6.

Table 5.6 [HYDRAULICS] section attributes

Column	**Value**	**Required**	**Default Value**
START_ELEMENT	Identifier for beginning element of the reach where the hydraulic data it to be applied	Yes	N/A
END_ELEMENT	Identifier for the end element of the reach where the hydraulic data is to be applied	Yes	N/A
VARIABLE	Options include: DEPTH WIDTH MC_ADVECTION_COEFFICIENT	Yes	N/A

	GR_DEPTH		
TYPE	VALUE/TIMESERIES indicating whether a constant value is to be applied or a timeseries	Yes	N/A
VALUE/TIMESERIES	Constant value or name for time series file to be applied. In units of m for depth and width of HTS Zone, and depth of ground conduction zone, and m^3/s advection coefficient If the number of columns in the time series matches the number of computational elements in the reach, each column is matched to an element. Otherwise, the first column is applied to all elements.	Yes	N/A

5.1.9 RADIATIVE_FLUXES Section

The [RADIATIVE_FLUXES] section is used to provide external radiative heat fluxes to the model. Table 5.7 provides details for how this section is prescribed.

Table 5.7 [RADIATIVE_FLUXES] section attributes

Column	**Value**	**Required**	**Default Value**
START_ELEMENT	Identifier for beginning element of the reach where the radiation flux data it to be applied	Yes	N/A
END_ELEMENT	Identifier for the end element of the reach where the radiation flux is to be applied	Yes	N/A
TYPE	VALUE/TIMESERIES indicating whether a constant value is to be applied or a timeseries	Yes	N/A
VALUE/TIMESERIES	Constant value or name for time series file to be applied.	Yes	N/A

	Data must be provided in units of W/m^2. If the number of columns in the time series matches the number of computational elements in the reach, each column is matched to an element. Otherwise, the first column is applied to all elements.		

An example snippet of this section is shown below:

```
[RADIATIVE_FLUXES]
;;START_ELEMENT    END_ELEMENT    TYPE        VALUE/TIMESERIES
;;===========================================================================
L1                 L1            VALUE        800.0
L2                 L100          TIMESERIES   attn_shortwave_radiation
```

5.1.10 BOUNDARY_CONDITIONS

The [BOUNDARY_CONDITIONS] section is used to prescribe boundary conditions for the computational elements. Table 5.8 provides details about this section.

Table 5.8 [BOUNDARY_CONDITIONS] section attributes

Column	Value	Required	Default Value
START_ELEMENT	Identifier for beginning element of the reach where the boundary data it to be applied	Yes	N/A
END_ELEMENT	Identifier for the end element of the reach where the boundary data is to be applied	Yes	N/A
VARIABLE	Options include TEMPERATURE Solute Identifier	Yes	N/A

	If TEMPERATURE is specified, the flux must be provided in J/s (i.e., energy per unit time per unit length of the reach) If the name of a Solute is provided, a value representing solute mass per unit time per unit length of the reach (kg/s).		
SOURCE	MC or GR if the boundary is at the interface of the main channel or ground conduction zone	Yes	N/A
TYPE	VALUE/TIMESERIES indicating whether a constant value is to be applied or a timeseries	Yes	N/A
VALUE/TIMESERIES	Constant value or name for time series file to be applied. If the number of columns in the time series matches the number of computational elements in the reach, each column is matched to an element. Otherwise, the first column is applied to all elements.	Yes	N/A

6 Radiative Heat Exchange Component (RHEComponent)

Following Maidment (1993), Magnusson et al. (2012), and Glose et al. (2017), the net shortwave solar radiation on the water surface is estimated as follows:

$$J_{sn} = (1 - R_S)J_{in}(1.0 - f_s) \tag{6.1}$$

where R_S is albedo (the fraction of shortwave radiation that is reflected), J_{in} is the incoming shortwave radiation $\left(\frac{W}{m^2}\right)$, and f_s is the fraction of the solar radiation that is removed through shading. The long wave radiation calculations for back radiation (J_{br}) from the surface of the water, atmospheric (J_{an}), and land cover (J_{lc}) are calculated using modified forms of the Stefan-Boltzmann law (McCutcheon, 1990) as follows:

$$J_{br} = \varepsilon_w \sigma {T_w}^4 \tag{6.2}$$

$$J_{an} = \varepsilon_{atm} \sigma {T_a}^4 (1 - R_L) \tag{6.3}$$

$$J_{lc} = \varepsilon_{lc} (1 - f_{sky}) \sigma {T_a}^4 \tag{6.4}$$

where ε is the emissivity of the material under consideration (i.e., ε_w for emissivity of water, ε_{atm} for emissivity of the atmosphere, and ε_{lc} for emissivity of land cover), T_w and T_a are temperatures of the water in the river channel and of air respectively (K), σ is the Stefan-Boltzmann constant $\left(\frac{W}{m^2K^4}\right)$, and f_{sky} is the sky view factor. The emissivity of the atmosphere (ε_{atm}) used in computing the atmospheric long wave radiation is computed from Brunt (1932):

$$\varepsilon_{atm} = A_a + A_b\left(\sqrt{e_a}\right) \tag{6.5}$$

where A_a is an empirical coefficient with typical values between 0.5 and 0.7, A_b is an empirical coefficient with a typical value of 0.0027, and $e_a$is the vapor pressure of air (Pa).

The vapor pressure of air (e_a) used to compute atmospheric emissivity (ε_{atm}) used in estimating atmospheric longwave radiation (J_{an}) is computed using Equation 6.6 (Raudkivi, 1979; Chapra et al., 2008):

$$e_a = \frac{H}{100\%} e_s \tag{6.6}$$

where H is the relative humidity (%) and e_s is the saturation vapor pressure (Pa) computed using Equation 6.7:

$$e_s = 0.61275e^{\left(\frac{17.27T_a}{237.3+T_a}\right)} \quad (6.7)$$

where T_a is air temperature in $(°C)$.

6.1 RHEComponent Input Files

As with the CSHComponent, the RHEComponent input file is also specified using the *.inp file format. The sections that must/can be prescribed are enumerated in the following sections.

6.1.1 OPTIONS Section

The [OPTIONS] section allows a user to prescribe the global options associated with a simulation including start and end times, solution methods, solvers etc. They are specified by providing an attribute tag followed by its value. These attributes and their acceptable values are provided in Table 6.1.

Table 6.1 [Options] section attributes

Tag	Description	Required	Default Value
START_DATETIME	Starting date and time for the simulation specified using the format MM/DD/YYYY hh:mm:ss	Yes	N/A
END_DATETIME	End date and time for the simulation specified using the format MM/DD/YYYY hh:mm:ss	Yes	N/A
REPORT_INTERVAL	Numeric value specifying how often to report outputs in seconds	Yes	N/A
TIME_STEP	Timestep in seconds	No	0.5
ALBEDO	Albedo	No	0
WATER_EMISSIVITY	Emissivity of waver	No	0.97

ATM_EMISSIVITY_COEFF	Atmospheric emissivity calculation coefficient A.	No	0.5
ATM_LW_REFLECTION	Atmospheric longwave radiation reflection factor	No	0.03
STEFANBOLTZMANN_CONSTANT	Stefan-Boltzmann constant $\left(\frac{W}{m^2K^4}\right)$,	No	5.67e-8
EXTINCTION_COEFF	Solar radiation extinction coefficient	No	0.9675
VERBOSE	YES/NO to indicate whether to print detailed data to the console during a simulation	No	No
PRINT_FREQ	Number of timesteps to skip before printing to console	No	10
FLUSH_TO_DISK_FREQ	Number of output timesteps to cache in memory before flushing to disk	No	10

6.1.2 OUTPUTS Section

```
[OUTPUTS]
NETCDF ./outputs/outputfile.nc
```

6.1.3 ELEMENTJUNCTIONS Section

The [ELEMENTJUNCTIONS] section is used to specify the coordinates of the downstream and upstream nodes of each computational element. Table 6.2. details how to specify the coordinates. While the coordinates are not used in computations, they must match the coordinates of computational elements of other components that are to be coupled to the RHEComponent so that correct spatial matching can be accomplished.

Table 6.2 [ELEMENTJUNCTIONS] section attributes

Column	**Value**	**Required**	**Default Value**
JUNCTION	Unique identifier for element junction	Yes	N/A
X	X coordinate (m). Must match coordinates of computational elements in other	Yes	N/A

	components to be coupled.		
Y	Y coordinate (m). Must match coordinates of computational elements in other components to be coupled.	Yes	N/A
Z	Z coordinate (m)	Yes	N/A

6.1.4 *ELEMENTS Section*

The [ELEMENTS] section is used to provide attributes of the computational elements as illustrated in Table 6.3.

Table 6.3 [ELEMENTS] section attributes

Column	**Value**	**Required**	**Default Value**
ELEMENT	Unique identifier for element	Yes	N/A
FROM_J	Identifier for upstream element junction	Yes	N/A
TO_	Identifier for downstream element junction	Yes	N/A
LENGTH	Length of the computational element (m)	Yes	N/A
DEPTH	Flow depth (m). This value is overridden when time varying depth data is supplied from a hydraulic model that is coupled to the CSHComponent.	Yes	N/A
WIDTH	Channel flow with (m). This value is overridden when time varying depth data is supplied from a hydraulic model that is		

	coupled to the CSHComponent.		
TEMPERATURE	Temperature of water in channel (°C)	Yes	N/A
SHADE	Solar radiation shading factor (f_s)	Yes	N/A
SKYVIEW	Skyview factor (f_{sky})	Yes	N/A
LC_EMISS	Land cover emissivity	Yes	N/A

6.1.5 TIMESERIES Section

The [TIMESERIES] section is used to provide time series file that are used to prescribe boundary condition and forcing data to the component. A snippet of a timeseries entry is shown below:

```
[TIMESERIES]
;;NAME                 FILE
;;==========================================================
peak_0.5m_temp         ./peak_0.5m_temp.csv
peak_1.0m_temp         ./peak_1.0m_temp.csv
```

Time series files are provided using comma-separated values files, where the first column is date and time and the remaining columns numeric values. Date time must be provided using the format MM/DD/YYYY hh:mm:ss.

6.1.6 BOUNDARY_CONDITIONS Section

The [BOUNDARY_CONDITIONS] section is used to prescribe boundary conditions for the computational elements. Table 6.4 provides details about this section.

Table 6.4 [BOUNDARY_CONDITIONS] section attributes

Column	**Value**	**Required**	**Default Value**

START_ELEMENT	Identifier for beginning element of the reach where the boundary data it to be applied	Yes	N/A
END_ELEMENT	Identifier for the end element of the reach where the boundary data is to be applied	Yes	N/A
VARIABLE	TEMPERATURE .	Yes	N/A
TYPE	VALUE/TIMESERIES indicating whether a constant value is to be applied or a timeseries	Yes	N/A
VALUE/TIMESERIES	Constant value or name for time series file to be applied. If the number of columns in the time series matches the number of computational elements in the reach, each column is matched to an element. Otherwise, the first column is applied to all elements.	Yes	N/A

6.1.7 HYDRAULICS Section

The hydraulic section is used to provide external constant or time varying hydraulic information to be used in the transport equations. Values provided in the section may be overridden using hydraulics supplied from another component. Details for this section are provided in Table 6.5.

Table 6.5 [HYDRAULICS] section attributes

Column	**Value**	**Required**	**Default Value**

START_ELEMENT	Identifier for beginning element of the reach where the hydraulic data it to be applied	Yes	N/A
END_ELEMENT	Identifier for the end element of the reach where the hydraulic data is to be applied	Yes	N/A
VARIABLE	Options include: DEPTH WIDTH	Yes	N/A
TYPE	VALUE/TIMESERIES indicating whether a constant value is to be applied or a timeseries	Yes	N/A
VALUE/TIMESERIES	Constant value or name for time series file to be applied. In units of m for depth and width of water in the channel. If the number of columns in the time series matches the number of computational elements in the reach, each column is matched to an element. Otherwise, the first column is applied to all elements.	Yes	N/A

6.1.8 RADIATIVE_FLUXES Section

The [RADIATIVE_FLUXES] section is used to provide external radiative heat fluxes to the model. Table 6.6 provides details for how this section is prescribed.

Table 6.6 [RADIATIVE_FLUXES] section attributes

Column	Value	Required	Default Value
START_ELEMENT	Identifier for beginning element of the reach where the radiation flux data it to be applied	Yes	N/A
END_ELEMENT	Identifier for the end element of the reach where the radiation flux is to be applied	Yes	N/A
TYPE	VALUE/TIMESERIES indicating whether a constant value is to be applied or a timeseries	Yes	N/A
VALUE/TIMESERIES	Constant value or name for time series file to be applied. Data must be provided in units of W/m^2. If the number of columns in the time series matches the number of computational elements in the reach, each column is matched to an element. Otherwise, the first column is applied to all elements.	Yes	N/A

An example snippet of this section is shown below:

```
[RADIATIVE_FLUXES]
;;START_ELEMENT    END_ELEMENT    TYPE        VALUE/TIMESERIES
;;==========================================================================
L1                L1          VALUE       800.0
L2                L100        TIMESERIES  attn_shortwave_radiation
```

6.1.9 METEOROLOGY Section

The [METEOROLOGY] section is used to provide the meteorology forcing data used to compute evaporation and convection. Table 6.7 provides details about how this section is prescribed.

Table 6.7 [METEOROLOGY] section attributes

Column	Value	Required	Default Value
START_ELEMENT	Identifier for beginning element of the reach where the met data it to be applied	Yes	N/A
END_ELEMENT	Identifier for the end element of the reach where the met data is to be applied	Yes	N/A
VARIABLE	Options include: RELATIVE_HUMIDITY AIR_TEMPERATURE	Yes	N/A
TYPE	VALUE/TIMESERIES indicating whether a constant value is to be applied or a timeseries	Yes	N/A
VALUE/TIMESERIES	Constant value or name for time series file to be applied. Values must be in units of % for relative humidity, °C for temperature. If the number of columns in the time series matches the number of computational elements in the reach, each column is matched to an element. Otherwise, the first column is	Yes	N/A

	applied to all elements.		

7 Groundwater Model Component (GWComponent)

This document describes the groundwater model GWComponent, developed to simulate mass, heat, and solute fluxes exchanged between a river channel and its adjacent shallow groundwater zone. The GWComponent solves the vertically-averaged unconfined saturated groundwater flow equations and the heat and solute transport equations using the semi-discrete finite volume approximation. The underlying assumption we make is that the principal directions of flow are perpendicular to the channel (i.e., lateral) and along the channel (i.e., longitudinal) as depicted in Figure 7.1. The GWComponent was developed to be primarily used and coupled with other components within the HydroCouple component-based modeling framework (Buahin and Horsburgh, 2016; Buahin and Horsburgh, 2018). However, it can be compiled and used as a standalone executable.

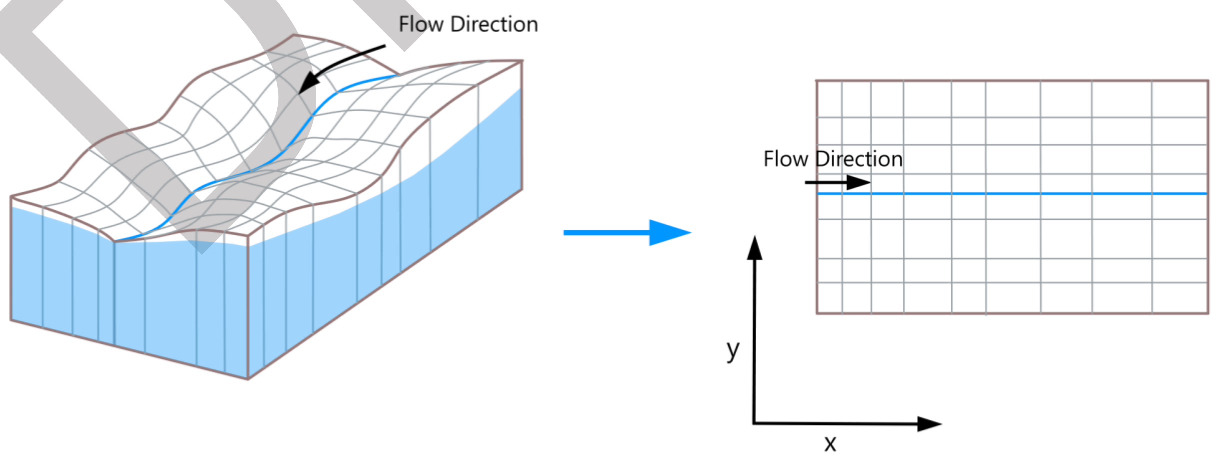

Figure 7.1. GWComponent spatial domain simplification schematic

7.1 Flow Formulations

The vertically-averaged unconfined saturated groundwater flow equations solved by the GWComponent is shown in equation 1:

$$\frac{\partial}{\partial x}\left(K_x b \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y b \frac{\partial h}{\partial y}\right) + bQ = S_O \frac{\partial h}{\partial t} \quad (1)$$

where x and y are distances in the longitudinal and lateral directions respectively (m), K_x and K_y and hydraulic conductivity values in the longitudinal and lateral directions respectively $\left(\frac{m}{s}\right)$, h is the hydraulic head (m), b is the saturated thickness of the aquifer (m), Q represent external water fluxes $\left(\frac{m^3}{s \cdot m^3}\right)$, S_O is the storage coefficient (i.e., specific yield for an unconfined aquifer) $\left(\frac{m}{m}\right)$, and t is time (s).

Applying the finite volume approximation over the control volume $CV_{i,j}$ in the model domain shown in Figure 2 over a time step Δt (s), yields equation 2.

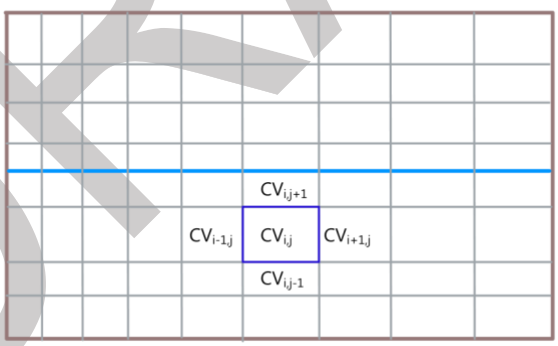

Figure 2. Control volume schematic

$$\int_{\Delta t}\int_{CV}\left[\frac{\partial}{\partial x}\left(K_x b \frac{\partial h}{\partial x}\right)\right] dV dt + \int_{\Delta t}\int_{CV}\left[\frac{\partial}{\partial y}\left(K_y b \frac{\partial h}{\partial y}\right)\right] dV dt + \int_{\Delta t}\int_{CV}(bQ) dV dt =$$

$$\int_{\Delta t}\left[\int_{CV}\left(S_O \frac{\partial h}{\partial t}\right) dV\right] dt \quad (2)$$

where V is the volume of the control volume CV (m^3). Using the explicit time marching method and applying the Gauss divergence theorem to equation 2 yields equation 3.

$$\sum_{k=1}^{NBx}\left(K_x b \frac{\partial h}{\partial x}\right) A_{NBx} + \sum_{k=1}^{NBy}\left(K_y b \frac{\partial h}{\partial y}\right) A_{NBy} + bQV = S_O\left(\frac{h^{t+\Delta t}-h^t}{\Delta t} V + \frac{V^{t+\Delta t}-V^t}{\Delta t} h\right) \tag{3}$$

where $\sum_{k=1}^{NBx}$ $and \sum_{k=1}^{NBy}$ represent the summation of their respective terms in the x and y directions respectively at the boundaries of the control volume, A_{NBx} and A_{NBy} represent the cross sectional area of flow in the x and y directions at the boundaries of the control volume respectively (m^2), and superscripts t and t+Δt represent the current and next time step a solution is being sought (s). The first two terms on the right-hand side of equation 3 are approximated numerically as follows for the control volume boundaries:

$$\sum_{k=1}^{NBx}\left(K_x b \frac{\partial h}{\partial x}\right) A_{NBx} = K_{i+\frac{1}{2},j} b\left(\frac{h_{i+1,j}-h_{i,j}}{\frac{\Delta x_{i+1,j}}{2}+\frac{\Delta x_{i,j}}{2}}\right) b\Delta y - K_{i-\frac{1}{2},j} b\left(\frac{h_{i,j}-h_{i-1,j}}{\frac{\Delta x_{i,j}}{2}+\frac{\Delta x_{i-1,j}}{2}}\right) b\Delta y \tag{4}$$

$$\sum_{k=1}^{NBy}\left(K_y b \frac{\partial h}{\partial y}\right) A_{NBy} = K_{i,j+\frac{1}{2}} b\left(\frac{h_{i,j+1}-h_{i,j}}{\frac{\Delta y_{i,j+1}}{2}+\frac{\Delta y_{i,j}}{2}}\right) b\Delta x - K_{i,j-\frac{1}{2}} b\left(\frac{h_{i,j}-h_{i,j-1}}{\frac{\Delta y_{i,j}}{2}+\frac{\Delta y_{i,j-1}}{2}}\right) b\Delta x \tag{5}$$

where the subscripts i and j represent the current control volume, the subscripts $i-1$, $i+1$, $j-1$, and $j+1$ represent neighboring control volumes on the left, right, south, and north of the current control volume respectively, and the subscripts $i-\frac{1}{2}$, $i+\frac{1}{2}$, $j-\frac{1}{2}$, $j+\frac{1}{2}$ represent boundaries of the control volume on the left, right, south, and north sides respectively, and Δx and Δy represent the sizes of the control volumes in the x and y directions respectively (m).

The effective hydraulic conductivity values at the boundary between any two cells that are used in equations 4 and 5 are calculated based on formulations by Leonards (1962) and are shown as follows:

$$K_{i+\frac{1}{2},j}=\left(\frac{\frac{\Delta x_{i,j}}{2}+\frac{\Delta x_{i+1,j}}{2}}{\frac{\frac{\Delta x_{i,j}}{2}}{K_{i,j}}+\frac{\frac{\Delta x_{i+1,j}}{2}}{K_{i+1,j}}}\right) \tag{6}$$

$$K_{i-\frac{1}{2},j}=\left(\frac{\frac{\Delta x_{i,j}}{2}+\frac{\Delta x_{i-1,j}}{2}}{\frac{\frac{\Delta x_{i,j}}{2}}{K_{i,j}}+\frac{\frac{\Delta x_{i-1,j}}{2}}{K_{i-1,j}}}\right) \tag{7}$$

$$K_{i,j+1}=\left(\frac{\frac{\Delta y_{i,j}}{2}+\frac{\Delta y_{i,j+1}}{2}}{\frac{\frac{\Delta y_{i,j}}{2}}{K_{i,j}}+\frac{\frac{\Delta y_{i,j+1}}{2}}{K_{i,j+1}}}\right) \tag{8}$$

$$K_{i,j+1}=\left(\frac{\frac{\Delta y_{i,j}}{2}+\frac{\Delta y_{i,j+1}}{2}}{\frac{\frac{\Delta y_{i,j}}{2}}{K_{i,j}}+\frac{\frac{\Delta y_{i,j+1}}{2}}{K_{i,j+1}}}\right) \tag{9}$$

7.1.1 Flow Exchanges with Channel

The mass exchanges between the aquifer and the channel is computed using formulations used in the River package of the U.S. Geological Survey Modular Ground-Water Model (MODFLOW), which assumes a partially penetrating river with a semi confining bed layer (Harbaugh, 2005). Flow into and out of the aquifer is computed as a function of the relative differences in hydraulic heads in the underlying groundwater cell and the channel as well as the elevation of the channel bottom. The three configurations for flux exchanges are depicted in Figure 3.

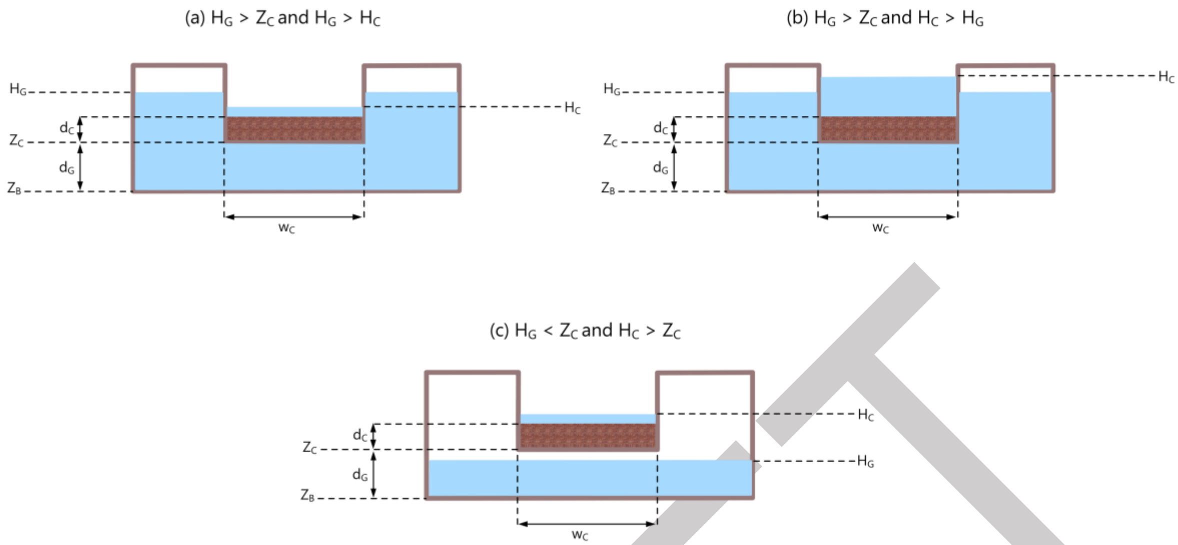

Figure 3. Groundwater-surface water exchange configurations

For configurations a and b, where the hydraulic head (H_G) in the underlying cell is greater than channel bottom elevation, the flow into/out of the aquifer is computed as follows:

$$Q_C = K_{eff}\left(\frac{H_C - H_G}{\frac{d_C}{2}+\frac{d_G}{2}}\right) w_c \Delta x \tag{10}$$

where K_{eff} is the effective hydraulic conductivity in the z direction $\left(\frac{m}{s}\right)$, H_C is the hydraulic head in the channel (m), d_C is the thickness of the semi-confining bed layer (m), d_G is the saturated thickness of the aquifer (m), and w_C is the width of the channel (m). K_{eff} is calculated in a similar fashion to the boundary hydraulic conductivities as follows:

$$K_{eff} = \frac{\frac{d_C}{2}+\frac{d_G}{2}}{\frac{\frac{d_C}{2}}{K_C}+\frac{\frac{d_G}{2}}{K_Z}} \tag{11}$$

where K_C is the hydraulic conductivity of the semi-confining bed layer in the z direction $\left(\frac{m}{s}\right)$ and K_Z is the hydraulic conductivity of the underlying groundwater cell in the z direction $\left(\frac{m}{s}\right)$.

For scenario c, the flow out of the channel into the aquifer is computed using the following equation:

$$Q_C = K_C\left(\frac{H_C - Z_C}{\frac{d_C}{2}}\right)w_c\Delta x \tag{12}$$

where Z_C is the elevation of the channel bed (m).

7.2 Heat Transport Formulations

The two-dimensional advection, dispersion, and conduction groundwater heat transport equations (de Marsily, 1986; Domenico and Schwartz, 1998) that the GWComponent solves is shown in equation 13:

$$n\rho_w c_w \frac{\partial T_w}{\partial t} + (1-n)\rho_s c_s \frac{\partial T_s}{\partial t} = \nabla \cdot [\,(\lambda_m + n\rho_w c_w \alpha v)\nabla T] - \nabla \cdot (n\rho_w c_w v T) + q_h \tag{13}$$

where n is the porosity, ρ_w and ρ_s are water and sediment density respectively $\left(\frac{kg}{m^3}\right)$, c_w and c_s are specific heat capacity of water and sediment respectively $\left(\frac{J}{kg°C}\right)$, T_w and T_s are temperatures of the water and sediment respectively $(°C)$, T is the temperature of both water and sediment $(°C)$, λ_m is effective thermal conductivity of the sediment and water $\left(\frac{W}{m°C}\right)$, α is the dispersivity(m), v is seepage velocity $\left(\frac{m}{s}\right)$, and q_h is the sum of external heat sources $\left(\frac{W}{m^3}\right)$.

A valid assumption to make for many cases is that the temperature of the sediment and water are the same and that there is no transfer of heat from one to the other (Hecht-

Méndez *et al.*, 2010; Nield and Bejan, 2013). Under this assumption, equation 13 can be expressed in the following form:

$$\rho_m c_m \frac{\partial T}{\partial t} = \overbrace{\nabla \cdot [\,(\lambda_m + n\rho_w c_w \alpha v)\nabla T]}^{Conduction\ and\ Dispersion} - \overbrace{\nabla \cdot (n\rho_w c_w v T)}^{Advection} + q_h \quad (14)$$

where $\rho_m c_m$ is the heat capacity per unit volume of the combined sediment and water medium $\left(\frac{J}{m^{3\circ}C}\right)$. $\rho_m c_m$ is computed as the weighted average of the sediment and pore water (Domenico and Schwartz, 1998; Hecht-Méndez *et al.*, 2010) as shown in equation 15. λ_m is calculated in a similar manner as shown in equation 16.

$$\rho_m c_m = n\rho_w c_w + (1-n)\rho_s c_s \quad (15)$$

$$\lambda_m = n\lambda_w + (1-n)\lambda_s \quad (16)$$

where λ_w and λ_s thermal conductivity of the water and sediment respectively $\left(\frac{W}{m^{\circ}C}\right)$.

The finite volume approximation of equation 14 is shown in equation 17. Adopting the explicit time marching approach yields equation 18.

$$\int_{\Delta t}\int_{CV} \rho_m c_m \frac{\partial T}{\partial t}\, dV dt = \int_{\Delta t}\int_{CV} \nabla \cdot [\,(\lambda_m + n\rho_w c_w \alpha v)\nabla T] dV dt - \int_{\Delta t}\int_{CV} \nabla \cdot (n\rho_w c_w v T)\, dV dt + \int_{\Delta t}\int_{CV} q_h\, dV dt \quad (17)$$

$$\rho_m c_m \left(\frac{T^{t+\Delta t} - T^t}{\Delta t} V + T \frac{V^{t+\Delta t} - V^t}{\Delta t}\right) = \int_{CV} \nabla \cdot [\,(\lambda_m + n\rho_w c_w \alpha v)\nabla T] dV - \int_{CV} \nabla \cdot (n\rho_w c_w v T)\, dV + \int_{CV} q_h\, dV \quad (18)$$

7.2.1 Heat Conduction and Dispersion

Applying the Gauss divergence theorem, the heat conduction and dispersion terms are discretized numerically for the control volume CV as follows:

$$\int_{CV} \nabla \cdot [\,(\lambda_m + n\rho_w c_w \alpha v)\nabla T]dV = \; (\lambda_m + n\rho_w c_w \alpha v)_{i+\frac{1}{2},j} \left(\frac{T_{i+1,j} - T_{i,j}}{\frac{\Delta x_{i+1,j}}{2} + \frac{\Delta x_{i,j}}{2}} \right) b\Delta y - (\lambda_m + n\rho_w c_w \alpha v)_{i-\frac{1}{2},j} \left(\frac{T_{i,j} - T_{i-1,j}}{\frac{\Delta x_{i,j}}{2} + \frac{\Delta x_{i-1,j}}{2}} \right) b\Delta y + (\lambda_m + n\rho_w c_w \alpha v)_{i,j+\frac{1}{2}} \left(\frac{T_{i,j+1} - T_{i,j}}{\frac{\Delta y_{i,j+1}}{2} + \frac{\Delta y_{i,j}}{2}} \right) b\Delta x - (\lambda_m + n\rho_w c_w \alpha v)_{i,j-\frac{1}{2}} \left(\frac{T_{i,j} - T_{i,j-1}}{\frac{\Delta y_{i,j}}{2} + \frac{\Delta y_{i-1,j}}{2}} \right) b\Delta x \tag{19}$$

7.2.2 Heat Advection

Again, the divergence theorem is applied to numerically discretize the heat advection term as follows:

$$-\int_{CV} \nabla \cdot (n\rho_w c_w v T)\, dV = -\sum_{k=1}^{NBx} \left(\rho_w c_w K_x \frac{\partial h}{\partial x} \right) T A_{NBx} - \sum_{k=1}^{NBy} \left(\rho_w c_w K_y \frac{\partial h}{\partial y} \right) T A_{NBy} \tag{20}$$

The heat advection terms may be discretized using any number of advective schemes provided in the GWComponent including the upwind, central, and hybrid differencing schemes. Many Total Variation Diminishing (TVD) schemes are also available for applications width sharp discontinuities in their solutions. Here, we only describe the upwind scheme. The upwind advective terms in the x and y direction are shown in equations 21 and 22 below:

$$-\sum_{k=1}^{NBx} \left(\rho_w c_w K_x \frac{\partial h}{\partial x} \right) T A_{NBx} = \left(\rho_w c_w K_x \frac{\partial h}{\partial x} \right)_{i-\frac{1}{2},j} T_{i-1,j} b\Delta y - \left(\rho_w c_w K_x \frac{\partial h}{\partial x} \right)_{i+\frac{1}{2},j} T_{i,j} b\Delta y \tag{21}$$

$$-\sum_{k=1}^{NBy} \left(\rho_w c_w K_y \frac{\partial h}{\partial y} \right) T A_{NBy} = \left(\rho_w c_w K_y \frac{\partial h}{\partial y} \right)_{i,j-\frac{1}{2}} T_{i,j-1} b\Delta x - \left(\rho_w c_w K_y \frac{\partial h}{\partial y} \right)_{i,j+\frac{1}{2}} T_{i,j} b\Delta x \tag{22}$$

7.2.3 Heat Exchanges with Channel

Heat fluxes exchanged between the channel and the shallow water zone are calculated as follows:

$$q_C = \rho_w c_w Q_C T_C \qquad for\ Q_C > 0 \tag{23}$$

$$q_C = \rho_w c_w Q_C T_G \qquad for\ Q_C < 0 \tag{24}$$

where T_C and T_G are the temperatures in the channel and the underlying groundwater cell respectively $(°C)$.

7.3 Solute Transport Formulations

The modified form of the groundwater solute transport equations (Domenico and Schwartz, 1998; Hecht-Méndez *et al.*, 2010) that the GWComponent solves is shown in equation 25:

$$R_f \frac{\partial C}{\partial t} = \nabla \cdot [\ (D_m + \alpha v)\nabla C] - \nabla \cdot (vC) + S_c - \lambda_1 C \tag{25}$$

where R_f is the retardation factor (a dimensionless value denoting the ratio between the total solute concentration and the mobile solution concentration given by the distribution of the contaminant in the fluid and solid phases), C is the concentration of the solute $\left(\frac{kg}{m^3}\right)$, D_m is the molecular diffusion coefficient $\left(\frac{m^2}{s}\right)$, S_c is the sum of external solute fluxes $\left(\frac{kg}{m^3 s}\right)$, and λ_1 is the first order reaction coefficient. The retardation factor R_f is computed using equation 26 (Domenico and Schwartz, 1998; Hecht-Méndez *et al.*, 2010):

$$R_f = 1 + \left(\frac{1-n}{n}\right)\rho_s K_d \tag{26}$$

where K_d is the distribution coefficient $\left(\frac{m^3}{kg}\right)$.

The integral version of equation 25 is shown in equation 26. This equation expands to equation 27 when the explicit time marching scheme is adopted.

$$\int_{\Delta t}\int_{CV} R_f \frac{\partial C}{\partial t} dVdt = \int_{\Delta t}\int_{CV} \nabla \cdot [\ (D_m + \alpha v)\nabla C]\, dVdt - \int_{\Delta t}\int_{CV} \nabla \cdot (vC) dVdt + \int_{\Delta t}\int_{CV} S_c dVdt - \int_{\Delta t}\int_{CV} \lambda_1 C dVdt \tag{26}$$

$$R_f\left(\frac{C^{t+\Delta t}-C^t}{\Delta t}V+\frac{V^{t+\Delta t}-V^t}{\Delta t}C\right)=\overbrace{\int_{CV}\nabla\cdot[\,(D_m+\alpha v)\nabla C]\,dV}^{Dispersion}-\overbrace{\int_{CV}\nabla\cdot(vC)dV}^{Advection}+S_cV-\lambda_1 CV \quad (27)$$

7.3.1 Solute Dispersion

The dispersion term in equation 27 is discretized in a similar fashion to the heat conduction & dispersion terms as follows:

$$\int_{CV}\nabla\cdot[\,(D_m+\alpha v)\nabla C]\,dV = (D_m+\alpha v)_{i+\frac{1}{2},j}\left(\frac{C_{i+1,j}-C_{i,j}}{\frac{\Delta x_{i+1,j}}{2}+\frac{\Delta x_{i,j}}{2}}\right)b\Delta y-(D_m+\alpha v)_{i-\frac{1}{2},j}\left(\frac{C_{i,j}-C_{i-1,j}}{\frac{\Delta x_{i,j}}{2}+\frac{\Delta x_{i-1,j}}{2}}\right)b\Delta y+(D_m+\alpha v)_{i,j+\frac{1}{2}}\left(\frac{C_{i,j+1}-C_{i,j}}{\frac{\Delta y_{i,j+1}}{2}+\frac{\Delta y_{i,j}}{2}}\right)b\Delta x-(D_m+\alpha v)_{i,j-\frac{1}{2}}\left(\frac{C_{i,j}-C_{i,j-1}}{\frac{\Delta y_{i,j}}{2}+\frac{\Delta y_{i-1,j}}{2}}\right)b\Delta x \quad (28)$$

7.3.2 Solute Advection

The solute advection term is discretized as follows by applying the divergence theorem:

$$-\int_{CV}\nabla\cdot(vC)dV=-\sum_{k=1}^{NBx}\left(K_x\frac{\partial h}{\partial x}\right)CA_{NBx}-\sum_{k=1}^{NBy}\left(K_y\frac{\partial h}{\partial y}\right)CA_{NBy} \quad (29)$$

Like the heat advection terms, the solute advection terms may be discretized using the upwind, the central, hybrid differencing schemes, or various TVD schemes. Here, we only describe the upwind scheme. The upwind advective terms in the x and y direction are shown in equations 30 and 31 below:

$$-\sum_{k=1}^{NBx}\left(K_x\frac{\partial h}{\partial x}\right)CA_{NBx}=\left(K_x\frac{\partial h}{\partial x}\right)_{i-\frac{1}{2},j}C_{i-1,j}b\Delta y-\left(K_x\frac{\partial h}{\partial x}\right)_{i+\frac{1}{2},j}C_{i,j}b\Delta y \quad (30)$$

$$-\sum_{k=1}^{NBy}\left(K_y\frac{\partial h}{\partial y}\right)CA_{NBy}=\left(K_y\frac{\partial h}{\partial y}\right)_{i,j-\frac{1}{2}}C_{i,j-1}b\Delta x-\left(K_y\frac{\partial h}{\partial y}\right)_{i,j+\frac{1}{2}}C_{i,j}b\Delta x \quad (31)$$

7.3.3 GWComponent Solvers

The GWComponent solves all the discretized equations using one of 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 (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.

7.4 GWComponent Validation

To verify that the model's predictions had an acceptable level of accuracy, we embarked on numerical experiments that compared results from the model with analytical solutions.

7.5 Flow Validation

To test the mass transport component of the GWComponent, we applied the analytical solution provided by (Singh, 2004) that predicts a semi-infinite aquifer's hydraulic head response to a sinusoidal stream stage excitation. For our application, we assumed no stream bed resistance. The Singh (2004) formulation for aquifer response for this configuration is shown below:

$$h(y,t) = Ae^{\left(-y\sqrt{\frac{\omega}{2\beta}}\right)} \sin\left(-y\sqrt{\frac{\omega}{2\beta}} + \omega t + \phi\right) \tag{32}$$

where h is the hydraulic head (m), y is the lateral distance away from the stream (m), t time (s), amplitude of the sinusoidal flood wave (m), ω angular frequency of sinusoidal flood wave (s^{-1}), β is hydraulic diffusivity of aquifer computed using equation 33 $\left(\frac{m^2}{s}\right)$, and ϕ is the dimensionless phase shift of the wave.

$$\beta = \frac{bK}{S} \tag{33}$$

For our test problem, we applied a sinusoidal wave with an amplitude of 1m to the channel depicted in Figure 4. Other parameters used in the model are shown in Table 1. The numerical model was executed twice, first using to mesh sizes of 1.0 m and the a mesh size of 0.5 m.

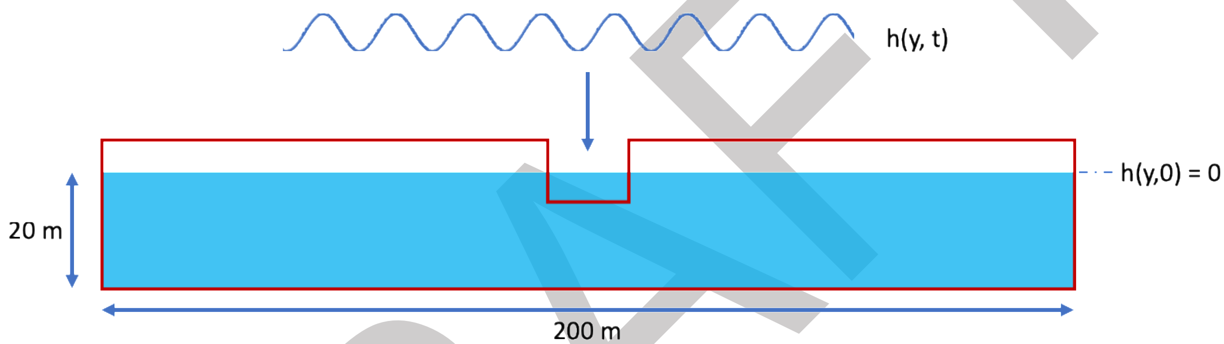

Figure 4. Aquifer Schematic

Table 1. Aquifer and sinusoidal wave parameters

Parameter	Value	Units
Amplitude (A) =	1	m
Angular Frequency (ω) =	0.00018981	s^{-1}
Phase Shift (ε) =	0	
Storage Coefficient (S) =	0.3	
Hydraulic Conductivity (K) =	0.0001	m/s
Hydraulic Diffusivity (β) =	0.00667	m^2/s
Bedrock Elevation =	-20	m

Results from the numerical model compared well with analytical solutions as shown Figures 5 and 6 for mesh sizes 1.0 m and 0.5 m respectively. The worst mean absolute error of 0.004m was observed at 0.75 meters from the channel. As one would expect, the high resolution 0.5 m mesh resulted in lower errors as shown in Table 2.

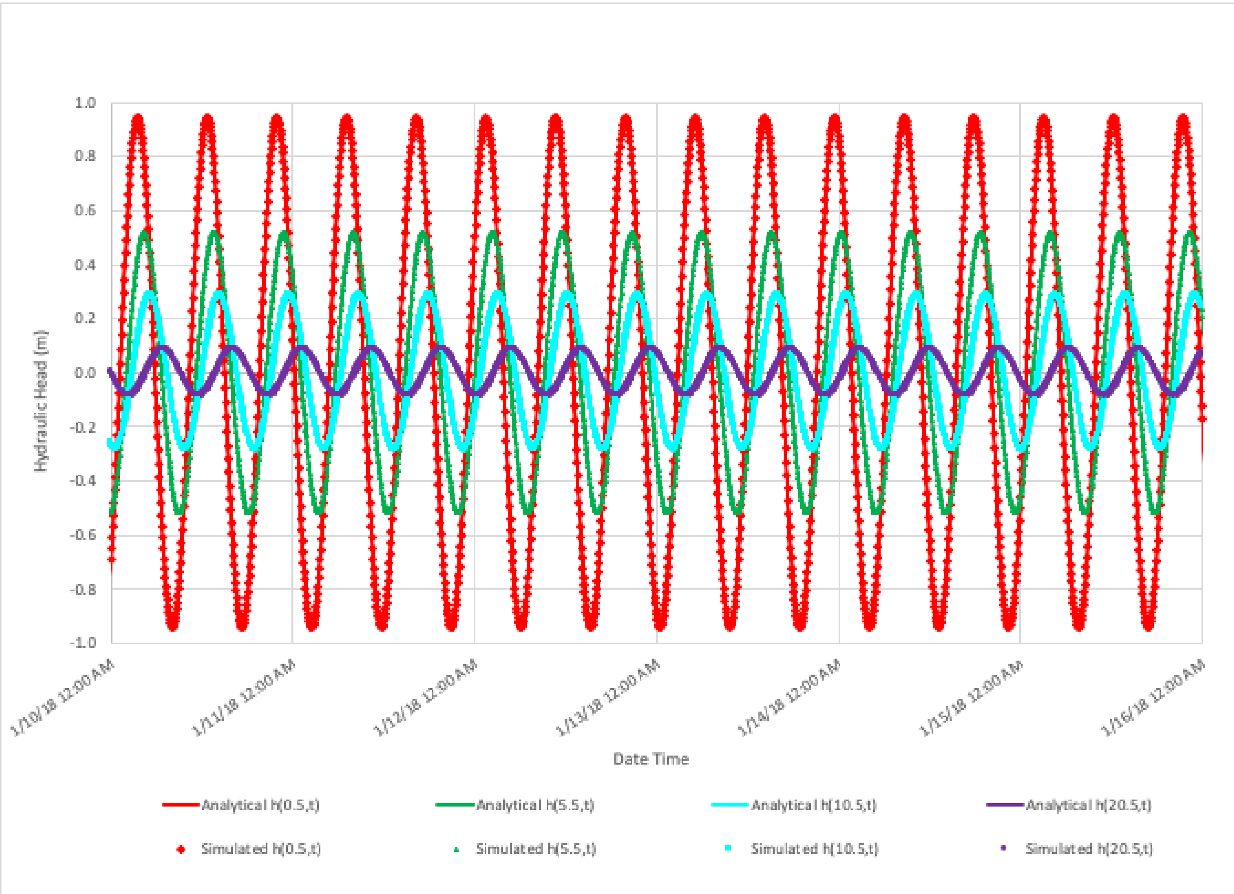

Figure 5. Simulated vs. analytical hydraulic head solution for 1.0 m cell resolution

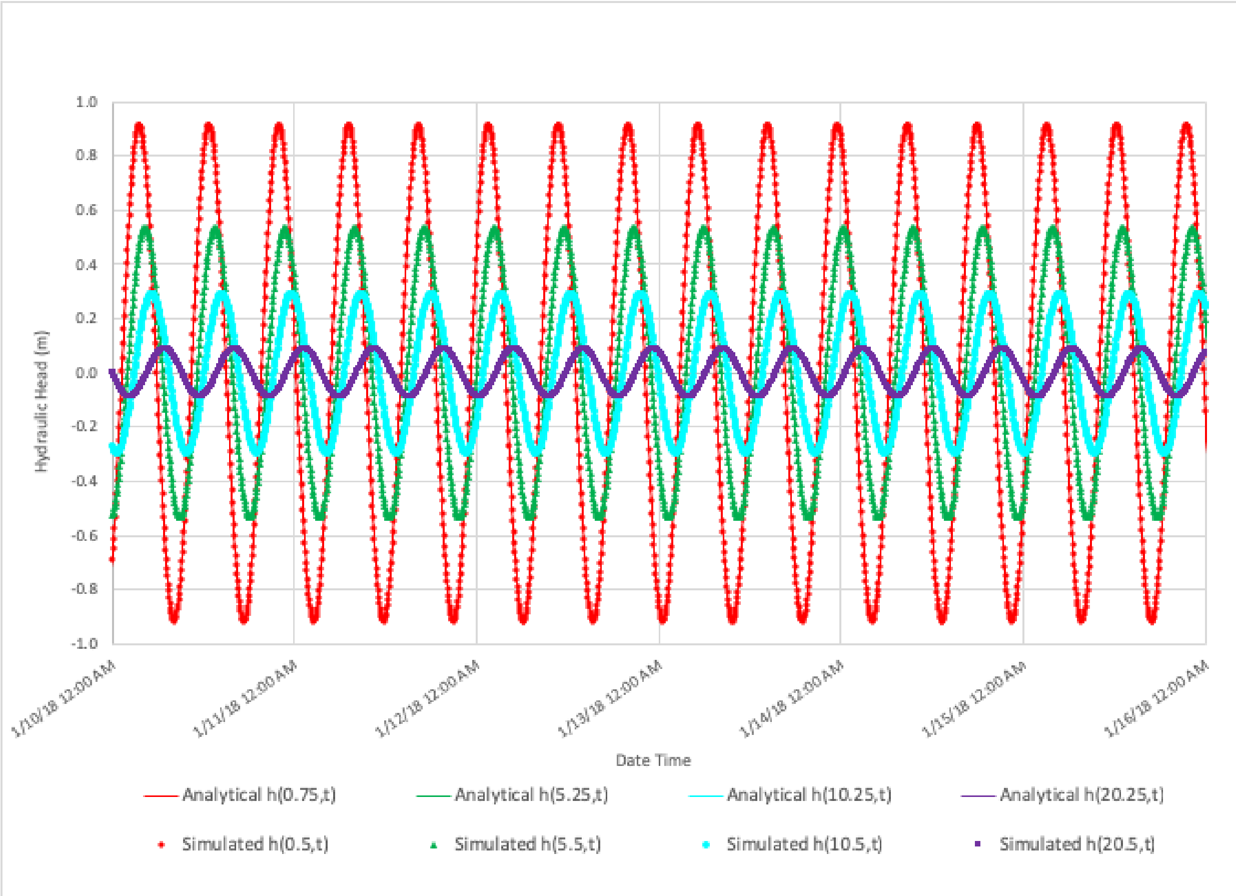

Figure 5. Simulated vs. analytical hydraulic head solution for 0.5 m cell resolution

Table 2. Mean absolute error for predicted hydraulic head

Mesh Size	Mean Absolute Error			
	h(0.75,t)	**h(5.25,t)**	**h(10.25,t)**	**h(20.25,t)**
1.0 m	0.004	0.002	0.001	0.0005
0.5 m	0.003	0.001	0.0007	0.0002

7.5.1 Heat Transport Validation

To test the heat transport component of the GWComponent, the analytical solution for heat transport of a line heat source representing a vertical ground heat exchanger (GHE) derived by Diao *et al.* (2004) was evaluated. Equations 33 and 34 represent the Diao *et* *al.* (2004) analytical solutions for conduction in space and time and both advection and conduction formulations in the steady state respectively:

$$\Delta T(r,t) = -\frac{q_l}{2\pi\lambda_m} Ei\left(-\frac{\rho_m c_m r^2}{4\lambda_m t}\right) \tag{33}$$

where $\Delta T(r,t)$ is the function for the increase or decrease in temperature over the initial temperature over space and time $(°C)$, r is the distance from the line source (m), t is time (s), q_l is the heat flow per unit length of line source $\left(\frac{W}{m}\right)$, and $Ei()$ is the exponential integral function.

$$\Delta T(x,y) = -\frac{q_l}{2\pi\lambda_m} e^{\left(\frac{\rho_m c_m v x}{2\lambda_m}\right)} K_0\left(\frac{\rho_m c_m v r}{2\lambda_m}\right) \tag{34}$$

where $\Delta T(x,y)$ is the increase or decrease over the initial temperature over space in the steady state, and $K_0()$ is the modified Bessel function of the second kind of order zero.

For our test problem, we applied a line heat source of 60 $\frac{W}{m}$ at the point shown in Figure 6. Other attributes for the aquifer used for this test problem are shown in Table 3. This represents a challenging problem because of the sharp temperature gradient created in the vicinity of the source.

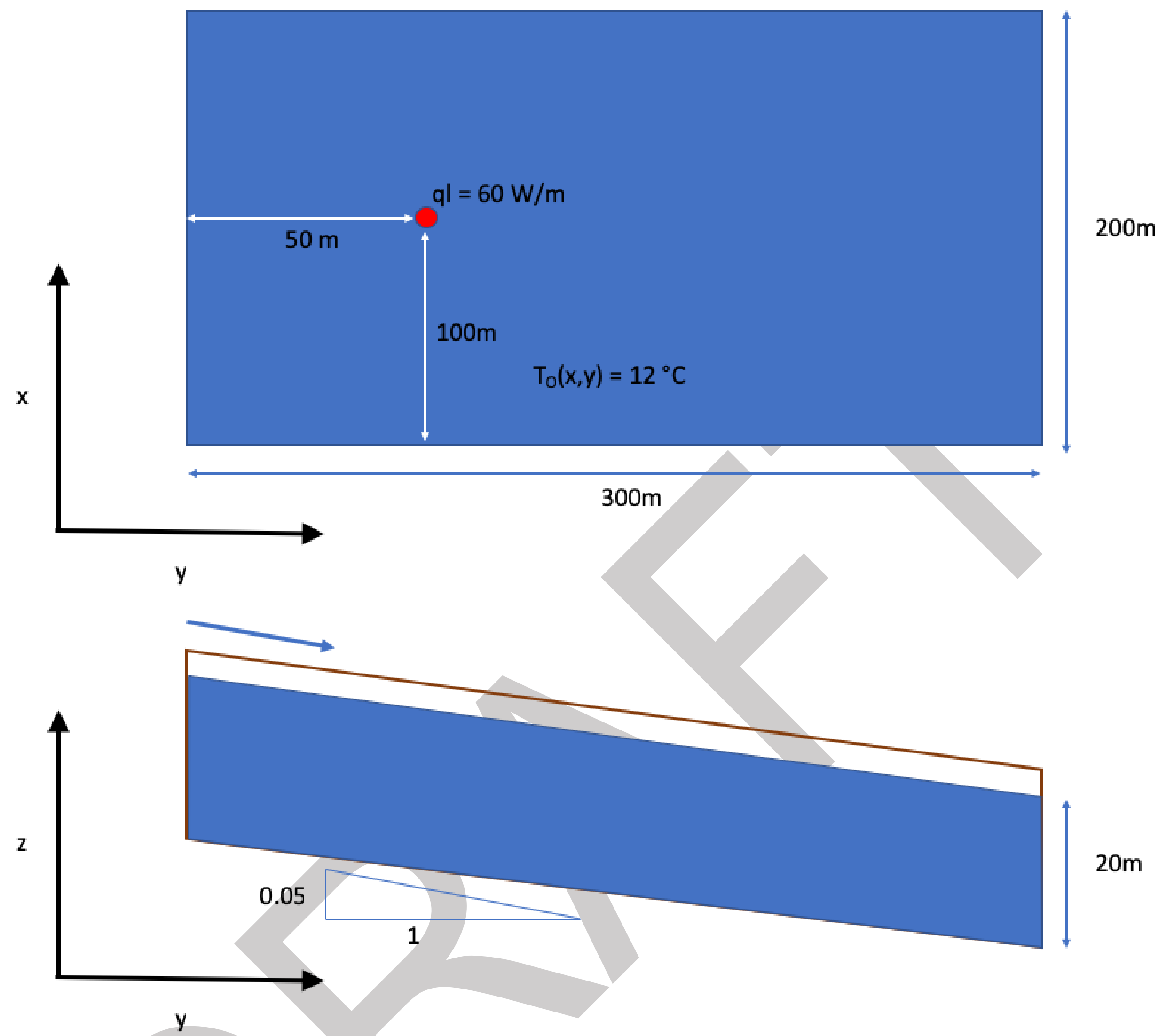

Figure 6. Line heat source experiment schematic

Table 3. Line heat source experiment aquifer parameters

Parameter	Value	Units
η =	**0.3**	
ρ_w =	**1000**	**kg/m^3**
c_w =	**4184**	**J/kg/C**
ρ_s =	**2650**	**kg/m^3**
c_s =	**880**	**J/kg/C**
$\rho_m c_m$ =	**2887600**	**kg/m^3**
grad H =	**0.05**	
T =	**20**	**m**
L =	**40**	**m**
w =	**1**	**m**
K_y and K_x =	**0.0001**	**m/s**
λ_w =	**0.6060000000**	**W/m/K**
λ_s =	**2.5974285714**	**W/m/K**
λ_m =	**2.0000000000**	**W/m/K**
α =	**0.0500000000**	**m**

Simulated results for the conduction simulation compared well with the analytic solution with a worst MAE of 0.03 °C (Figure 7). Results may be improved be further refining the mesh near the source location. Results for the advection and conduction simulation also compared well with the analytic solution with and MAE of 0.01 °C.

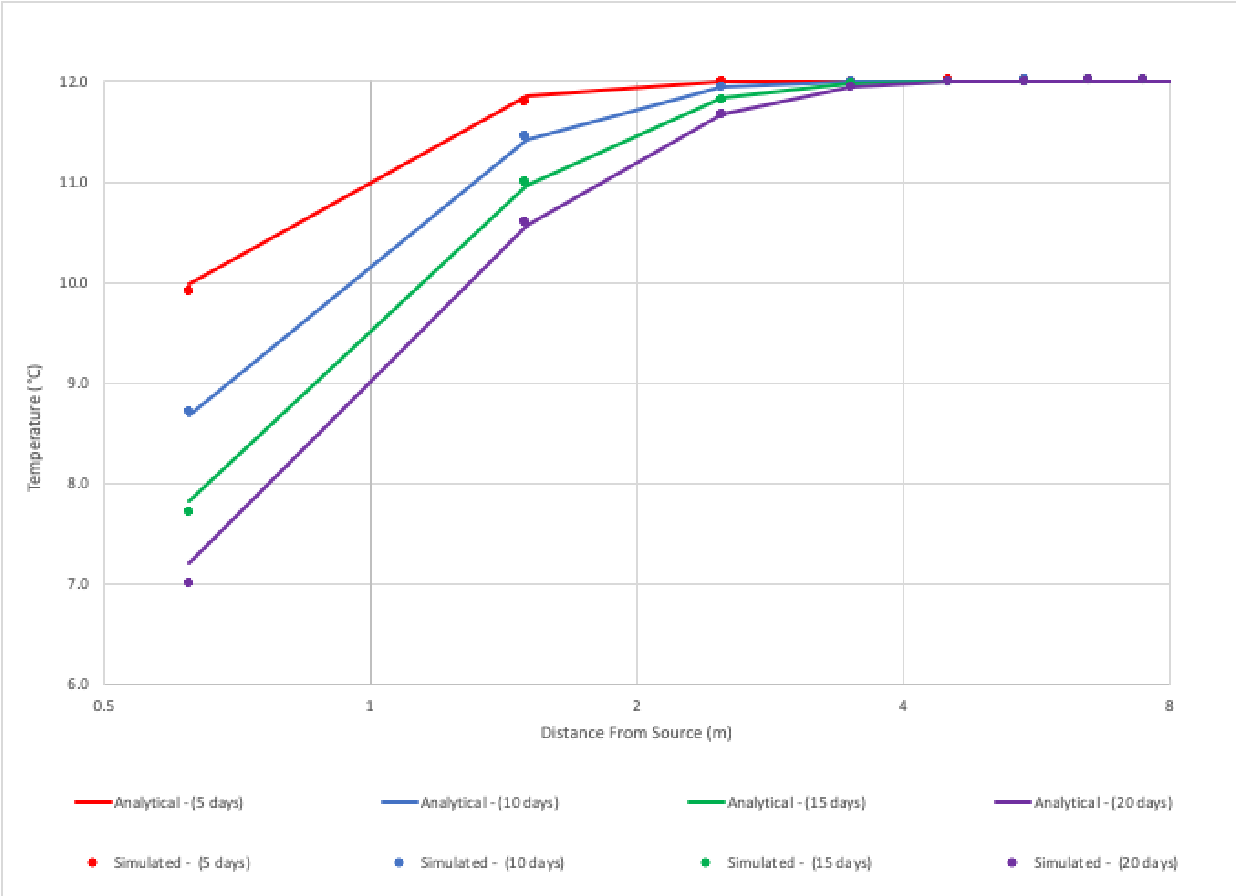

Figure 7. Simulated vs. analytical solution for conduction problem

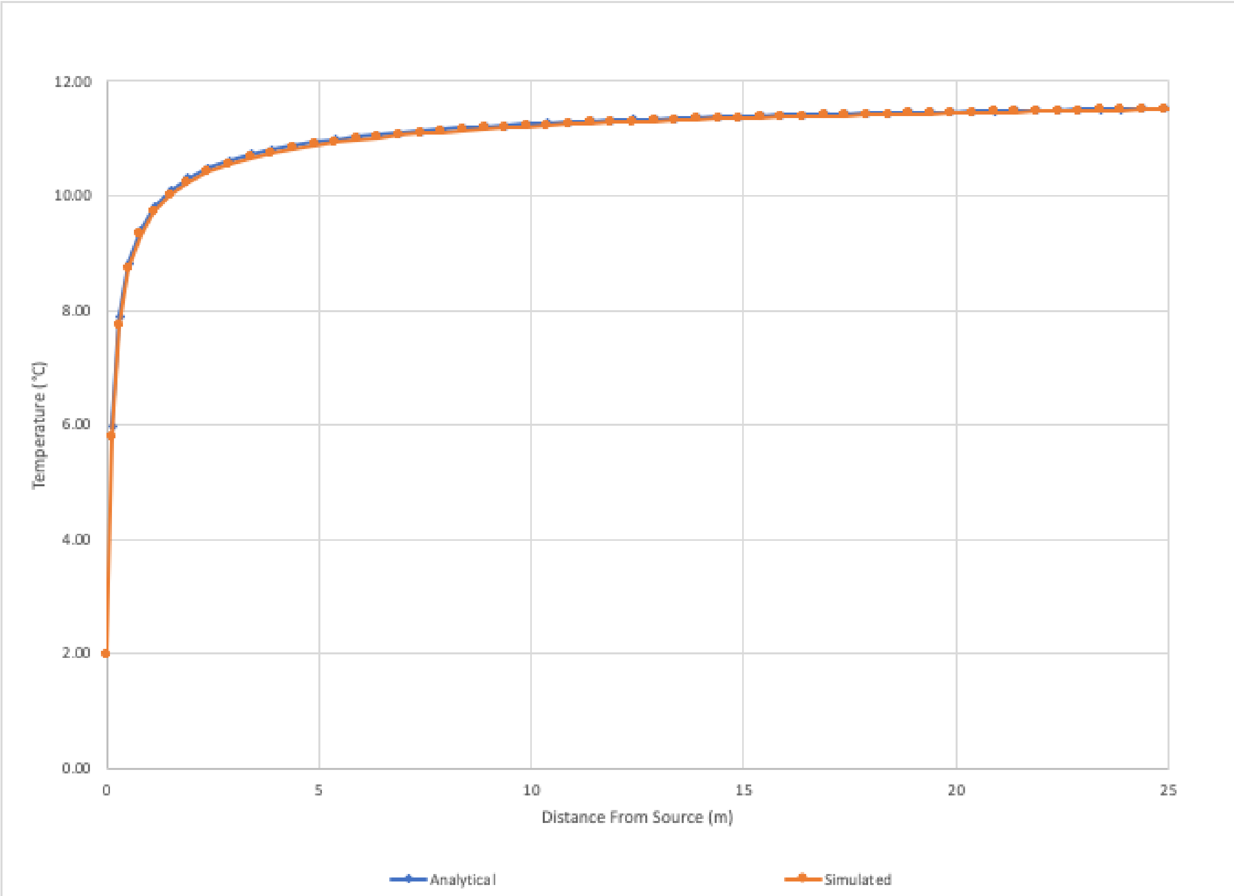

Figure 7. Simulated vs. analytical solution for advection & conduction problem

7.5.2 *Solute Transport Validation*

For testing for the solute transport formulations, the 1D advection and dispersion analytic solution for an infinitesimal aquifer with a Cauchy boundary condition (Domenico and Schwartz, 1998) was used:

$$C(y,t) = \left(\frac{1}{2}\right) erfc\left(\frac{y - vt}{2\sqrt{\alpha vt}}\right) C_o \qquad (35)$$

where $C(y,t)$ is the concentration of the solute in space and time $\left(\frac{mg}{L}\right)$ and C_o is the concentration specified at the boundary $\left(\frac{mg}{L}\right)$.

For our test problem, we applied a boundary condition of 10mg/L in an aquifer with a saturated thickness of 1m, a hydraulic gradient of 0.05 m/m, porosity of 0.3, hydraulic conductivity of 0.001, and a mesh resolution of 0.1m. Numerical results from the model compared well with the analytical solution with the largest MAE of 0.05 mg/L.

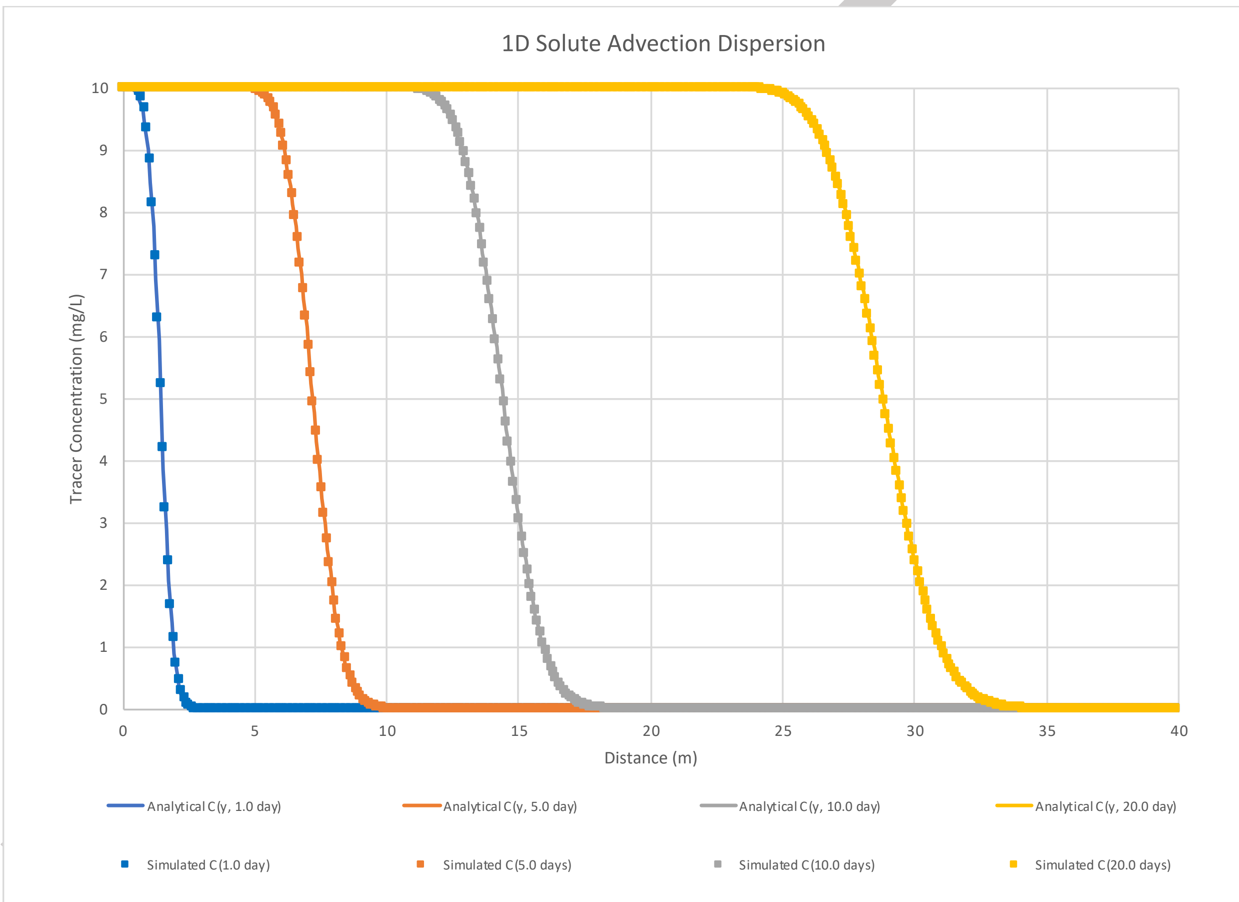

Figure 9. Simulated vs. analytic solution for 1D advection dispersion solute transport problem

7.6 GWComponent Input File Format

8 Time Series Provider Component (TimeSeriesProviderComponent)

9 Calibration/Optimization Component (CalibrationComponent)

10 Timeseries Objective Function Calculation Component (TSObjectiveFunctionComponent)

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