RECLAMATION

Managing Water in the West

SRH-WQ: A Water Quality and Mercury Transport Model for Streams and Reservoirs

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Final Report ST-2017-3425-02

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Mission Statements

Protecting America's Great Outdoors and Powering Our Future

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Mercury is a toxic metal that is found both naturally and as an introduced contaminant in an aquatic environment. Even very low concentrations of Methylmercury (MeHg) in water lead to bioaccumulation through food web and may cause high levels of mercury contamination in fish in aquatic systems. So, MeHg is the form of the greatest concern for both human health and ecosystems. In this research a two-dimensional (2D) depth-averaged mercury and water quality model is developed by integrating SRH-2D model and mercury modules (MMs). SRH-2D is a 2D depth-averaged flow and sediment transport model developed at the U.S. Bureau of Reclamation and widely used for engineering projects. MMs are developed at the US Army Corps of Engineer (USACE) which has been incorporated into HEC-RAS 1Dand AdH. Key techniques are developed that allow advective and dispersive transport of mercury and other water quality species in waterbody in a 2D space. In the report results are presented with regard to how the coupling of SRH-2D and MMs is achieved and how the new integrated mercury model is designed for robustness and ease-of-use for engineering applications. The proposed method allows independent time steps being used by SRH-2D and MMs so that long-term mercury and water quality modeling may be realized. The integrated model is tested and verified with cases having known solutions. A number of tutorial cases are provided so that this report alone may be used as model User's Manual.

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SRH-WQ: A Water Quality and Mercury Transport Model for Streams and Reservoirs Title_

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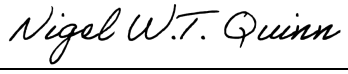

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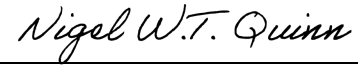

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Executive Summary

Mercury is a toxic metal that is found both naturally and as an introduced contaminant in an aquatic environment. Besides elementary mercury (Hg0), major mercury forms in water are inorganic and organic mercury, particularly methylmercury (MeHg). Inorganic mercury is bound to chloride, sulfide, or organic acids and it is lumped together by most mercury-cycling models into a single species identified by reactive mercury (HgII). MeHg is the most toxic form. Even very low concentrations of MeHg in water lead to bioaccumulation through food web and may cause high levels of mercury contamination in fish in aquatic systems. So, MeHg is the form of the greatest concern for both human health and ecosystems and has led to the identification of state-level water quality standards and control programs. Reclamation will be required to comply with these new standards as they need to develop and implement various reservoir mercury management practices. Untested management practices may be ineffective at providing the appropriate level of mitigation and can be cost prohibitive for large reservoir operators at Reclamation.

In this study, a two-dimensional (2D) depth-averaged mercury and water quality model is developed by integrating SRH-2D model and mercury modules (MMs) through a collaboration with the US Army Corps of Engineer (USACE). SRH-2D is a 2D depth-averaged flow and sediment transport model developed at the U.S. Bureau of Reclamation and widely used for engineering projects. MMs are developed at USACE which has been incorporated into HEC-RAS 1D and AdH. Key techniques are developed that allow advective and dispersive transport of mercury and other water quality species in waterbody in a 2D space.

In this report, the mathematical equations governing all physical and biochemical equations are presented. The numerical algorithms developed to solve the 2D transport of mercury and water quality species are described. In particular results are presented with regard to how the coupling of SRH-2D and MMs is achieved and how the new integrated model is designed for robustness and ease-of-use for engineering applications. The proposed method allows independent time steps being used by SRH-2D and MMs so that long-term mercury and water quality modeling may be realized. In Chapter 3, the mercury and the associated water quality modules are briefly described; focus is to summarize what users need to know about the model inputs as mercury and water quality modeling can be complex and data intensive. Chapter 4 provides three tutorial cases to help readers understand what a typical mercury and water quality modeling looks like, in particular, learn how to carry out such a modeling themselves with SRH-WQ. In this sense the report may also be used as the User's Manual of SRH-WQ. In the final Chapter 5, test and verification cases are presented and model results are compared with known solutions.

SRH-WQ has been developed and tested with relatively simple cases. In the future we plan to advance the model in several areas as follows: (a) Find practical streams having sufficient water quality and/or mercury data so that the model may be further verified and validated; (b) extension of SRH-WQ to basin level modeling since there are mercury data set compiled already at the basin scale; and (c) application of the model to Reclamation projects.

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1. Introduction

Water quality constituents and contaminants such as mercury are introduced into aquatic systems through both natural means, such as atmospheric deposition and weathering of soils and rocks, and human activities, such as mining, processing, or use of toxic substances. The U.S. Environmental Protection Agency (EPA) and State EPAs have developed water quality objectives and standards for the nation's impaired waterbodies. In order to more fully understand the factors affecting water quality and to control water quality to meet these water quality criteria, numerical modeling tools have been developed. These tools are used to evaluate and predict the fate and transport of contaminants and water quality constituents in the environment. For example, the CE-Qual-ICM (Cerco and Cole 1993) and EFDC-WASP (Zou et al. 2006; Xia et al. 2010) numerical models have been used for environmental management of mercury in lakes and streams.

Water quality models are often coupled with existing hydrologic and hydraulic (H&H) models for environmental analysis or water quality forecasting. Differing levels of H&H models have been developed over the last three decades (Bahadur et al. 2013). In the area of stream and reservoir models, a number of recent H&H models have been mature enough to be used extensively on a number of applications. Examples include the Hydrologic Engineering Center-River Analysis System (HEC-RAS) (HEC 2010), two-dimensional hydrodynamics and water quality (CE-QUAL-W2) model (Cole and Wells 2011), Adaptive Hydraulics (AdH) (Berger et al. 2012), and Sedimentation and River Hydraulics – 2D model (SRH-2D) (Lai, 2008, 2010). These models, however, still lack the capability to perform water quality and contaminant fate and transport analysis. Recognizing this need, the Environmental Quality Technology Research Program at the U.S. Army Corp of Engineers (USACE) sponsored research and development into water quality and contaminant simulation modules designed to be coupled to the above H&H models. The final products of these efforts are the NSM, CSM and HgSM modules reported by Zhang and Johnson (2016a; b). Through a Reclamation-USACE collaborative project, funded through the Reclamation Science and Technology Program, the water quality module NSMI and the mercury module HgSM have been coupled to the Reclamation SRH-2D model.

In this report the two-dimensional (2D) depth-averaged scalar transport module, named SRH-WQ, is developed and described. SRH-WQ provides a coupling between the water quality and mercury modules and the H&H model. It solves any number of constituents (or scalars) that are transported by water in streams or within reservoirs. On one hand, SRH-WQ is linked to SRH-2D (Lai, 2008; 2010) which provides the needed water flux to enable constituent transport. SRH-2D is a widely used 2D flow and sediment transport model developed at the U.S. Bureau of Reclamation (Reclamation). It is robust and reliable in predicting flow and sediment transport which enhances its capability for water quality and mercury modeling. The model-associated source and sink terms (i.e., the kinetics) of water quality and mercury constituent transport equations are computed by the NSMI and HgSM modules, developed by USACE. NSMI is an aquatic nutrient simulation module (Zhang and Johnson, 2016a) and HgSM is a mercury simulation module (Zhang and Johnson, 2016b). For water quality modeling, the availability and

the accuracy of the underlying hydrodynamics model are of great importance, and the method of model linkage can affect the efficiency and computer run time of the water quality model.

This work is part of a collaborative research among multiple agencies to develop a mercury simulation model to address mercury issues in reservoirs. Team members include the U.S. Bureau of Reclamation and the U.S. Army Corps of Engineers.

2. Governing Equations and Numerical Methods

2.1 Flow Equations

Only water flow in streams and reservoirs are considered. The water flow module is based on SRH-2D whose details may be found in Lai (2008; 2010). The basic equations and the associated numerical models presented in this previous work are the same equations and algorithms used for the water quality and mercury constituents modeling theoretical development presented in this report.

Most open channel flow is relatively shallow and the effect of vertical motion can be assumed to be negligible. The three-dimensional Navier-Stokes equations may be vertically averaged to obtain a set of depth-averaged two-dimensional (2D) equations, leading to the following well known 2D St. Venant (or dynamic-wave) equations:

$$\frac{\partial h}{\partial t}+\frac{\partial hU}{\partial x}+\frac{\partial hV}{\partial y}=0 \tag{1}$$

$$\frac{\partial hU}{\partial t}+\frac{\partial hUU}{\partial x}+\frac{\partial hVU}{\partial y}=\frac{\partial hT_{xx}}{\partial x}+\frac{\partial hT_{xy}}{\partial y}-gh\frac{\partial z}{\partial x}-\frac{\tau_{bx}}{\rho} \tag{2}$$

$$\frac{\partial hV}{\partial t}+\frac{\partial hUV}{\partial x}+\frac{\partial hVV}{\partial y}=\frac{\partial hT_{xy}}{\partial x}+\frac{\partial hT_{yy}}{\partial y}-gh\frac{\partial z}{\partial y}-\frac{\tau_{by}}{\rho} \tag{3}$$

In the above, t is time, x and y are horizontal Cartesian coordinates, h is water depth, U and V are depth-averaged velocity components in x and y directions, respectively, g is the gravitational acceleration, T_{xx}, T_{xy}, and T_{yy} are depth-averaged diffusion stresses owing to turbulence and dispersion caused by depth averaging, $z = z_b + h$ is the water surface elevation, z_b is the bed elevation, ρ is the water density, and τ_{bx}, τ_{by} are the bed shear stresses (friction).

Bed friction in the above equations is calculated using the Manning's roughness equation as follows:

$$\begin{pmatrix}\tau_{bx}\\ \tau_{by}\end{pmatrix}=\rho C_f\begin{pmatrix}U\\ V\end{pmatrix}\sqrt{U^2+V^2}; \qquad C_f=\frac{gn^2}{h^{1/3}} \tag{4}$$

where n is the Manning's roughness coefficient.

Turbulence stresses are based on the Boussinesq equations as follows:

$$T_{xx} = 2(\upsilon + \upsilon_t)\frac{\partial U}{\partial x} - \frac{2}{3}k$$
$$T_{xy} = (\upsilon + \upsilon_t)(\frac{\partial U}{\partial y} + \frac{\partial V}{\partial x}) \quad (5)$$
$$T_{yy} = 2(\upsilon + \upsilon_t)\frac{\partial V}{\partial y} - \frac{2}{3}k$$

where υ is the kinematic viscosity of water; υ_t is the turbulent eddy viscosity; and *k* is the turbulent kinetic energy.

Two turbulence models may be used to compute the turbulent eddy viscosity: (a) the depth-averaged parabolic model; and (b) the two-equation *k*-ε model. With the parabolic model, $\upsilon_t = C_t U_* h$ is adopted in which U_* is bed friction velocity and C_t is a model constant ranging from 0.3 to 1.0. Note that terms with *k* are dropped in Equation (5).

If the *k*-ε model is used, turbulent viscosity is calculated using: $\upsilon_t = C_\mu k^2 / \varepsilon$. Two additional equations are solved as follows:

$$\frac{\partial hk}{\partial t} + \frac{\partial hUk}{\partial x} + \frac{\partial hVk}{\partial y} = \frac{\partial}{\partial x}(\frac{h\upsilon_t}{\sigma_k}\frac{\partial k}{\partial x}) + \frac{\partial}{\partial y}(\frac{h\upsilon_t}{\sigma_k}\frac{\partial k}{\partial y}) + P_h + P_{kb} - h\varepsilon \quad (6)$$

$$\frac{\partial h\varepsilon}{\partial t} + \frac{\partial hU\varepsilon}{\partial x} + \frac{\partial hV\varepsilon}{\partial y} = \frac{\partial}{\partial x}(\frac{h\upsilon_t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x}) + \frac{\partial}{\partial y}(\frac{h\upsilon_t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial y}) + C_{\varepsilon 1}\frac{\varepsilon}{k}P_h + P_{\varepsilon b} - C_{\varepsilon 2}h\frac{\varepsilon^2}{k} \quad (7)$$

Where P_h, P_{kb} and C_u are coefficients defined as follows:

$$P_h = h\upsilon_t\left[2\left(\frac{\partial U}{\partial x}\right)^2 + 2\left(\frac{\partial V}{\partial y}\right)^2 + \left(\frac{\partial U}{\partial y} + \frac{\partial V}{\partial x}\right)^2\right] \quad (8)$$

$$P_{kb} = C_f^{-1/2}U_*^3; \quad P_{\varepsilon b} = C_{\varepsilon\Gamma}C_{\varepsilon 2}C_\mu^{1/2}C_f^{-3/4}U_*^4 / h \quad (9)$$

$$C_\mu = 0.09,\ C_{\varepsilon 1} = 1.44,\ C_{\varepsilon 2} = 1.92, \sigma_k = 1, \sigma_\varepsilon = 1.3, C_{\varepsilon\Gamma} = 1.8 \sim 3.6 \quad (10)$$

The additional coefficients P_{kb} and $P_{\varepsilon b}$ are added to account for the generation of turbulent energy and dissipation due to bed friction for the case of uniform flows.

2.2 Scalar Transport Equations

Any constituents, solids or chemical species are transported using the 2D shallow-water transport equation. The scalar transport equation is written in a general form for mass conservation as follows:

$$\frac{\partial hC}{\partial t}+\frac{\partial hUC}{\partial x}+\frac{\partial hVC}{\partial y}=\frac{\partial}{\partial x}\left(hD\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(hD\frac{\partial hC}{\partial y}\right)+S \qquad (11)$$

where C is the depth-averaged value of the scalar, $D=\frac{\upsilon_t}{\sigma_C}$ is the diffusivity, and σ_C is the Schmidt number. If the scalar is a water quality constituent, C is the depth-averaged volume concentration (m^3/m^3) and hC is the scalar volume per unit bed area. The volume concentration (C) can be converted to a mass concentration measured in kilograms per unit volume by multiplying C and the density of the constituent.

The scalar is one of the advection state variables used by the various USACE water quality modules for temperature (TEMP and general constituents (GC) as well as for the NSMI and HgSM modules.

2.3 Discretization of the Scalar Equation

A detailed presentation of the numerical method for the flow equations has been described previously by Lai (2008) and is not repeated in this report. Briefly, the equations are solved with the finite volume method that guarantees mass conservation locally and globally. An implicit time marching scheme is used with the arbitrarily shaped unstructured mesh methodology of Lai (2003).

Each scalar equation is similar to the momentum equation and is discretized and solved using the same techniques. The discretization and solution of the scalar equation is described below.

For the 2D depth-averaged model using SRH-2D and SRH-WQ - a solution domain is selected and then covered with an unstructured mesh. Each mesh cell may assume the shape of an arbitrarily shaped polygon. Only triangular and quadrilateral polygons have been tested and verified at present. All dependent variables are assigned to the geometric center of a polygon. The governing equation of each scalar equation may be written in the following convection-diffusion form:

$$\frac{\partial h\Phi}{\partial t}+\nabla\bullet(h\vec{V}\Phi)=\nabla\bullet(\Gamma\nabla\Phi)+S_\Phi^* \qquad (12)$$

Here Φ denotes a scalar, Γ is the diffusivity, and S_Φ^* is the source/sink term. Integration over an arbitrarily shaped polygon *P* shown in Figure **1** leads to:

$$\frac{(h_P^{n+1}\Phi_P^{n+1} - h_P^n\Phi_P^n)A}{\Delta t} + \sum_{all-sides}(h_C V_C |\vec{s}|)^{n+1}\Phi_C^{n+1} = \sum_{all-sides}(\Gamma_C^{n+1}\nabla\Phi^{n+1} \bullet \vec{n}|\vec{s}|) + S_\Phi \qquad (13)$$

In the above, Δt is time step, A is polygon area, $V_C = \overrightarrow{V_C} \bullet \vec{n}$ is the velocity component normal to the polygonal side (e.g., P_1P_2 in Figure **1**) and is evaluated at the side center C, $\vec{n}$ is polygon side unit normal vector, $\vec{s}$ is the polygon side distance vector(e.g., from P_1 to P_2 in Figure 1), and $S_\Phi = S_\Phi^* A$. Subscript C represents a value located at the center of one side of a polygon and assigned the superscript, n (or n+1) denoting the time step. In the remaining discussion, superscript n+1 will be dropped for ease of notation. Note that the first-order Euler implicit time discretization is adopted. The main task of the discretization is to obtain appropriate expressions for the convective and diffusive fluxes at each polygon side.

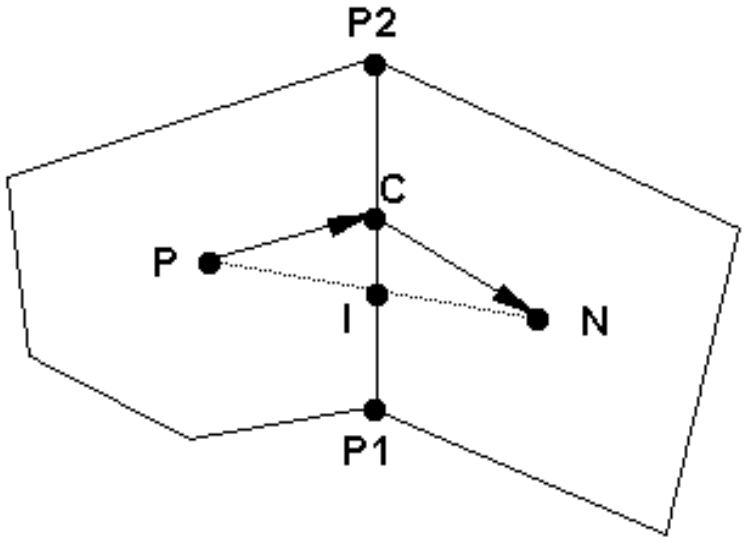

Figure 1. Schematic showing adjacent polygons P and N with labelled distances to the common boundary between polygon centroids.

Discretization of the diffusion term, the first term on the right hand side of equation (13), can be simplified further. The final expression for $\nabla\Phi \bullet \vec{n}$ can be written as:

$$\nabla\Phi \bullet \vec{n}\,|\vec{s}| = D_n(\Phi_N - \Phi_P) + D_c(\Phi_{P2} - \Phi_{P1}) \qquad (14)$$

where

$$D_n = \frac{|\vec{s}|}{(\vec{r}_1 + \vec{r}_2) \bullet \vec{n}}; \qquad D_c = -\frac{(\vec{r}_1 + \vec{r}_2) \bullet \vec{s}\,/|\vec{s}|}{(\vec{r}_1 + \vec{r}_2) \bullet \vec{n}} \qquad (15)$$

In the above, $\vec{r}_1$ is the distance vector from P to C and $\vec{r}_2$ is from C to N. The normal and cross diffusion coefficients, D_n and D_c , along the common boundaries of each polygon involve only geometric variables -they are calculated only once in the beginning of the computation.

Interpolation is often required for a number of spatial variables. With reference to Figure 1 – the calculation of a variable, *Y*, at the center C of a polygon side may be required. A point I is defined as the intercept point between line PN and line P_1P_2. A second-order interpolation for point I is provided by the following expression:

$$Y_I = \frac{\delta_1 Y_N + \delta_2 Y_P}{\delta_1 + \delta_2} \tag{16}$$

for which $\delta_1 = \vec{r}_1 \bullet \vec{n}$ and $\delta_2 = \vec{r}_2 \bullet \vec{n}$. In this instance, Y_I is used to approximate a parameter value at location C between adjacent polygons. The expression does not guarantee second-order accuracy unless $\vec{r}_1$ and $\vec{r}_2$ are parallel.

Φ_C in the convective term in equation (12) needs further discussion. A damping term Φ_C has been added to the convective term of equation (12) to emulate the concept of artificial viscosity. The damped schema is derived by blending the first-order upwind schema with the second-order central difference schema – it can be expressed as follows:

$$\Phi_C = \Phi_C^{CN} + d(\Phi_C^{UP} - \Phi_C^{CN}) \tag{17}$$

where

$$\Phi_C^{UP} = \frac{1}{2}(\Phi_P + \Phi_N) + \frac{1}{2} sign(V_C)(\Phi_P - \Phi_N) \tag{18}$$

and Φ_C^{CN} is from the interpolation equation (16). In the above expression, *d* defines the amount of damping employed. In most applications, *d* is given values of between 0.2 and 0.3.

Including expressions for the diffusion and convection terms, the final discretized governing equation for an element P can be arranged according to the following linear equation:

$$A_P \Phi_P = \sum_{nb} A_{nb} \Phi_{nb} + S_{diff} + S_{conv} + S_\Phi \tag{19}$$

where "nb" refers to all neighboring polygons surrounding the polygon P. The coefficients in this equation are as follows:

$$A_{nb} = \Gamma_C D_n + Max(0, -h_C V_C |\vec{s}|) \tag{20a}$$

$$A_P = \frac{h_P^n A}{\Delta t} + \sum_{nb} A_{nb} \tag{20b}$$

$$S_{diff} = \frac{h_P^n A}{\Delta t} + \sum_{all\ sides} \Gamma_C D_c \left(\Phi_{P2} - \Phi_{P1}\right) \tag{20c}$$

$$S_{conv} = \sum_{all\ sides} (h_C V_C |\vec{s}|) \left\{ (1-d) \left[\frac{\delta_1}{\delta_1 + \delta_2} - \frac{1 - sign(V_C)}{2} \right] (\Phi_N - \Phi_P) \right\}$$
$$- \sum_{all\ sides} (h_C V_C |\vec{s}|) \left[(1-d) C_{side} (\Phi_{P2} - \Phi_{P1}) \right] \tag{20d}$$

Equation (19) forms the basis for a set of linear algebraic equations. An efficient and robust linear equation solver, the conjugate gradient squared solver (Lai 2008), was chosen for running model simulations.

2.4 Treatment of Source Terms

The treatment of the source/sink terms in the scalar equations has been subject os considerable past research. Two options have been developed for the SRH-WQ model.

The first is a linearization method for which the source/sink terms are linearized according to the following equation:

$$S = Su - Sp\,C \tag{21}$$

Su represents all the erms that are treated explicitly, while *Sp* includes all terms that are treated implicitly. This method is highly suitable for the temperature equation for which source/sink terms may be expressed in the form of $k(T_{eq} - T)$ where T_{eq} represents the equilibrium temperature and k is the rate of recovery.

The second method is the operating splitting technique developed by Savant and Berger (2012) for which the scalar equation (11) is split into two separate solution procedures:

$$\frac{\partial hC}{\partial t} + \frac{\partial hUC}{\partial x} + \frac{\partial hVC}{\partial y} = \frac{\partial}{\partial x}\left(hD \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y}\left(hD \frac{\partial hC}{\partial y} \right) \tag{22}$$

$$\frac{\partial hC}{\partial t} = hS(C,t) \tag{23}$$

The first equation (22) is the convection-diffusion equation with zero sources/sinks which can be viewed as a typical hyperbolic initial value problem. The implicit numerical procedure discussed above may be used to obtain an intermediate solution C_* from the prior-time solution C_n. Since an implicit scheme is used, a very large time step may be used for the first model simulation iteration.

The second equation (23) is a typical non-linear ordinary differential equation and we follow the recommendation of Savant and Berger (2012) for the solution of the model at time C_{n+1} given C_*.The embedded fifth-order Runge-Kutta (RK5E) numerical integration scheme has been adopted combined with the use of adaptive time-stepping. A detailed description of RK5E procedure and program was provided by Cash and Karp (1990) and Press et al. (1992) – these procedures are described below.

For instance – in order to solve the equation $\frac{dY}{dt} = S(Y,t)$ and when Y_n a time t_n is already known - we need to find Y_{n+1} at $t_{n+1} = t_n + h$. The general form of the fifth-order Runge-Kutta schema is as follows:

$$
\begin{aligned}
k_1 &= h\,S(Y_n, t_n) \\
k_2 &= h\,S(Y_n + b_{21}k_1, t_n + a_2 h) \\
k_3 &= h\,S(Y_n + b_{31}k_1 + b_{32}k_2, t_n + a_3 h) \\
k_4 &= h\,S(Y_n + b_{41}k_1 + b_{42}k_2 + b_{43}k_3, t_n + a_4 h) \\
k_5 &= h\,S(Y_n + b_{51}k_1 + b_{52}k_2 + b_{53}k_3 + b_{54}k_4, t_n + a_5 h) \\
k_6 &= h\,S(Y_n + b_{61}k_1 + b_{62}k_2 + b_{63}k_3 + b_{64}k_4 + b_{65}k_5, t_n + a_6 h)
\end{aligned} \qquad (24)
$$

$$
Y_{n+1} = Y_n + c_1k_1 + c_2k_2 + c_3k_3 + c_4k_4 + c_5k_5 + c_6k_6 + O(h^6) \qquad (25)
$$

The imbedded fourth-order schema can be represented as:

$$
Y^*_{n+1} = Y_n + c^*_1k_1 + c^*_2k_2 + c^*_3k_3 + c^*_4k_4 + c^*_5k_5 + c^*_6k_6 + O(h^5) \qquad (26)
$$

The accumulated error at the current time step may be estimated to be:

$$
\Delta = \sum_{i=1}^{6} \left(c_i - c_i^*\right) k_i \qquad (27)
$$

If we know using a time step of h_1 produces an error Δ_1, then time step needed to keep the error below Δ_0 can be estimated to be:

$$
h_0 = h_1 \left| \frac{\Delta_0}{\Delta_1} \right|^{1/5} \qquad (28)
$$

This schema provides adaptive time step in order to satisfy the desired maximum error. It schema can be applied in two ways: If Δ_1 is larger than Δ_0 in magnitude, the equation provides a revised time step decrement to convergence to a solution. Conversely, if Δ_1 is smaller than Δ_0, then the equation suggests a time step increment for the next step to speed up the simulation.

Table 1. The constants used in the RK5E is listed below according to Cash and Karp (1990):

i	a_i	b_{i1}	b_{i2}	b_{i3}	b_{i4}	b_i	c_i	c_i^*
1							$\frac{37}{378}$	$\frac{2825}{27648}$
2	$\frac{1}{5}$	$\frac{1}{5}$					0	0
3	$\frac{3}{10}$	$\frac{3}{40}$	$\frac{9}{40}$				$\frac{250}{621}$	$\frac{18575}{48384}$
4	$\frac{3}{5}$	$\frac{3}{10}$	$-\frac{9}{10}$	$\frac{6}{5}$			$\frac{125}{594}$	$\frac{13525}{55296}$
5	1	$-\frac{11}{54}$	$\frac{5}{2}$	$-\frac{70}{27}$	$\frac{35}{27}$		0	$\frac{277}{14336}$
6	$\frac{7}{8}$	$\frac{1631}{55296}$	$\frac{175}{512}$	$\frac{575}{13824}$	$\frac{44275}{110592}$	$\frac{253}{4096}$	$\frac{512}{1771}$	$\frac{1}{4}$

3. Water Quality and Mercury Modules

The source/sink terms for all advected (or transported) state variables are represented as nonlinear, complex functions within water quality and mercury cycling models. These functions are governed by physical, chemical and biological processes and, in this study, computed using the water quality and mercury modules developed by U.S. Army Corps of Engineers (USACE) through a collaborative program between Reclamation and USACE. Detailed descriptions of these USACE water quality and mercury modules are documented in two reports by Zhang and Johnson (2016a; b); and they are enclosed as attachments. Only the most relevant main variables and processes simulated by the Reclamation WQ model are provided in this report. The report does describe, in detail, the model input parameters required to run SRH-WQ model. A primary purpose of the report is to facilitate application of SRH-WQ model to appropriate sites.

At present, four USACE water quality and mercury modules are incorporated into SRH-WQ: the temperature module (TEMP), the general constituent module (GC), the nutrient simulation module (NSMI), and the mercury simulation module (HgSM). They are developed as dynamic link libraries (DLLs) so that their integration into any hydrological and hydraulic models can be accommodated. A further benefit is that the water quality and mercury modules can be made independent of the specific model adopted for integration. In this study, SRH-2D is the hydraulic model for integration with the USACE modules. A separate 2D depth-averaged scalar transport module, SRH-WQ, has been developed that achieves two goals: (1) solve all advected water quality state variables; and (2) provide the integration between the SRH-2D and USACE modules.

With the SRH-WQ model, a typical mercury or water quality simulation proceeds as follows. First, the SRH-2D model is used to simulate water flow in a stream and/or reservoir without considering the mercury or water quality processes. Such a flow simulation has been carried out routinely for numerous water resource projects, as documented by Lai (2008; 2010). Simulated flow variables such as water depth, velocity and bed shear stress are saved to memory at user-specified time intervals. In addition, the model domain and relevant 2D mesh information are also saved. These flow simulation outputs become inputs to the SRH-WQ model. Next, the SRH-WQ model is used to simulate the physical and biochemical processes represented by the mercury and water quality state variables. The SRH-WQ transport module simulates the physical processes of advection and dispersion of all advected state variables, along with inflows and outflows represented by these variables across open boundaries. The 2D transport module is responsible for transport represented by these state variables throughout the model domain. The internal sources and sinks at each water quality mesh cell are computed using the USACE mercury and water quality modules (TEMP, GC, NSMI and HgSM). These modules simulate the chemical speciation, chemical reactions, and transformations of state water quality variables. In the final step, the SRH-WQ model writes out simulated state variables, along with other dependent, derived and pathway variables, at a user-specified time interval so that the model results may be graphically processed for interpretation and project-specific applications. A typical mercury and water quality simulation may involve more than 30 state variables and hundreds of dependent, derived and pathway variables. Such a simulation requires a large number of input parameters, significant computer memory and storage capacity and other computing resources.

Major inputs for a mercury and water quality simulation include a simulation domain, a network of model cells arranged in a 2D mesh, flow variables, meteorological data, measured state variables from all inflow sources (boundary conditions), state variables at the start of simulation (initial condition), and a large number of model parameters representing physical and biochemical processes. Additional mercury and water quality data are required for model calibration and validation – these data, where available, are typically chosen for a range of flow conditions and other environmental conditions. Availability of reliable and comprehensive input data sets is limited although critical to ensure model validity for project applications.

Reliable simulation of the complex hydrochemistry of mercury and other water quality parameters demands a great number of parameters and coefficients, used to describe many biochemical reactive and transformation processes within each cell of the model mesh. Many of these model input parameters are user-specified.

3.1 A General Description

SRH-WQ conceptualizes the water body as follows. At each water quality mesh cell (a spatial location in the waterbody), two vertical zones are assumed: (a) a well-mixed water column; and (b) an active sediment layer at the top surface of the lake or riverbed. The active sediment layer represents a shallow, biologically active layer of surficial sediments. The depth of the sediment layer and other bed properties are user inputs and selected according to the problem at hand. The kinetics of water quality constituents is simulated by the model in both the water column and the sediment layer. Transport represented by state variables is simulated in the water column only.

3.1.1 Temperature Module (TEMP)

The TEMP module simulates two state variables: (a) the vertically averaged temperature in the water column; and (b) the average temperature in the active sediment layer. Only water temperature is simulated spatially by SRH-WQ.

Temperature is one of the most important simulation parameters in an aquatic system. It is an important water quality measure by itself. Most mercury and other water quality hydrochemistry parameters are functions of water and sediment temperatures which affect most biological and chemical reactions. In general the TEMP module is always included when other modules are included in the model simulation.

The TEMP module applies the energy balance equation to each cell in the model mesh. Heat inputs and outputs at the water surface and at the water-sediment interface are the heat processes considered in the energy balance. Simulated heat exchange at the water surface includes: (a) solar radiation, (b) atmospheric radiation, (c) back radiation from water to atmosphere; (d) evaporation/condensation (latent heat); and (e) heat conduction (sensible heat). Direct heat inputs/outputs through the open flow boundaries are treated separately.

In the water column, the energy balance equation can be written as follows:

$$q_{net} = q_s + q_{atm} - q_b + q_h - q_l + q_{sed}$$

where

- q_{net} = net heat flux entering the water column ($W\ m^{-2}$)
- q_s = short-wave solar radiation flux entering the water ($W\ m^{-2}$)
- q_{atm} = atmospheric long-wave radiation flux ($W\ m^{-2}$)
- q_b = back long-wave radiation flux ($W\ m^{-2}$)
- q_h = sensible heat flux ($W\ m^{-2}$)
- q_l = latent heat flux ($W\ m^{-2}$)
- q_{sed} = heat flux at the water-sediment interface ($W\ m^{-2}$)

The TEMP module, through use of the equilibrium water temperature concept, provides an alternative simpler equation to compute the net heat flux in the water column. The equilibrium temperature is defined as the water temperature at which all meteorological conditions remain constant with respect to time and space. This approach needs only three meteorological parameters: solar radiation, dew point temperature and wind speed. The net heat flux in a water column is simplified as:

$$q_{net} = K_T\left(T_{eq} - T_w\right)$$

where

- T_{eq} = equilibrium temperature (^oC) computed using an empirical function dependent on K_T , dew point temperature, and the solar radiation.
- K_T = overall heat exchange coefficient ($W\ m^{-2}\ {}^oC^{-1}$) which is an empirical function of wind speed, dew point temperature, and water temperature

Details of each parameter and how they are computed are described by Zhang and Johnson (2016a) and are not repeated in this report.

There is typically little heat exchange between the water column and the active sediment layer although heat exchange can become important in shallow areas. The heat balance for the active sediment layer can be written as follows:

$$\rho_s C_{ps} \frac{\partial T_{sed}}{\partial t} = \frac{q_{sed}}{h_2} = \rho_s C_{ps} \frac{\alpha_s}{h_2} \frac{T_{sed} - T_w}{0.5 h_2}$$

where

- T_{sed} = sediment temperature (^oC)
- t = time (s)
- ρ_s = sediment density ($kg\ m^{-3}$)
- C_{ps} = specific heat capacity of sediment ($J\ kg^{-1}\ {}^oC^{-1}$)
- h_2 = active layer thickness (m)
- α_s = sediment thermal diffusivity ($m^2\ s^{-1}$)

The above equation is used to compute both the sediment temperature and the heat exchange between water and sediment. Note that no heat exchange is assumed between the active layer and subsurface bed layer beneath (adiabatic).

Net heat flux is computed within the water column and water temperature is computed using the following transport equation:

$$\frac{\partial h T_w}{\partial t} + \frac{\partial h U T_w}{\partial x} + \frac{\partial h V T_w}{\partial y} = \frac{\partial}{\partial x}\left[\frac{h \nu_t}{\sigma_t}\frac{\partial T_w}{\partial x}\right] + \frac{\partial}{\partial y}\left[\frac{h \nu_t}{\sigma_t}\frac{\partial T_w}{\partial y}\right] + \frac{q_{net}}{C_{pw}\rho_w}$$

where

- T_w = water temperature (^oC)
- t = time (s)
- x and y = horizontal Cartesian coordinates (m)
- h = water depth *(m)*
- U and V = depth-averaged velocity components (m/s) in x and y directions, respectively
- ν_t = turbulent viscosity for dispersion (m^2/s)
- σ_t = thermal Prandtl number
- ρ_w = water density ($kg\ m^{-3}$)
- C_{pw} = specific heat capacity of water ($J\ kg^{-1}\ {}^oC^{-1}$)

The above equations establish the input parameters needed for the TMEP module, which will be discussed later. It should be noted that most chemical reaction coefficients for the mercury and water quality state variables are user-specified input parameters specified at a reference

temperature (usually at 20°*C*). These coefficients are corrected by the modules based on the difference between the actual temperature and the reference temperature. Three methods are used by the USACE water quality and mercury modules: the Arrhenius equation; Q10 equation; and the modified Arrhenius equation. Refer to Zhang and Johnson (2016b; p.17) for details.

The TEMP module requires several additional inputs besides the meteorological inputs that are described below..

A wind function is used to compute the latent and sensible heats and is expressed as:

$$f_W = (a + bW^c) f(R_i)$$

where

- a and b are user defined coefficients with the units of $bar^{-1}\ s^{-1}$ (the order of magnitude is 10^{-6}).
- c is a user defined coefficient close to 1 (dimensionless)
- W is the wind speed (m/s) at a 2 m height. It can be converted from speed at any height using eq. (2.12) from Zhang and Johnson (2016a).
- R_i is the Richardson number

The three coefficients (a, b and c) are user inputs applied through the USACE module control file and are geographical region dependent. The Richardson number function may use one of two options: (a) Option 1 is to use equation (2.14) in Zhang and Johnson (2016a); (b) Option 2 is to use a simple constant of 1.0.

The sensible heat describes the flux of heat through molecular or turbulent transfer between air and water surface. The amount of heat gained or lost through sensible heat depends on the temperature gradient in the vertical direction. The sensible heat flux (q_h) is computed using:

$$q_h = \left(\frac{K_h}{K_W} \right) C_p \rho_W (T_a - T_w) f_W$$

where

- C_p = specific heat capacity of air at a constant pressure (J kg-1 C-1)
- T_a = air temperature (°C)

- $\left(\frac{K_h}{K_W}\right)$ = diffusivity ratio (dimensionless). It is a user input parameter through the control file. The ratio allows users to partition the heat flux between latent and sensible heat. The diffusivity ratio is generally set to unity but the user may choose between 0.5 and 1.5 (values between 0.9 and 1.1 is recommended).

The TEMP module has no derived variables.

3.1.2 General Constituent Module (GC)

The GC module can be used to simulate variables not in the NSMI or HgSM modules. The state variables that can be simulated include TDS, salinity, user-definable dissolved constituents and suspended solids in the water column (they are advected), and user-definable particulate solids in the active sediment layer. They may be needed by other modules such as the HgSM module.

A user-specified number of dissolved constituents may be simulated in the water column resulting from the application of simple kinetic expressions. A dissolved constituent may represent a dissolved contaminant in the water column. The simple kinetic expressions include up to three processes: zero-order decay, first-order decay, and net settling loss. The rate equation is expressed as follows:

$$\frac{dC_i}{dt} = -k_{0i}(T) - k_{1i}(T)C_i - \frac{v_{si}}{h}C_i$$

where

- C_i = concentration of the constituent *i* (*mg L*$^{-1}$)
- k_{0i} = zero-order decay rate (*mg L*$^{-1}$*d*$^{-1}$)
- k_{1i} = first-order decay rate (*d*$^{-1}$)
- T = water temperature (*Celsius*)
- v_{si} = net settling loss rate (*m d*$^{-1}$)
- h = water depth (*m*)

Users need to supply the temperature dependent zero- and first-order decay rates for the constituent as well as the net settling loss rate. The net settling rate of a constituent can be negative depending on the degree of sediment re-suspension; a negative rate means that more constituent is added into the water column over time. Other contaminants with more complex reactions and transformations may be simulated using specialized modules such as HgSM or CSM (note: CSM is the contaminant module and is not incorporated into the current SRH-WQ).

User-selected numbers of particulate, inorganic, suspended solids can also be simulated in a water column. Suspended solids can provide adsorbing surfaces so that mercury in the water column may be lost or gained due to the settling and re-suspension of solids. A realistic simulation of suspended solids mass balance is, therefore, important for predicting mercury transport and suggesting the ultimate fate of mercury in aquatic systems. In the SRH-WQ model, these suspended solids represent the inorganic solids that are not simulated by the GC or NSMI modules and onto which mercury may be adsorbed.

Suspended solids simulated by the GC module may consist of both the inorganic fraction (silts and clays) and the organic fraction (e.g., algae, zooplankton, bacteria, and detritus). Both are important in creating turbidity and limiting light within the water column. In general, fine solids (silt, clay, POM, etc) are of greater importance than larger solids in water quality modeling due to their significantly higher adsorbing capacity and greater impact on underwater light attenuation.

An overview of the major processes of solids modeled by the GC module is shown in Figure 2 at a mesh cell. The water column and the underlying active sediment layer are assumed to be well-mixed. Suspended solids and attached contaminants such as mercury in the water column can be transferred to the sediment layer by settling. Contaminants such as mercury may also be released to water column through sediment re-suspension, mixing by benthic organisms and diffusion from the sediment pore water. A single sediment layer assumption with a constant thickness is used by the model because of its potential interactions with the overlying water column. The three most important sediment processes associated with contaminant modeling are settling, re-suspension (or “erosion”) and “burial”. In addition to these processes, the fate of solids in an aquatic system is also affected by physical transport.

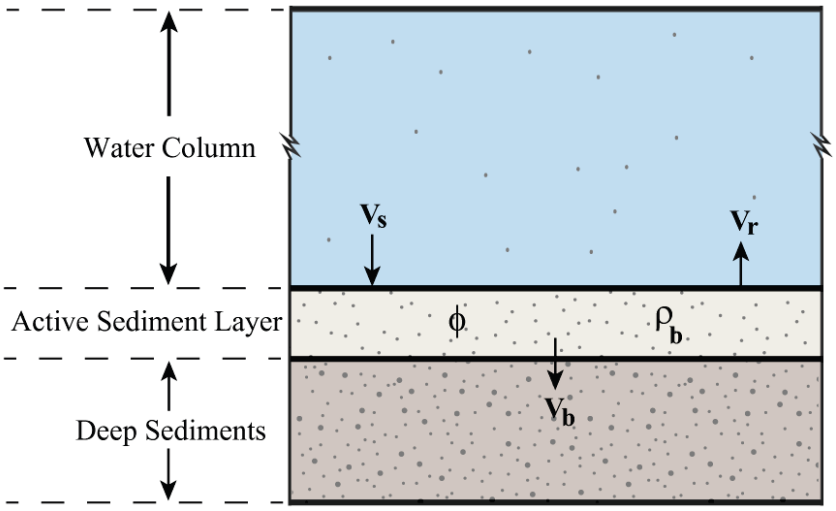

Figure 2. Conceptual representation of water column and bed sediment interactions for solids (V_s is the settling velocity; V_r is the re-suspension velocity; V_b is burial rate; ϕ is porosity; ρ_b is bulk density of the sediment layer) (source: Zhang and Johnson 2016b)

The GC module considers both sources and sinks in the water column and sediment layer. The time varying input parameters such as solids settling, re-suspension, and solids concentrations may be estimated or computed.

3.1.3 Nutrient Simulation Module (NSMI)

The NSMI module simulates aquatic eutrophication using simplified hydrochemistry processes and a minimal number of state variables. It computes biochemical reactive processes affecting state variables within each cell within the model mesh. The time rate of production (source) or destruction (sink) of constituent mass for each state variable is computed and utilized by the hydrologic model to simulate constituent fate and transport. The NSMI module includes up to 16 state variables to simulate water quality within a waterbody. These state variables can include algae, nitrogen and phosphorus cycles, carbon cycle, carbonaceous biochemical oxygen demand, dissolved oxygen, and pathogens within a water column. The NSMI module does not simulate benthic sediment processes through sediment diagenesis; such a simulation requires use of another USACE module named NSMII. This module is not yet developed and, upon completion, will be incorporated into the model in future.

The 16 state variables simulated by NSMI are as follows (see Table 2 from Zhang and Johnson 2016a):

- 3 nitrogen cycle state variables: organic nitrogen, ammonium, and nitrate (OrgN; NH4; NO3)

- 2 phosphorus cycle state variables: organic phosphorus and inorganic phosphorus (OrgP; TIP)
- 3 carbon cycle state variables: particulate and dissolved organic carbon and dissolved inorganic carbon (POC, DOC, DIC)
- 2 algae state variables: benthic algae (A_b) and floating algae (A_p -phytoplankton)
- 6 other state variables: dissolved oxygen (DO); carbonaceous biochemical oxygen demand (CBOD); particulate organic matter (POM); sediment particulate organic matter (POM2); pathogens (PX); and alkalinity(Alk)

Among the 16 state variables only 14 state variables represent the result of advection by the SRH-WQ transport module. Ab and POM2 are sediment layer variables and are therefore excluded.

A benthic sediment layer variable used by the NSMI module is the sediment oxygen demand (SOD). SOD is the rate of oxygen consumption exerted by benthic sediments and is a user input. Accounting for exchange fluxes of inorganic nutrients (NH4, NO3 and TIP) between the water column and sediment layer are also provided by the NSMI module.

The pH of the water column in aquatic environments is an important factor because some chemical processes are initiated only after the water column exceeds certain pH thresholds. The pH of the water column determines the solubility and biological availability of chemical constituents such as nutrients (nitrogen, phosphorus and carbon) and heavy metals (lead, copper, cadmium, etc.). The pH affects the ionization and hydrolysis of organic chemicals which have effects on chemical fate and the degree of chemical toxicity to biota. The pH is computed in the NSMI module based on DIC and alkalinity.

Not all 16 state variables need to be simulated for a specific project application. Users can select or deselect each state variable as needed inputs to the model. When a state variable is selected (On) - all internal source and sink terms associated with that state variable are computed for every time step. When not selected (Off) - no calculations are conducted for the source and sink terms for the state variable. When a state variable is ommitted, users do not need to provide any parameter inputs, boundary concentration values, or initial conditions for the state variables.

3.1.4 Mercury Simulation Module (HgSM)

The HgSM module is specifically included to simulate mercury cycling and mercury speciation kinetics in an aquatic system. Many of the concepts and kinetic expressions employed were adopted from the U.S. EPA developed Water Quality Analysis Simulation Program (WASP) (Wool et al. 2006) and the Electric Power Research Institute (EPRI) developed Dynamic Mercury Cycling Model (D-MCM) (EPRI 2013).

The HgSM module simulates three major Hg species: elemental mercury (abbreviated as Hg0), divalent inorganic mercury (abbreviated as HgII), and methylmercury (referred to as MeHg). Hg0 exists only in a water column in the dissolved phase while HgII and MeHg exist in both the water column and the sediment layer in the dissolved phase and the solid phase – adsorbed to either inorganic solids (simulated by the GC module) or organic solids such as DOC, POM and algae (simulated by the NSMI module). DOC and inorganic solids were found to be the two principal vehicles for MeHg and HgII transport (Lyon et al. 1997). Inorganic solids can be categorized as mineral abiotic solids, detrital solids, or miscellaneous solids of various size classes. The concentration of various mercury species are typically expressed in terms of nanograms per volumetric units of liter ($ng\ L^{-1}$).

Physical and biochemical processes simulated in the HgSM modeule include:

- adsorption and desorption
- volatilization
- atmospheric deposition
- diffusive exchange between the water column and sediment layer
- deposition and re-suspension
- sediment burial
- biogeochemical transformations between the three mercury species

The HgSM module computes only the kinetics of the mercury state variables in an aquatic system. An overview of the model representation of the mercury species and cycling processes in both water column and active sediment layer is shown in Figure 3 (labelled as Figure 6 of the report by Zhang and Johnson (2016b). Detailed equations for all the cycling and mercury species transformation processes were previously discussed by Zhang and Johnson (2016b) and are not covered in this report.

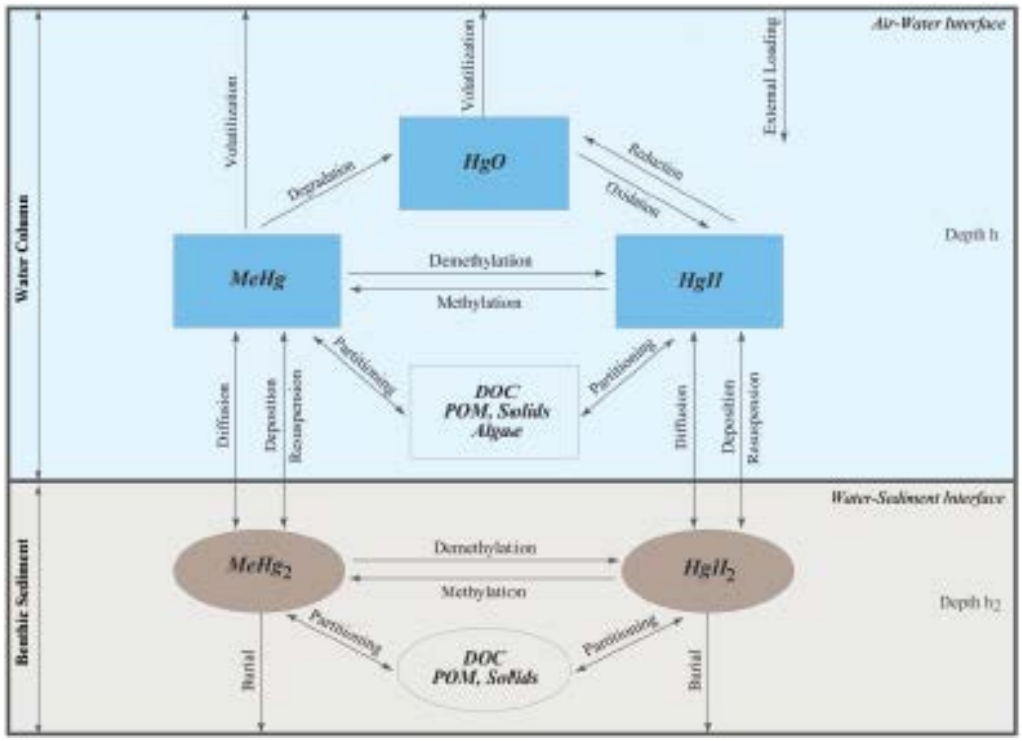

Figure 3. Conceptual representation of mercury speciation and hydrochemical processes (source: Zhang and Johnson 2016b)

3.2 General User Inputs

A list of general user-supplied model inputs are discussed first for a typical mercury and water quality simulation since they are shared by all associated model modules and are not tied to any specific module. These inputs are the dependent variables used in each module to compute values for the state variables.

Users are able to partition the model domain into a number of distinct subregions using the SMS material IDs (nRegion). Within a subregion, a uniform set of user-defined inputs are assigned for enable the simulation of water quality and mercury fate and transport. The subregion topology can be independent of the domain partitions used by the SRH-2D flow model which is typically used to assign unique flow roughness characteristics for each region.

The thickness of the active sediment layer should also be specified together with other bed layer properties. Note that different sediment layer thicknesses may be used by different modules as specified within the module control file. The sediment layer thickness can be varied as a calibration parameter for specific applications such as for certain important biochemical processes that occur in the sediment layer.

Initial and Boundary Conditions for all State Variables

Constant values of all state variables, both in water column and active sediment layer, are typically used by SRH-WQ transport module as initial conditions for unsteady (transient) modeling. These values can be spatially distributed within the model domain.

Time series data sets of all advected state variable are required at all model inflow boundaries to capture diurnal thermal processes and water quality dynamics. These time series inputs are used as boundary inflow/outflow conditions by the SRH-WQ transport model. Sufficient, high quality, temperature and water quality data must be collected at inflow boundaries and tributary inflow locations to ensure good model performance.

Meteorological Data:

Hourly meteorological data sets are typically required for modeling water quality and mercury transport in water bodies due to large potential fluctuations in air temperature and solar radiation. National weather stations (NWS) and nearby local meteorological stations are often able to provide these data. In general, meteorological stations installed near the water body specifically for modeling purposes tend to produce the best results. The following meteorological data is required for a full energy balance temperature simulation:

- solar radiation (W/m^2)
- atmospheric pressure (*atm*)
- air temperature (*Celsius*)
- vapor pressure of air (*mb*). The vapor pressure is a function of the moisture content of air (humidity). The actual vapor pressure of the air is the saturation vapor pressure at the dewpoint temperature. It can be computed from the dew point temperature, but normally is measured directly.
- cloud cover (dimensionless)
- wind speed (*m/s*)

Dependent Variables

Dependent variables are those which are used as inputs to compute the state variables contained in each module but that are also available from other modules. They are not user provided module inputs but are documented in this report to help users understand the combined data requirements of all the modules.

The TEMP Module needs the following dependent variables:

- water column depth and surface area for each mesh cell (from the Flow Module)
- depth-averaged water flow velocity for each mesh cell (from the Flow Module)
- Shear velocity at the base of the water column (from the Flow Module)

The GC Module needs the following dependent variables:

- Water column depth (from the Flow Module)
- Shear velocity at the base of the water column (from the Flow Module)
- Water column temperature (from the TEMP module)

The NSMI Module needs the following dependent variables:

- Water column depth, water flow velocity, shear velocity at base of the water column (from the Flow Module)
- Water and bed sediment temperature (from the TEMP Module)
- Salinity and suspended solids concentration (from the GC Module)

The HgSM Module uses the following dependent variables:

- Water column depth, shear velocity at the base of the water column, surface area of each mesh cell (from the Flow Module)
- Water and bed sediment temperature (from the TEMP Module)
- Suspended solids concentration in water and solids concentration in the active sediment layer, along with their properties such as settling velocity, resuspension velocity, and sediment burial velocity (from the GC Module)
- Apd, DOC, POM and POM2 (from the NSMI Module)
- Lambda and ka (from the NSMI Module as derived variables)

3.3 TEMP Module Specific Inputs

Additional inputs are required for the TEMP module besides the general inputs discussed above. The scalar values that need to be selected are listed below:

- Three coefficients for the wind function (see 3.1.1)
- Diffusivity ratio and Richardson function coefficients (see 3.1.1)
- Active sediment layer properties
    - Layer thickness
    - Layer bulk density, specific heat capacity, and thermal diffusivity (a default value for heat capacity $\rho_s C_{ps}$ is 0.64 $cal\ cm^{-3}\ ^oC^{-1}$)

If the water temperature and sediment temperature are not computed by the TEMP module, constant values are specified by default and used by the NSMI and the HgSM modules. This is not a recommended option.

Only 3 meteorological parameters are needed if the equilibrium temperature method is used: Solar radiation, dew point temperature, and wind speed. This option is not operational with the TEMP module at present.

The thermal diffusivity and heat capacity of the sediment layer may be obtained following the recommendations of Chapra et al. (2008). A list of their values are provided in Table **2** and were adapted from the report by Zhang and Johnson (2016a).

Table 2. Thermal properties of various sediment materials based on Chapra et al. (2008) (adapted from Zhang and Johnson 2016a)

Material	Conductivity	Diffusivity	ρ	Cp	$P \cdot Cp$
	cal s−1 cm−1 °C-1	cm2 s−1	g	cal (g °C)	cal (cm3 °C)
Sediment samples					
Mud flat (a)	0.0044	0.0048			0.906
Sand (a)	0.006	0.0079			0.757
Mud sand (a)	0.0043	0.0051			0.844
Mud (a)	0.0041	0.0045			0.903
Wet sand (b)	0.004	0.007			0.57
Sand 23% saturation with water (c)	0.0044	0.0126			0.345
Wet peat (b)	0.0009	0.0012			0.717
Rock (d)	0.0042	0.0118			0.357
Loam 75% saturation with water (c)	0.0043	0.006			0.709
Lake, gelatinous sediment (e)	0.0011	0.002			0.55
Concrete (e)	0.0037	0.008			0.46
Average of sediment samples	0.0037	0.0064			0.647
Component materials					
Water	0.0014	0.0014	1.00	0.999	1.000
Clay	0.0031	0.0098	1.49	0.210	0.310
Soil (dry)	0.0026	0.0037	1.50	0.465	0.700
Sand	0.0014	0.0047	1.52	0.190	0.290
Soil (wet)	0.0043	0.0045	1.81	0.525	0.950
Granite	0.0069	0.0127	2.70	0.202	0.540
Average of sediment samples	0.0033	0.0061	1.67	0.432	0.632

a Andrews and Rodvey (1980)
b Geiger (1965)
c Nakshabandi and Kohnke (1965)
d Chow et al. (1988 and Carslaw and Jaeger (1959)
e Hutchinson (1957), Jobson (1977), Likens and Johnson (1969)

3.4 GC Module Specific Inputs

Potential state variables of the GC module include salinity, TDS, dissolved constituents, suspended solids in water column, and solids in the active sediment layer. All state variables in the water column are advected. All state variables need initial conditions to be specified while only those in the water column require the selection of boundary conditions for the SRH-WQ transport module.

Salinity and suspended solids in water are used by the NSMI module; suspended solids in water and solids in the active layer are used by the HgSM module.

Additional user-specified inputs that need to be specified to enable model simulation are described below.

Dissolved Constituents

- The number of dissolved constituents simulated
- Zero-order decay rate for each dissolved constituent
- First-order decay rate for each dissolved constituent
- The net settling loss rate ($m\ d^{-1}$) for each dissolved constituent

Solids

The number of solid size classes is required; for each of these size classes the list of specified inputs is provided below:

- Solid density and diameter
- Deposition features:
    - Settling velocity (water column to active layer)
    - The lower and upper water column critical shear stresses for solid deposition
- Erosion features:
    - Re-suspension velocity (active layer to water column)
    - Critical shear stress for erosion
    - Critical shear stress for the initiation of movement of non-cohesive solids
    - Sediment surface erosion rate
    - Sediment erosion exponent
- The active sediment layer properties:
    - thickness (typically 10 cm)
    - sediment dry density (typically 2.7 $g\ cm^{-3}$)
    - sediment porosity (0.3 to 0.9)

- The sediment burial velocity: it is the rate of settling from the active layer to the deep sediments; it is normally computed automatically by the GC module based on the requirement that the active layer thickness remains constant.

The settling velocity for each solid can be obtained from field and laboratory measurements or the use of suggested values in Table 1 based on recommendations p.7) by Zhang and Johnson (2016b). The GC module also offers two empirical equations to compute the settling velocity: (a) the van Rijn formula and (b) the Cheng formula. The settling velocity may have to be calibrated for cohesive sediments since all the above methods do not consider concentration-dependent flocculation.

The sediment re-suspension velocity (equivalent to the erosion rate in $g\ cm^{-2}s^{-1}$) is a user-defined input parameter. Alternatively, using estimates for bottom shear stress, the GC module can compute the re-suspension velocity using one of three equations: (a) Lick et al. (1995); (2) Parchure and Mehta (1985); and (3) Lick (2009). The first two equations are applicable to cohesive sediment while the third equation is applicable to both. All three equations require inputs of critical shear stress and the erodibility coefficient. Typical values of critical shear stresses are on the order of 0.1-0.4 $N\ m^{-2}$.

The density of solids in the model is assigned a value of 2.65 *g m-3* which is applicable for most sediments (sands, silts, and clays). However, the solids density for carbon-occluded minerals ranges from 1.5 to 2.2 *g m-3* (Di Toro 2001). The porosity of the upper few centimeters of the sediment layer typically ranges from 0.7 to 0.9 or higher. The sediment porosity is known to decrease with solid particle diameter, where values range from approximately 0.7 - 0.9 for 0.001 mm to 0.3 for 1.0 mm (Di Toro 2001).

Note that the user-specified constant values of the following variables are needed if not simulated in the GC module give that they are used by the NSMI and HgSM modules. These variable are as follows:

- Salinity in the water column
- Solids concentration in both the water column and the sediment layer
- Settling velocity and the resuspension velocity of all solids

All relevant parameters related to the user-defined constituents and solids in the GC module are listed in Table 2 (p.15) of Zhang and Johnson (2016b).

3.5 NSMI Module Specific Inputs

Primary inputs to the NSMI module include the initial conditions for all 16 state variables and boundary conditions of all 14 advected state variables in the water column (as discussed in

Section 3.1.2). Additional module inputs are related to the biochemical processes that are mathematically simulated as described in Zhang and Johnson (2016a). All model input parameters associated with the NSMI module are listed below - details can be found in Table 6 of the report by Zhang and Johnson (2016a). These parameters can be accessed through the USACE WQ module control file.

Global Inputs

- Fraction of carbon in organic matter (focm)
  - It can range from 0 to 1.0 *mg-C mg-D*$^{-1}$ (0.4 is the default value)
- Partition coefficient (kdpo4) for inorganic P uptake by suspended solids (*L kg*$^{-1}$)
  - default value is 0.0
- Sediment oxygen demand (SOD; *mg-O*$_2$ *m*$^{-2}$ *d*$^{-1}$). It is expressed as a zero-order reaction. It ranges from 0.2 to 10.0 *mg-O*$_2$ *m*$^{-2}$ *d*$^{-1}$, and a default value of 0.5 *mg-O*$_2$ *m*$^{-2}$ *d*$^{-1}$ is recommended for natural SOD, and a value of 1.5 *mg-O*$_2$ *m*$^{-2}$ *d*$^{-1}$ for the total oxygen demand. The SOD rates are adjusted according to the local water depth and temperature. Some *in-situ* SOD values for some rivers and streams are also listed in Table 5 of Zhang and Johnson (2016a).
- The half saturation oxygen attenuation constant for SOD (KsSod; *mg-O*$_2$ *L*$^{-1}$) and 1.0 is the default.
- Method to compute pH (as a function of temperature, DIC and Alk)
  - 1 for Newt-Raphson method
  - 2 for Bisection method
- Hydraulic O_2 reaeration rate (kah; unit=*d*$^{-1}$)
  - It can range from 0.4 to 1.5 with temperature correction (default is 1.0) or 4.0 to 10 without temperature correction.
  - A constant may be specified, or a number of methods may be used to compute the rate. Options include: O'conner-Dobbins; Owens et al. and Churchill et al.; Melching-Flores (Pool&riffle); Melching-Flores (channel); Tsivoglou-Neal; Thackston-Dawson.
- Wind velocity effect on O_2 reaeration rate (kaw; unit=*m d*$^{-1}$)
  - It may be temperature corrected and the default is zero
  - Various kaw options may be used: 1=constant value; 2=Broecher et al.; 3=Gelda et al.; 4=Banks&Herrera; 5=Wanninkhof et al.; 6=Cole&Buchak; 7=Banks; 8=Smith; 9=Liss; 10=Downing&Truesdale; 11=Kanwisher; 12=Yu et al.; 13=Weiler
- Settling velocity (m/d) due to:
  - Suspended sediments
  - Organic N; Organic P; POC
- Light extinction coefficients due to:
  - lambda0: Background

- lambdas: Inorganic suspended sediment (GC)
- lambdam: Organic matter
- lambda1: algae with linear model
- lambda2: algae with nonlinear model

Algae in Water Column

- Algal stoichiometry for
  - Biomass (dry weight) (AWd; mg-D)
  - Carbon (AWc; mg-C)
  - Nitrogen (Awn; mg-N)
  - Phosphorus (AWp; mg-P)
  - Chlorophyll-a (Awa; µg-Chla)
- Algal growth
  - Maximum algal growth rate (mu_max; 1/d)
  - Light limiting constant for algal growth (KL; W m^{-2})
  - Algal growth rate formulation option: Multiplicative; Limiting and Nutrient; or Harmonic and Mean
  - Algal growth light limiting factor formulation option: Half and Saturation, Smith, or Steele
- Algal respiration and mortality rates (krp; kdp; 1/d)
- Algal settling velocity (vsap; m/d)
- Algal growth light limiting factor formulation (Half&Saturation|Smith|Steele)
- Half-saturation N and P limiting constants for algal growth (KsN; mg-N L^{-1}; KsP; mg-P L^{-1})
- NH4 preference factor for algal growth (PN)
- Fraction of algal mortality into POC (Fpocp)

Algae in Benthic Active Layer

- Benthic Algae Stoichiometry:
  - dry weight biomass (BWd; mg-D)
  - carbon (BWc; mg-C)
  - nitrogen (BWn; mg-N)
  - phosphorus (BWp; mg-P)
  - chlorophyll-a (BWa; µg-Chla)
- Benthic Algal Growth
  - Maximum benthic algal growth rate (mub_max; 1/d)
  - Light limiting constant for benthic algal growth (KLb; W m-2)
  - Benthic algal growth rate formulation option: Multiplicative; or Limiting-Nutrient

    - Benthic algal growth light limiting factor formulation option: Half and Saturation, Smith, or Steele
- Benthic algae base respiration rate (krb; 1/d)
- Benthic algae mortality rate (kdb; 1/d)
- Half-saturation limiting constant for benthic algal growth for N and P (KsNb; KsPb; mg/L)
- Half-saturation density constant for benthic algae growth (KSb; g-D m^{-2})
- NH4 preference factor for benthic algal growth (PNb)
- Fraction of benthic algae mortality into POC (Fpocb)
- Fraction of benthic algae mortality into water column (Fw)
- Fraction of bottom area available for benthic algae growth (Fb)

Nitrogen Cycle

- Organic nitrogen hydrolysis rate (KON; 1/d)
- Nitrification rate (KNit; 1/d)
- Denitrification rate (KDNit; 1/d)
- Sediment denitrification velocity (VNO3; m/d)
- Half-saturation oxygen inhibition constant for denitrification (KsOxdn; mg-O2/L)
- Benthos NH4 release rate (RNH4; g-N m^{-2} d^{-1}) (or sediment release rate of NH4)

Phosphorus Cycle

- Organic P decay/hydrolysis rate to DIP (KOP; 1/d)
- Benthic sediment release rate of DIP (RPO4; g-P m^{-2} d^{-1})

Carbon Cycle

- POC hydrolysis rate (KPOC; 1/d)
- DOC oxidation rate (KDOC; 1/d)
- Half-saturation oxygen attenuation constant for DOC oxidation (KsOxmc; mg-O2/L)
- Fraction of total inorganic carbon (DIC) in CO2 (FCO2)
- Partial pressure of CO2 (PCO2; ppm)

Carbonaceous biochemical oxygen demand (CBOD)

- CBOD oxidation rate (KBOD; 1/d)
- CBOD sedimentation rate (KsBOD; m/d)
- Half-saturation oxygen attenuation constant for CBOD oxidation (KsOxBOD; mg-O/L)

Pathogens (Px)

- Pathogen death rate (Kdx; 1/d)
- Light efficiency factor for pathogen death (Apx)
- Pathogen settling velocity (Vx; m/d)

Particulate Organic Matter (POM)

- POM settling velocity (Vsom; m/d)
- POM dissolution rate (KPOM; 1/d)
- Sediment POM dissolution rate (KPOM2; 1/d)
- Active sediment layer thickness (h2; m)
- Sediment burial velocity (Vb; m/d)

The NSMI module outputs include the concentrations of water quality state variables and other intermediate variables. (See Table 2 in Zhang and Johnson (2016a) for a complete list of all water quality state variables, Table 7 for all derived variables, and Table 8 for all pathway fluxes).

The following variables are user-specified if they are not simulated by the NSMI module and if the HgSM module is included in the simulation:

State Variables:

- Algae in the water column (Apd)
- DOC in the water column (DOC)
- POM in both the water column and sediment layer (POM; POM2)

Derived Variables:

- Lambda
- Ka
- pH
- Burial velocity (Vb)

3.6 HgSM Module Inputs

General user inputs for the HgSM module include the air concentrations of Hg0 and MeHg as well as DOC and SO4 in the active sediment layer (SO42; DOC2)

HgII and MeHg are partitioned into dissolved phase and solid phases adsorbed to inorganic suspended sediments in the GC module and organic solids in the NSMI module representing algae, DOC and POM. Both equilibrium and non-equilibrium approaches can be used to determine the phase partition. The related partition parameters are user inputs and they are described in Section 4.2.2 (p.66) of Zhang and Johnson (2016b).

Mercury species can be transformed through a number of reactive processes including oxidation, reduction, methylation and demethylation. Some of the reaction processes are not well understood and thus are not well defined. Hence simplified transformation processes are simulated in the HgSM module. Table 3 below summarizes the key reaction and transformation processes considered by HgSM. The input parameters include the rate constants for transformations that are mostly temperature dependent but include those that are also sunlight dependent. Section 4.3 of Zhang and Johnson (2016b) provides additional details on these transformations.

Table 3. Mercury species and their transformations modeled by HgSM (Source: Zhang and Johnson 2016b)

Species	Water column			Sediment layer	
	Hg0	HgII	MeHg	HgII	MeHg
Hg0		Oxidation (Hg0-->HgII)			
HgII	Photoreduction (HgII-->Hg0)		Methylation (HgII-->MeHg)		Methylation (HgII-->MeHg)
MeHg	Photoreduction (MeHg-->Hg0)	Demethylation (MeHg-->HgII)		Demethylation (MeHg-->HgII)	

Several studies have indicated that HgII methylation is the primary source of MeHg in aquatic systems (USEPA 1997; EPRI 2013). Methylation takes place mainly in surface layers of sediments although it can also take place in the water column but at a reduced rate (Regnell et al. 1996). HgII can be methylated to MeHg in the water phase through biotic pathways or abiotic pathways and is simulated by considering the dissolved phase and the DOC sorbed phase. In the active sediment layer sulfate reducing bacteria (SRB) are the most important catalysts of biological methylation of HgII. Strong relationships were observed between sulfate reduction rates and HgII methylation rates in sediments (Benoit et al. 1999; King et al. 1999; King et al. 2001). This relationship is non-linear and has been adopted by the HgSM module. Sulfate (SO4) concentration, therefore, is an important factor affecting methylation rates and needs to be considered in the simulation.

Atmospheric deposition of HgII and MeHg into the water column are represented by the sum of wet and dry mercury deposition. Areal atmospheric deposition rates are necessary module inputs.

The volatilization of Hg0 and MeHg from the water column to air are simulated at the surface of the water column but volatilization of HgII is ignored since HgII has a much lower Henry's Law Constant (USEPA 1997). Volatilization rates, referenced to a standard temperature of 20° C, can be user defined..Mercury species concentrations in the atmosphere and the Henry's Law constant are the required user inputs.

HgII and MeHg may settle to the sediment layer or be re-suspended as solid particles. In addition, HgII and MeHg may also be buried to occur at deeper sediment layers. The settling velocities of POM, algae and solids, the re-suspension velocities of solids, and the burial velocity for POM and solids are the relevant module input parameters.

The dissolved forms of HgII and MeHg may also exchange mass through diffusion at the sediment-water interface. The mass-transfer velocities are either user specified parameters or are internally computed. Four internal equations are available to the HgSM module, namely: (1) Thibodeaux et al. (2001), (2) Di Toro et al. (1981), (3) Boyer et al. (1994), and (4) Schink and Guinasso (1977). The report of Zhang and Johnson (2016b) contains additional details.

The summary of model parameter input values that should be entered through the control file are summarized below:

Mercury Global Parameters:

- Algae settling velocity (VsAp; m/d)
- POM settling velocity (VsOM; m/d)
- Active sediment layer thickness (h2; m)
- Sediment layer porosity (Por)
- Sediment average bioturbed depth (z2; cm)
- Sediment dry density (ps; g/cm3)
- Biodiffusion coefficient representing particle diffusivity in the bed (Db; cm2/d)
- Water-side benthic boundary layer mass transfer coefficient (Beta; cm/d)
- Coefficient to adjust light attenuation (Alpha)
- Maximum relative error of the numerical solution (res)

Elementary Mercury (Hg0) Parameters:

- Hg0 molecular weight (MW; g/mol)
- Hg0 solubility (Hgds; ng/L)

- Hg0 oxidation rate (k12; 1/d)
- Hg0 oxidation yield coefficient (Y12; g/g)
- Hg0 activation energy of oxidation rate (Ea12; kJ/mol)
- Hg0 oxidation correction reference temperature (Tr12; oC)
- Hg0 Henry's constant (KH; Pa m3/mol)
- Hg0 volatilization velocity (Vv; m/d)
- Hg0 volatilization velocity option: 1=Constant above; 2=Computed

Inorganic Mercury (HgII) Parameters:

- General Parameters
    - HgII molecular weight (MW; g/mol)
    - HgII solubility (Hgds; ng/L)
    - HgII molecular diffusivity (Dm; m2/d)
    - HgII sediment-water mass transfer velocity (Vm; m/d)
    - HgII sediment-water mass transfer velocity option: 1=Constant above; 2=Thibodeaux et al. (2001); 3=Boyer et al. (1994); 4=Di Toro et al. (1981); 5=Schink&Guinasso(1977)

- The water column with the equilibrium partitioning (all phases lumped together)
    - HgII equilibrium partition coefficient for DOC in water (Kdoc; L/kg)
    - HgII equilibrium partition coefficient for DOC in sediment (Kdoc2; L/kg)
    - HgII equilibrium partition coefficient for algae (Kap; L/kg)
    - HgII equilibrium partition coefficient for POM in water (Kpom; L/kg)
    - HgII equilibrium partition coefficient for POM in sediment (Kpom2; L/kg)
    - HgII equilibrium partition coefficient for solid i in GC module in water (Kp_i; L/kg)
    - HgII equilibrium partition coefficient for solid i in GC module in sediment (Kp2_i; L/kg)

- Water column under non-equilibrium partitioning (each phase is done separately)
    - Algae adsorbed HgII
        - Langmuir adsorption constant for algae (Klap; L/ug)
        - Algae adsorption capacity (qcap; ug/g)
        - Freundlich adsorption constant for algae [Kfap; (ug/g)(L/ug)b]
        - Freundlich exponent for algae (bap)
    - POM adsorbed HgII
        - Langmuir adsorption constant for POM in water (Klpom; L/ug)
        - POM adsorption capacity in water (qcpom; ug/g)
        - Freundlich adsorption constant for POM in water [Kfpom; (ug/g)(L/ug)b]

        - Freundlich exponent for POM in water (bpom)
        - Langmuir adsorption constant for POM in sediment (Klpom2; L/ug)
        - POM adsorption capacity in sediment (qcpom2; ug/g)
        - Freundlich adsorption constant for POM in sediment [Kfpom2; (ug/g)(L/ug)b]
        - Freundlich exponent for POM in sediment (bpom2)
    - Solids adsorbed HgII
        - Langmuir adsorption constant for solid i in water (Klp_i; L/ug)
        - Solid i adsorption capacity in water (qcp_i; ug/g)
        - Freundlich adsorption constant for solid i in water [Kfp_i; (ug/g)(L/ug)b]
        - Freundlich exponent for solid i in water (bp_i)
        - Langmuir adsorption constant for solid i in sediment (Klp2_i; L/ug)
        - Solid i adsorption capacity in sediment (qcp2_i; ug/g)
        - Freundlich adsorption constant for solid i in sediment [Kfp2_i; (ug/g)(L/ug)b]
        - Freundlich exponent for solid i in sediment (bp2_i)
    - Numerical method selection for computing nonlinear partition: 1=Newton-Raphson; 2=Bisection.

- Photoreduction
    - Photoreduction rate for dissolved HgII (kd21; 1/d)
    - Photoreduction rate for DOC sorbed HgII (kdoc21; 1/d)
    - Light intensity when aquatic photolysis rate is measured (I0pht; W/m2)
    - Photoreduction yield coefficient in water (Y21; g/g)

- Methylation
    - Methylation rate for dissolved HgII in water (kd23; 1/d)
    - Methylation rate for DOC sorbed HgII in water (kdoc23; 1/d)
    - Methylation yield coefficient in water (Y23; g/g)
    - Sediment sulfate reduction rate (kso42; 1/d)
    - Ratio of methylation rate and sulfate reduction rate in sediment (rmso4; (L/mg)
    - Half saturation constant for the effect of sulfate on methylation (Kso4; mg-O2/L)

Methylmercury (MeHg) Parameters:

- General Parameters
    - MeHg molecular weight (MW; g/mol)
    - MeHg solubility (Hgds; ng/L)
    - MeHg molecular diffusivity (Dm; m2/d)

- MeHg sediment-water mass transfer velocity (Vm; m/d)
- MeHg sediment-water mass transfer velocity option: 1=Constant above; 2=Thibodeaux et al. (2001); 2=Boyer et al. (1994); 3=Di Toro et al. (1981); 4=Schink&Guinasso (1977)
- MeHg Henry's constant (KH; Pa m3/mol)
- MeHg volatilization velocity (Vv; m/d)
    - MeHg volatilization velocity option: 1=Constant above; 2=Computed

- Partition Parameters
    - MeHg equilibrium partition coefficient for DOC in water (Kdoc; L/kg)
    - MeHg equilibrium partition coefficient for DOC in sediment (Kdoc2; L/kg)
    - MeHg equilibrium partition coefficient for algae (Kap; L/kg)
    - MeHg equilibrium partition coefficient for POM in water (Kpom; L/kg)
    - MeHg equilibrium partition coefficient for POM in sediment (Kpom2; L/kg)
    - MeHg equilibrium partition coefficient for solid i in water (Kp_i; L/kg)
    - MeHg equilibrium partition coefficient for solid i in sediment (Kp2_i; L/kg)
    - Numerical method for computing nonlinear partition: 1=Newton-Raphson; 2=Bisection

- Adsorption Parameters
    - Langmuir adsorption constant for algae (Klap; L/ug)
        - Algae adsorption capacity (qcap; ug/g)
    - Langmuir adsorption constant for POM in water (Klpom; L/ug)
        - POM adsorption capacity in water (qcpom; ug/g)
    - Langmuir adsorption constant for POM in sediment (Klpom2; L/ug)
        - POM adsorption capacity in sediment (qcpom2; ug/g)
    - Langmuir adsorption constant for solid i in water (Klp_i; L/ug)
        - Solid i adsorption capacity in water (qcp_i; ug/g)
    - Langmuir adsorption constant for solid i in sediment (Klp2_i; L/ug)
        - Solid i adsorption capacity in sediment (qcp2_i; ug/g)
    - Freundlich adsorption constant for algae [Kfap; (ug/g)(L/ug)b]
        - Freundlich exponent for algae (bap)
    - Freundlich adsorption constant for POM in water [Kfpom; (ug/g)(L/ug)b]
        - Freundlich exponent for POM in water (bpom)
    - Freundlich adsorption constant for POM in sediment [Kfpom2; (ug/g)(L/ug)b]
        - Freundlich exponent for POM in sediment (bpom2)
    - Freundlich adsorption constant for solid i in water [Kfp_i; (ug/g)(L/ug)b]
        - Freundlich exponent for solid i in water (bp_i)
    - Freundlich adsorption constant for solid i in sediment [Kfp2_i; (ug/g)(L/ug)b]
        - Freundlich exponent for solid I in sediment (bp2_i)

- Photoreduction
    - Photoreduction rate for dissolved MeHg (kd31; 1/d)
    - Photoreduction rate for DOC sorbed MeHg (kdoc31; 1/d)
    - Light intensity when aquatic photolysis rate is measured (I0pht; W/m2)
    - Photoreduction yield coefficient (Y31; g/g)

- Demethylation
    - Demethylation rate from dissolved MeHg to HgII in water (kd32; 1/d)
    - Demethylation rate from DOC sorbed MeHg to HgII in water (kdoc32; 1/d)
    - Demethylation yield coefficient in water (Y32; g/g)
    - Demethylation rate from dissolved MeHg to HgII in sediment (kd32_2; 1/d)

A compilation of all HgSM parameters are listed in Table 25 (p.93) of the report by Zhang and Johnson (2016b) – that table is reproduced in this report for convenient reference. The original report also provides detailed on the equations used in the model and appropriate parameter values for these equations. Literature values were used from a number of available published studies; most are model parameters obtained from model calibration in real-world applications. The parameters for the water column and sediment layer can be specified as either a uniform constant for all mesh cells, or spatially-varying values in different user specified regions. There are three groups of parameters: global, water column and sediment layer. The table will be repeated for each water quality region, allowing the user to choose appropriate values for input parameters.

Table 4. List of all input parameters of HgSM (Source: Zhang and Johnson 2016b)

Symbol	Definition	Default values	Approximate range	Units	Temp correction	
Global						
D_m	Molecular diffusivity	-	n/a	$m^2\ d^{-1}$		
v_m	Sediment-water mass transfer velocity	-	n/a	$m\ d^{-1}$		
h_2	Sediment layer thickness	0.1 – 0.15	m			
z_2	Sediment bioturbation layer thickness	0.05 – 0.1	m			
v_{ss}	Solids settling velocity	-	n/a	$m\ d^{-1}$		
v_{som}	Organic matter settling velocity	-	n/a	$m\ d^{-1}$		
$k_{pht}(T)$	Aquatic photolysis rate	-	n/a	d^{-1}	E_a	n/a
I_{0pht}	Light intensity when kpht is measured	-	n/a	$W\ m^{-2}$		
α_I	Light attenuation adjusting coefficient	1.33	1.2 - 1.6	unitless		
Water column - elemental mercury						
MW	Hg0 molecular weight[a]	200.6	-	$g\ mol^{-1}$		
S_{Hg0}	Hg0 solubility	56	-	$\mu g\ L^{-1}$		
$v_{v\text{-}Hg0}(T)$	Hg0 volatilization velocity[f]	0.006	0.0059 – 0.45	$m\ hr^{-1}$	θ	n/a
K_H	Hg0 Henry's Law constant	0.09[l]	-	$Pa\ m^3\ mol^{-1}$		
$Hg0_0$	Hg0 air concentration	2.10^{-3}	n/a	$ng\ L^{-1}$		
$k_{12}(T)$	Hg0 oxidation rate[b]	10^{-3}	10^{-3} - 10^{-1}	d^{-1}	E_a	n/a
Y_{12}	Hg0 oxidation yield coefficient	1.0	0 - 2.0	unitless		
Water column - inorganic mercury						
MW	HgII molecular weight[a]	271.52	232.68 (HgS) 271.52 ($HgCl_2$)	$g\ mol^{-1}$		
$K_{p\text{-}HgII}$	HgII equilibrium partition coefficient for algae[c]	-	10^5 - 10^6	$L\ kg^{-1}$		
$K_{p\text{-}HgII}$	HgII equilibrium partition coefficient for silt[b]	2.10^5	10^3 - 10^6	$L\ kg^{-1}$		
$K_{p\text{-}HgII}$	HgII equilibrium partition coefficient for clay[b]	2.10^5	10^3 - 10^6	$L\ kg^{-1}$		
$K_{p\text{-}HgII}$	HgII equilibrium partition coefficient for solids[e]	$10^{5.3}$	$10^{4.2}$ - $10^{6.9}$	$L\ kg^{-1}$		
b_{HgII}	HgII Freundlich exponent[h]	-	0.4 – 1.2	unitless		
$K_{f\text{-}HgII}$	HgII Freundlich adsorption constant[h]	-	$4.5{\cdot}10^4$ – $2.52{\cdot}10^8$	$(\mu g\ g^{-1})\ (\mu g\ L^{-1})^{-b}$		

$K_{I\text{-}HgII}$	HgII Langmuir adsorption constant[h]	-	10^{6} – $7{\cdot}10^{6}$	L μg^{-1}		
$q_{cn\text{-}HgII}$	HgII adsorption capacity for solid "n"[h]	-	$2.8{\cdot}10^{2}$ – $3.58{\cdot}10^{3}$	μg g^{-1}		
$k_{adn\text{-}HgII}$	HgII adsorption coefficient	-	n/a	L μg^{-1} d^{-1}		
Symbol	Definition	Default values	Approximate range	Units	Temp correction	
$k_{dan\text{-}HgII}$	HgII desorption rate	1.0	n/a	d^{-1}		
$k_{doc\text{-}HgII}$	HgII partition coefficient for DOC[e]	$10^{5.3}$	$10^{5.3}$ - $10^{5.6}$	L kg^{-1}		
k_{d21}	Dissolved HgII photoreduction rate[b]	5.10^{-2}	10^{-3} - $5{\cdot}10^{-1}$	d^{-1}		
k_{doc21}	DOC adsorbed HgII photoreduction rate[b]	0.0	10^{-3} - $5{\cdot}10^{-1}$	d^{-1}		
Y_{21}	HgII photoreduction yield coefficient	1.0	0 - 2.0	unitless		
$k_{d23}(T)$	Dissolved HgII methylation rate[b]	10^{-3}	10^{-5} - $5{\cdot}10^{-2}$	d^{-1}	θ	1.14
$k_{doc23}(T)$	DOC adsorbed HgII methylation rate[b]	10^{-3}	10^{-5} - $5{\cdot}10^{-2}$	d^{-1}	θ	1.14
Y_{23}	HgII methylation yield coefficient	1.07	0 - 2.0	unitless		
Water column – methymercury						
MW	MeHg molecular weight[a]	230.66 ($CH3_2Hg$)	n/a	g mol^{-1}		
$K_{p\text{-}MeHg}$	MeHg equilibrium partition coefficient for algae[g]	10^{5}	10^{5} - 10^{7}	L kg^{-1}		
$K_{p\text{-}MeHg}$	MeHg equilibrium partition coefficient for silt[b]	$2{\cdot}10^{5}$	10^{3} - 10^{6}	L kg^{-1}		
$K_{p\text{-}MeHg}$	MeHg equilibrium partition coefficient for caly[b]	$2{\cdot}10^{5}$	10^{3} - 10^{6}	L kg^{-1}		
$K_{p\text{-}MeHg}$	MeHg equilibrium partition coefficient for solids[e]	$10^{5.4}$	$10^{4.2}$ - $10^{6.2}$	L kg^{-1}		
$K_{doc\text{-}MeHg}$	MeHg equilibrium partition coefficients for DOC[b]	$2{\cdot}10^{5}$	10^{5} - 10^{6}	L kg^{-1}		
b_{MeHg}	MeHg Freundlich exponent	-	n/a	unitless		
$K_{f\text{-}MeHg}$	MeHg Freundlich adsorption constant	-	n/a	(μg g^{-1}) (μg L^{-1})$^{-b}$		
$K_{I\text{-}MeHg}$	MeHg Langmuir adsorption constant[h]	-	n/a	L μg^{-1}		
$q_{cn\text{-}MeHg}$	MeHg adsorption capacity for solid "n"	-	n/a	μg g^{-1}		
k_{d31}	Dissolved MeHg photoreduction rate into Hg0[b]	-	10^{-3} - $5{\cdot}10^{-1}$	d^{-1}		
k_{doc31}	DOC adsorbed MeHg photoreduction rate into Hg0[b]	0.0	10^{-3} - $5{\cdot}10^{-1}$	d^{-1}		

Y_{31}	MeHg photoreduction yield coefficient	0.93	0 - 2.0	unitless		
k_{d32}	Dissolved MeHg demethylation rate into HgII[b]	$5{\cdot}10^{-2}$	10^{-3} - $5{\cdot}10^{-1}$	d^{-1}		
k_{doc32}	DOC adsorbed MeHg demethylation rate into HgII[b]	0.0	10^{-3} - $5{\cdot}10^{-1}$	d^{-1}		
Symbol	Definition	Default values	Approximate range	Units	Temp correction	
Y_{32}	MeHg demethylation yield coefficient	0.93	0 - 2.0	unitless		
$v_{v\text{-}MeHg}(T)$	MeHg volatilization velocity	$1.9{\cdot}10^{-5}$	n/a	$m\ d^{-1}$	θ	n/a
K_H	MeHg Henry's constant	$4.5{\cdot}10^{-6}$ [l]	n/a	$Pa\ m^3\ mol^{-1}$		
$MeHg_0$	MeHg air concentration	0.0	n/a	$ng\ L^{-1}$		
Sediment layer - inorganic mercury						
$K_{p\text{-}HgII2}$	HgII equilibrium partition coefficient for silt[b]	-	10^{3} - 10^{6}	$L\ kg^{-1}$		
$K_{p\text{-}HgII2}$	HgII equilibrium partition coefficient for clay[b]	-	10^{3} - 10^{6}	$L\ kg^{-1}$		
$K_{p\text{-}HgII2}$	HgII equilibrium partition coefficient for solids[e]	$10^{4.9}$	$10^{3.8}$ - 10^{6}	$L\ kg^{-1}$		
b_{HgII2}	HgII Freundlich exponent	-	n/a	unitless		
$K_{f\text{-}HgII2}$	HgII Freundlich adsorption constant	-	n/a	$(\mu g\ g^{-1})\ (\mu g\ L^{-1})^{-b}$		
$K_{l\text{-}HgII2}$	HgII Langmuir adsorption constant[d]	-	51 - 390	$L\ \mu g^{-1}$		
$q_{cn\text{-}HgII2}$	HgII adsorption capacity for solid "n"	-	n/a	$\mu g\ g^{-1}$		
$k_{adn\text{-}HgII2}$	HgII adsorption coefficient	-	n/a	$L\ \mu g^{-1}\ d^{-1}$		
$k_{dan\text{-}HgII2}$	HgII desorption rate	0.1	n/a	d^{-1}		
$k_{doc\text{-}HgII2}$	HgII partition coefficient for DOC[b]	-	10^{4} - 10^{5}	$L\ kg^{-1}$		
$k_{so42}(T)$	Sediment SO4 reduction rate	-	-	d^{-1}	θ	n/a
K_{SO4}	Half-saturation constant for the effect of SO4 on methylation	-	-	$mg\text{-}O_2\ L^{-1}$		
r_{mso4}	Ratio of sediment methylation rate and sulfate reduction rate	-	-	$L\ mg^{-1}$		
Sediment layer - methymercury						
$K_{p\text{-}MeHg2}$	MeHg equilibrium partition coefficient for silt[b]	-	10^{3} - 10^{6}	$L\ kg^{-1}$		
$K_{p\text{-}MeHg2}$	MeHg equilibrium partition coefficient for clay[b]	-	10^{3} - 10^{6}	$L\ kg^{-1}$		
$K_{p\text{-}MeHg2}$	MeHg equilibrium partition coefficient for solids[e]	$10^{3.6}$	$10^{2.8}$ - 10^{5}	$L\ kg^{-1}$		
$K_{doc\text{-}MeHg2}$	MeHg equilibrium partition coefficients for DOC[b]	-	10^{5} - 10^{6}	$L\ kg^{-1}$		

b_{MeHg2}	MeHg Freundlich exponent	-	n/a	Unitless		
$K_{f–MeHg2}$	MeHg Freundlich adsorption constant	-	n/a	$(\mu g\ g^{-1})\ (\mu g\ L^{-1})^{-b}$		
$K_{l–MeHg2}$	MeHg Langmuir adsorption constant[d]	-	n/a	$L\ \mu g^{-1}$		
$q_{cn–MeHg2}$	MeHg adsorption capacity for solid "n"	-	n/a	$\mu g\ g^{-1}$		
$k_{d32\text{-}2}(T)$	Sediment MeHg demethylation rate	0.2[j]	-	d^{-1}	E_a	n/a

a. ATSDR (2005).

b. Wool (et al. 2006).

c. Hudson et al. (1994).

d. Tsiros and Ambrose (1999).

e. Allison and Allison (2005).

f. Loux (2004).

g. Miles et al. (2001).

h. Chen et al. (2009).

l. Lin et al. (2012).

j. Gilmour et al. (2007).

Note that the active sediment layer retains a constant volume and thickness during a model simulation. Sediment particle density and porosity are fixed. Settling velocities of solid particles and the particle re-suspension rate are computed from the GC module.

4. Tutorial Cases to Illustrate the Procedure to Run SRH-WQ

Running simulations of water quality and mercury with the SRH-WQ model follows the following steps:

1. Select model domain and generate an appropriate 2D model mesh for simulation.
2. Run the SRH-2D model to obtain flow outputs at a user-specified time interval
3. Run the SRH-WQ model to obtain updated values for all state variables

Two tutorial cases are presented in this chapter to illustrate the entire modeling process using both SRH-2D and SRH-WQ. These tutorials can be followed by novice users to learn the general principles of carrying out a water quality and mercury simulation. The first tutorial uses the TEMP module only while the second covers the setup of a mercury transport and cycling simulation.

4.1 A Tutorial Case Running TEMP Module

4.1.1 Model Domain and Mesh Generation

A simple example has been formulated to run the TEMP module. The model domain consists of a simple channel with length of 100 miles and width of 2 miles. Mesh generation is simple and final mesh has a total of 100 cells in the flow direction and 2 cells in the lateral direction (one mile in mesh size). The 2D mesh is generated using Aquaveo's SMS software. The water flow is from left to right and the two lateral boundaries (top and bottom) are given the labels "Symmetry" within the SRH-2D model. The channel is assumed flat and bed elevation is zero. The model domain and the mesh are shown in Figure 4.

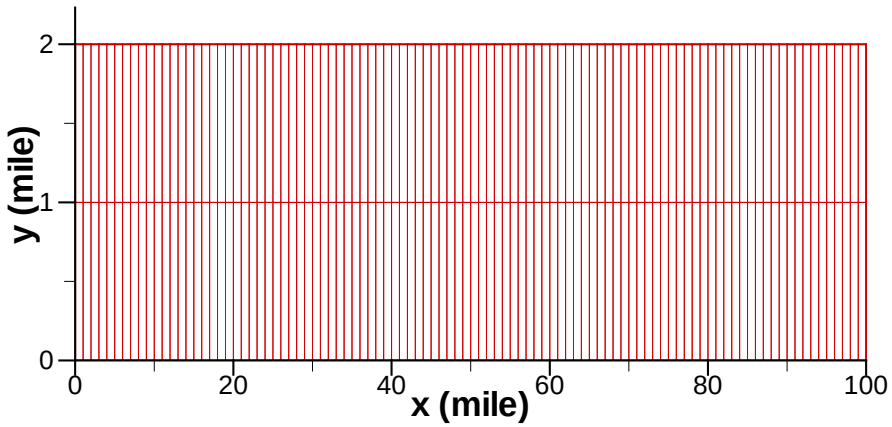

Figure 4. Model domain and the mesh for the TEMP module tutorial case (1:20 scale between x and y axis)

4.1.2 Flow Modeling with the SRH-2D model

Unsteady (time varying) flow simulations are performed as part of all water quality and mercury model simulations even if the actual flow does not change with time (steady). Before initiating an unsteady run, a steady-state model analysis should be completed so that the results of the steady run may be used as the initial condition to the unsteady simulation. For this tutorial example a constant flow discharge of 645.3 ft^3/s, leading to a flow velocity of 1 mile/day, is imposed on the left side of the model domain.The fixed water stage on the right boundary of the domain is set to 1.0. A constant flow velocity of 1 mile/day was obtained by SRH-2D assuming zero channel friction.

Lai (2008; 2010) has performed SRH-2D simulations for many years and the results of these simulations have been well documented - hence no model details are included in this report. It is sufficient to list the input data file (_SIF.dat) created by SRH-2D preprocessor (shown below) since this file, plus the 2D mesh file, are the only inputs needed to perform a steady flow simulation.

Below is a list of the _SIF.dat file:

```
// Simulation Description (not used by SRH-2D):
Steady Run for Case1
// Module/Solver Selected (FLOW MOB TEM TC WQ)
FLOW
// Monitor-Point-Info: NPOINT
1
99.99 1.0
// Steady-or-Unsteady (STEADY/UNS)
STEADY
0 360 25000
// Turbulence-Model-Selection(PARA or KE)
PARA
0.7
// Initial Condition Method (DRY RST AUTO ZONAL)
DRY
// Mesh-Unit (FOOT METER INCH MM MILE KM GSCALE)
MILE
mesh1.2DM SMS
// Manning Roughness Input Method(1=uniform 2=2DM 3=(x y) distributed
1
1.e-10
// Any-Special-Treatments? (0 or empty = NO; 1=YES)

// Boundary Type (INLET-Q EXIT-H etc)
INLET-Q
   645.33333 EN V
EXIT-H
   1.0 EN
SYMM
SYMM
MONITOR
// Wall-Roughess-Height-Specification (empty-line=DONE)

// Any In-Stream Flow Obstructions? (empty-line or 0 = NO)

// Results-Output-Format-and-Unit(SRHC/TEC/SRHN/XMDF;SI/EN) + Optional STL
TEC EN
// Headers of Output Variables specified by the User: EMPTY line means default is used

// Intermediate Result Output Control: INTERVAL(hour) OR List of T1 T2 ...  EMPTY means
-1
```

The solution process can be monitored by examining the residual file (_RES.dat). The residual velocity U for the model run is shown in Figure 5.

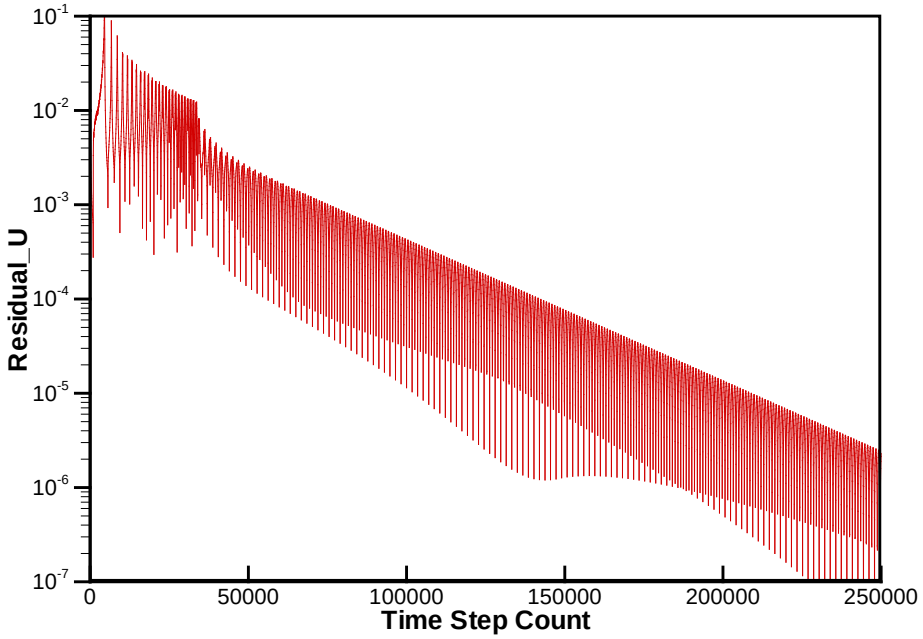

Figure 5. Residual of the U momentum equation for the steady flow run

Next the unsteady flow run is simulated using the steady run output as the initial condition. The unsteady model runs serve two purposes. First, the model run generates flow results at a user-specified time interval (e.g., hourly or daily). These flow results are typically stored in a format accessible to SRH-WQ for water quality and mercury simulations. Second, the input file to run SRH-WQ may be generated using the SRH-2D preprocessor while setting up unsteady flow models

In setting up an unsteady flow run, values for the following additional input parameters are needed to perform a SRH-WQ simulation – even though these parameters are not used for SRH-2D flow simulations:

- SRH-WQ Time Parameters
    - DT_WQ = Model time step in seconds for SRH-WQ simulations.
    - TIME_DURATION_FLOW = the time duration or interval in hours for which flow results are stored for use by the SRH-WQ model. During the specified time interval flow variables are held constant by the SRH-WQ model - primarily to carry out an unsteady water quality and mercury simulations.
    - N_DURATION = the total number of time steps to carry out the SRH-WQ model simulation; so the total simulation time is N_DURATION*TIME_DURATION_FLOW (in hours).

  Comments: It should be obvious that the time step (DT_WQ) of the WQ module should be smaller than TIME_DURATION_FLOW. The flow is simulated by the SRH-2D,

model results are stored in files named _WQFi.dat (i refers to results at i-th flow time duration).

- Meteorological Data
  - The simple analytical equilibrium temperature model is used for heat flux at the water-air interface; complete meteorological data sets are not needed. Only four constants are entered: $K_T = 0.2$ (1/day); $T_{eq} = 0$ (Celsius).

- SRH-WQ Diffusion or Dispersion Parameter
  - SCHMIDT = a list of Schmidt numbers (denoted as Sc) for all advected state variables that simulate transport within the SRH-WQ module. It is used to compute the diffusivity/dispersion of the state variable as υ_t / Sc where υ_t is the turbulent viscosity of the flow.

- SRH-WQ Initial Condition
  - C_INIT = a list of constant values representing the initial values of all advected state variables. They are used to set up the initial condition of the advected state variables by SRH-WQ.

- SRH-WQ Boundary Condition

  General Comment: At each inflow boundary of the model domain, the Dirichlet boundary condition is used. That is, the time series values of all advected state variables are needed at all inflow boundaries. With SRH-2D inflow boundaries include types of INLET-Q and INLET-SC. These boundary condition values should use measured data where available. The input is either a constant value or a time series file containing the transient data. Some examples are discussed below:

  - Example #1: “INLET-Q 10.0 0.1 SI” where 10.0 is the flow discharge in m3/s at the inlet and 0.1 is the scalar value at the inlet (if there is only one advected state variable)
  - Example #2: “INLET-SC 10.0 5.0 0.1 SI” where 10.0 is the flow discharge in m3/s, 5.0 is the stage in meters, and 0.1 is the value of the advected state variable.
  - Example #3: “INLET-Q 10.0 c_wq_data.dat SI” where the advected state variable is changing with time and the data is inside the file named c_wq_data.dat. The content and format of a time series data file are as follows: (a) at the beginning, any lines starting with // are comment lines and they are not used by the model; (b) pairs if (time, C) data follows the comment lines. Time is always in hours while the units of the scalar input depends on the requirement of the model preprocessor. Listed below is a sample time series data file:

```
//
// time(hour)  Sediment_Concentration(dimensionless)
//
0    0.1
6    0.08
12  0.04
18  0.05
24  0.06
30  0.08
36  0.1
42  0.11
48  0.11
```

For our tutorial example, the only advected state variable is water temperature and the transport equation to be solved is written as follows:

$$\frac{\partial T}{\partial t}+\frac{\partial UT}{\partial x}=-kT$$

where U velocity is 1.0 mile/day and the rate coefficient *k* is 0.2/day. The 100 mile domain has an initial temperature of 20 Celsius, uses a high Schmidt number indicate of near zero diffusivity, and maintains a constant temperature of 20 Celsius over time at the left boundary (specified as INLET-Q).

The SRH-WQ model simulation is runt using a one hour time step for a total of 50 days (1200 hours). Since the flow velocity is constant, only one flow result file, _WQF1.dat, is needed. The flow result file is obtained by running the unsteady SRH-2D modeling for one hour; i.e. the flow code uses a time step of 360 seconds.

The unsteady SRH-2D model flow simulation is performed using the following _SIF.dat file:

```
// Simulation Description (not used by SRH-2D):
Case1_Temperature_Analytical --> Unsteady Run
// Module/Solver Selected (FLOW MOB TEM TC WQ)
WQ
// WQ(Water Quality) Time Parameters: DT_WQ(s) TIME_Duration(Hr) N_Duration
3600 1200 1
// Meterological data (empty=not supplied as they are not used) Means Simple Equilibrium Temp

// WQ: SIMPLE-EQUILIBRIUM-TEMPERATURE-PARAMETERS: Keq(1/day) T0(C) TA(C) Period(day)
0.2 0.0 0.0 1.0
// WQ(Water Quality) Other Parameters: SCHMIDT SC_INIT
1.0e20  20.0
// Monitor-Point-Info: NPOINT
1
99.99 1.0
// Steady-or-Unsteady (STEADY/UNS)
UNS
0 360 1.0
// Turbulence-Model-Selection(PARA or KE)
PARA
0.7
// Initial Condition Method (DRY RST AUTO ZONAL)
RST
flow_RST.dat
// Mesh-Unit (FOOT METER INCH MM MILE KM GSCALE)
MILE
mesh1.2DM SMS
// Manning Roughness Input Method(1=uniform 2=2DM 3=(x y) distributed
1
1.e-10
// Any-Special-Treatments? (0 or empty = NO; 1=YES)

// Boundary Type (INLET-Q EXIT-H etc)
INLET-Q
   645.33333 inlet_tem.dat EN V
EXIT-H
   1.0 EN
SYMM
SYMM
MONITOR
// Wall-Roughess-Height-Specification (empty-line=DONE)

// Any In-Stream Flow Obstructions? (empty-line or 0 = NO)

// Results-Output-Format-and-Unit(SRHC/TEC/SRHN/XMDF;SI/EN) + Optional STL
TEC EN
// Headers of Output Variables specified by the User: EMPTY line means default is used

// Intermediate Result Output Control: minus for none
-1
```

The execution of the SRH-2D model preprocessor and the unsteady simulation with the SRH-2D model produce two types of model input file which are used by the SRH-WQ simulation model. The first file provides input to the SRH-WQ model transport module (casename_WQ_input.dat); the second produces flow output files (only one is generated for the tutorial case named casename_WQF1.dat).

The casename_WQ_input.dat file generated by the SRH-2D preprocessor is shown below for the tutorial. The unsteady SRH-2D simulation model results are identical to the steady state run output. These analyses are not discussed further.

```
// ========================================
// = Water Quality Module Input Parameters =
// ========================================
// Time Parameters: Dt_WQ(s) Time_Duration_Flow(hr) N_Duration MOD_RK5E
    3.60000000E+03    1.20000000E+03           1  0
// Meterology data file name & SIMPLE-EQUILIBRIUM-TEMP-PARAMETERS: Keq(1/day) T0(C) TA(C) Period(day)
NO_USE
    2.00000000E-01    0.00000000E+00    0.00000000E+00    1.00000000E+00
// Miscelleneous: Schmidt Number
    1.00000000E+20
// Initial Scalar Field: C_Init
    2.00000000E+01
// Boundary Condition: N_FIXED_BD  N_FIXED_NBDF
         1          2
// Time_Series_ID;    <0 for constant; >0 for TVF
         1
// List of L_fixed() array (IBDF IDBD) at each boundary face
   1   1   2   1
// TVF Info: ntvf ntvfsz
         1          4
// INTVF() array for each TVF: (ID_TVF SIZE) pair for each TVF
         1          3
// Time(s) Sc arrays for TVF =          1 and SIZE=          3
    0.00000000E+00  2.00000000E+01  8.64000000E+04  2.00000000E+01  1.29600000E+09  2.00000000E+01
// Monitoring Point Info: Number_of_Points & then list of CELL_ID x(m) y(m) data
   1
      199      1.6091862840E+05    1.6093472187E+03
```

4.1.3 Temperature Modeling with SRH-WQ

Performing SRH-WQ model simulations is straightforward. In the following example three input files are needed:

(1) Input File for the SRH-WQ model: This input file is generated while setting up the SRH-2D model flow run as discussed above;

(2) SRH-2D model Flow Results: These are the model output files, in the form of _WQFi.dat, representing model results after a user-specified time interval. For the tutorial case, only one file is needed (_WQF1.dat) since the flow simulation is a constant discharge case.

(3) WQ Control File: This is a WQ module file, named _WQ_controlfile.dat, used by the USACE WQ modules. The control file for this this tutorial example is shown below – it is used for the TEMP module only. For the definitions of the file parameters – the user is directed to a new manual under development by the USACE.

```
! WQ input file

! Test HgSM.dll only -- 2/14/17 Zhong

! WQ DLL ON/OFF
'TEMP.DLL',    ON        ! Water Temperature Simulation Module (TEMP)
'GC.DLL',      OFF       ! General Constituent Simulation Module (GC)
'NSMI.DLL',    OFF       ! Nutrient Simulation Module (NSMI)
'HgSM.DLL',    OFF       ! Mercury Simulation Module (HgSM)

! WQ region
  2

!-----------------------------------------------------------------------------------------------------------
! TEMP.DLL - Inputs

! TEMP State Variables ON/OFF
  'TwaterC',    ON        ! Water Temperature (oC)     'TwaterC' must be ON if TEMP.DLL is ON.
  'TsedC',      off       ! Sediment Temperature (oC)

! TEMP Pathway ON/OFF
  'Pathway',    off       ! All pathways are output if Pathway is ON. Otherwise, no pathway is output.

! TEMP Parameters: number of parameter lines = 10. (Real Real_Theta); Last isTC=True or False --> Temperature-
  'Temperature'
    'wind_a',     1.0,      0.0,   1.522,    0.0,      .false.    ! Coefficient a in wind function
    'wind_b',     1.0,      0.0,   3.323,    0.0,      .false.    ! Coefficient b in wind function
    'wind_c',     1.0,      0.0,   1.069,    0.0,      .false.    ! Coefficient c in wind function
    'wind_kh_kw', 1.0,      0.0,   0.958,    0.0,      .false.    ! Diffusivity ratio
    'Richardson Number Function Option',     2,        1,          ! Define whether Richardson Number Function
    'h2',         0.1,      0.0,   0.123,    0.0,      .false.    ! Sediment layer thickness (m)
    'pb',         1600.0,   0.0,   1800.0,   0.0,      .false.    ! Sediment bulk density (kg/m^3)
    'Cps',        1674.72,  0.0,   1673.0,   0.0,      .false.    ! Sediment specific heat capacity (J/kg/m^3)
    'alphas',     0.0432,   0.0,   0.0437,   0.0,      .false.    ! Sediment thermal diffusivity (m^2/d)
```

The model simulated temperature on the right side of the flow domain was compared to the analytical solution (Figure 6). The model results match the analytical solution very well.

Both implicit and Runge-Kutta methods were compared – the model produced the same solution.

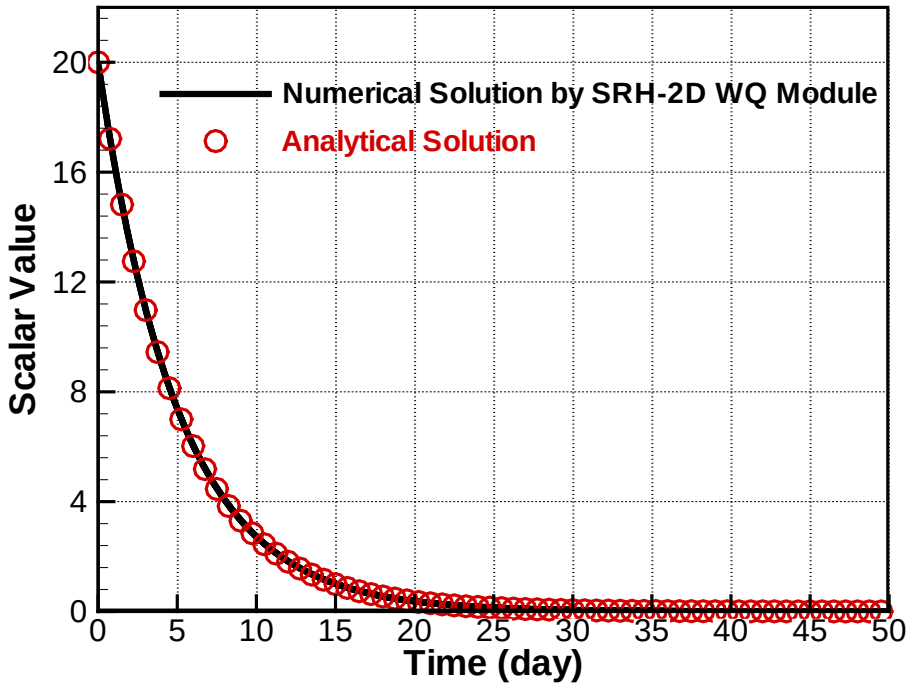

Figure 6. Figure. Comparison of temperature at 100-mile location between model and analytical solution

4.2 A Tutorial Case Running the NSMI Module

4.2.1 Model Domain and Mesh Generation

A simple channel flow example was set up and used as a tutorial for running the NSMI module. All model inputs follow the lumped point model test case configuration proposed by Dr. Zhang at U.S. Army Corp of Engineers (USACE). The example serves as an additional purpose to verify that the 2D transport model developed at Reclamation and the integration of the SRH-2D model with the water quality modules were successfully realized.

The model domain represents a straight channel with a length of 200 meters and a width of 20 meters. The mesh has square cells and there are a total of 20 cells in the flow direction and 2 cells in the lateral direction (for a total of 200 cells). The flow moves from left to right with two lateral boundaries specified as “Symmetry” within the SRH-2D model. The channel has a slope of 0.02% allowing normal flow to occur in the channel with inlet discharge of 30 m^3/s (1.0 m/s

velocity), a normal depth of 1.5 m, and a Manning's "n" coefficient of 0.0185. The model domain and the mesh are shown in Figure 7.

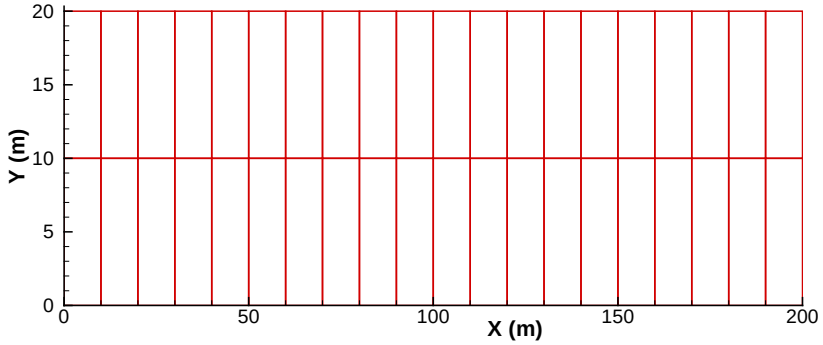

Figure 7. Model domain and the mesh for the NSMI module tutorial case (1:4 scale between x and y axis)

4.2.2 Flow Modeling with the SRH-2D model

A steady-state flow simulation was performed first so that the results could be used as the initial condition for the unsteady state simulation. The unsteady (time varying) flow simulation is always carried out first if the results are to be linked to the SRH-WQ model simulation - this condition is true even if the flow does not change with time (steady). For the steady-state run, a constant flow discharge of 30 m^3/s is imposed at the left boundary of the domain, leading to a flow velocity of 1 m/s. A 1.5 m water depth is the boundary condition imposed on the right boundary. With a Manning's roughness coefficient of 0.0185, a normal flow condition prevails which is simulated by the SRH-2D model.

Flow modeling with SRH-2D has been well established and documented by Lai (2008; 2010); so details are omitted. The input file (_SIF.dat) used for the steady run is listed before as a reference.

```
// Simulation Description (not used by SRH-2D):
Steady Run: Normal Flow through a channel
// Module/Solver Selected (FLOW MOB TEM TC WQ)
FLOW
// Monitor-Point-Info: NPOINT
1
100.5 9.8
// Steady-or-Unsteady (STEADY/UNS)
STEADY
0 100 5
// Turbulence-Model-Selection(PARA or KE)
PARA
0.7
// Initial Condition Method (DRY RST AUTO ZONAL)
zonal
// 1 for constant setup; 1.5m for Depth
1
0 0 1.5
// Mesh-Unit (FOOT METER INCH MM MILE KM GSCALE)
meter
mesh2.2DM SMS
// Manning Roughness Input Method(1=uniform 2=2DM 3=(x y) distributed
1
0.0185
// Any-Special-Treatments? (0 or empty = NO; 1=YES)

// Boundary Type (INLET-Q EXIT-H etc)
INLET-Q
   30 SI V
EXIT-H
   1.5 SI
SYMM
SYMM
MONITOR
// Wall-Roughess-Height-Specification (empty-line=DONE)

// Any In-Stream Flow Obstructions? (empty-line or 0 = NO)

// Results-Output-Format-and-Unit(SRHC/TEC/SRHN/XMDF;SI/EN) + Optional STL
TEC SI
// Headers of Output Variables specified by the User: EMPTY line means defau

// Intermediate Result Output Control: INTERVAL(hour) OR List of T1 T2 ...
-1
```

Next an unsteady flow simulation is carried out using the steady run flow results as initial conditions. The unsteady run serves two purposes. First, the simulation produces flow results at a user-specified time interval (e.g., hourly or daily); these flow results are stored in files to be used by the SRH-WQ model for the water quality and Hg simulation. Second, the unsteady flow modeling setup process, using the SRH-2D model preprocessor, creates the input file needed to run the SRH-WQ model.

In addition to the inputs needed for the flow simulation, following additional inputs were used for setting up the SRH-WQ model for the NSMI simulation:

- SRH-WQ Module Time Parameters

    - DT_WQ = Time step, in seconds, used by SRH-WQ
    - TIME_PERIOD = Time interval, in hours, for which flow results are stored. During the time interval, the flow variables are held constant by the SRH-WQ model for carrying out the unsteady water quality and Hg simulations.

- N_PERIOD = Total number of time periods (intervals) used to carry out the SRH-WQ simulation. The total water quality simulation time is N_PERIOD*TIME_PERIOD (hours).

  Comments: For the WQ model time step, DT_WQ, should be smaller than the specified TIME_PERIOD and it used to enhance temporal accuracy of the results. The flow variables during TIME_PERIOD are simulated by the SRH-2D model and stored in files named _WQFi.dat (i refers to results at i-th flow period).

- Meteorological Data

  - A input data file, named data_meteorology.dat, contains a time stamp and six meteorological variables: Time (hour), Cloud Cover, Air Temperature (Celsius), Vapor Pressure at Saturation (mb), Atmospheric Pressure (Atm), Wind Speed (m/s), and Solar Radiation (W/m2). For the tutorial example, constant inputs were used and the six meteorological inputs are (in order): 0.6, 18.0, 26.0, 1.0, 3.0, 500.0.

- State Variable Information

  - The total number of state variables for all WQ modules and the total number of state variables that are advected by the SRH-WQ transport module need to be specified. For the tutorial case, they are 56 and 24, respectively.
  - For each state variable in the SRH-WQ transport module the following information should be provided: Name, Schmidt Number, and Initial Value. (The Schmidt number is the ratio of effective turbulence eddy viscosity to effective scalar transport diffusivity, and used only for advected state variables). For non-advected state variables, -999 should be entered as a flag to signal that it is a non-advected variable. For a given the Schmidt number, Sc , the diffusivity/dispersion of the state variable is estimated by υ_t / Sc with υ_t being the flow viscosity.

- Boundary Conditions for Advected State Variables

  General Comment: At each inflow boundary of the model domain (INLET-Q), boundary conditions for all advected state variables are needed. Two options are available to specify the boundary condition of a variable: (a) a zero flux condition implemented as the symmetry condition or (b) the Dirichlet condition. With (b), the Dirichlet condition, a constant or a time series boundary flux data set is specified. The boundary condition data is normally derived from recorded gauge data. A sample boundary condition input where the SYMM option is used for all variables is listed below.

- TwaterC SYMM
  TDS SYMM
  Salinity SYMM
  Constituent1 SYMM
  Constituent2 SYMM
  SuspendedSolid1 SYMM
  SuspendedSolid2 SYMM
  SuspendedSolid3 SYMM
  SuspendedSolid4 SYMM
  SuspendedSolid5 SYMM
  Ap SYMM
  NH4 SYMM
  NO3 SYMM
  OrgN SYMM
  TIP SYMM
  OrgP SYMM
  POC SYMM
  DOC SYMM
  DIC SYMM
  CBOD1 SYMM
  DO SYMM
  Alk SYMM
  PX SYMM
  POM SYMM

For the tutorial example, the flow velocity is constant, hence only one flow result file, _WQF1.dat, is needed. The flow result file is obtained by running the unsteady SRH-2D model using the following _SIF.dat file.

```
// Simulation Description (not used by SRH-2D):
Unsteady Run: 1 m/s Flow with 1.5m Depth
// Module/Solver Selected (FLOW MOB TEM TC WQ)
WQ
// WQ(Water Quality) Time Parameters: DT_WQ(s) TIME_Period(Hr) N_Period
300 8.33333333334 1
// Meterological data file name
data_meteorology.dat
// WQ: Number of total & Advected State Variables
56 24
// List of 56 State Variables: NAME SC_INIT SCHMIDT
TwaterC           25.0       1.e20
TsedC             21.0       -999
TDS               68.0       1.e20
Salinity          1.6        1.e20
Constituent1      125.35     1.e20
Constituent2      137.35     1.e20
SuspendedSolid1   100.0      1.e20
SuspendedSolid2   50.0       1.e20
SuspendedSolid3   20.0       1.e20
SuspendedSolid4   15.0       1.e20
SuspendedSolid5   10.0       1.e20
SedimentSolid1    1000000.0  -999
SedimentSolid2    500000.0   -999
SedimentSolid3    200000.0   -999
SedimentSolid4    100000.0   -999
SedimentSolid5    50000.0    -999
Ap        36.77       1.e20
Ab        24.0        -999
NH4       0.063       1.e20
NO3       5.54        1.e20
OrgN      1.726       1.e20
TIP       0.071       1.e20
OrgP      0.24        1.e20
POC       4.356       1.e20
DOC       5.234       1.e20
DIC       0.003       1.e20
CBOD1     5.0         1.e20
DO        8.0         1.e20
Alk       100.0       1.e20
PX        100.0       1.e20
POM       10.89       1.e20
NH41      0.0     -999
NO31      0.0     -999
CH41      0.0     -999
SO41      0.0     -999
TH2S1     0.0     -999
DIC1      0.0     -999
TIP1      0.0     -999
```

```
POC2G1   56.22667     -999
PON2G1   10.86837     -999
POP2G1   0.8344222    -999
POC2G2   1072.333     -999
PON2G2   208.3411     -999
POP2G2   9.252676     -999
POC2G3   24966.554    -999
PON2G3   3114.917     -999
POP2G3   98.3023      -999
NH42     7.763713     -999
NO32     0.06930469   -999
CH42     0.019309528  -999
SO42     1031.67      -999
TH2S2    3590.369     -999
DIC2     0.0          -999
TIP2     112.4662     -999
ST',       22.55192   -999
HSO4',     0.0        -999
// HgSM Extra Input: Initial Values of Hg00 MeHg0 SO42 DOC2

// Monitor-Point-Info: NPOINT
1
100.5 9.8
// Steady-or-Unsteady (STEADY/UNS)
UNS
0 360 1.0
// Turbulence-Model-Selection(PARA or KE)
PARA
0.7
// Initial Condition Method (DRY RST AUTO ZONAL)
RST
flow_RST.dat
// Mesh-Unit (FOOT METER INCH MM MILE KM GSCALE)
meter
mesh2.2DM SMS
// Manning Roughness Input Method(1=uniform 2=2DM 3=(x y) distributed
1
0.0185
// Any-Special-Treatments? (0 or empty = NO; 1=YES)
```

```
// Boundary Type (INLET-Q EXIT-H etc)
INLET-Q
   30 SI V
   TwaterC  SYMM
   TDS      SYMM
   Salinity SYMM
   Constituent1     SYMM
   Constituent2     SYMM
   SuspendedSolid1  SYMM
   SuspendedSolid2  SYMM
   SuspendedSolid3  SYMM
   SuspendedSolid4  SYMM
   SuspendedSolid5  SYMM
   Ap       SYMM
   NH4      SYMM
   NO3      SYMM
   OrgN     SYMM
   TIP      SYMM
   OrgP     SYMM
   POC      SYMM
   DOC      SYMM
   DIC      SYMM
   CBOD1    SYMM
   DO       SYMM
   Alk      SYMM
   PX       SYMM
   POM      SYMM
//
EXIT-H
   1.5 SI
SYMM
SYMM
MONITOR
// Wall-Roughess-Height-Specification (empty-line=DONE)

// Any In-Stream Flow Obstructions? (empty-line or 0 = NO)

// Results-Output-Format-and-Unit(SRHC/TEC/SRHN/XMDF;SI/EN) + Optional STL
TEC SI
// Headers of Output Variables specified by the User: EMPTY line means default is used

// Intermediate Result Output Control: minus for none
-1
```

The execution of the SRH-2D model preprocessor using the above _SIF.dat file and the unsteady simulation with the SRH-2D model create two types of files which are used by the SRH-WQ model. The first is the input file for SRH-WQ transport module (_WQ_input.dat); the second is(are) the flow results file(s) (only one is generated for the tutorial example and is labelled casename_WQF1.dat).

The _WQ_input.dat file generated by SRH-2D model preprocessor is shown below for the tutorial example while the unsteady output results file, _WQF1.dat, is stored in binary format (used directly by SRH-WQ without the need of user intervention).

```
// ========================================
// = Water Quality Module Input Parameters =
// ========================================
// Time Parameters: Dt_WQ(s) Time_Duration_Flow(hr) N_Duration MOD_RK5E
    3.00000000E+02    8.33333333E+00           1  0
// Meterology data file name + 6 TVF IDs: CC Tair(C) VPAir(mb) Pair(Atm) WS(m/s) Solar(W/m2)
data_meteorology.dat
   1   2   3   4   5   6
// Number of Advected/Transported State Variables & Total number of scalars
     24     56
// State Variable Name & Initial Condition Scalar Value
TwaterC                    2.50000000E+01    1.00000000E+20
TsedC                      2.10000000E+01   -9.99000000E+02
TDS                        6.80000000E+01    1.00000000E+20
Salinity                   1.60000000E+00    1.00000000E+20
Constituent1               1.25350000E+02    1.00000000E+20
Constituent2               1.37350000E+02    1.00000000E+20
SuspendedSolid1            1.00000000E+02    1.00000000E+20
SuspendedSolid2            5.00000000E+01    1.00000000E+20
SuspendedSolid3            2.00000000E+01    1.00000000E+20
SuspendedSolid4            1.50000000E+01    1.00000000E+20
SuspendedSolid5            1.00000000E+01    1.00000000E+20
SedimentSolid1             1.00000000E+06   -9.99000000E+02
SedimentSolid2             5.00000000E+05   -9.99000000E+02
SedimentSolid3             2.00000000E+05   -9.99000000E+02
SedimentSolid4             1.00000000E+05   -9.99000000E+02
SedimentSolid5             5.00000000E+04   -9.99000000E+02
Ap                         3.67700000E+01    1.00000000E+20
Ab                         2.40000000E+01   -9.99000000E+02
NH4                        6.30000000E-02    1.00000000E+20
NO3                        5.54000000E+00    1.00000000E+20
OrgN                       1.72600000E+00    1.00000000E+20
TIP                        7.10000000E-02    1.00000000E+20
OrgP                       2.40000000E-01    1.00000000E+20
POC                        4.35600000E+00    1.00000000E+20
DOC                        5.23400000E+00    1.00000000E+20
DIC                        3.00000000E-03    1.00000000E+20
CBOD1                      5.00000000E+00    1.00000000E+20
DO                         8.00000000E+00    1.00000000E+20
Alk                        1.00000000E+02    1.00000000E+20
PX                         1.00000000E+02    1.00000000E+20
POM                        1.08900000E+01    1.00000000E+20
NH41                       0.00000000E+00   -9.99000000E+02
NO31                       0.00000000E+00   -9.99000000E+02
CH41                       0.00000000E+00   -9.99000000E+02
SO41                       0.00000000E+00   -9.99000000E+02
TH2S1                      0.00000000E+00   -9.99000000E+02
DIC1                       0.00000000E+00   -9.99000000E+02
TIP1                       0.00000000E+00   -9.99000000E+02
POC2G1                     5.62266700E+01   -9.99000000E+02
PON2G1                     1.08683700E+01   -9.99000000E+02
POP2G1                     8.34422200E-01   -9.99000000E+02
POC2G2                     1.07233300E+03   -9.99000000E+02
PON2G2                     2.08341100E+02   -9.99000000E+02
POP2G2                     9.25267600E+00   -9.99000000E+02
POC2G3                     2.49665540E+04   -9.99000000E+02
PON2G3                     3.11491700E+03   -9.99000000E+02
POP2G3                     9.83023000E+01   -9.99000000E+02
NH42                       7.76371300E+00   -9.99000000E+02
NO32                       6.93046900E-02   -9.99000000E+02
CH42                       1.93095280E-02   -9.99000000E+02
SO42                       1.03167000E+03   -9.99000000E+02
TH2S2                      3.59036900E+03   -9.99000000E+02
DIC2                       0.00000000E+00   -9.99000000E+02
TIP2                       1.12466200E+02   -9.99000000E+02
ST'                        2.25519200E+01   -9.99000000E+02
HSO4'                      0.00000000E+00   -9.99000000E+02
// HgSM Module Extra Inputs: Hg00 MeHg0 SO42 DOC2
    2.00000000E-03    0.00000000E+00    0.00000000E+00    0.00000000E+00
// Boundary Condition: N_BD_having_FixedValues  N_of_BDF_having_FixedValues
         1         2
// BD Type for all Advected State Variable (-999=SYMM; 0=Constant; >0=TVF) at BD_ID =    1
  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999
// BD Auxillary Array: L_fixed() = (IBDF IDBD) at each boundary face of the BD
   1   1   2   1
// TVF Info: Ntvf Ntvfsz <-- used for Time Dependent BC, MeteorologyData, ...
         6        25
// TVF Info: (ID_TVF NP) for each TVF; NP=number of data points
         1         4
         2         4
         3         4
         4         4
         5         4
         6         4
// [Time(s) Value] for TVF =  1 and SIZE=         4
    0.00000000E+00  6.00000000E-01  2.16000000E+06  6.00000000E-01  4.32000000E+06  6.00000000E-01
    1.29600000E+07  6.00000000E-01
// [Time(s) Value] for TVF =  2 and SIZE=         4
    0.00000000E+00  1.80000000E+01  2.16000000E+06  1.80000000E+01  4.32000000E+06  1.80000000E+01
    1.29600000E+07  1.80000000E+01
// [Time(s) Value] for TVF =  3 and SIZE=         4
    0.00000000E+00  2.60000000E+01  2.16000000E+06  2.60000000E+01  4.32000000E+06  2.60000000E+01
    1.29600000E+07  2.60000000E+01
// [Time(s) Value] for TVF =  4 and SIZE=         4
    0.00000000E+00  1.00000000E+00  2.16000000E+06  1.00000000E+00  4.32000000E+06  1.00000000E+00
    1.29600000E+07  1.00000000E+00
// [Time(s) Value] for TVF =  5 and SIZE=         4
    0.00000000E+00  3.00000000E+00  2.16000000E+06  3.00000000E+00  4.32000000E+06  3.00000000E+00
    1.29600000E+07  3.00000000E+00
// [Time(s) Value] for TVF =  6 and SIZE=         4
    0.00000000E+00  5.00000000E+02  2.16000000E+06  5.00000000E+02  4.32000000E+06  5.00000000E+02
    1.29600000E+07  5.00000000E+02
// Monitoring Point Info: Number_of_Points & then list of CELL_ID x(m) y(m) data
   1
      19      1.0050000000E+02    9.8000000000E+00
```

4.2.3 Running the NSMI Module

Simulation using the NSMI Module with the SRH-WQ model is simple. For the tutorial example the following input data files are required:

(1) SRH-WQ Input File: This input file, named _WQ_input.dat, is generated while setting up the SRH-2D unsteady flow run as discussed above.
(2) SRH-2D Model Flow Results: The model flow results for user-specified time interval/periods, named _WQFi.dat, are generated while running the unsteady flow model with SRH-2D. For the tutorial example, only one file is generated and required (_WQF1.dat).
(3) SRH-WQ Control File: This is a water quality module specification file, named _WQ_controlfile.dat, produced by the USACE WQ modules. The file specifies information such as: (a) whether the modules are turned on or off; (b) the state variables activated for each module: (c) specification of relevant water quality model scalars for each module; (d) output options of derived and pathway variables, etc. This control file is not listed in this report due to its length. A detailed description of the control file is under development by the USACE and documentation will be available in the future.

Running the SRH-WQ model is accomplished by copying the executable file SRH-WQ.exe, along with all USACE WQ module DLLs (TEMP.dll, GC.dll, and NSMI.dll) for the tutorial example, to the project directory - then starting the simulation by clicking on the SRH-WQ.exe executable file.

4.2.4 Output from NSMI Module Simulation

For the tutorial example, several output files are generated once the simulation has completed. They include _PTi.dat (i starts from 1), _TECi.dat (i starts from 1), and _WQ_RESULT.dat.

For the tutorial example, _PT1.dat contains the time series simulation results at user specified monitoring points. All 56 state variables are reported in the file. Two plots displaying the simulated temperature, NO3 and DOC concentrations are shown in Figure 8 for the tutorial example. The _TEC1.dat contains a 2D spatial distribution of all 56 state variables at the end of the model simulation. The data can be graphically displayed and post-processed using visualization software such as TECPLOT. A sample plot of the NO3 distribution for the tutorial example is shown in Figure 9. In Figure 9, the spatial distribution appears almost uniform in the channel. Finally, the _WQ_RESULT.dat file contains output information from the USACE WQ modules.

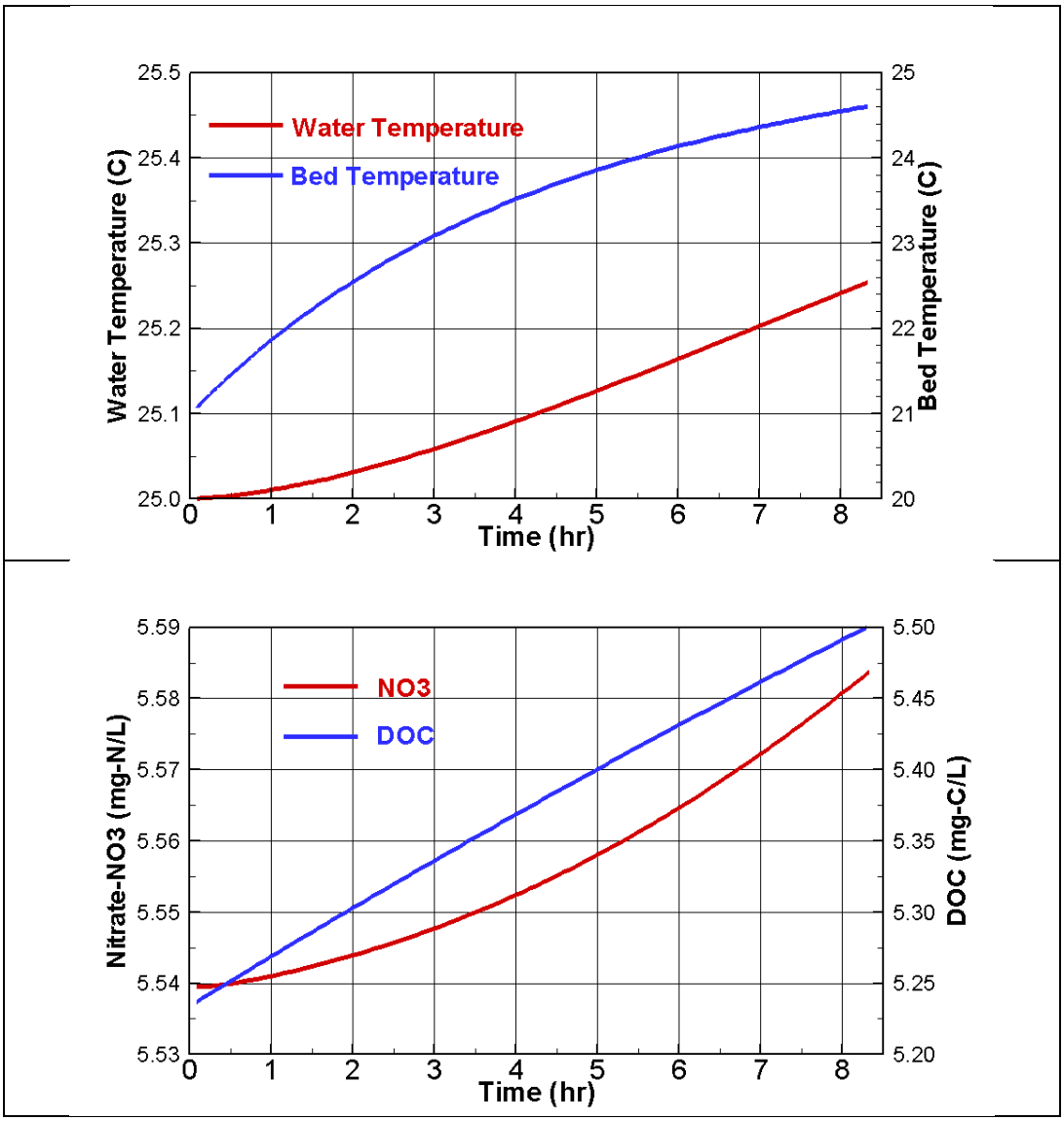

Figure 8. Simulated temporal change in temperature in the water column and in the bed sediments as well as simulated changes in NO3 and DOC concentrations in the water column for the tutorial example

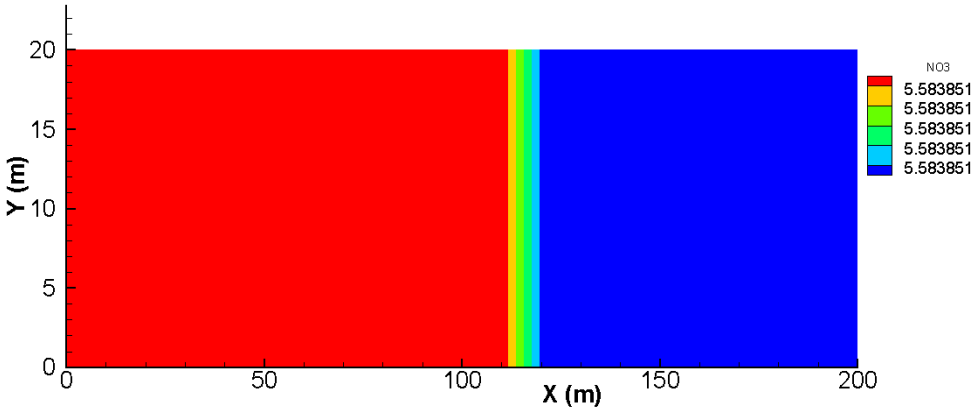

Figure 9. Distribution of simulated NO3 concentration (mg-N/L) in the water column of the channel at the end of the simulation for the tutorial example

4.3 A Tutorial Example Running the HgSM Module

4.3.1 Model Domain and Mesh Generation

The same simple channel flow example used in the NSMI tutorial example in Section 4.2 was used as a tutorial on how to run the HgSM module. All model inputs follow the lumped point model test case set up and supplied by Dr. Zhang (USACE). The model simulation serves also to verify the formulation of the 2D transport model developed at Reclamation and its successful integration with the SRH-2D module and HgSM module.

Details of the model domain and mesh are discussed in Section 4.2.1 and not repeated herein.

4.3.2 Flow Modeling with the SRH-2D model

The process of running the flow simulation model was previously presented in Section 4.2.2 for the NSMI module tutorial example. The only difference in this instance is that additional inputs are used to set up the unsteady flow simulation so that the input data file for the HgSM simulation is generated.

Additional inputs are required for setting up the SRH-WQ model run that includes the Hg simulation (Section 4.2.2 provides a complete tutorial overview of the steps required to run the HgSM module). The additional inputs required are listed below:

- SRH-WQ Time Parameters
    - DT_WQ = Time step (seconds), used by SRH-WQ

- TIME_PERIOD = Time interval (hours) for which the flow results are stored. During the time interval, flow variables are held constant by the SRH-WQ model carrying out the unsteady water quality and Hg simulation.
- N_PERIOD = Total number of time periods (intervals) used to complete the SRH-WQ simulation. The total water quality simulation time is calculated as: N_PERIOD*TIME_PERIOD (hours).

Comments: The WQ time step, DT_WQ, should be smaller than TIME_PERIOD and it is primarily needed to ensure accurate results. The flow output produced by the SRH-2D model simulation during the TIME_PERIOD are stored in files named _WQFi.dat (i refers to results for i-th flow period).

- Meteorological Data

  - A data file, named data_meteorology.dat, contains the input data as well as six meteorological variables including: Time (hour), Cloud Cover, Air Temperature (Celsius), Vapor Pressure at Saturation (mb), Atmospheric Pressure (Atm), Wind Speed (m/s), and Solar Radiation (W/m2). For the tutorial example, constant inputs are used and the six meteorological inputs are (in order): 0.6, 18.0, 26.0, 1.0, 3.0, 500.0.

- State Variable Information

  - The total number of state variables for all WQ modules along with the total number of state variables that are advected by the SRH-WQ transport module. For the tutorial example, the totals are 33 and 25, respectively.
  - For each state variable in the SRH-WQ transport module the following information should be provided: Name, Schmidt Number, and Initial Value. (The Schmidt number is the ratio of effective turbulence eddy viscosity to effective scalar transport diffusivity, and used only for advected state variables). For non-advected state variables, -999 should be entered as a flag to signal that it is a non-advected variable. For a given the Schmidt number, Sc , the diffusivity/dispersion of the state variable is estimated by υ_t / Sc with υ_t being the flow viscosity.

- Initial Condition of Auxiliary Variables

  - The HgSM Module needs the following initial values: Gaseous elemental Hg (Hg0) concentration in the air (ng/L), Gaseous methyl mercury (MeHg) concentration in the air (ng/L), Sulfate (SO4) concentration in the bed pore water (mg-O2/L), and DOC concentration in the bed pore water (mg-C/L)

- Boundary Conditions for Advected State Variables

  General Comment: At each inflow boundary of the model domain (INLET-Q), boundary conditions for all advected state variables are needed. Two options are available to specify the boundary condition of a variable: (a) a zero flux condition implemented as the symmetry condition or (b) the Dirichlet condition. With (b), the Dirichlet condition, a constant or a time series boundary flux data set is specified. The boundary condition data is normally derived from recorded gauge data. A sample boundary condition input where the SYMM option is used for all variables is listed below.

  - TwaterC SYMM
    TDS SYMM
    Salinity SYMM
    Constituent1 SYMM
    Constituent2 SYMM
    SuspendedSolid1 SYMM
    SuspendedSolid2 SYMM
    SuspendedSolid3 SYMM
    Ap SYMM
    NH4 SYMM
    NO3 SYMM
    OrgN SYMM
    TIP SYMM
    OrgP SYMM
    POC SYMM
    DOC SYMM
    DIC SYMM
    CBOD1 SYMM
    DO SYMM
    Alk SYMM
    PX SYMM
    POM SYMM
    Hg0 SYMM
    HgII SYMM
    MeHg SYMM

For the tutorial example, the flow velocity is constant, hence only one flow result file, _WQF1.dat, is needed. The flow result file is obtained by running the unsteady SRH-2D model using the following _SIF.dat file.

```
// Simulation Description (not used by SRH-2D):
Unsteady Run: 1 m/s Flow with 1.5m Depth
// Module/Solver Selected (FLOW MOB TEM TC WQ)
WQ
// WQ(Water Quality) Time Parameters: DT_WQ(s) TIME_Period(Hr) N_Period
300 8.33333333334 1
// Meterological data file name
data_meteorology.dat
// WQ: Number of total & Advected State Variables
33 25
// All WQ State Variables:  NAME  SCHMIDT  SC_INIT (NOTE: Schmidt number = 0
TwaterC           25.0       1.e20
TsedC             21.0       -999
TDS               68.0       1.e20
Salinity          1.6        1.e20
Constituent1      125.35     1.e20
Constituent2      137.35     1.e20
SuspendedSolid1   100.0      1.e20
SuspendedSolid2   50.0       1.e20
SuspendedSolid3   20.0       1.e20
SedimentSolid1    1000000.0  -999
SedimentSolid2    500000.0   -999
SedimentSolid3    200000.0   -999
Ap        36.77       1.e20
Ab        24.0        -999
NH4       0.063       1.e20
NO3       5.54        1.e20
OrgN      1.726       1.e20
TIP       0.071       1.e20
OrgP      0.24        1.e20
POC       4.356       1.e20
DOC       5.234       1.e20
DIC       0.003       1.e20
CBOD1     5.0         1.e20
DO        8.0         1.e20
Alk       100.0       1.e20
PX        100.0       1.e20
POM       10.89       1.e20
POM2      60000.0     -999
Hg0       0.01        1.e20
HgII      0.1         1.e20
HgII2     0.2         -999
MeHg      0.01        1.e20
MeHg2     0.02        -999
// HgSM Extra Input: Initial Values of Hg00 MeHg0 SO42 DOC2
0.001  0.001  0.001  50.3
// Monitor-Point-Info: NPOINT
1
100.5 9.8
// Steady-or-Unsteady (STEADY/UNS) & Turbulence-Model-Selection(PARA or KE)
UNS
0 360 1.0
PARA
0.7
```

```
// Initial Condition Method (DRY RST AUTO ZONAL)
RST
flow_RST.dat
// Mesh-Unit (FOOT METER INCH MM MILE KM GSCALE)
meter
mesh2.2DM SMS
// Manning Roughness Input Method(1=uniform 2=2DM 3=(x y) distributed
1
0.0185
// Any-Special-Treatments? (0 or empty = NO; 1=YES)

// Boundary Type (INLET-Q EXIT-H etc)
INLET-Q
   30 SI V
   TwaterC  SYMM
   TDS      SYMM
   Salinity SYMM
   Constituent1     SYMM
   Constituent2     SYMM
   SuspendedSolid1  SYMM
   SuspendedSolid2  SYMM
   SuspendedSolid3  SYMM
   Ap       SYMM
   NH4      SYMM
   NO3      SYMM
   OrgN     SYMM
   TIP      SYMM
   OrgP     SYMM
   POC      SYMM
   DOC      SYMM
   DIC      SYMM
   CBOD1    SYMM
   DO       SYMM
   Alk      SYMM
   PX       SYMM
   POM      SYMM
   Hg0      SYMM
   HgII     SYMM
   MeHg     SYMM
EXIT-H
   1.5 SI
SYMM
SYMM
MONITOR
// Wall-Roughess-Height-Specification (empty-line=DONE)

// Any In-Stream Flow Obstructions? (empty-line or 0 = NO)

// Results-Output-Format-and-Unit(SRHC/TEC/SRHN/XMDF;SI/EN) + Optional STL
TEC SI
// Headers of Output Variables specified by the User: EMPTY line means default is used

// Intermediate Result Output Control: minus for none
-1
```

The execution of the SRH-2D model preprocessor using the above _SIF.dat file and the unsteady simulation with the SRH-2D model create two types of files which are used by the SRH-WQ model. The first is the input file for SRH-WQ transport module (_WQ_input.dat); the second is(are) the flow results file(s) (only one is generated for the tutorial example and is labelled casename_WQF1.dat).

The _WQ_input.dat file generated by SRH-2D model preprocessor is shown below for the tutorial example while the unsteady output results file, _WQF1.dat, is stored in binary format (used directly by SRH-WQ without the need of user intervention).

```
// ========================================
// = Water Quality Module Input Parameters =
// ========================================
// Time Parameters: Dt_WQ(s) Time_Duration_Flow(hr) N_Duration MOD_RK5E
    3.00000000E+02    8.33333333E+00           1  0
// Meterology data file name + 6 TVF IDs: CC Tair(C) VPAir(mb) Pair(Atm) WS(m/s) Solar(W/m2)
data_meteorology.dat
   1   2   3   4   5   6
// Number of Advected/Transported State Variables & Total number of scalars
      25    33
// State Variable Name & Initial Condition Scalar Value
TwaterC                    2.50000000E+01    1.00000000E+20
TsedC                      2.10000000E+01   -9.99000000E+02
TDS                        6.80000000E+01    1.00000000E+20
Salinity                   1.60000000E+00    1.00000000E+20
Constituent1               1.25350000E+02    1.00000000E+20
Constituent2               1.37350000E+02    1.00000000E+20
SuspendedSolid1            1.00000000E+02    1.00000000E+20
SuspendedSolid2            5.00000000E+01    1.00000000E+20
SuspendedSolid3            2.00000000E+01    1.00000000E+20
SedimentSolid1             1.00000000E+06   -9.99000000E+02
SedimentSolid2             5.00000000E+05   -9.99000000E+02
SedimentSolid3             2.00000000E+05   -9.99000000E+02
Ap                         3.67700000E+01    1.00000000E+20
Ab                         2.40000000E+01   -9.99000000E+02
NH4                        6.30000000E-02    1.00000000E+20
NO3                        5.54000000E+00    1.00000000E+20
OrgN                       1.72600000E+00    1.00000000E+20
TIP                        7.10000000E-02    1.00000000E+20
OrgP                       2.40000000E-01    1.00000000E+20
POC                        4.35600000E+00    1.00000000E+20
DOC                        5.23400000E+00    1.00000000E+20
DIC                        3.00000000E-03    1.00000000E+20
CBOD1                      5.00000000E+00    1.00000000E+20
DO                         8.00000000E+00    1.00000000E+20
Alk                        1.00000000E+02    1.00000000E+20
PX                         1.00000000E+02    1.00000000E+20
POM                        1.08900000E+01    1.00000000E+20
POM2                       6.00000000E+04   -9.99000000E+02
Hg0                        1.00000000E-02    1.00000000E+20
HgII                       1.00000000E-01    1.00000000E+20
HgII2                      2.00000000E-01   -9.99000000E+02
MeHg                       1.00000000E-02    1.00000000E+20
MeHg2                      2.00000000E-02   -9.99000000E+02
// HgSM Module Extra Inputs: Hg00 MeHg0 SO42 DOC2
    1.00000000E-03    1.00000000E-03    1.00000000E-03    5.03000000E+01
// Boundary Condition: N_BD_having_FixedValues  N_of_BDF_having_FixedValues
         1         2
// BD Type for all Advected State Variable (-999=SYMM; 0=Constant; >0=TVF) at BD_ID =    1
  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999  -999
// BD Auxillary Array: L_fixed() = (IBDF IDBD) at each boundary face of the BD
   1   1   2   1
// TVF Info: Ntvf Ntvfsz <-- used for Time Dependent BC, MeteorologyData, ...
         6        25
// TVF Info: (ID_TVF NP) for each TVF; NP=number of data points
         1         4
         2         4
         3         4
         4         4
         5         4
         6         4
// [Time(s) Value] for TVF =  1 and SIZE=         4
    0.00000000E+00  6.00000000E-01  2.16000000E+06  6.00000000E-01  4.32000000E+06  6.00000000E-01
    1.29600000E+07  6.00000000E-01
// [Time(s) Value] for TVF =  2 and SIZE=         4
    0.00000000E+00  1.80000000E+01  2.16000000E+06  1.80000000E+01  4.32000000E+06  1.80000000E+01
    1.29600000E+07  1.80000000E+01
// [Time(s) Value] for TVF =  3 and SIZE=         4
    0.00000000E+00  2.60000000E+01  2.16000000E+06  2.60000000E+01  4.32000000E+06  2.60000000E+01
    1.29600000E+07  2.60000000E+01
// [Time(s) Value] for TVF =  4 and SIZE=         4
    0.00000000E+00  1.00000000E+00  2.16000000E+06  1.00000000E+00  4.32000000E+06  1.00000000E+00
    1.29600000E+07  1.00000000E+00
// [Time(s) Value] for TVF =  5 and SIZE=         4
    0.00000000E+00  3.00000000E+00  2.16000000E+06  3.00000000E+00  4.32000000E+06  3.00000000E+00
    1.29600000E+07  3.00000000E+00
// [Time(s) Value] for TVF =  6 and SIZE=         4
    0.00000000E+00  5.00000000E+02  2.16000000E+06  5.00000000E+02  4.32000000E+06  5.00000000E+02
    1.29600000E+07  5.00000000E+02
// Monitoring Point Info: Number_of_Points & then list of CELL_ID x(m) y(m) data
   1
      19      1.0050000000E+02    9.8000000000E+00
```

4.3.3 Running HgSM Module

Simulation using the NSMI Module with the SRH-WQ model is simple. For the tutorial example the following input data files are required:

(1) SRH-WQ Input File: This input file, named _WQ_input.dat, is generated while setting up the SRH-2D unsteady flow run as discussed above.
(2) SRH-2D Model Flow Results: The model flow results for user-specified time interval/periods, named _WQFi.dat, are generated while running the unsteady flow model with SRH-2D. For the tutorial example, only one file is generated and required (_WQF1.dat).
(3) SRH-WQ Control File: This is a water quality module specification file, named _WQ_controlfile.dat, produced by the USACE WQ modules. The file specifies information such as: (a) whether the modules are turned on or off; (b) the state variables activated for each module: (c) specification of relevant water quality model scalars for each module; (d) output options of derived and pathway variables, etc. This control file is not listed in this report due to its length. A detailed description of the control file is under development by the USACE and documentation will be available in the future.

Running the SRH-WQ model is accomplished by copying the executable file SRH-WQ.exe, along with all USACE WQ module DLLs (TEMP.dll, GC.dll, and NSMI.dll) for the tutorial example, to the project directory - then starting the simulation by clicking on the SRH-WQ.exe executable file.

4.3.4 Output from HgSM Module Simulation

For the tutorial example, several output files are generated once the simulation has completed. They include _PTi.dat (i starts from 1), _TECi.dat (i starts from 1), and _WQ_RESULT.dat.

For the tutorial example, _PT1.dat contains the time series simulation results at user specified monitoring points. All 56 state variables are reported in the file. Two plots displaying the simulated temperature, NO3 and DOC concentrations are shown in 10 for the tutorial example. The _TEC1.dat contains a 2D spatial distribution of all 56 state variables at the end of the model simulation. The data can be graphically displayed and post-processed using visualization software such as TECPLOT. A sample plot of the NO3 distribution for the tutorial example is shown in 11. In Figure 11, the spatial distribution appears almost uniform in the channel. Finally, the WQ_RESULT.dat file contains output information from the USACE WQ modules.

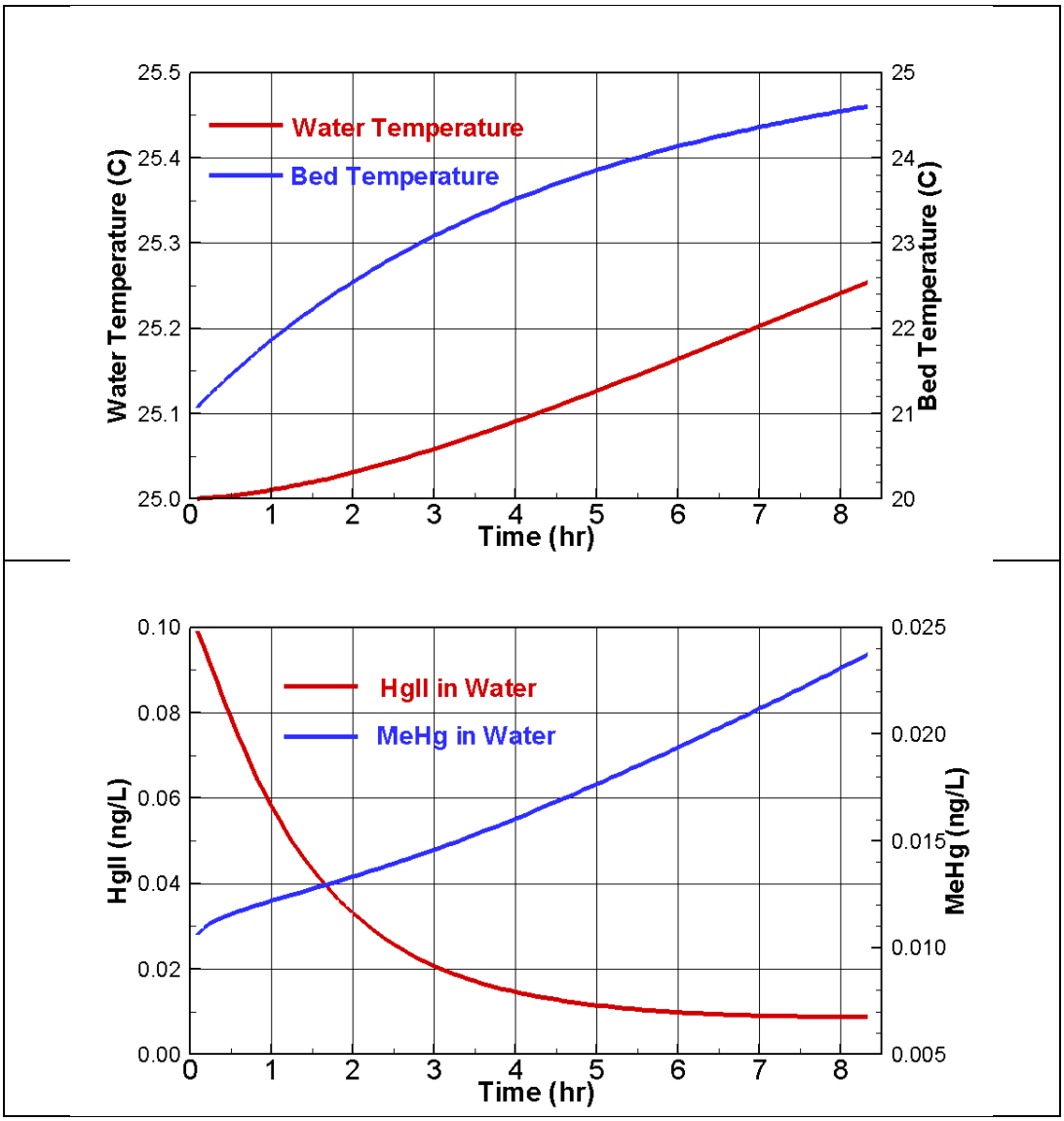

Figure 10. Time history of temperature change in water column and bed sediment and the simulated inorganic Hg (HgII) and methylmercury (MeHg) change in water column for the tutorial case.

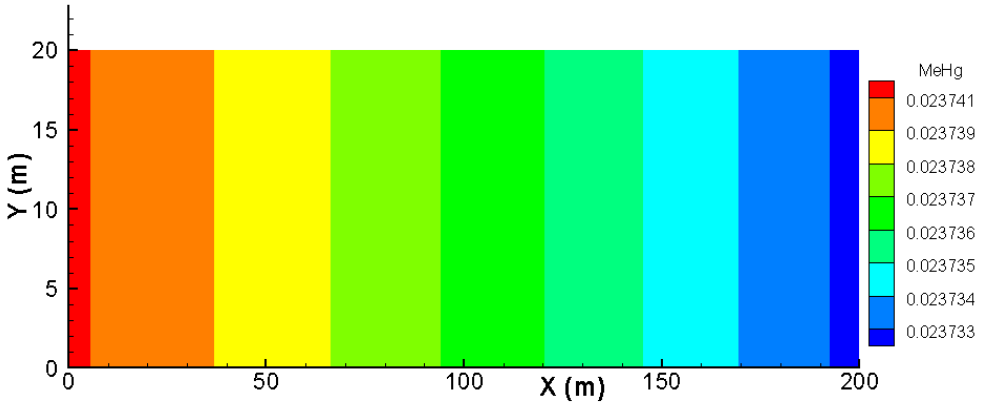

Figure 11. Distribution of simulated MeHg concentration (ng/L) in water column of the channel at the end of the simulation for the tutorial case.

5. Model Test and Verification

This section describes a number of case examples used to test and verify the SRH-WQ model. They are presented, in detail, below.

5.1 TEMP Module Verification Using Analytical Solutions

Two example cases presented below use SRH-WQ to solve the temperature equation which may be expressed as:

$$\frac{\partial T}{\partial t}+\frac{\partial UT}{\partial x}=k(T_{eq}-T)$$

The above temperature equation can be solved analytically and has the following exact solution:

$$T(t,x)=T_0(t-\tau)e^{-\kappa\tau}+T_{avg}(1-e^{-\kappa\tau})+\kappa T_\Delta\frac{\cos[\omega(t-\tau)]}{\omega^2+\kappa^2}\left[\omega e^{-\kappa\tau}-\omega\cos(\omega\tau)+\kappa\sin(\omega\tau)\right]$$
$$+\kappa T_\Delta\frac{\sin[\omega(t-\tau)]}{\omega^2+\kappa^2}\left[-\kappa e^{-\kappa\tau}+\kappa\cos(\omega\tau)+\omega\sin(\omega\tau)\right]$$

In the above, $T_0(t)$ is boundary condition at x=0, κ is a first-order rate constant which can be a function of meteorological parameters and water depth, $T_{eq}=T_\Delta\sin\left(\frac{2\pi t}{P_\Delta}\right)+T_{avg}$ is the equilibrium water temperature, $\tau=x/U$, and $\omega=\frac{2\pi}{P_\Delta}$.

The first test case has the following parameters: a constant flow velocity of U=1.0 mile/day, a zero equilibrium temperature in Celsius $T_{eq}=0$, and zero rate constant k=0.0. This case has flow source term that is zero and is designed to check the ability of the model to transport a scalar wave through use of the convection term only. A 100-mile straight channel is used. The initial temperature is zero Celsius everywhere - however the temperature at $x=0$ changes with time according to $T(x=0)=10+10\sin\left(\frac{2\pi t}{P}\right)$ in Celsius with the period of P = 20 days. The same model mesh is used as for the example in Chapter 4 and shown in Figure **4**. The model estimated temperature variation with time at $x=40$ miles is compared with the exact analytical solution in Figure **12**. The model-simulated temperature remains at zero Celsius until about day 35. The analytical solution predicts that the temperature wave would reach the location at day 40. The discrepancy between SRH-WQ prediction and the exact solution is most likely due to the numerical discretization errors.

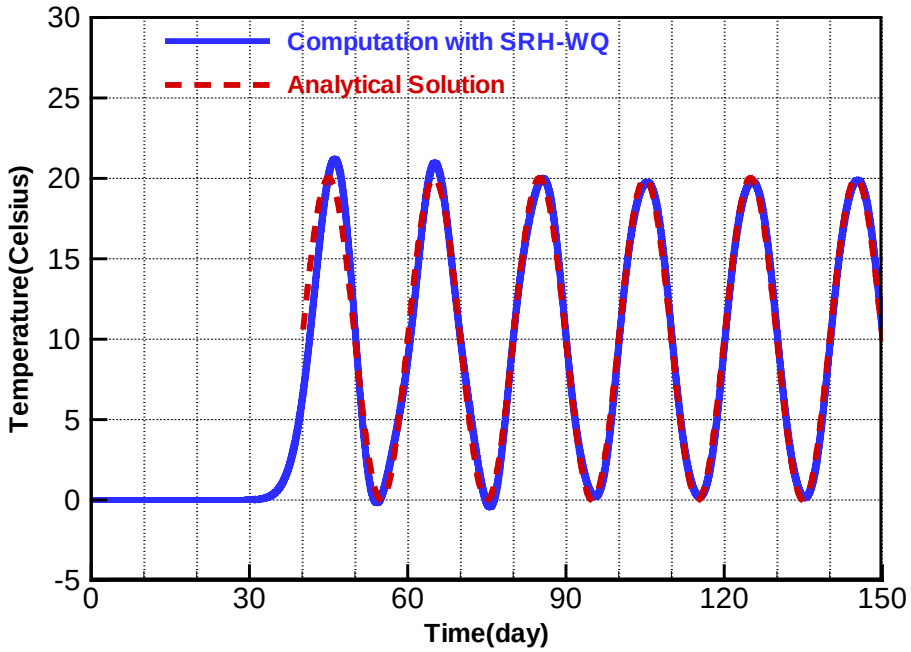

Figure 12. Comparison of simulated temperature and the exact solution at a location of 40 miles for case 1

The second case example has the following parameters: a constant flow velocity of *U*=1.0 mile/day, T_Δ=10 Celsius, T_{avg}=15 Celsius, and P_Δ =360 day, and a constant rate coefficient *k* = 0.2/day. This case has a first-order source term combined with scalar transport achieved through convection. A 100-mile straight channel is used for model simulation. The model mesh contains 100 or 300 cells in the flow direction (x) and 2 cells in the lateral direction (y). The temperature is 11.51 Celsius everywhere; the temperature at $x = 0$ is maintained according to the equation: $T_0(t) = 10\sin(\frac{2\pi t}{10}) + 10$. The equilibrium temperature varies according to the equation: $T_{eq} = 10\sin\left(\frac{2\pi t}{360}\right) + 15$. The model simulation is carried out for 150 days with a time step of 6 minutes. The model prediction and the analytical solution are compared in Figure 13 for temperature at $x = 4.5\ miles$. Figure 13 shows good agreement between the numerical and theoretical solutions..

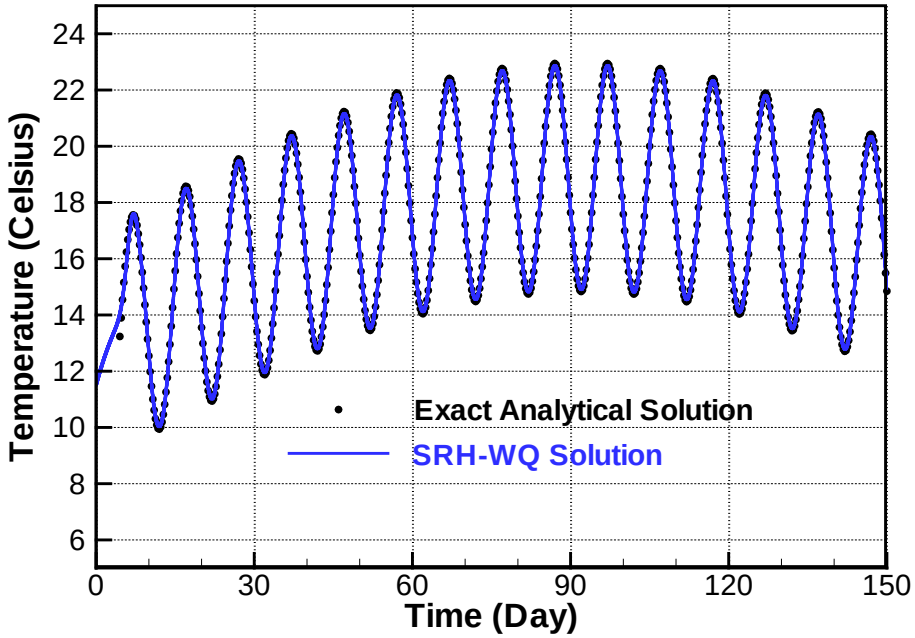

Figure 13. Case example 2 shows a comparison of simulated and exact analytical solutions for temperature in a 100 mile channel at mile 4.5.

5.2 TEMP Module Validation with McKay Dam Tailwater Data

The TEMP module is used to simulate temperature on a river reach downstream of the McKay Dam. The simulated model reach incorporates a section of McKay Creek and the first 2.57 miles of the Umatilla River.

5.2.1 Case Description

The McKay Dam and Reservoir are located on McKay Creek about 6 miles south of Pendleton, northeast Oregon. Downstream of the dam, the McKay Creek flows into the middle Umatilla River (at about RM 52). The Umatilla River drains into the Columbia River at about Columbia River Mile 289. Flows in the 2.57-mile reach of the Umatilla River from the confluence of the Umatilla River and McKay Creek to the Reith Bridge were controlled to provide a water temperature profile to benefit the fishery. In particular, the flat slope and pools within the first mile of the Umatilla River downstream of the confluence with McKay Creek provides potential habitat for fish.

A cross-sectional channel survey downstream of the McKay Creek was conducted in March and November 2000 by Reclamation staff. The U.S. Army Corp of Engineers (Walla Walla District Office) provided sparse background cross-section data of the Umatilla River collected in 1950. Around 64 cross-sections were assembled by Bender (2001) who carried out a temperature study for a 9-mile reach from McKay Dam to downstream of the Reith Bridge on the Umatilla River.

The same cross sectional data were used in the present study to construct a 2D model mesh for the SRH-WQ model simulation.

The simulation starts from midnight July 27, 2000 and continues for 5 days. Temperature measurements at selected locations provide the data for comparison with the TEMP module prediction. Continuous McKay Creek and Umatilla River temperature data were collected by the Umatilla tribes.

5.2.2 Mesh and Model Input

The simulation domain consists of about 6 miles of McKay Creek downstream of the McKay Dam and 3 miles of Umatilla River downstream of the confluence between McKay Creek and Umatilla River. The developed 2D mesh consists of 4,024 cells with both quadrilateral cells and triangular cells. The topography is interpolated from the cross sectional survey data.

Boundary conditions include water discharge and temperature downstream of the McKay Dam and upstream of the confluence in the Umatilla River. The hourly McKay Dam release discharge and temperature are used as upstream boundary conditions for the modeling period. The discharge downstream of the McKay Dam varies from 242 to 257 cfs and temperature ranges from 8.3 to 9.1 Celsius. The hourly flow, from 40 to 49 cfs, at Pendleton, Oregon is used as the upstream condition of the Umatilla River. The temperature, ranging from 24 to 27 Celsius, at the Umatilla River is based on a synoptic survey taken on July 28, 2000.

Initial conditions of the modeling used a steady state flow discharge of (257 cfs) at midnight of July 27, 2000. The initial temperature varies depending on the location of the cross section from 8.4 C downstream of the McKay Dam to 23.0 C at the Reith Bridge.

Hourly meteorological data, including cloud cover, air temperature, air vapor pressure, air pressure, and wind speed, are based on the National Weather Service (NWS) data from Pendleton, Oregon; and Agrimet solar radiation data from Hermiston, Oregon (station HMRO). Vegetation shading is not considered in the model because the TEMP module does not offer such an option. However we do not believe that the impact of shade is significant compared to other factors considered at the site.

5.2.3 Result and Comparison

Model simulation was initiated at midnight July 27, 2000 and continued for five days. The simulated temperature was cross-sectionally averaged where measured temperature data was available. Comparisons of the model simulated and measured temperature observations are shown in Figure **14** and Figure **17** at four measurement locations.

It is clear that the TEMP module over-predicts the temperature diurnal variation for the river reach when compared to measured temperature data. The reason is unclear and future discussion with the USACE will be necessary since the TEMP module was a product of USACE, not Reclamation. This case example does show that the integrated SRH-WQ model performs adequately when applied to a candidate river. An assessment of model accuracy study will be considered in ongoing and future research and development.

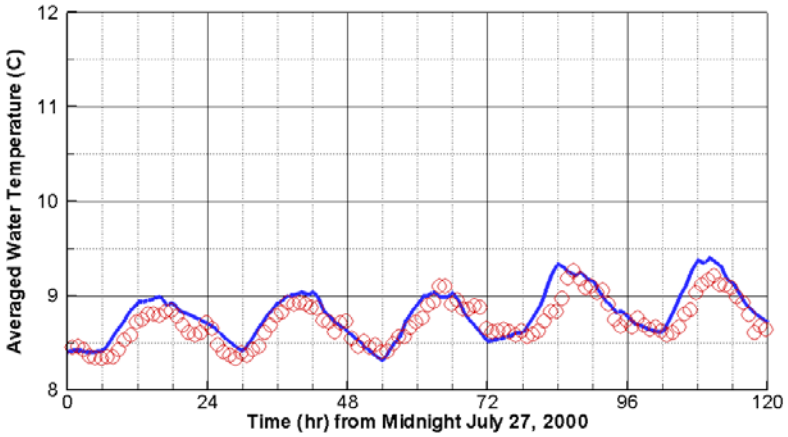

Figure 14. Comparison of model simulated and theoretical temperature near McKay Dam (McKay RM 6.0) from July 28 through August 1, 2000 (Solid: Simulated; Symbol: Measured)

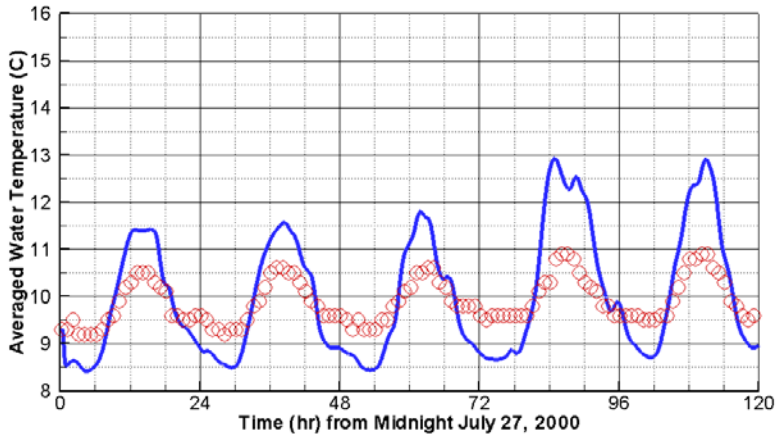

Figure 15. Comparison of model simulated and theoretical temperature at Scheeler (McKay RM 3.7) from July 28 through August 1, 2000 (Solid: Simulated; Symbol: Measured)

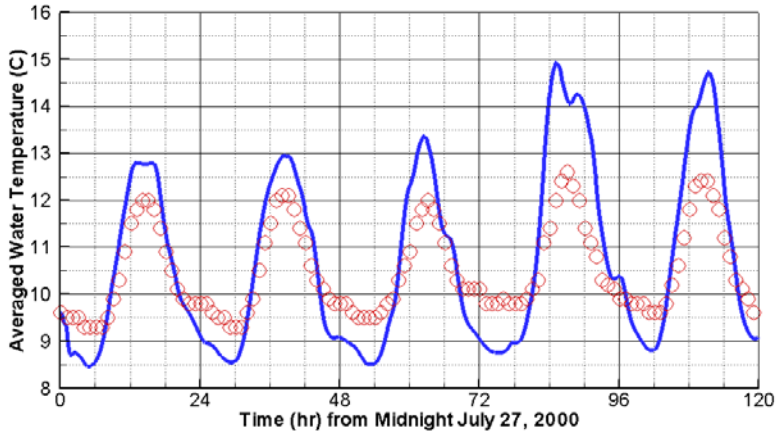

Figure 16. Comparison of model simulated and theoretical temperature at School (McKay RM 1.9) from July 28 through August 1, 2000 (Solid: Simulated; Symbol: Measured)

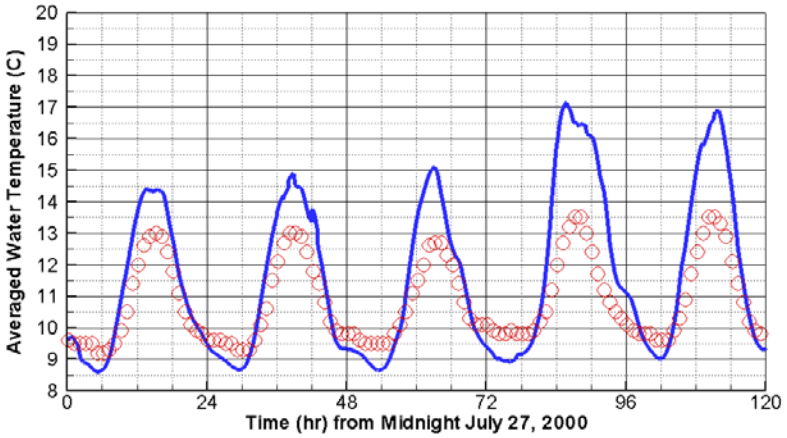

Figure 17. Comparison of model simulated and theoretical temperature at Fish Barrier (McKay RM 0.01) from July 28 through August 1, 2000 (Solid: Simulated; Symbol: Measured)

A validation study of the NSMI module was initiated and is ongoing - simulating more than 50 miles of the lower Minnesota River. Due to the complexity of the modeling, the completion of this study isn't anticipated until FY 2018 and the final results documented as an amendment or additional technical appendix to the current report.

5.3 HgSM Module Demonstration for the Trinity River

In the course of this study, considerable effort was spent seeking streams and/or reservoirs that have sufficient mercury data for HgSM module verification and validation. No suitable site with comprehensive Hg data was found although sites do exist where inferences can be made from adjacent watersheds to supplement a sparse database. This strategy is documented in a companion report entitled,

"An Integrated Model for Mercury Transport and Transformation at Reservoirs - 2017 Progress". This report describes new datasets that have not been reviewed for the Putah and Cache Creek watersheds in the Sacramento River Basin in Northern California and a strategy for combining datasets using inference mapping of characteristics. This report also presents some preliminary model development work using the WARMF model mercury module.

For this report, a HgSM simulation was carried out and analyzed after applying the model to a section of the Trinity River, in California. For model demonstration purposes the integrated model was applied to actual rivers and streams rather than just simple channels. The model developers plan to continue to collaborate with researchers and agency personnel in developing comprehensive Hg datasets that will allow more rigorous HgSM module calibration, validation and verification for realistic streams and reservoirs – especially those managed by Reclamation and other federal agencies where there is an acute need for mercury management decision support.

5.3.1 Model Domain, 2D Mesh and Terrain Data

Developing a 2D simulation model of water quality begins by defining a model domain of the study site and then generating a mesh to cover the model domain. The model domain is often constrained by the available terrain data. For the study example, a section of the Trinity River near the Upper Junction City (UJC) was selected for SRH-WQ model simulation. The model domain selected is displayed in Figure 18. The model domain covers an area of 4,100 ft in length (stream reach) and 120 ft in width (stream width at cross-section)..

Model meshes were generated using the AquaVeo Surface-water Modeling System software (SMS). The following website link provides the information about the SMS software: http://www.aquaveo.com. Additionally, SRH-2D manual (Lai, 2008) may be used for instructions on generating an appropriate 2D mesh. The 2D mesh generated is also shown in Figure 18. It consists of mixed quadrilaterals and triangles with a total of 3,166 mesh cells and 3,408 mesh points.

The stream terrain of the UJC section was surveyed by engineers at the Trinity River Restoration Program in 2009 and the terrain is displayed in Figure 19. The terrain incorporated data from two sources. Terrestrial and bathymetric LiDAR was flown in early April 2009 before flow started going up for the 2009 release. This data was very good in emergent areas but poor in shallow submerged areas. Therefore, sonar data was obtained in areas deeper than about a meter in November and December, 2009. The 2009 terrain data was interpolated onto the 2D mesh so that the stream can be simulated with SRH-WQ.

Figure 18. Model domain (red) and the mesh (black) used for the Trinity River UJC section case

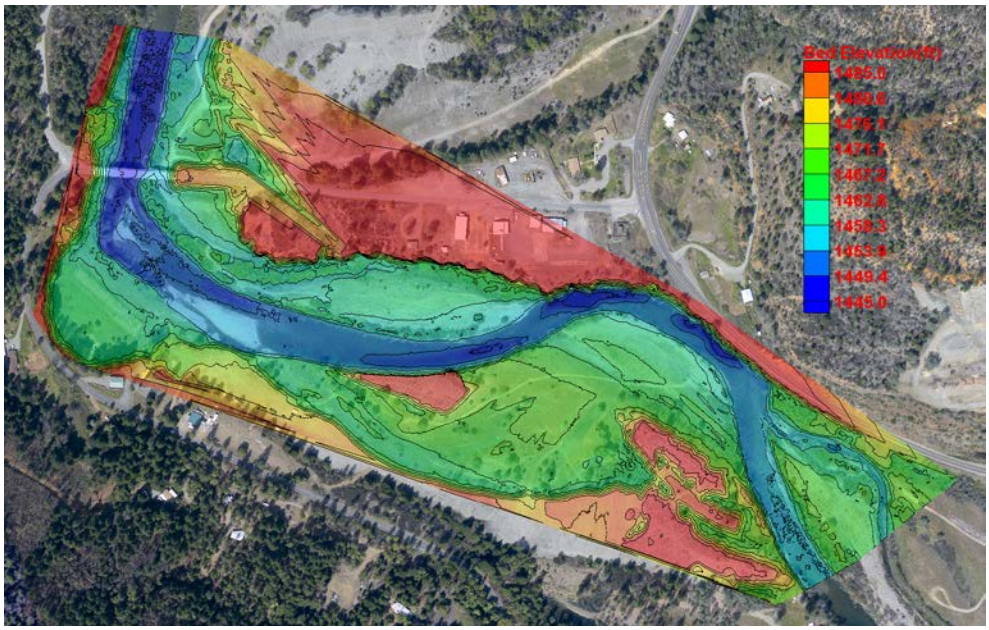

Figure 19. 2009 surveyed terrain of the UJC section represented by the bed elevation contours (aerial photo in April 2009)

5.3.2 SRH-2D Flow Modeling and Inputs for SRH-WQ

A steady-state flow model with a constant flow discharge was developed first given that the flow output is needed to establish the initial conditions for the unsteady-state simulation. Unsteady flow simulation is always performed to simulate mercury and other water quality constituents with the SRH-WQ model because of the dynamic nature of mercury hydrochemistry.

For the steady-state model run, a constant flow discharge of 4,160 ft^3/s was imposed on the upstream boundary of the domain representing the flow on May 1, 2009. A rating curve was used as the downstream boundary condition (obtained through a separate 1D HEC-RAS simulation). A Manning's roughness coefficient of 0.035 was applied to the entire model domain.

Flow modeling with SRH-2D is well established and documented by Lai (2008; 2010); so details have been omitted. The input file (_SIF.dat), used for the steady-state model run is listed (as previously) as a reference.

```
// Simulation Description (not used by SRH-2D/3D):
Trinity UJC Section
// Module/Solver Selected (FLOW MOB TEM TC WQ)
FLOW
// Monitor-Point-Info: NPOINT --> 4 Points near(downstream) 4 monitor lines from upstream to downstream
4
6269592 2149398 6268952 2149863.2 6267967.4 2149716 6267410 2150695
// Steady-or-Unsteady (STEADY/UNS)
STEADY
// Tstart Time_Step and Total_Simulation_Time: TSTART DT T_SIMU [FLAG]
0 1 10
// Turbulence-Model; and A_TURB for the PARA Model (0.05 to 1.0)
PARA
0.7
// Initial Flow Condition Method (DRY RST AUTO ZONAL VWSE/VWD)
DRY
// Mesh-Unit (FOOT METER INCH MM MILE KM GSCALE); Mesh FILE_NAME and FORMAT(SMS...)
FOOT
mesh.2DM SMS
// Bed Friction. ISpace for 2D; ISpace Imethod for 3D. Ispace=1=uniform 2=2DM. Imethod=1=n 2=ks
1
// Manning-n or ks(mm) Entry: a real value or a WD~n file name
0.035
// Any-Special-Treatments? (0 or empty = NO; 1=YES)

// Boundary Type (INLET-Q EXIT-H etc)
INLET-Q
   4160 EN C
// Boundary Type (INLET-Q EXIT-H etc)
EXIT-H
   exit_rating_curve.dat EN
// 4 Monitor Lines from Upstream to Downstream
monitor
monitor
monitor
monitor
// Wall-Roughess-Height-Specification (empty-line=DONE)

// Any In-Stream Flow Obstructions? (empty-line or 0 = NO)

// Results-Output-Format-and-Unit(SRHC/TEC/SRHN/XMDF/XMDFC/PARA;SI/EN) + Optional STL
TEC EN
// Headers of Output Variables specified by the User: EMPTY line means default is used

// Intermediate Result Output Control: INTERVAL(hour) OR List of T1 T2 ...  EMPTY means the end
-1
```

The next task was to perform an unsteady flow simulation using the flow hydrograph from May 1 to 10, 2009 (10 days of stream flow simulation). The unsteady-state run serves two purposes. First, the simulation produces flow results at a user-specified time interval (24 hours or daily for the current example) which are stored in computer memory and used by the SRH-WQ model for the Hg simulation. Second, the unsteady flow modeling setup process, using the SRH-2D model preprocessor, helps to create the input file to run the SRH-WQ model.

In addition to the inputs needed for flow simulation, the following additional inputs were used to set up the input file for the SRH-WQ HgSM model simulation:

- SRH-WQ Model Time Parameters

    - Time step (DT_WQ) is 36 seconds for SRH-WQ
    - Time interval (TIME_PERIOD) is 24 hours for which flow results are stored
    - Total number of time periods (N_PERIOD) is 10. This equates to a 240 hour (10 day) WQ simulation

- Meteorological Data

    - A file named meteorology_data.dat, was used for the meteorological data inputs. The time series solar radiation and air temperature data, are 2 out of the 6 meteorological variables, plotted in Figure 20.

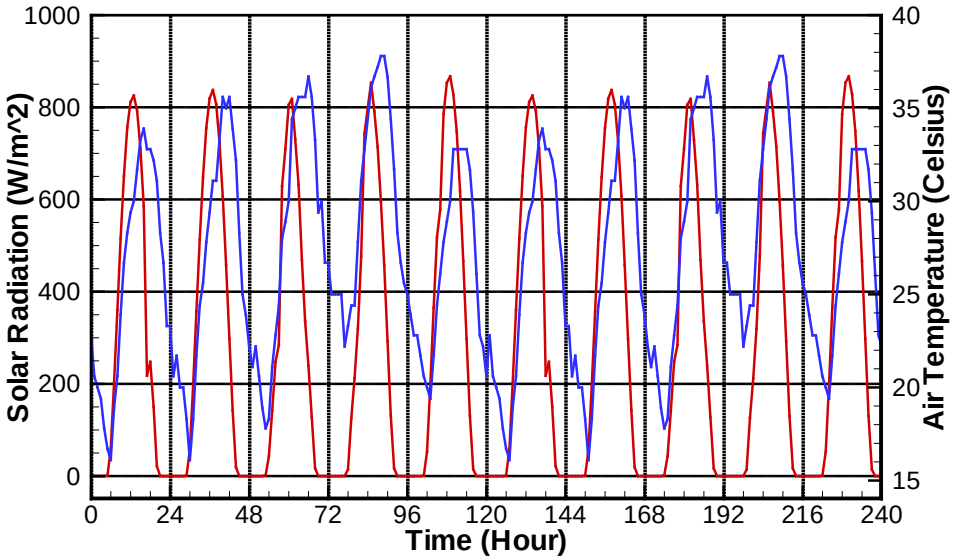

Figure 20. Temporal variation of solar radiation and air temperature used for the 10-day SRH-WQ Model simulation

- State Variable Information

    - A total of 33 state variables wereused for the SRH-WQ simulation; and 25 state variables were advected by SRH-WQ transport module.
    - A list of all state variable names, Schmidt number, and initial values were specified and listed later in the _SIF.dat file.
    - Initial Hg0 and MeHg concentrations in air and concentrations of SO4 and DOC in the active sediment layer were also supplied as model inputs.

- Boundary Condition of Advected State Variables

    Two open boundaries were used for the flow simulation: upstream and downstream boundaries. At the upstream flow boundary, water enters the model domain and the boundary conditions for all advected state variables were supplied. As previously discussed, two options are available to specify the boundary condition of a variable: (a) a zero flux condition implemented as the symmetry condition or (b) the Dirichlet condition. With (b), the Dirichlet condition, a constant or a time series boundary flux data set is specified. The boundary condition data is normally derived from recorded gauge data.

    Dirichlet conditions were used for flow discharge, water temperature, Hg0, HgII, MeHg; and the symmetry condition was used for the remaining state variables. The flow hydrograph and the water temperature boundary conditions are shown in Figure 21. Hg0=0.01, HgII=0.1 and MeHg=0.01 were used as constant value boundary conditions. At the downstream boundary, a rating curve was used and the data obtained through a separate 1D HEC-RAS simulation.

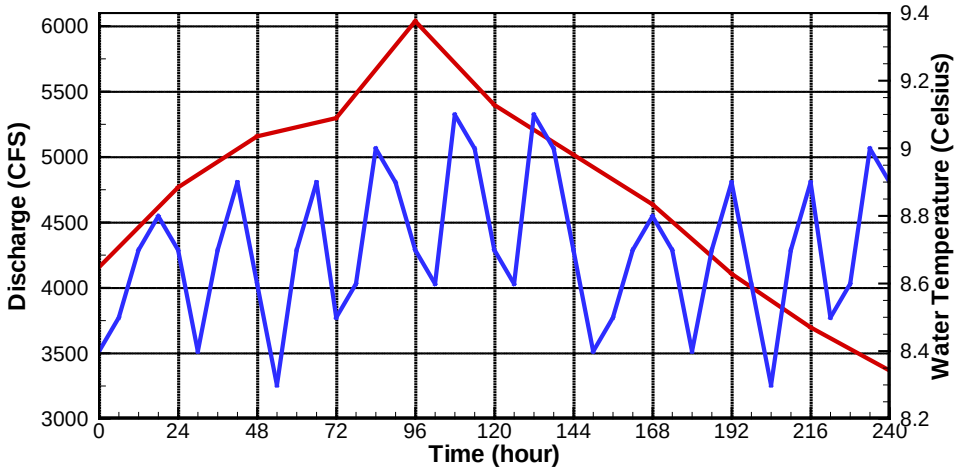

Figure 21. Temporal variation of flow discharge (red) through the UJC section from May 1 to 10, 2009. The water temperature (blue) is simulated at the upstream boundary

The _SIF.dat file used to run the SRH-2D preprocessor is shown below, which produces not only the needed inputs to run the SRH-2D unsteady flow simulation, it also creates the input data file to run the SRH-WQ model.

```
// Simulation Description (not used by SRH-2D):
Trinity River UJC Section: Flow Run + HgSM Modeling Setup
// Module/Solver Selected (FLOW MOB TEM TC WQ)
WQ
// WQ(Water Quality) Time Parameters: DT_WQ(s) TIME_Period(Hr) N_Period
36 24.0 10
// Meterological data file name & Option(1=USACE; 2=Reclamation)
meteorology_data.dat
// WQ: Number of total & Advected State Variables
33 25
// All WQ State Variables:  NAME  SCHMIT  SC_Initial (-999 signals non-Advected)
TwaterC          1.0      8.4
TsedC            -999     8.4
TDS              1.0e20   68.0
Salinity         1.0e20   1.6
Constituent1     1.0e20   125.35
Constituent2     1.0e20   137.35
SuspendedSolid1  1.0e20   100.0
SuspendedSolid2  1.0e20   50.0
SuspendedSolid3  1.0e20   20.0
SedimentSolid1   -999     1000000.0
SedimentSolid2   -999     500000.0
SedimentSolid3   -999     200000.0
Ap       1.e20    36.77
Ab       -999     24.0
NH4      1.e20    0.063
NO3      1.e20    5.54
OrgN     1.e20    1.726
TIP      1.e20    0.071
OrgP     1.e20    0.24
POC      1.e20    4.356
DOC      1.e20    5.234
DIC      1.e20    0.003
CBOD1    1.e20    5.0
DO       1.e20    8.0
Alk      1.e20    100.0
PX       1.e20    100.0
POM      1.e20    10.89
POM2     -999     60000.0
Hg0      1.e20    0.01
HgII     1.e20    0.1
HgII2    -999     0.1
MeHg     1.e20    0.01
MeHg2    -999     0.01
// HgSM Extra Input: Initial Values of Hg00 MeHg0 SO42 DOC2
0.001  0.001  0.001  50.3
// Monitor-Point-Info: NPOINT --> 4 Points near(downstream) 4 monitor lines from upstream to downstream
4
// Monitor Point Coordinates: x1 y1 x2 y2 ...
6269592 2149398 6268952 2149863.2 6267967.4 2149716 6267410 2150695
// Steady-or-Unsteady (STEADY/UNS)
UNS
0 1 240
// Turbulence-Model-Selection(PARA or KE)
PARA
0.7
// Initial Condition Method (DRY RST AUTO ZONAL)
RST
flow_RST.dat
// Mesh-Unit (FOOT METER INCH MM MILE KM GSCALE)
foot
mesh.2DM SMS
// Manning Roughness Input Method(1=uniform 2=2DM 3=(x y) distributed
1
0.035
// Any-Special-Treatments? (0 or empty = NO; 1=YES)

// Boundary Type (INLET-Q EXIT-H etc);  TwaterC  inlet_tem.dat; TwaterC  uma_tem.dat
INLET-Q
   qcfs_2009.dat EN C
// STart of WQ Boundary Values
   TwaterC  inlet_tem.dat
   TDS      SYMM
   Salinity SYMM
   Constituent1     SYMM
   Constituent2     SYMM
   SuspendedSolid1  SYMM
   SuspendedSolid2  SYMM
   SuspendedSolid3  SYMM
```

```
   Ap        SYMM
   NH4       SYMM
   NO3       SYMM
   OrgN      SYMM
   TIP       SYMM
   OrgP      SYMM
   POC       SYMM
   DOC       SYMM
   DIC       SYMM
   CBOD1     SYMM
   DO        SYMM
   Alk       SYMM
   PX        SYMM
   POM       SYMM
   Hg0       0.01
   HgII      0.1
   MeHg      0.01
//
EXIT-H
  exit_rating_curve.dat EN
// 4 Monitor Lines from Upstream to Downstream
monitor
monitor
monitor
monitor
// Wall-Roughess-Height-Specification (empty-line=DONE)

// Any In-Stream Flow Obstructions? (empty-line or 0 = NO)

// Results-Output-Format-and-Unit(SRHC/TEC/SRHN/XMDF;SI/EN) + Optional STL
TEC SI
// Headers of Output Variables specified by the User: EMPTY line means default is used

// Intermediate Result Output Control: minus for none
-1
```

Model simulation runs made with the SRH-2D model preprocessor uses the _SIF.dat file listed above; the unsteady-state simulation with the SRH-2D model creates two types of files used by the SRH-WQ model: (a) the input file for SRH-WQ (_WQ_input.dat) and (b) the flow output files (_WQFi.dat). For the present example , ten _WQi.dat files were created.

The SRH-2D model flow simulation is shown in Figure 22 when the total discharge estimated for the stream is 4,160 cfs.

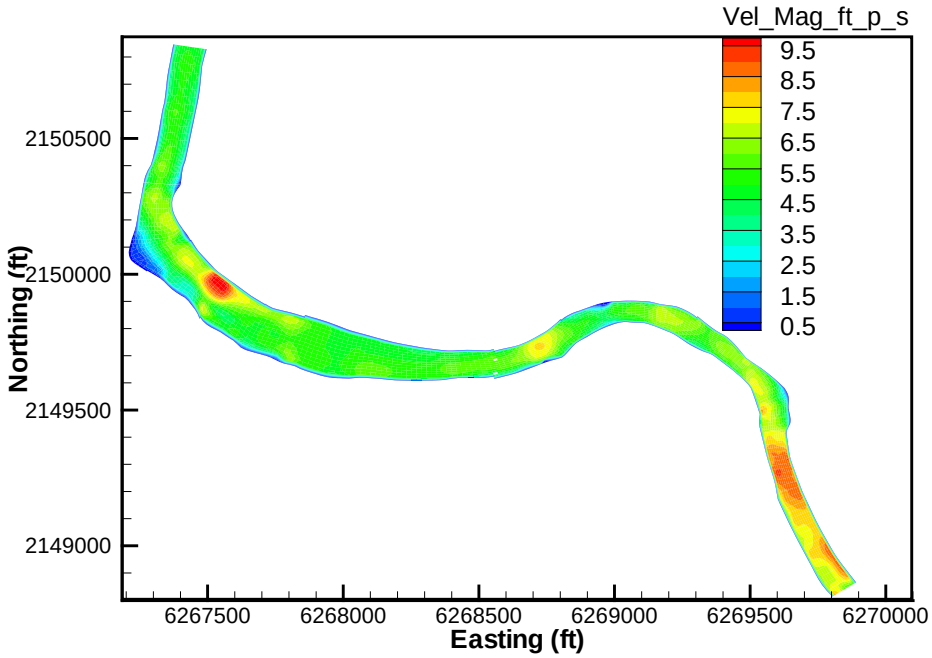

Figure 22. Simulated channel velocity vectors (ft/sec) when discharge is estimated to be 4,160 cfs

5.3.3 HgSM Modeling

The SRH-WQ model simulation using the HgSM module was carried out for 10 days using the inputs previously described. The following scalar inputs are used for the simulation:

(1) SRH-WQ Input File: This input file, named _WQ_input.dat, is generated while setting up the SRH-2D unsteady flow run as discussed above.
(2) SRH-2D Flow Results: Ten flow (outputs) results at an interval of 24 hours are generated by the SRH-2D model unsteady simulation (_WQFi.dat).
(3) SRH-WQ Control File

Running the SRH-WQ model is accomplished by copying the SRH-WQ.exe, file along with all the USACE module DLLs (TEMP.dll, GC.dll, NSMI.dll and HgSM.dll) for the tutorial example, to the project directory. The SRH-WQ.exe model file executable can then be run to complete the simulation.

5.3.4 Results of SRH-WQ HgSM Simulation

Selected model simulation results are presented in this section, however no interpretation or performance evaluation is offered owing to the lack of field observations for model validation.

The example is intended more as a demonstration to show the successful integration of the SRH-2D model with the USACE WQ modules, the further development of the SRH-WQ 2D transport module, and the potential model application to streams and rivers implicated in mercury fate and transport, especially those water bodies that flow into reclamation reservoirs.

Temporal variations of several important model state variables were plotted at two monitoring locations (cross-sections) lines (#1 and #2) shown in Figure 23. The time series data for water temperature, DOC, POM, Hg0, HgII, and MeHg at the two monitoring sites are shown in Figure 24 through Figure 32.

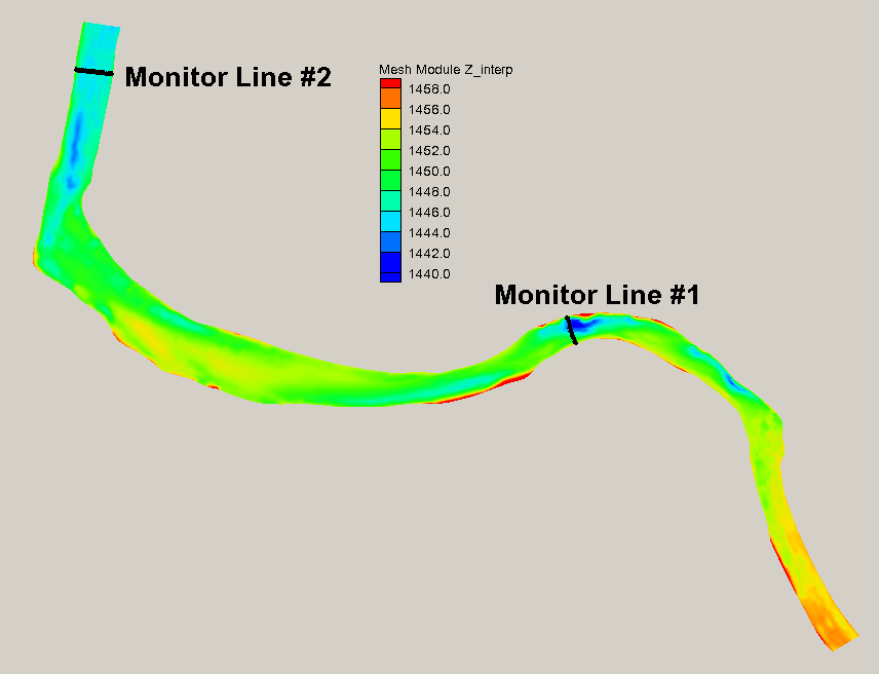

Figure 23. Locations of two monitoring locations (cross sections) for the UJC reach of the Trinity River, California.

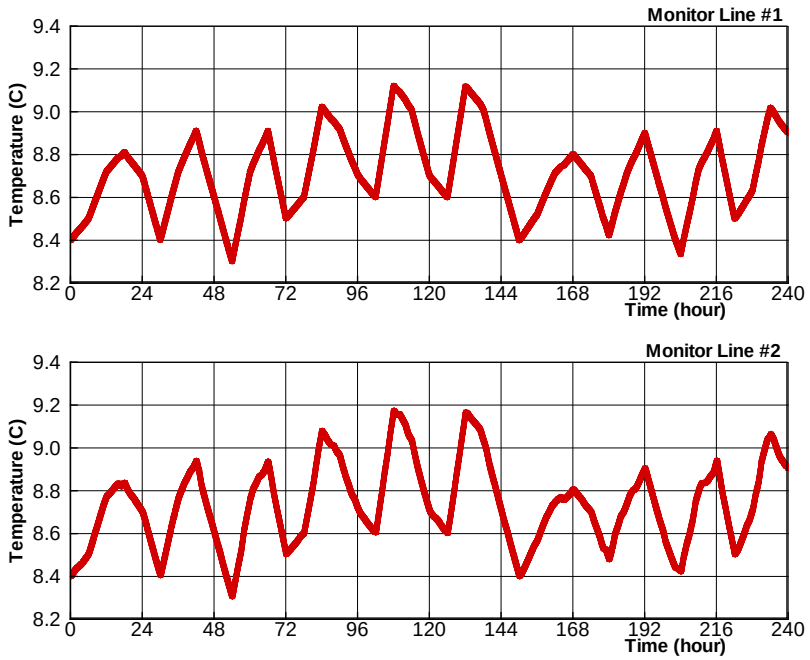

Figure 24. Simulated water temperature time series at two water quality monitoring stations on the Trinity River, California.

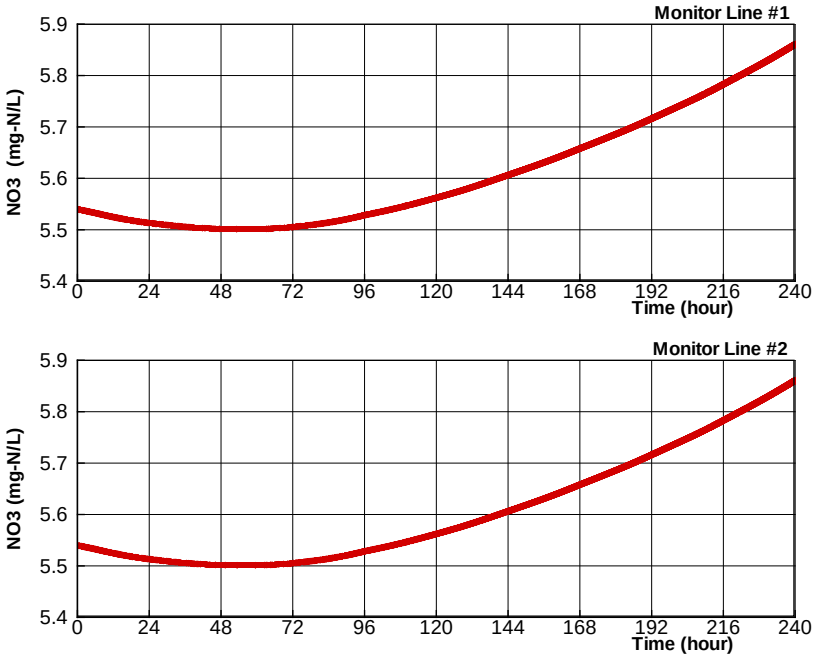

Figure 25. Simulated NO3 concentration time series at two water quality monitoring stations on the Trinity River, California.

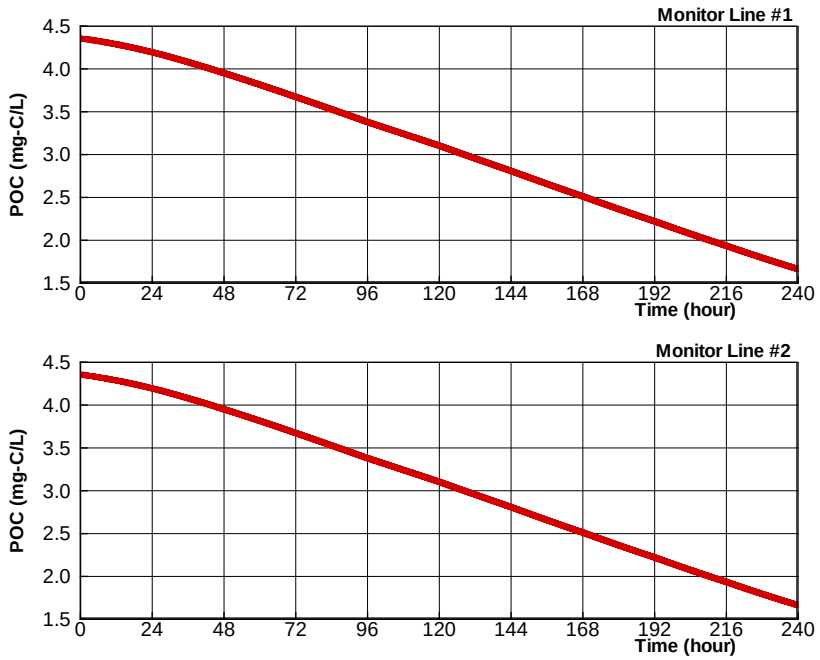

Figure 26. Simulated POC concentration time series at two water quality monitoring stations on the Trinity River, California.

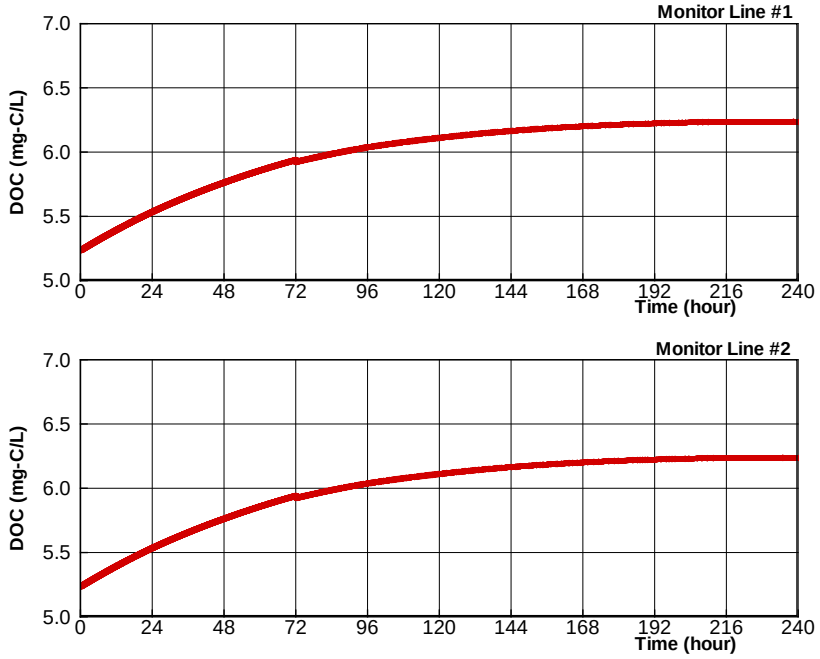

Figure 27. Simulated DOC concentration time series at two water quality monitoring stations on the Trinity River, California.

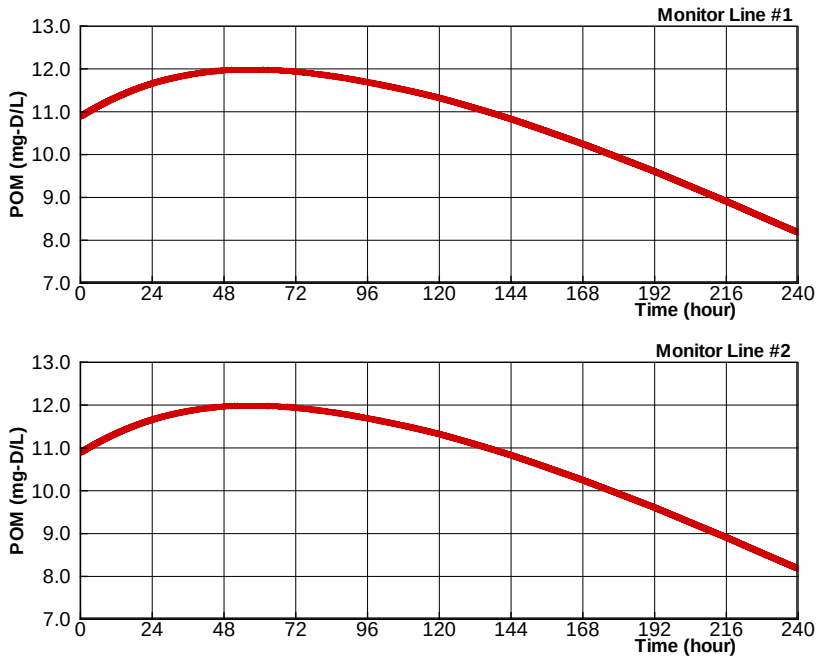

Figure 28. Simulated POM concentration time series at two water quality monitoring stations on the Trinity River, California.

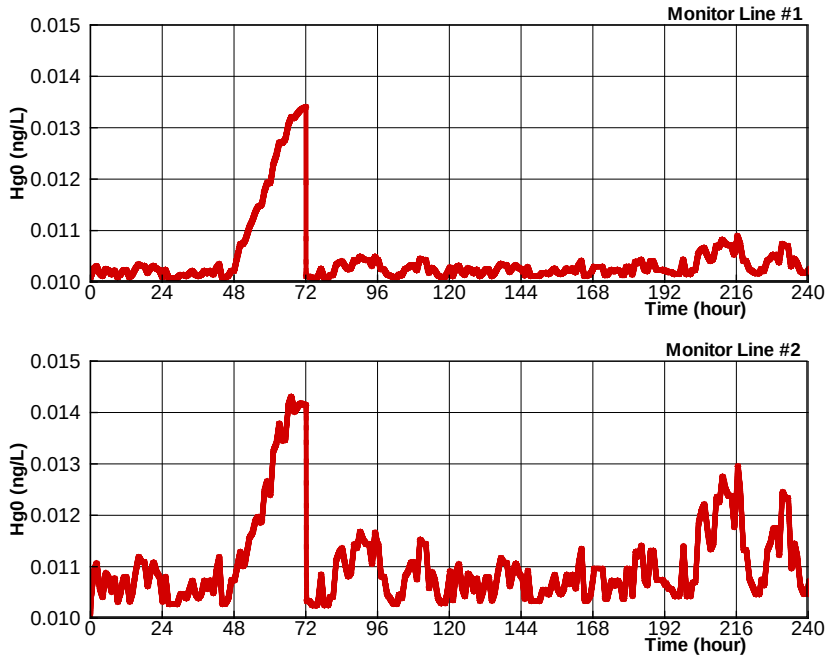

Figure 29. Simulated Hg0 concentration time series in water at two water quality monitoring stations on the Trinity River, California.

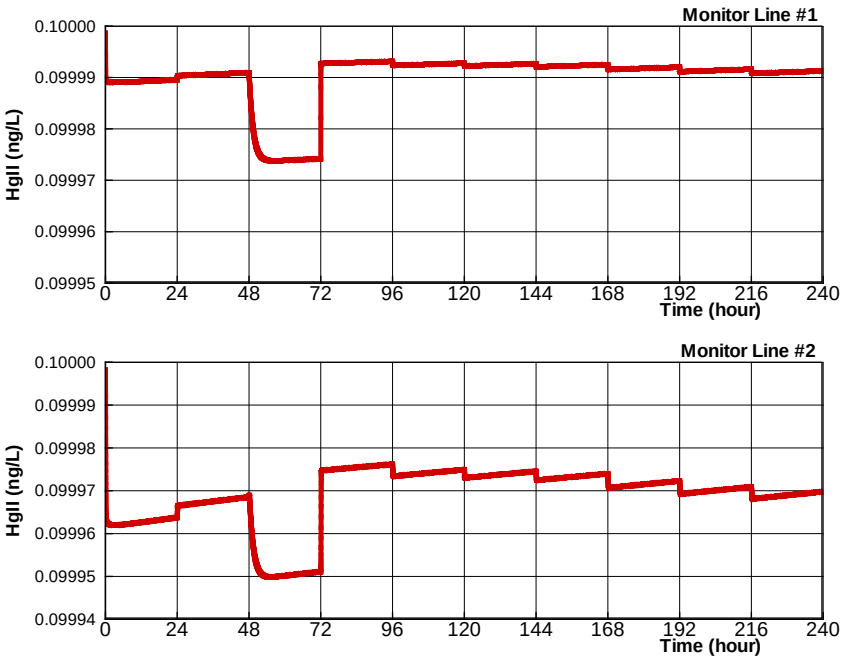

Figure 30. Simulated HgII concentration time series in water at two water quality monitoring stations on the Trinity River, California.

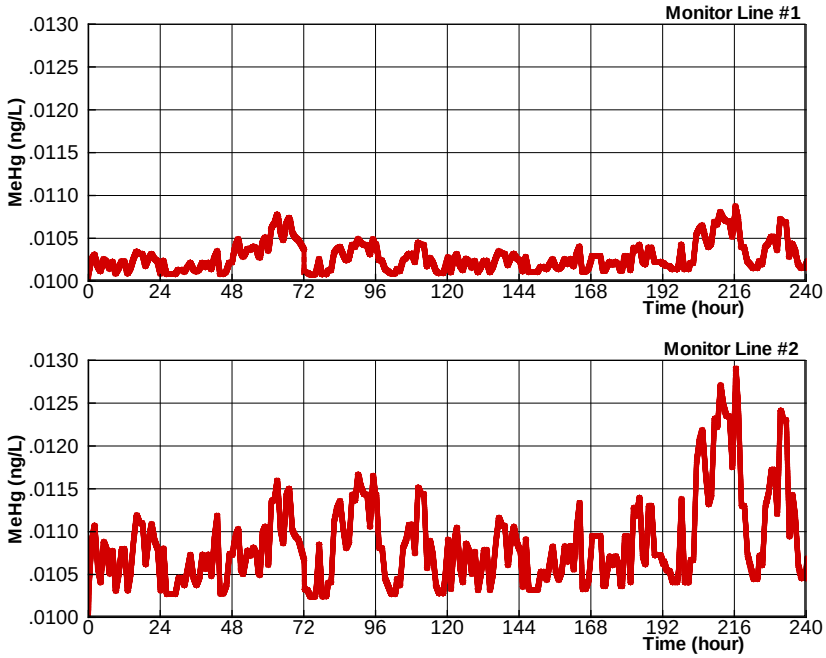

Figure 31. Simulated MeHg concentration time series in water at two water quality monitoring stations on the Trinity River, California.

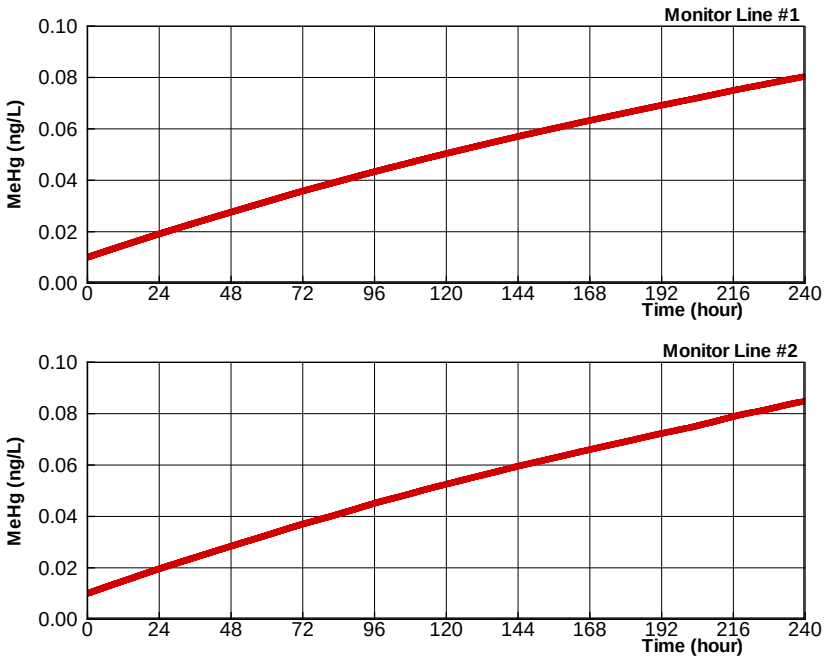

Figure 32. Simulated MeHg concentration time series in the active sediment layer at two water quality monitoring stations on the Trinity River, California.

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