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# Numerical Framework to Link the Adaptive Hydraulics (AdH) Code to the Nutrient Simulation Module-I (NSMI)

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**PURPOSE:** This Coastal and Hydraulics Engineering Technical Note (CHETN) describes the numerical framework for linking the U.S. Army Engineer Research and Development Center, Environmental Laboratory-developed Nutrient Simulation Module-I (NSMI) kinetics library to the Coastal and Hydraulics Laboratory-developed Adaptive Hydraulics (AdH) hydrodynamic code.

**BACKGROUND:** The AdH hydrodynamic code is a linear element-based finite element code that is capable of solving the saturated/unsaturated groundwater equations, the Reynolds Averaged Navier-Stokes equations, Diffusive Wave equations as well as the two/three-dimensional (2D/3D) Shallow Water Equations (SWE). This CHETN provides the framework for linking NSMI to the AdH-2D/3D SWE code (hereafter referred to as AdH).

A variety of 2D/3D reservoir, riverine, coastal, and estuarine models exist (e.g., AdH, CH3D, TABS-MDS). These models solve some form of the Reynolds Averaged Navier-Stokes equations using the hydrostatic and Bousinnesq assumptions. The computed flow field is then used within the transport advection-diffusion-reaction equation to numerically simulate the transport of constituents. The governing equations for the advection-diffusion-reaction of constituents are written as

$$\text{3D-SWE: } \frac{\partial c_i}{\partial t}+\frac{\partial c_i u}{\partial x}+\frac{\partial c_i v}{\partial y}+\frac{\partial c_i w}{\partial z}-\frac{\partial D_x \frac{\partial c_i}{\partial x}}{\partial x}-\frac{\partial D_y \frac{\partial c_i}{\partial y}}{\partial y}-\frac{\partial D_z \frac{\partial c_i}{\partial z}}{\partial z}\pm \text{source/sink}+R\left(c_i,t\right)=0 \quad (1)$$

and

$$\text{2D-SWE: } \frac{\partial c_i}{\partial t}+\frac{\partial c_i u}{\partial x}+\frac{\partial c_i v}{\partial y}-\frac{\partial D_x \frac{\partial c_i}{\partial x}}{\partial x}-\frac{\partial D_y \frac{\partial c_i}{\partial y}}{\partial y}\pm \text{source/sink}+R\left(c_i,t\right)=0 \quad (2)$$

Where $c_i$ is the concentration (depth averaged in 2D) of the $i^{th}$ constituent, $h$ is the fluid depth, $u$ is the x-direction velocity, $v$ is the y-direction velocity, $w$ is the z-direction velocity, $D_x$ is the x-direction diffusivity, $D_y$ is the y-direction diffusivity, $D_z$ is the z-direction diffusivity, and $R\left(c_i,t\right)$ are the reaction rate terms.

Historically, the reaction rate, $R\left(c_i,t\right)$, terms in Equations 1 and 2 have been provided by water quality equations implicitly embedded into the advection-diffusion-reaction equation. This can add non-linearity to what is otherwise a simple linear initial value problem, and the benefits of such tight coupling are not sufficient to justify the increased computational burden. This is especially true for water quality constituents as the rate of change is small compared to the temporal scale of the advection-diffusion component. In these cases, the mathematical technique of operator splitting (OS) is beneficial.

**OPERATOR SPLITTING:** OS is a mathematical technique that involves splitting an equation into two or more separate equations that when added together reformulate the original equation. The strategy behind OS is particularly beneficial for equations with terms whose temporal or spatial rates of change are not the same as that of the other terms in the equation. In this document, only the temporal rate of change is of interest. Ignoring source/sink terms and writing Equations 1 and 2 as described yields

$$\Delta c_i = c_i\left(t+\Delta t\right) - c\left(t\right) = \int_{t}^{t+\Delta t} \nabla.\left(D\nabla c_i - \vec{V}c_i\right)dt + \int_{t}^{t+\Delta t} R_i dt \qquad (3)$$

The above equation is an OS equation and has divided Equations 1 and 2 into two distinct parts. The first part is the integral consisting of the advection-diffusion component of the transported constituent, and the second integral consists of the growth or decay of the constituent with the rate of this growth or decay determined by NSMI.

The first integral consisting of the advection-diffusion equation calculates the intermediate solution ($c_i^*$); this intermediate solution then provides the input to the second integral consisting of the growth/decay reaction (NSMI).

With Equation 3, the complete advection-diffusion-reaction equation has essentially been split into two distinct parts that have disparate rates of change, and the benefit of doing so is that two separate solution strategies can now be utilized. The first part may be solved using finite difference, finite volume, finite element, or some other method, and the second can be solved as an ordinary differential equation (ODE). Splitting Equations 1 and 2 using OS provides the following benefits:

1. The non-linearity imparted to the complete advection-diffusion-reaction equation is now relegated to the ODE represented by the second term in Equation 3, and the advection-diffusion is purely linear.
2. The time-step used for the two parts in Equation 3 can be different as allowed by the robustness of advection-diffusion and/or reaction.
3. Solution strategies that maximize accuracy and efficiency for the two separate parts can be selected instead of a single solution technique for both.
4. The global advection-diffusion-reaction solve has been split into a global advection-diffusion and a local reaction rate solve.
5. For rapid reaction rates, the combined advection-diffusion-reaction equation becomes stiff due to extreme differences in the temporal scales of the advection-diffusion and reaction parts; OS relegates the solution of the stiff reaction ODE to efficient solution techniques such as the Runge-Kutta method (Hairer and Wanner 1996).
6. The possible choice of the source of the reaction rate is greatly expanded for just one. The source in this note is NSMI but could be any number of water quality or other reaction rate models.

Wheeler and Dawson (1987) used a second-order Runge-Kutta method for the ODE and obtained reasonable results and illustrated that the order of error introduced by the OS procedure is equal to the order of integration.

The complete solution procedure (after the calculation of adequate hydrodynamics) is therefore as illustrated in Figure 1.

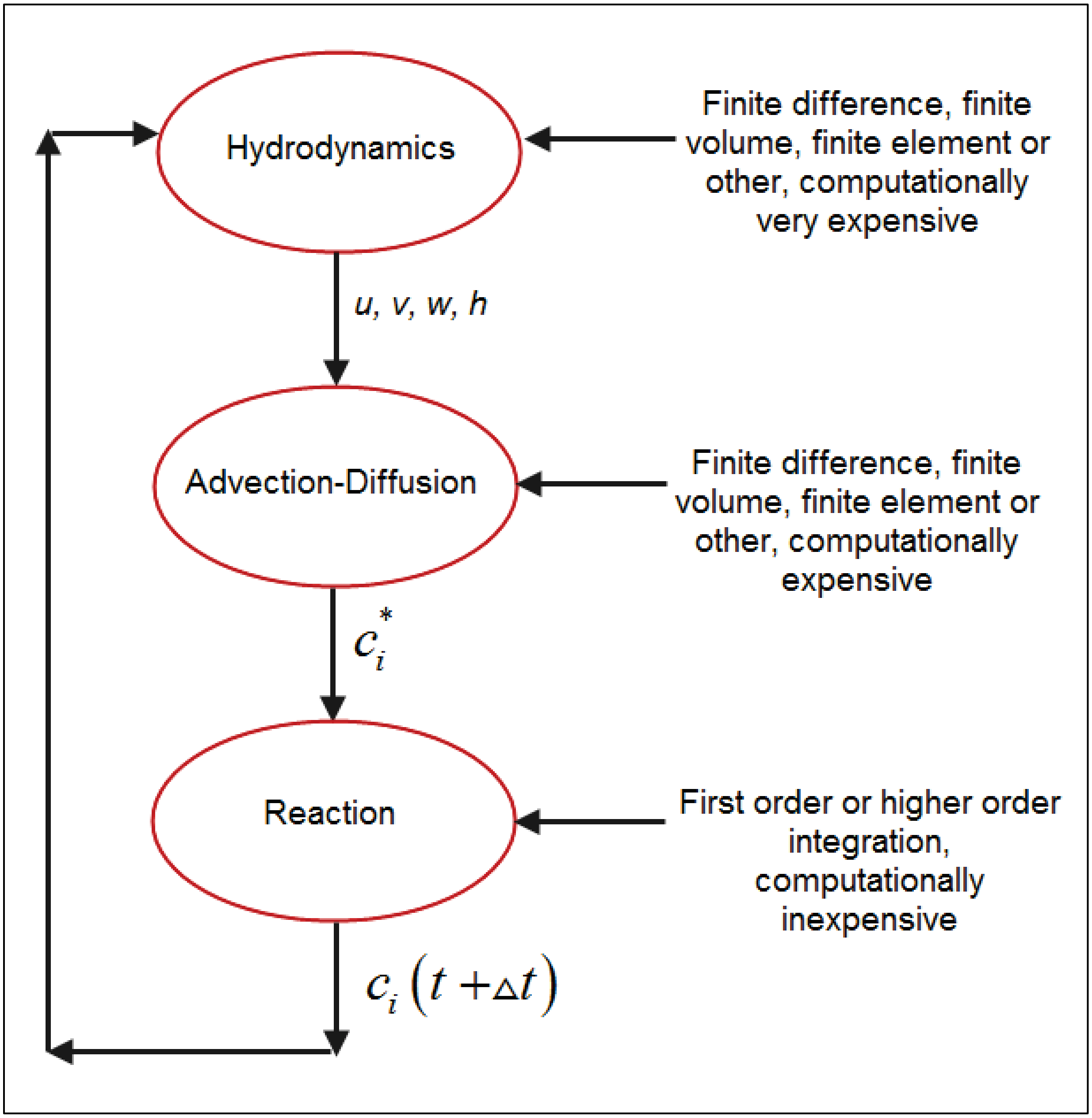

Figure 1. Complete computation and OS strategy.

**ADH LINKAGE TO REACTION RATE MODELS:** The linkage of AdH to a reaction rate model/library must adhere to the following:

1. AdH is a modular code wherein all input and output (I/O) is standardized for intra-model operability; therefore the, OS strategy for AdH must extend beyond the numerical implementation and incorporate the I/O for the model or library providing the reaction rates.
2. AdH is linked to several reaction rate models/libraries; the incorporation of a new model/library must not interfere with the functionality of others already operational.
3. The model/library being linked to AdH must be able to function in the presence of other models/libraries.
4. The model/library being linked to AdH must be spatially agnostic (i.e., it must not require the knowledge of how the mesh/grid is connected, and any information required must be communicable from AdH to the model/library. This is of special interest as AdH is a spatially and temporally adaptive code.
5. AdH is a massively parallel numerical code, and care must be exercised that the model/library providing the reaction rates is incorporated in a fashion that does not impede the AdH parallel computing capabilities.
6. AdH is used by researchers, engineers, and scientists on several operating systems, and therefore the library being linked must not be written using operating system-specific language protocols.

Figure 2 illustrates the linkage protocol followed by AdH in linking to all process/reaction rate models/libraries.

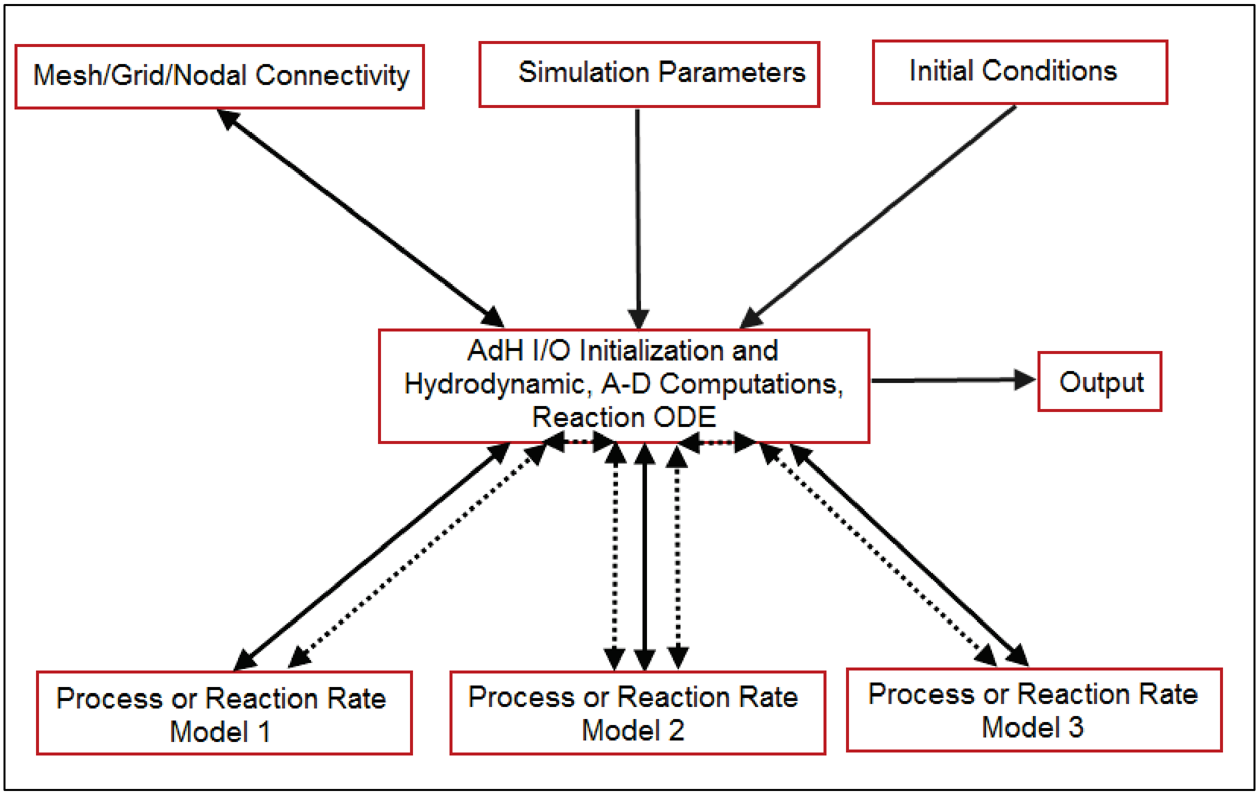

Figure 2. AdH linkage strategy (dashed lines indicate interlibrary communication).

An analysis of Equation 3 shows that it is not required or necessary that the advection-diffusion solution occur before the reaction rate step. In fact, for reactions that are extremely sensitive to parameter values such as velocities, depths, antecedent values, it might be beneficial to solve the reaction first before the advection-diffusion solve. This is primarily an artifact of visualization; extremely sensitive reactions tend to exhibit *splotches* in visualization when the reaction is solved secondary to the advection-diffusion solve. These splotches tend to be smoothed out if the reaction step is solved prior to the advection-diffusion solve. Currently, NSMI is being implemented to solve the reaction rate after the advection-diffusion solve, but this may be modified based on results obtained during model testing.

**ODE INTEGRATION:** The accuracy of the OS method is dependent upon the order of integration performed on the reaction term of the OS, and several integration techniques such as the Euler, midpoint, Runge-Kutta, predictor-Corrector, Bulirsch-Stoer, etc., are available and widely used in standard OS situations.

AdH uses the 4th-order Runge-Kutta (RK-4) integration technique for the reaction term in the OS. The RK-4 integrator is an advancement over the Euler and midpoint methods and uses four evaluations to obtain the next time value. Mathematically this is illustrated as follows:

$$\begin{aligned}
k_1 &= \Delta t f\left(t_n, c_{i,n}\right) \\
k_2 &= \Delta t f\left(t_n + \frac{\Delta t}{2}, c_{i,n} + \frac{k_1}{2}\right) \\
k_3 &= \Delta t f\left(t_n + \frac{\Delta t}{2}, c_{i,n} + \frac{k_2}{2}\right) \\
k_4 &= \Delta t f\left(t_n + \Delta t, c_{i,n} + k_3\right) \\
c_{i,n+1} &= c_{i,n} + \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6} + O\left(\Delta t^5\right)
\end{aligned} \tag{4}$$

The method in Equation 4 provides a 5th-order accurate integrator and in general is computationally inexpensive.

The RK-4 method as shown in Equation 4 requires four estimations of the right-hand side per time-step to obtain the value at the next time-step; this can get computationally expensive if several reaction rates are being computed with constituent values being updated. In such cases, AdH allows the user to apply a simple Euler integrator provided in Equation 5:

$$c_{i,n+1} = c_{i,n} + \Delta t f\left(t_n, c_{i,n}\right) \tag{5}$$

Note that the Euler method is only 1st-order accurate and has the least accuracy of any ODE integrator because it uses the slope of the function at the present time to estimate the new time value.

**NSMI INTEGRATION:** NSMI (Zhang and Johnson 2016) is a water quality kinetics module consisting of 16 state variables to model algae and other water quality phenomenon of interest. NSMI provides information necessary for water quality simulations by providing rate of change information for the modeled state variables in a unit volume of water. As previously noted, RK-4 integration can become computationally cost prohibitive when a large number of reactions are incorporated. NSMI with all 16 state variables activated is one such case, and therefore Euler integration is the preferred choice for the NSMI ODE solution. The 1st-order accuracy of the Euler method is not of concern as the reaction rates for NSMI reactions are linear or quasi-linear and occur at an extremely slow rate. This will reduce the computational cost of ODE integration by one-fourth without sacrificing accuracy of the solution obtained.

NSMI requires the concentration of inorganic suspended sediment be provided as an input to compute the light attenuation coefficient. The light attenuation coefficient is essential to accurately compute the change in reaction rates associated with increasing turbidity or depth. AdH is linked to the SEDLib sediment processes library, and this linkage provides the concentration of the inorganic suspended sediment. The concentration of inorganic suspended sediment is subsequently communicated to NSMI by AdH.

In addition, NSMI also requires the temperature of the water to incorporate the impact of temperature on the water quality reactions. AdH has the capability to simulate temperature using the complete heat balance equation or through a basic equilibrium temperature relationship. Using one of these options, AdH communicates the temperature of the water to NSMI.

NSMI is linked to AdH using information exchange and not through explicit memory coupling. This is done to ensure that the library format is maintained. Explicit memory linkage would require either AdH or NSMI to follow a certain data format, and this is not conducive to NSMI or AdH as both are linked to other models. The information exchange format requires that AdH convert data in the form NSMI requires and then convert data provided by NSMI into a format AdH can use; this is done within a wrapper. This wrapper is the data translator between AdH and NSMI and performs the ODE integration to update the concentrations of active NSMI constituents.

The NSMI process library is called by AdH for every node, and therefore the process can be computationally taxing for simulations with a large number of nodes. To alleviate some of the computational overhead, AdH allows the user to specify a call interval for NSMI; this interval can be the same as the A-D time-step or can be several times larger. It must be remembered that a change of the call interval from the A-D time-step will cause the loss of accuracy, and this loss is proportional to the reaction rate of the constituents (e.g., a constituent with a reaction rate on the order of seconds will be adversely effected by a call time-step larger than the A-D time-step whereas a constituent with a reaction rate on the order of hours or days will not be adversely effected by a call time-step larger than the A-D time-step. There is a possibility that the A-D time-step is too big to obtain the correct behavior for a rapidly changing constituent; in such cases, the wrapper allows the call to NSMI using a time-step smaller than the A-D time-step. If this is done, the wrapper will increment the time until the cumulative NSMI time-step is equal to the A-D time-step. One area of future research is the application of adaptive RK methods to internally modify the size of the time-step when the change in the reaction rate is greater than certain specified limits.

Figure 3 illustrates the linkage of NSMI with AdH.

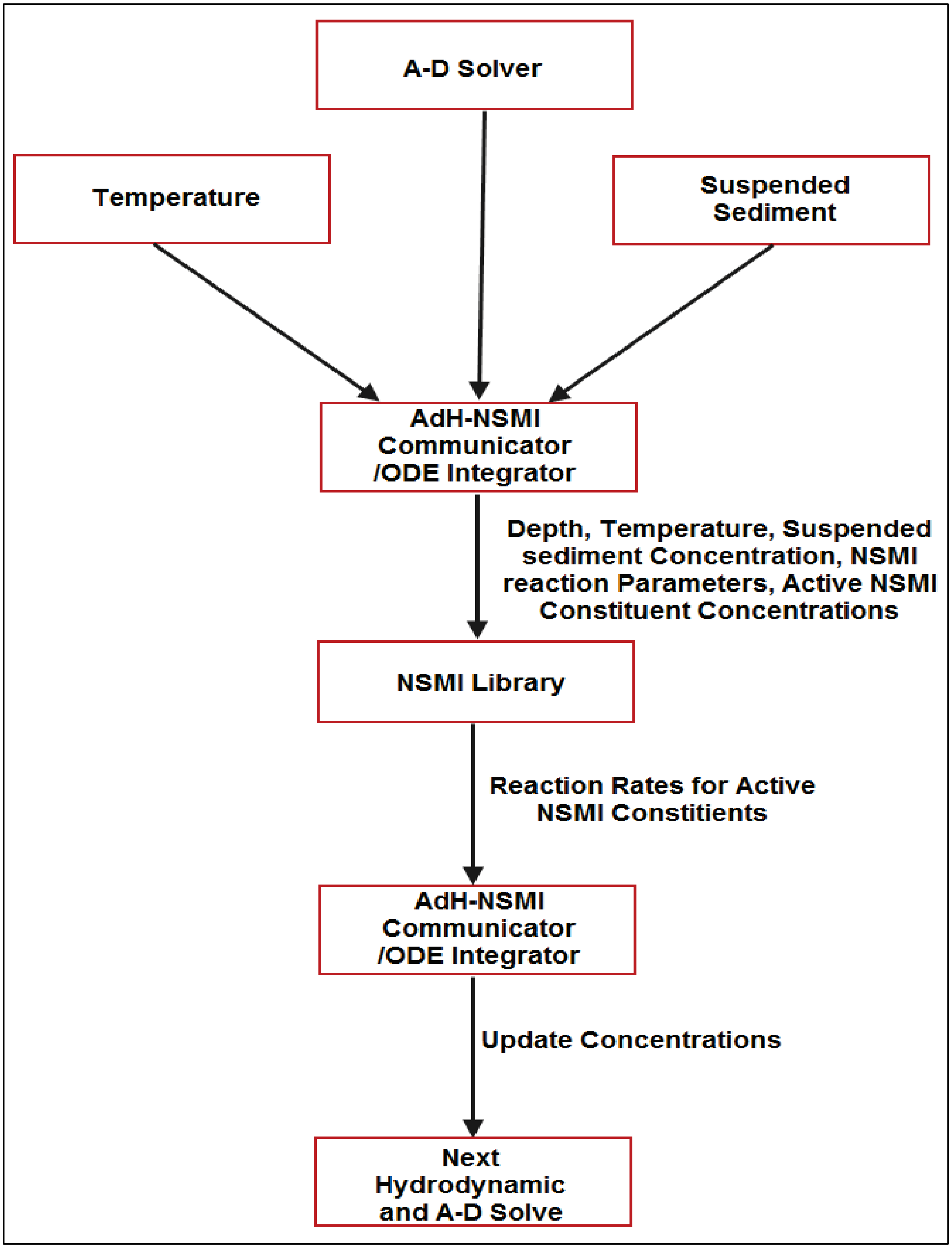

Figure 3. AdH linkage to NSMI.

**SOURCES OF ERROR:** The previous sections presented how AdH is linked with NSMI using an OS strategy. In this section, there is an expansion upon the possible sources of error in this strategy.

There are three possible sources of errors:

1. Time-step size. Time-step convergence is essential for the accuracy of the OS step, Figure 4 illustrates the result of using two different time-steps (10 and 100 seconds) to simulate a simple exponential decay. Even though both time-steps achieve the same steady state solution, the transient solution is substantially different. For an implicit method, the OS split time-step is the physically limiting time-step and can introduce substantial errors into the solution.

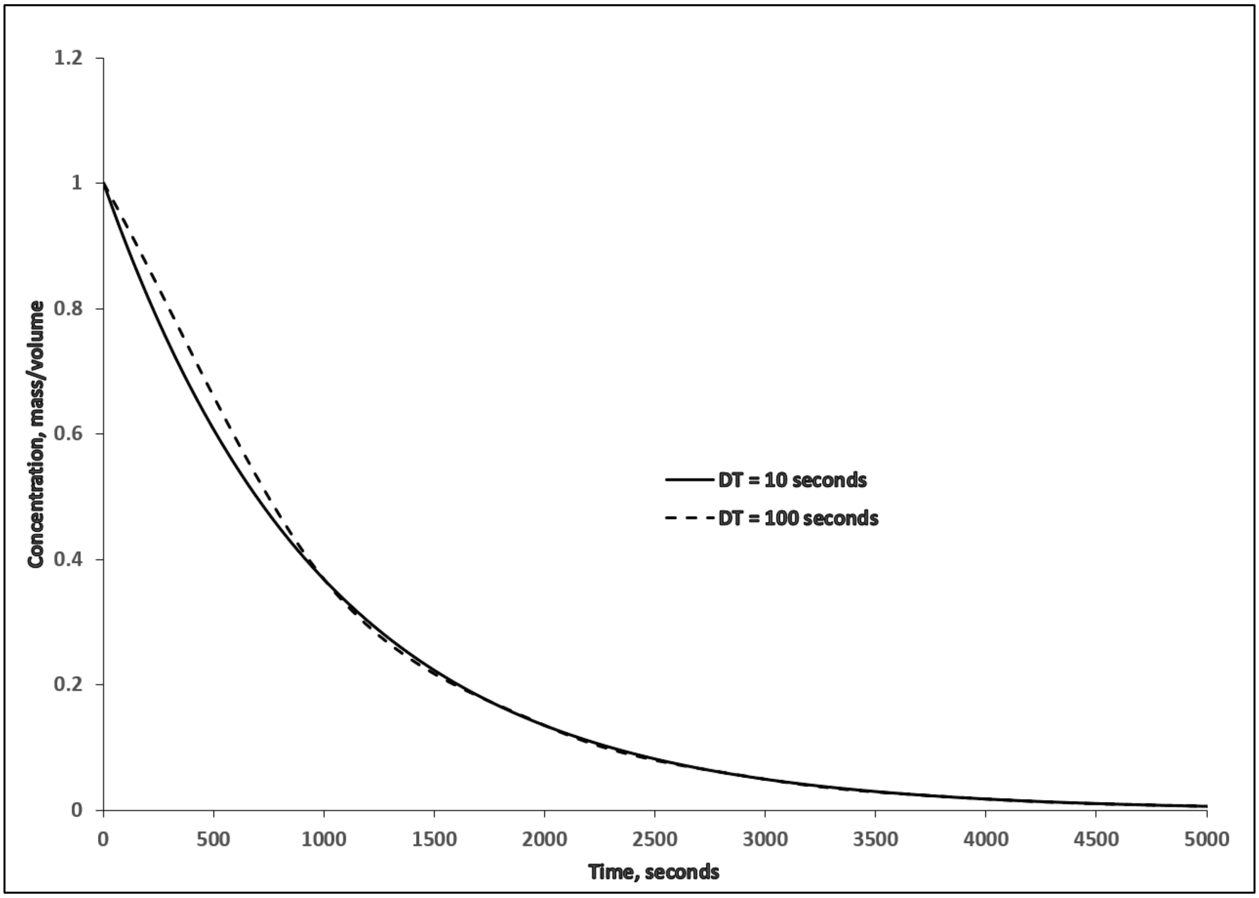

Figure 4. Influence of time-step on results from an exponential decay function.

2. Too large of a time difference between the A-D call and the OS call. This error comes into play when the OS step is not performed for every A-D step; this might be done for computational efficiency or convenience. In this case, the A-D step is performed multiple times before the next OS step and assumes that the reaction term is extremely slow compared to the changes brought on by the A-D. Even when this assumption holds true, there is a feedback to the A-D step from the OS step that can have a substantial impact on the distribution of the transported constituent. This feedback is through the diffusion terms

in the A-D equation. The diffusion terms are linear, but they are dependent upon the gradients in the concentration; calling the OS step once for several A-D steps could result in the contribution from the diffusion terms to be erroneous.

3. The A-D time-step is too large. In rare situations, the reaction terms might be fast enough that the A-D time-step becomes too large to accurately capture the influence of the reaction term. In these cases, the adaptive RK methods might be of use to internally reduce the time-step used by the OS ODE integrator to arrive at the correct solution.

**SUMMARY and CONCLUSIONS:** This CHETN describes the numerical framework linking the Adaptive Hydraulics (AdH) modeling suite to the Nutrient Simulation Model-I (NSMI). AdH linkage with NSMI through OS is presented, and the mathematical formulations behind the linkage are presented in detail. This CHETN also presents the common sources of error that might influence the accuracy and validity of the OS strategy.

**POINTS OF CONTACT:** This CHETN was prepared as part of the Flood and Coastal Storm Damage Reduction (FCSDR) Program of the U.S. Army Corps of Engineers. The point of contact for technical inquiries is Gaurav Savant (gaurav.savant@erdc.dren.mil). For information about the FCSDR program, please contact the FCSDR Program Manager, Julie Rosati (Julie.D.Rosati@erdc.dren.mil). This technical note should be referenced as follows:

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