BASIS FOR THE CE-QUAL-W2 VERSION 3 RIVER BASIN HYDRODYNAMIC AND WATER QUALITY MODEL

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Abstract: CE-QUAL-W2 Version 3, a 2-D (longitudinal-vertical) hydrodynamic and water quality model for river basins combining both river and stratified river-estuary and lake-reservoir flow, is a development product of the Waterways Experiment Station in Vicksburg, MS, USA. With the development and release of any revised or reformulated model codes, significant model validation is required. This includes comparison of model results to simple analytical solutions for hydrodynamics and water quality transport, as well as comparison to laboratory and field data. In this paper, the model is compared to numerous analytical solutions for mass transport (1-D advective mass transport) and hydrodynamics (impulsive wind stress on water surface, seiching). Suggestions are presented for proper validation protocols for hydrodynamic and water quality models.

INTRODUCTION

CE-QUAL-W2 Version 3 (Cole and Wells, 2001) is a two-dimensional water quality and hydrodynamic model capable of modelling watersheds with interconnected rivers, reservoirs and estuaries. A typical model domain is shown in Figure 1. The model is based on solving the two-dimensional unsteady hydrodynamic and advective-diffusion equations as shown in Table 1.

CE-QUAL-W2 Version 3 allows the model user to include riverine branches in conjunction with reservoir/lake and estuary branches. This code also allows the user to insert hydraulic elements between branches (pipes, weirs, weirs with flashboards, spillways, gates with dynamic gate openings), use up-to-date reaeration (including spillway effects) and evaporation theoretical models, view model results graphically as they are being computed, use a variety of turbulence closure schemes, insert internal weirs in the computational domain, use the updated numerical scheme ULTIMATE-QUICKEST for advective transport of mass/heat, add float-activated pumps, use a dynamic vegetative and topographic controlled shading algorithm, and include a user-defined number of algal, epiphyton/periphyton, CBOD, suspended solids, and generic model water quality constituents.

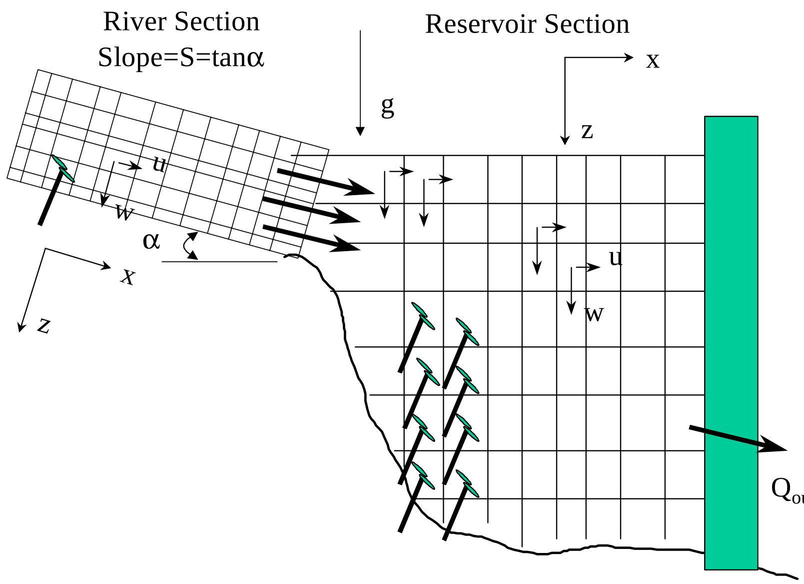

Figure 1 CE-QUAL-W2 Model Grid.

Table 1 CE-QUAL-W2 Governing equations.

Equation	Version 3 governing equations
x- momentum	$\frac{\partial UB}{\partial t}+\frac{\partial UUB}{\partial x}+\frac{\partial WUB}{\partial z}=gB\sin\alpha+g\cos\alpha B\frac{\partial\eta}{\partial x}-\frac{g\cos\alpha B}{\rho}\int_{\eta}^{z}\frac{\partial\rho}{\partial x}dz+\frac{1}{\rho}\frac{\partial B\tau_{xx}}{\partial x}+\frac{1}{\rho}\frac{\partial B\tau_{xz}}{\partial z}+qBU_x$
z-momentum	$0=g\cos\alpha-\frac{1}{\rho}\frac{\partial P}{\partial z}$
free surface equation	$B_\eta\frac{\partial\eta}{\partial t}=\frac{\partial}{\partial x}\int_{\eta}^{h}UBdz-\int_{\eta}^{h}qBdz$
continuity	$\frac{\partial UB}{\partial x}+\frac{\partial WB}{\partial z}=qB$
equation of state	$\rho = f(T_w, \Phi_{TDS}, \Phi_{ss})$
Conservation of mass/heat	$\frac{\partial B\Phi}{\partial t}+\frac{\partial UB\Phi}{\partial x}+\frac{\partial WB\Phi}{\partial z}-\frac{\partial\left(BD_x\frac{\partial\Phi}{\partial x}\right)}{\partial x}-\frac{\partial\left(BD_z\frac{\partial\Phi}{\partial z}\right)}{\partial z}=q_\Phi B+S_\Phi B$
where B is the width, U is the longitudinal velocity, W is the vertical velocity, q is the inflow per unit width, α is the channel angle, Φ is the concentration or temperature, η is the water surface elevation, P is the pressure, h is the depth, T_w is the water temperature, Φ_{TDS} is the concentration of TDS, Φ_{ss} is the concentration of suspended solids, ρ is the density	

All numerical modelling studies usually assume that the underlying model has been tested extensively to analytical solutions and other test cases to ensure that the model does not have any serious programming, theoretical, and/or numerical errors. This process is often termed “validation” or sometimes “verification” of a numerical model (Smith and Larock, 1999). In general, this process consists of comparison of simple theoretical analytical models to results predicted by the numerical model. This paper was meant to provide a basis for testing of the new model code CE-QUAL-W2 and to suggest approaches for proper validation of water quality and hydrodynamic models.

MASS/HEAT TRANSPORT

The simplest test of any code (but not necessarily the easiest) is to advect sharp concentration gradients. In CE-QUAL-W2 the model user can choose between 3 numerical formulations for testing the advective (both vertical and longitudinal) transport properties of the solution: UPWIND, QUICKEST (Leonard, 1979), and ULTIMATE-QUICKEST (Leonard, 1991) schemes. The UPWIND and QUICKEST schemes are used primarily for illustrative purposes since the ULTIMATE-QUICKEST scheme is an excellent technique for capturing sharp-front gradients and eliminating spurious oscillations at the leading and trailing edge of a gradient. Using a numerical upwind scheme introduces a tremendous amount of numerical diffusion (of order $0.5|u|\Delta x$ where u is the velocity and Δx is the segment spacing), analogous to physical diffusion (Vreugdenhil, 1989). While the QUICKEST scheme eliminates the numerical diffusive errors, it can cause spurious wiggles at the leading edge and following edge of a sharp front gradient.

Figure 2 shows a comparison of CE-QUAL-W2 predictions using these 3 different numerical schemes to the analytical solution for sharp front advection. This figure is for a worse case situation where the Courant number ($U\Delta t/\Delta x$) is much less than 1. As the Courant # $\Rightarrow$ 1, numerical diffusion decreases, and the model should more closely represent the numerical solution. In most multi-dimensional dynamic models though, one has a large spectrum of Courant numbers throughout the model domain, and validation tests with very small Courant numbers show potential code numerical inaccuracies.

WIND DRIVEN WATER CURRENTS

Hansen (1975) developed a simple analytical model of the growth of the velocity in a water body subjected to a sudden wind shear. Assuming that there is a balance between acceleration and vertical shear stresses in the x-momentum equation and that the turbulent eddy viscosity is constant with respect to z, the governing x-momentum equation becomes

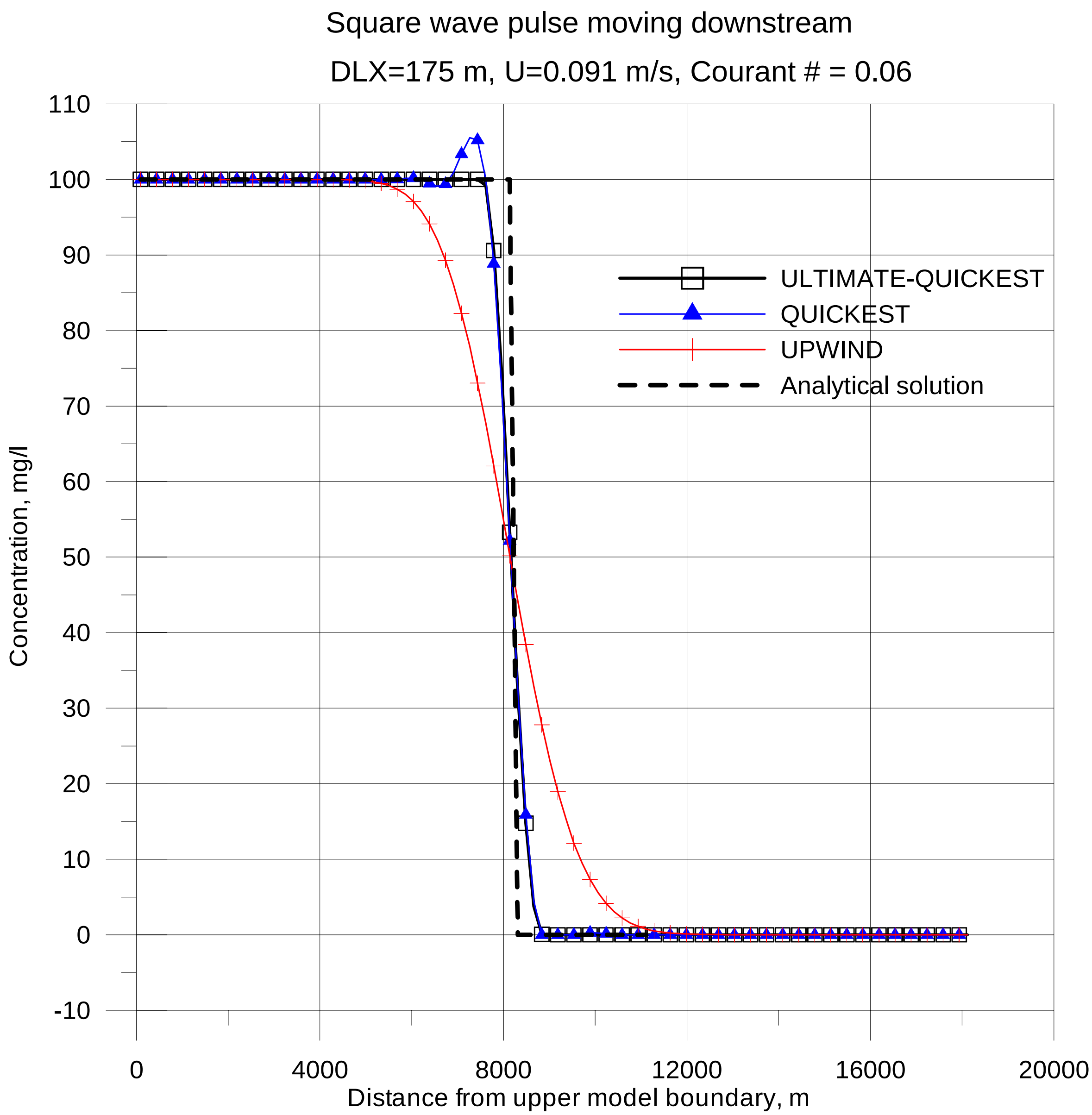

Figure 2. Comparison of sharp front advection of concentration predictions using CE-QUAL-W2 to the analytical solution.

$$\frac{\partial U}{\partial t} = \nu_t \frac{\partial^2 U}{\partial z^2}$$

where ν_t is the turbulent eddy viscosity and U is the longitudinal velocity as a function of z and t.

By using an empirical relationship for the turbulent eddy viscosity, $\nu_t = \frac{1}{28}\int_0^h U dz$ where h is the depth, the solution for the velocity over time is then

$$\frac{U}{U_*} = 6.65\left\{1 - erf\left(\frac{z}{0.267 U_* t}\right)\right\}$$

where U_* is the shear velocity = $\sqrt{\frac{\tau_{surface}}{\rho}}$.

For a vertical grid spacing of 0.1 m, the comparison of the analytical model and W2 are shown in Figure 3. In comparing CE-QUAL-W2 to this analytical solution, several adjustments were necessary for the model to agree with the assumptions of the analytical solution:

- Set the horizontal transport of momentum from horizontal advection to zero
- Set the vertical transport of momentum to zero
- Set the horizontal transport of momentum by longitudinal eddy diffusion to zero
- Set the eddy viscosity to $\nu_t = \frac{1}{28} U_*^2 t$ over the entire water depth
- Use an impulsive wind of 10 m/s measured at a 10 m height

Also, in order to agree with the momentum equation used in the analytical solution, the horizontal pressure gradient would need to be set to zero. Since the simulation was run for only 200 s, it was deemed that sufficient water surface pressure effects would still be negligible so there were no efforts to turn these off in the model. In W2 a decay function is used to transfer momentum from the wind to lower computational layers (see Cole and Wells, 2001). This also accounted for the wind-wave effect and was based on an empirical formula for the rate of decay of the wind energy with depth. This was originally proposed as a way to allow the results to be more grid-independent. If this were not implemented, a model with a fine grid near the surface would experience a greater shear and impulsive velocity than a model with a coarser grid spacing at the surface. To match the analytical solution, this was turned off in CE-QUAL-W2.

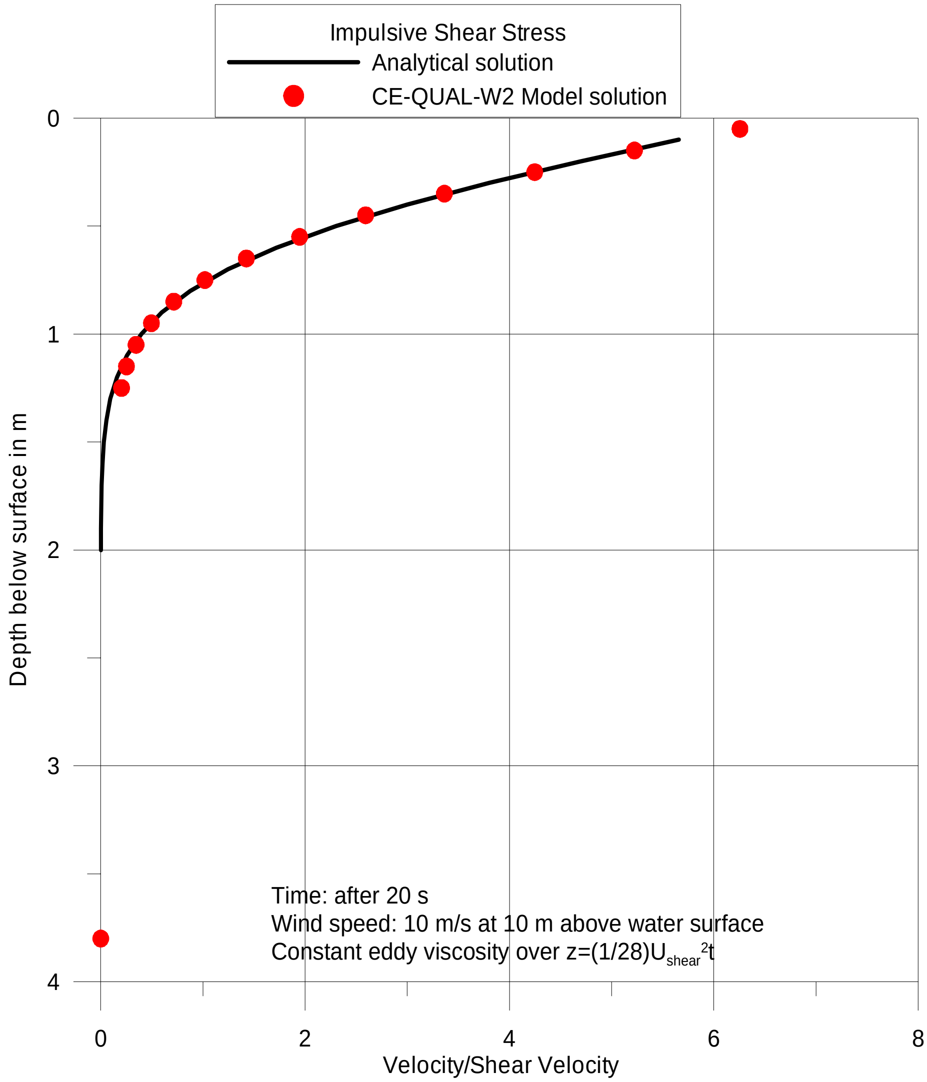

Figure 3. Comparison of CE-QUAL-W2 and analytical model solution for impulsive wind shear.

SEICHES

The shallow-water equations can be simplified to produce useful analytical solutions for comparison to numerical models. Using the following assumptions: frictionless bottom and sidewalls, hydrostatic and Boussinesq approximations, negligible non-linear terms in the momentum equation, and no turbulent or viscous fluid stresses, the simplified shallow water equations are

$$\frac{\partial \eta}{\partial t} + \frac{\partial Uh}{\partial x} = 0 \quad \text{continuity equation}$$

$$\frac{\partial U}{\partial t} = -g\frac{\partial \eta}{\partial x} + \frac{\tau_{sx}}{\rho_o h} \quad \text{x-momentum equation}$$

where η is the water surface elevation, U is the cross-sectionally averaged longitudinal velocity, h is the fluid depth, g is the acceleration due to gravity, x and t are independent variables of longitudinal distance and time, respectively, ρ is the fluid density and τ_{sx} is the surface shear stress in the x-direction.

By cross-differentiating and equating the above 2 equations, we obtain the 1-D wave equation,

$$\frac{\partial^2 \eta}{\partial t^2} - (gh)\frac{\partial^2 \eta}{\partial x^2} = 0 \ .$$

Assuming that there is no surface shear stress (τ_{sx}=0), the solution of the wave equation assuming an initially sinusoidal distribution in x and a sinusoidal distribution in time at the 2 ends of the domain (i.e., $\eta = \eta_o \cos\left(\frac{\pi c_o t}{L}\right)$ at x=0 and x=L), Eliason and Bourgeois (1997) showed analytical solutions to the shallow water equations for water surface and velocity respectively as

$$\eta = \eta_o \cos\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi c_o t}{L}\right)$$
$$U = \frac{\eta c_o}{H}\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{\pi}{L}c_o t\right)$$

where L is the closed basin length, η is the water surface elevation, η_o is the amplitude of the surface elevation, c_o is the gravity wave speed or $\sqrt{gH}$, U is the cross-sectionally averaged velocity, and H is the basin depth. This represents a seiche that continues ad infinitum since there is no frictional resistance. This condition would be similar to a wind that stops blowing after reaching a steady-state set-up, and the water surface begins to oscillate back and forth without any surface shear stress. In reality, the seiche is damped by friction. A comparison of CE-QUAL-W2 to this solution is shown in Figure 4 for water surface and Figure 5 for flow rate (based on velocity) for the following conditions: L=30 km, Δx=500m, η_o= 0.145 m, and H=5.0m. In order to agree with the governing equations of the analytical model, CE-QUAL-W2 was run with one-vertical layer (hence, no vertical flows), no friction (Chezy friction coefficient=0.0), no longitudinal dispersion of momentum, segment widths of 100 m, maximum time step of 2 s, and no non-linear advective terms in the momentum equation.

The model predictions agree well with the analytical solution even though one sees that the amplitude and phase of the numerical model begin to deviate from the analytical solution over time. For any numerical scheme, there will be some deterioration of the signal over time in amplitude and phase. The important aspect or test here of a numerical code is that we are true to the original signal for several wave periods. Even though the CE-QUAL-W2 model could have been run at a larger time step and still have been stable, the accuracy of the solution would have been degraded as shown in the next example.

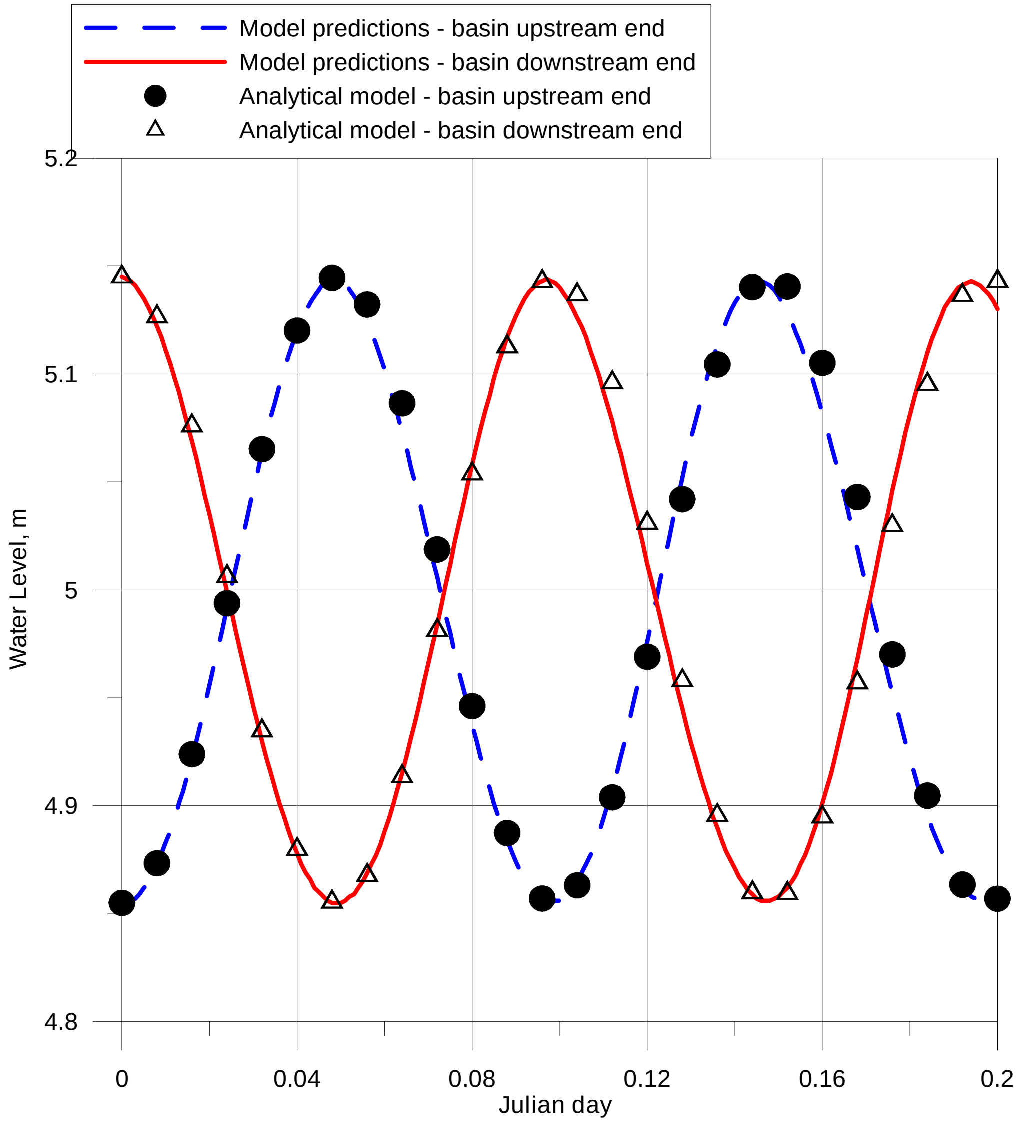

Figure 4 Comparison of CE-QUAL-W2 with analytical solution for a dynamic seiche in a narrow rectangular basin.

Another comparison to an analytical model is that provided by solving the 1-D wave equation above, subject to the following conditions:

Boundary conditions: $\frac{\partial \eta}{\partial x} = \frac{u_*^2}{gh}$ at $x = b$ and $x = -b$

Initial conditions: $u_* = 0$ for $t < 0$ and $u_* = u_*(t)$ for $t \geq 0$

and $\eta = 0$ at $t = 0$ for all x where u_* is the surface shear velocity, b is the half basin length, and x=0 is defined at the center of the basin.

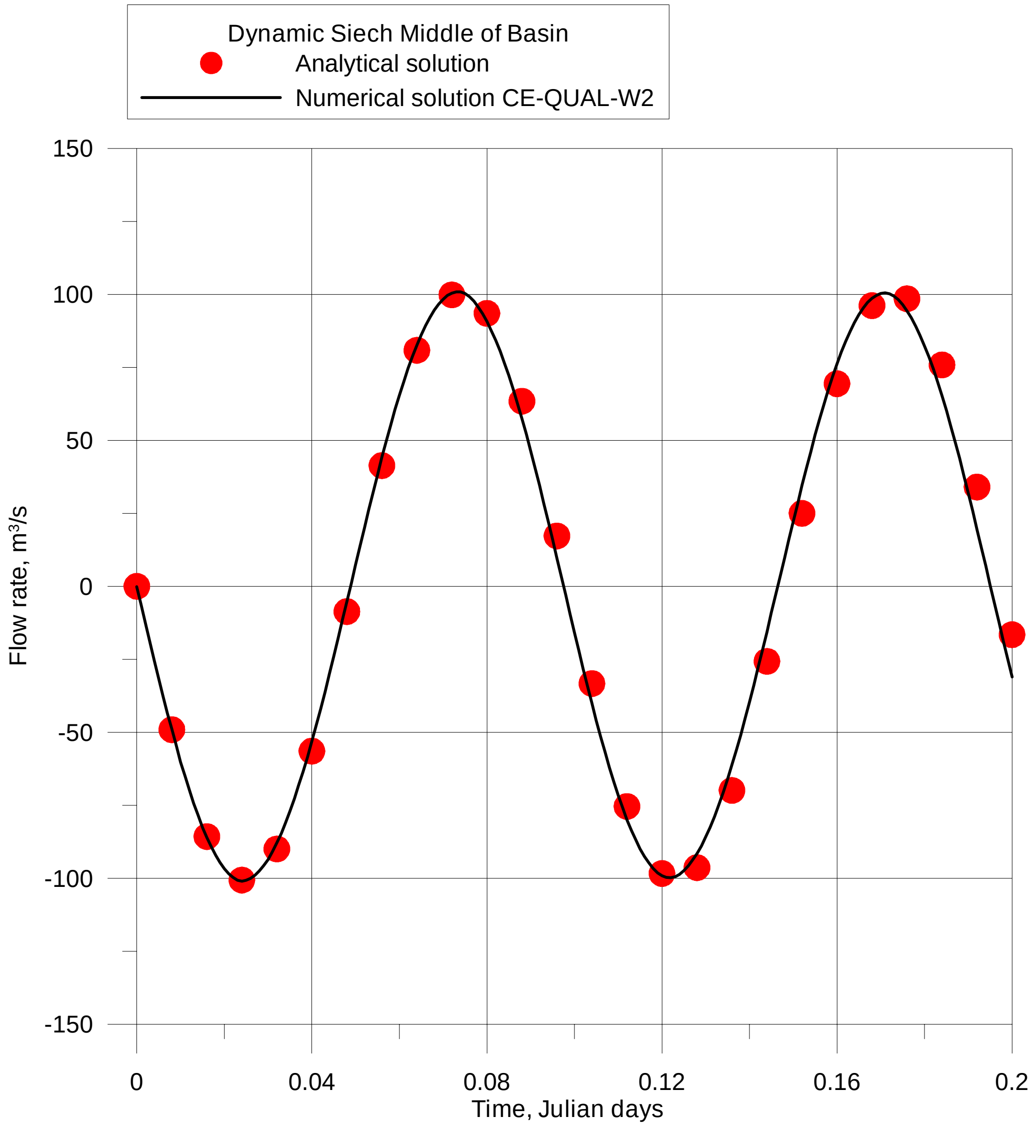

Figure 5. Flow rate predicted by numerical solution compared to CE-QUAL-W2 model predictions for a dynamic seiche in a narrow rectangular basin.

The analytical solution for the water surface was then

$$\eta = \frac{u_*^2}{gh}x - \frac{8bu_*^2}{\pi^2 gh}\left\{ \cos\frac{\pi c_o t}{2b}\sin\frac{\pi x}{2b} - \frac{1}{9}\cos\frac{3\pi c_o t}{2b}\sin\frac{3\pi x}{2b} + \frac{1}{25}\cos\left(\frac{5\pi c_o t}{2b}\right)\sin\frac{5\pi x}{2b} - ... + ... \right\}$$

The analytical model was compared to a CE-QUAL-W2 simulation for a basin of length of 30 km, segment widths of 100 m, segment lengths of 1000 m, 1 vertical layer, an initially flat water surface, and an impulsive wind velocity at 10 m height of 20 m/s. The comparison of the numerical and analytical solutions is shown in Figure 5 for a model time step of 100 s and 5 s.

An issue with numerical codes that solve the water surface equation by implicit techniques (which was done to eliminate the gravity wave speed stability criterion) is that the time step for numerical stability does not guarantee numerical accuracy. The model at higher time steps leads to very "diffusive" water level predictions and does not maintain the infinite seiche in the frictionless environment like the model with the lower time step. In Figure 5, a comparison is made using CE-QUAL-W2 at a numerically stable time step of 100 s compared to a reduced time step of 5 s (see also the model comparison to the analytical model in Figure 4 where the time step limit was 2 s). In this case though, the implicit numerical scheme of CE-QUAL-W2 leads to a numerically diffusive approximation to the water surface. This implies that modellers should always check the model results by doing sensitivity analyses with the model time step. If the model results are not sensitive to the time step, then the modeller can be confident that his hydrodynamic calibration (usually performed by adjustment of bottom friction) is not a function of the model numerical accuracy. In all practical applications of CE-QUAL-W2, sensitivity analyses evaluating the time step have never been shown to affect the solution even under estuary conditions like that shown for the Columbia-Willamette River system (Berger, Annear, and Wells, 2001).

SUMMARY

The model CE-QUAL-W2 was compared to analytical solutions for mass transport, wind driven currents, and dynamic seiching in order to validate that the model is reproducing known analytical solutions. All numerical solutions are approximations to the exact governing equations, and this step of validation is essential in testing new computer codes. Other comparisons not shown in this paper are also important – laboratory scale and field scale comparisons. These also provide a framework for evaluating mathematical models of water quality and transport. Some laboratory-scale studies that are useful comparisons to numerical models include:

- Baines and Knapp (1965) carried out experiments of wind driven currents in an experimental flume (length of 10 m, depth of 0.6 m, width 1 m)
- Kirkgoz, M. S. (1989) determined detailed velocity measurements in a rectangular sub-critical flow channel for both smooth and rough channels
- Johnson (1981) conducted dye tracer tests in a sloping channel reservoir flume (24.38 m X 0.91 m X 0.91 m) and used these data to compare to numerical model predictions of density driven inflows

An important assessment tool in the reliability of a model is its ability to reproduce field data with as little "calibration" or parameter estimation as is possible. These have been demonstrated for the CE-QUAL-W2 model as shown in Wells (2000) and Cole (2000) where field data from numerous reservoirs, estuaries and rivers were compared to model predictions of hydraulics and temperature under diverse conditions.

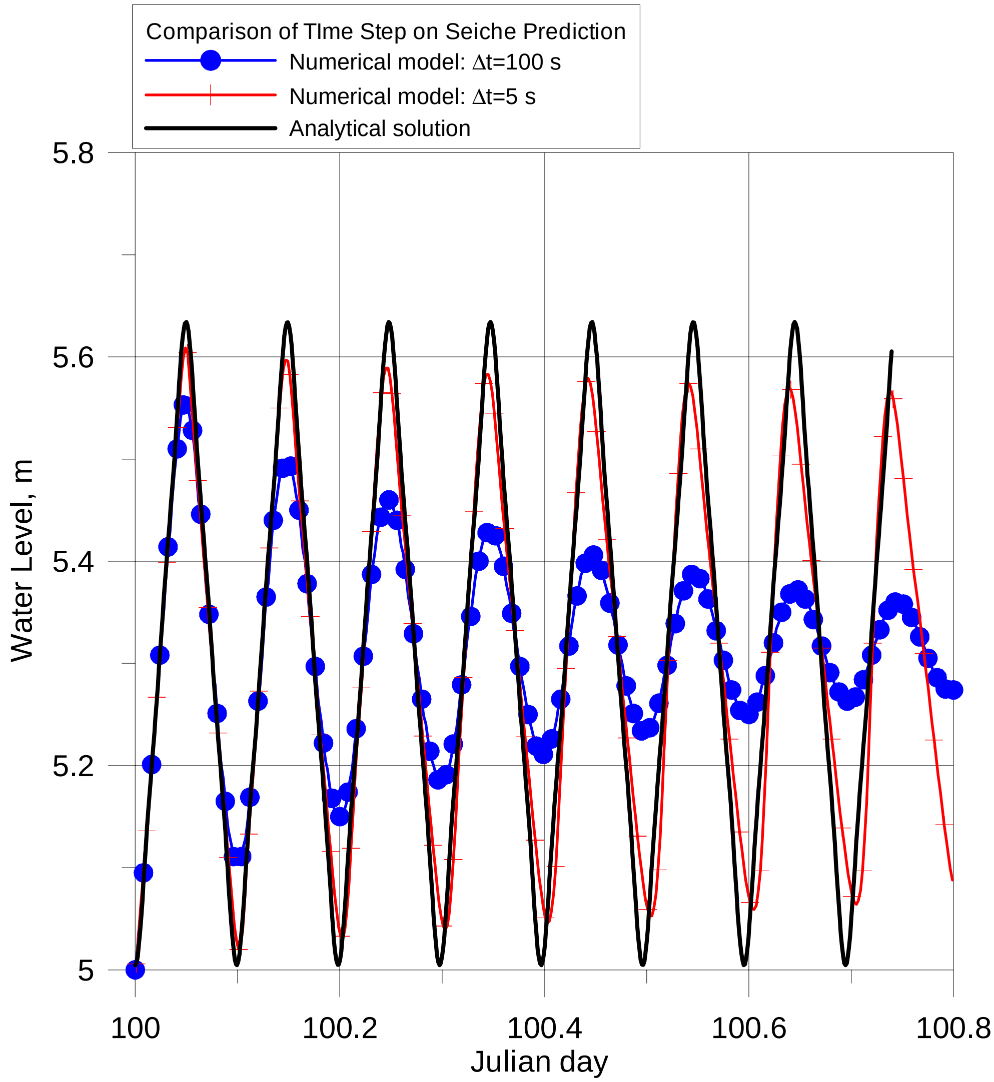

Figure 6. Effect of time step on CE-QUAL-W2's ability to maintain a seiche. Water level is at the uppermost end of basin.

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