Validation of 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.
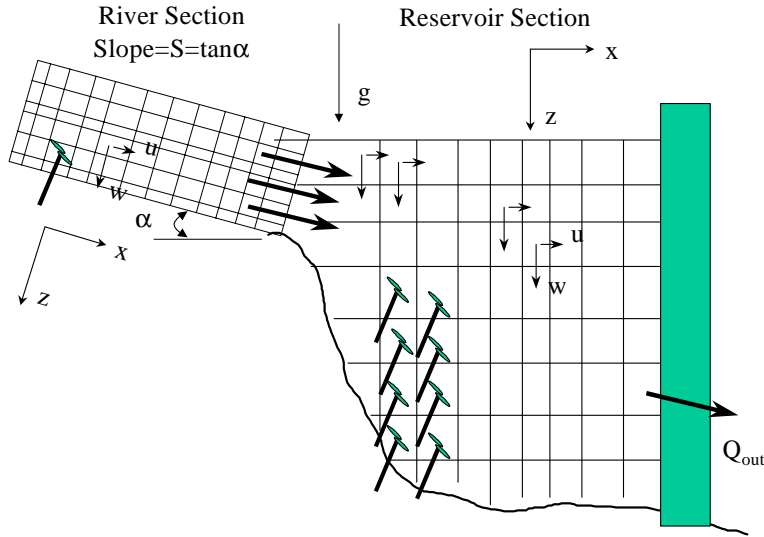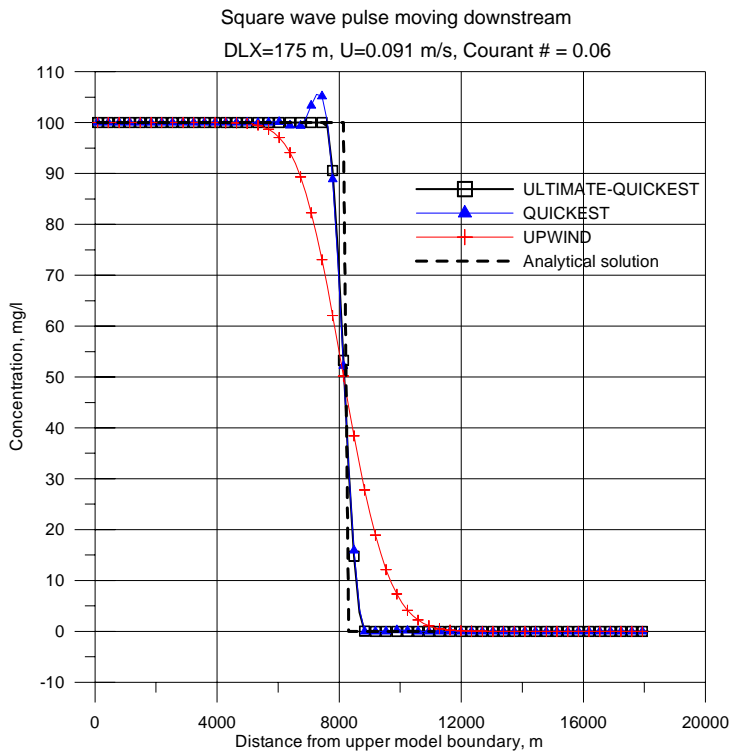

Figure 1 CE-QUAL-W2 Model Grid.

Table 1 CE-QUAL-W2 Governing equations.

Equation	Version 3 governing equations
x- momentum	$\dfrac{\partial\,UB}{\partial\,t}+\dfrac{\partial\,UUB}{\partial\,x}+\dfrac{\partial\,WUB}{\partial\,z}=gB\sin\alpha+g\cos\alpha B\,\dfrac{\partial\eta}{\partial x}-\dfrac{g\cos\alpha B}{\rho}\int_{\eta}^{z}\dfrac{\partial\rho}{\partial x}\,dz+$ $\dfrac{1}{\rho}\dfrac{\partial B\tau_{xx}}{\partial\,x}+\dfrac{1}{\rho}\dfrac{\partial\,B\,\tau_{xz}}{\partial\,z}+qBU_{x}$
z-momentum	$0=g\cos\alpha-\dfrac{1}{\rho}\dfrac{\partial P}{\partial z}$
free surface equation	$B_{\eta}\dfrac{\partial\eta}{\partial t}=\dfrac{\partial}{\partial x}\int_{\eta}^{h}UBdz-\int_{\eta}^{h}qBdz$
continuity	$\dfrac{\partial\,UB}{\partial\,x}+\dfrac{\partial\,WB}{\partial\,z}=qB$
equation of state	$\rho=f(T_{w},\Phi_{TDS},\Phi_{ss})$
Conservation of mass/heat	$\dfrac{\partial\,B\,\Phi}{\partial\,t}+\dfrac{\partial\,UB\,\Phi}{\partial\,x}+\dfrac{\partial\,WB\,\Phi}{\partial\,z}-\dfrac{\partial\left(BD_{x}\dfrac{\partial\Phi}{\partial\,x}\right)}{\partial\,x}-\dfrac{\partial\left(BD_{z}\dfrac{\partial\Phi}{\partial\,z}\right)}{\partial\,z}=q_{\Phi}\,B+S_{\Phi}\,B$
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, and ULTIMATE-QUICKEST schemes. The UPWIND are QUICKEST schemes are used primarily for illustrative purposes since the ULTIMATE-QUICKEST scheme of Leonard is an excellent technique for capturing sharp-front gradients and eliminating spurious oscillations at the leading and trailing edge of a 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 errors.

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

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

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
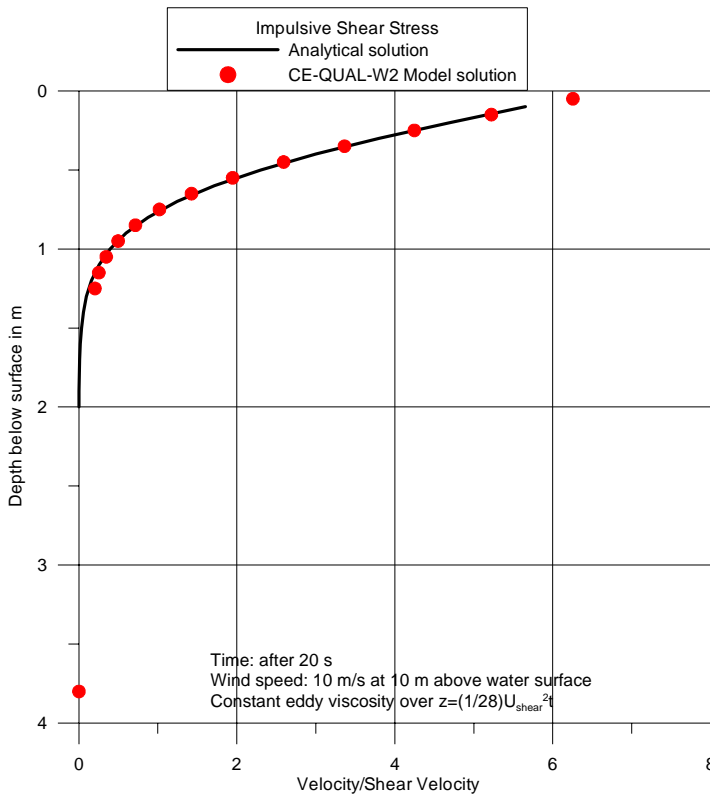- Use an impulsive wind of 10 m/s measured at a 10 m height

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

Also, in order to agree with the momentum equation used in the analytical solution, the 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.

Seiches

Eliason and Bourgeois (1997) showed analytical solutions to the shallow water equations. These equations included the following assumptions: frictionless bottom and side walls, no surface shear stress, hydrostatic and Boussinesq approximations, negligible non-linear terms in the momentum equation, and no turbulent or viscous fluid stresses.

The solution of the governing equations (continuity and x-momentum) resulted in a wave equation that has the following analytical solution:

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

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 $\sqrt{gH}$, and H is the basin depth. This represents a seiche that continues ad infinitum since there is no frictional resistance. A typical comparison of CE-QUAL-W2 to this solution is shown in Figure 4.

An issue though 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 (as shown in Figure 4). 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.

Summary

The tests made with CE-QUAL-W2 to analytical solutions for mass transport, wind driven currents, and dynamic seiching were made 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. 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.

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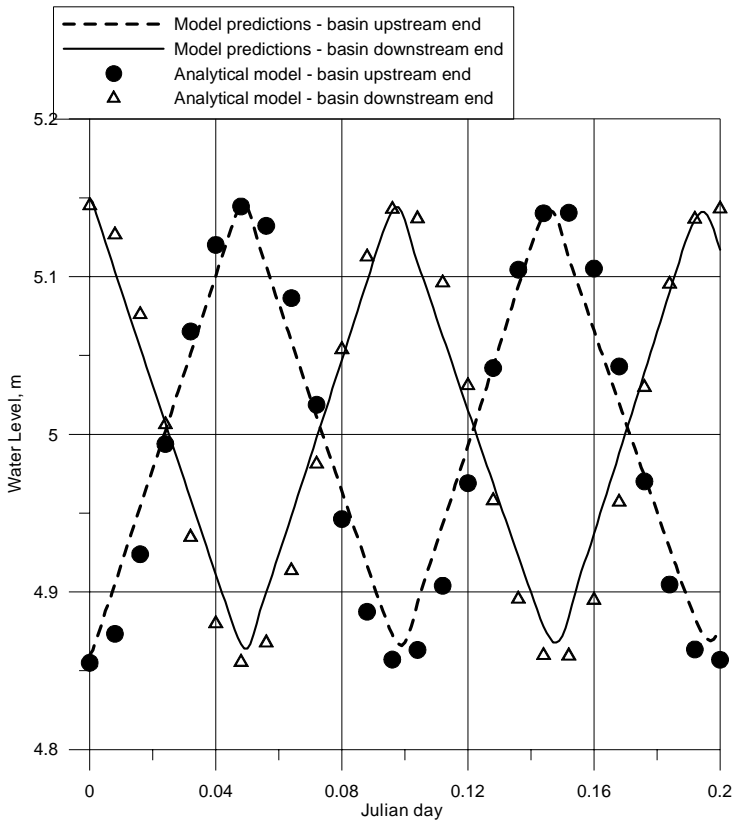
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Figure 4 Comparison of CE-QUAl-W2 with analytical solution for a dynamic seiche in a narrow rectangular basin.