Chapter 17

A Time Adaptive Grid on the QUAL2E Water Quality Model

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Water quality models are used extensively for maintaining and monitoring the waste assimilative capacity of water bodies when these bodies are exposed to contaminant inputs. Because of the sensitivity of DO concentrations over temporal and spatial steps, an accurate time dependent solution is required from the finite-difference model. To maintain numerical accuracy and efficiency, it is well known that the smaller the grid size, the more accurate the solution will be because of the decrease in the local truncation error. But this will lead to an excessive number of grid points requiring an increase in computational time. The opposite practice would be to decrease the computational time by decreasing the number of grid points. Of course, this will decrease the accuracy of the solution. Local grid clustering about areas of large physical gradients can help to solve this dilemma.

The first step in utilizing an adaptive grid in conjunction with a water quality model is to incorporate a grid generation technique that will adequately discretize the physical domain. However, this is often difficult to do since the initial physics of the solution are unknown and the initial grid may be unsuitable for the solution needed. An adaptive grid generator can concentrate the grid lines in areas where physical gradients are large, and disperse lines where the gradients

Jin, K-R. and J.K. Hasson. 1994. "A Time Adaptive Grid on the QUAL2E Water Quality Model." *Journal of Water Management Modeling* R176-17. doi: 10.14796/JWMM.R176-17.
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are smooth. Since the accuracy of the finite-difference solution is dependent upon the suitability of the grid used to compute the solution, the adaptive grid can help to increase the accuracy of the solution. Using an elliptic grid generator based upon the Poisson equations, control functions can be fashioned to control the spacing and orientation of the coordinate grid lines, thus achieving the adaptive grid.

A time dependent solution is often used in water quality modelling. However, the solution over the domain will change as time marches forward. Therefore, a dynamically adaptive grid generator is incorporated to follow the large physical gradients in time. A dynamically adaptive grid generator is a very powerful tool for time dependent solutions.

The purpose of this research is to modify an existing water quality model to perform more accurate, more representative calculations in tracking gradients in water quality variables. The model utilized in the research is The Enhanced Stream Water Quality Model QUAL2E distributed by the USEPA (Brown and Barnwell, 1987). In this model's original form, the grid lengths are set initially by the user to a uniform spacing across a stream reach, thus introducing the possibility of errors and inaccuracies in computation in areas of large physical water quality gradients. This model will be modified to have the initial grid generated automatically with a Poisson type elliptic grid generator with user-specified packing capabilities. For this study, the flow rate of the point source remains constant throughout the simulation. Unsteady water quality simulations will have the dynamically adaptive grid generation technique incorporated to accurately track all pertinent physical gradients, and the model will be converted to a multi-block computational environment with accurate time-differencing across block boundaries. These modifications will enable the QUAL2E model to more accurately simulate water quality variables over a variety of different physical and temporal situations.

The QUAL2E model is a basic one dimensional advection-dispersion mass transport model, numerically integrated over space and time for each physical water quality variable. For this research, no changes were made to the latter two elemental relationships of hydrogeometric and biokinetic properties. However, the mass transport relationships have to be modified to handle the general curvilinear coordinate system. All relationships of the water quality model represented by PDE's must be converted to the general curvilinear coordinate system.

17.1 Water Quality Model Equations in General Curvilinear Coordinates

The QUAL2E model is a basic one dimensional advection-dispersion mass transport model, numerically integrated over space and time for each

physical water quality variable. The mass balance is based upon advective transport into and out of the element, dispersive forces into and out of the element, external sources and withdrawals, and elemental sources and sinks. The governing equation used by the water quality model in the curvilinear coordinates is

$$\frac{\delta C}{\delta \tau} - \left(\frac{\delta C}{\delta \xi} \frac{\delta x}{\delta \tau} \right) = \frac{\delta \left(\frac{A_x D_L}{J} \frac{\delta C}{\delta \xi} \right)}{A_x J \delta \xi} - \frac{\delta (A_x \bar{u} C)}{A_x J \delta \xi} + \frac{dc}{dt} \pm \frac{S}{V} \quad (1)$$

where:

- A_x = cross-sectional area of a cell,
- c = transformation coefficient,
- C = conservative or non-conservative substance concentration,
- D_L = diffusion coefficient,
- J = Jacobian of transformation,
- S = sources or sinks of river cell,
- t = time,
- $\bar{u}$ = mean velocity,
- x = spatial coordinate,
- ξ = 1-D spatial curvilinear coordinate, and
- τ = temporal curvilinear coordinate.

There is a basic assumption that the flow in the stream, headwaters, and point sources remains steady throughout time. The unsteady simulations used in the research are unsteady in concentration, not in flow rates. By operating the model dynamically (unsteady), the user can observe the effects of biokinetics and other physical relationships on D.O. concentrations. However, the effects of dynamic forcing functions on the D.O. concentration, such as headwater and point load flow rates, cannot be modelled dynamically (Shindala et al. 1991). The water quality model utilizes an implicit backwards finite-difference technique that provides unconditional stability.

The new model generated by the coupling of the grid generator and the water quality model, operating on a multi-blocked computational domain is named QUAL2E-DAMB (QUAL2E-Dynamically Adaptive Multi-Blocked).

17.2 Dynamic Adaptive Grid Generator in Curvilinear Coordinates

The accuracy of a finite-difference solution is dependent upon the suitability of the grid used to compute the solution. Over a time-dependent solution, a dynamically adaptive grid can help to increase the accuracy of the

solution without a considerable increase in the amount of grid points used in the discretized domain. Using an elliptic grid generator based upon the Poisson equation,

$$\nabla^2 \xi = P(\xi) \quad (2)$$

control functions can be fashioned to control the spacing and orientation of the coordinate grid lines, achieving the dynamically adaptive grid (Eiseman 1987).

The adaptive grid generator can concentrate lines where the variations of the physical properties or pollutants are large, and disperse lines where physical properties or pollutants are slowly varying. The model can march the adaptive grid along the strong physical gradients, and update the grid at each time step to trace the physical properties and pollutants such as velocity, salinity, DO, BOD and chemicals. In this research, the dynamic adaptive grid generator could generate and update the new grid utilizing the strong variance of DO concentration gradients for each time step. The water quality model then recalculates the solution on the new grid and the cycle is repeated. The end result will have the grid packing following the large physical gradients along the domain for the duration of the temporal solution. The sensing of the physical solution is accomplished by the use of a weight function approach (Jin and Hasson 1992). Due to the new grid generated for each time step, an additional term which is called grid speed will be added to the model (Thompson et. al. 1985).

To develop the weight function approach, the equidistribution principle is utilized. The weight function is taken to be equally distributed over the entire physical field. In one dimension,

$$\int_{x_i}^{x_{i+1}} W(x) dx = \text{constant} \quad (3)$$

which, in discrete form equals

$$\Delta x_i W_i = \text{constant} \quad (4)$$

where $W(x)$ is the weight function, and Δx_i is the grid interval. Observing this definition, it can be seen that if the weight function is large, the grid interval must be small, and vice versa. The weight function is large in the areas of strong physical gradients, therefore, the grid interval will be smaller in the areas of these

gradients.

The control function is determined by observing the relationship between the one dimensional Poisson equation,

$$x_{\xi\xi} + Px_{\xi} = 0 \quad (5)$$

where

$$P = \frac{W_{\xi}}{W} \quad (6)$$

This results in

$$Wx_{\xi\xi} + W_{\xi}x_{\xi} = 0 \quad (7)$$

This formulation of the control function has been discussed extensively by Jin (1991). The weight function used above is determined by the physical gradient values over the physical domain. The weight function, used in the current research, is computed by the adaptation to a D.O. gradient formula,

$$W = 1 + |\nabla D.O.| \quad (8)$$

Using the definitions of the weight function and control function given above, the elliptic grid generation equation given by equation (2) becomes an adaptive grid generation system for dynamic D.O. concentration simulations for use on arbitrary one dimensional domain.

where

$$|\nabla D.O.| = \sqrt{\left(\frac{\delta D.O.}{\delta x}\right)^2} \quad (9)$$

The partial derivative of D.O. must be changed to the curvilinear coordinate system to be consistent with the elliptic grid generator. Making

$$\frac{\delta D.O.}{\delta x} = D.O._{\xi} \frac{1}{J} \quad (10)$$

the curvilinear transformation results in the weight function being expressed as the following,

$$W=1 + \sqrt{\left(D.O._\xi \frac{1}{J}\right)^2} \quad (11)$$

Equation (11), in finite difference equation becomes

$$W = 1 + \sqrt{\left(\frac{D.O._{i+1} - D.O._{i-1}}{2\Delta\xi J}\right)^2} \quad (12)$$

Using the definitions of the weight function and control function given above, the elliptic grid generation equation becomes an adaptive grid generation system for dynamic D.O. concentration simulations for use on arbitrary one dimensional domains (Luong et al. 1991).

17.3 Results of Unsteady Simulations

The main objective of the dynamic simulation on the QUAL2E-DAMB model is to demonstrate the ability of the modified model to handle a multiblock grid scheme in a dynamic, time-dependent simulation. A general data set is used containing a total number of four blocks. The data set, provided by the USEPA represents a fictional river section (Brown and Barnwell 1987). The Dirty River is the mainstream section containing two blocks of the grid running from river kilometre 66.0 to river kilometre 27.0 for a total length of 39.0 kilometres. Clear Creek is the tributary to the mainstream, and contains the remaining two blocks of the grid. The length of Clear Creek is a total of 22.0 kilometres from river kilometre 22.0 to river kilometre 0.0 where, at this point, the tributary flows into the mainstream. The junction element on the mainstream is located between mainstream river kilometre 46.0 and 45.0. Figures 17.1 and 17.2 show the geometry and the multiblock configuration of the river system, respectively. The dynamic simulation is run for a total of thirty hours at time steps of two hours, thus giving a total of fifteen solutions over the total simulation period.

Block 3 (as shown in Figure 17.2) possesses the possibility of having an impulse point load applied along its length at stream kilometre 9.0. The impulse is applied at any time step during the simulation depending upon the input by the user. During the startup of the model, the user inputs the time of impulse loading. When the time counter in the model reaches this point in time, the waste load is released into the stream for a total of one time period. The only variables changed to accomplish the impulse load are the D.O. value and the B.O.D. value of the point load. The flow rate of the point source remains constant throughout the simulation. This variable can not be changed because of the assumption in the derivation of the governing equation that the input flow

Figure 17.1
Geometry of the dynamic simulation river section

Figure 17.2
Block structure of dynamic simulation data

Figure 17.3
Dynamic simulation results after 12 hours

Figure 17.4
Dynamic simulation results after 16 hours

Figure 17.5
Dynamic simulation results after 18 hours

Figure 17.6
Dynamic simulation results after 20 hours

Figure 17.7
Dynamic simulation results after 24 hours

Figure 17.8
Dynamic simulation results after 28 hours

rate boundary conditions remain steady. The waste input represents a very strong pollutant with a B.O.D. concentration of 750.0 mg/l and a D.O. concentration of 0.0 mg/l. These concentrations are used to provide a sufficiently sharp D.O. gradient at the point of the waste input. All other variables are kept constant in the simulation.

The main driving forces in the simulation are the advective effects of the river, tributary, and point source flow rates. The river and tributary have headwater sources at the beginning of the respective reaches. Reaeration of the stream provides for the rebound of the D.O. drop at subsequent time steps after the impulse load. The results of the dynamic simulation are shown in Figure 17.3 to Figure 17.8.

The initial boundary conditions used for the dynamic simulation include only the headwater conditions along with the constant physical and kinetic coefficients. At the beginning of the dynamic simulation, the initial conditions along the reaches are set equal to zero. This is why the warmup period is mentioned earlier. The solution must be solved for several time periods to allow it to reach a condition where the conditions across the reach do not change considerably over a time step. The warmup period was determined to be approximately six to eight hours in simulation time.

Results of the dynamic simulation are presented beginning at a simulation time of twelve hours (Figure 17.3), and are presented at subsequent two hour intervals up to 30 hours of simulation. The representations presented are of the D.O. concentrations along the entire river system, and the adaptive grid corresponding to the respective river reaches and time levels. The D.O. concentrations are represented by the colours given in the legend with white being the highest D.O. concentration and black being the lowest. The waste point source is input into the model at a time of sixteen hours (Figure 17.4).

The most obvious observation shown in Figure 17.3 to Figure 17.8 is that the grid adapts very well to the D.O. gradients in the solution. Gradients are defined as the change in the concentration per change in distance. Where there are very sharp D.O. drops over relatively short distances, the gradients are very large. The grid adapts more in these areas than in others with weaker gradients. For instance, over every time step solution, a strong gradient occurs in the vicinity of the mainstream and tributary junction. The grid is packed at the junction. The effect of the gradient sensing across block interfaces can be seen at the junction point. The grids on both Blocks 1 and 4 on the mainstream are adapted, as well as Block 3 on the tributary. This effect is very desirable.

The grids also adapt dynamically between time intervals. This effect is shown beginning at a time of eighteen hours (Figure 17.5). Recall that the impulse load is released at a time level of sixteen hours (Figure 17.4). The grid does not adapt to the sharp D.O. gradient caused by the impulse load until a time level of eighteen hours. This illustrates the lag of the dynamic grid generator of one time step. The reason for this occurrence is clear. The grid adapts based on

the D.O. concentrations solved at the previous time level. Thus, the grid at time eighteen hours is adapted based on the gradients at time sixteen hours.

At a time level of eighteen hours (Figure 17.5), the grid begins to adapt to the sharp D.O. gradient in Block 3. As the simulation time progresses, the sharp gradient is changed by two processes. Advection moves the gradient downstream toward the mainstream junction and reaeration causes the D.O. sag curve to rebound. Both processes cause the gradient to be lessened, and the grid responds by relaxing the packing at the gradient. This can be observed as time progresses past eighteen hours (Figure 17.6 to Figure 17.8).

Figure 17.3 to Figure 17.8 reveal very well the nature of the operation of the dynamic grid generator. Due to the quality of the results obtained by the use of the dynamic grid generator, the process is shown to be successful in the tracking of physical gradients.

17.4 Conclusions and Discussion

The dynamically adaptive, multiblocked water quality model, QUAL2E-DAMB, can accurately predict desired physical concentrations over complex river systems. The finite difference grids used by the solution algorithm can adapt to either user specified locations, as used in the QUAL2E-AG model, or automatically to any user specified physical gradient or variable, as used in the QUAL2E-DAMB model. Excellent simulations of impulse waste loads, and the associated waste plume, have been achieved using the model.

An obvious recommendation for further research is the verification of the D.O. solutions for the dynamic, multiblocked model. As stated earlier, the dynamic model has been applied to an experimental, nonexistent river section for demonstration. For accurate verification of the results, application to actual river sections, with extensive field verification of the results must be conducted.

Further research should also include the modification of the one dimensional model to a two dimensional, and possibly three dimensional, mode of operation. After this modification, the model would be able to simulate reactions in directions normal to the axial direction of flow. For example, the effects of vertical mixing due to depth variations and horizontal mixing due to directional inputs could be modelled accurately.

Acknowledgements

Some of the numerical results will be published in 1993 International Conference on Hydro-Science & Engineering.

Variables

A_x	cross-sectional area of a cell, L^2
c	transformation coefficient
C	conservative or non-conservative substance concentration, M/L^3
D_L	diffusion coefficient, L^2/T
J	Jacobian of transformation
S	sources or sinks of river cell, M/T
t	time, T
$\bar{u}$	mean velocity, L/T
V	volume, L^3
$W(x)$	weight function
x	spatial coordinate, L
Δx_i	grid interval, L
ξ	1-D spatial curvilinear coordinate, L
τ	temporal curvilinear coordinate, T

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