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Hydrodynamics for Water Quality Models

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Abstract

During the past decade, the US Army Engineer Waterways Experiment Station (WES) has developed and applied a variety of numerical water quality models for surface waters. In most cases, the transport terms of these models have been computed using output from numerical hydrodynamic models. This paper summarizes the experience of linking water quality models to hydrodynamic models and examines the need for such linkages.

Introduction

Mechanistic, numerical water quality models are based upon the conservation of mass, i.e., the mass transport or advection-diffusion equation. This equation, which is solved for each water quality state variable, requires estimates for advective velocities or flows and eddy diffusivities. Although these hydrodynamic variables can be estimated by a variety of methods, such as calibration through a conservative tracer, the most direct, and usually the most accurate method, is application of a numerical hydrodynamic model. However, the application of a hydrodynamic model adds time and cost to conduct the study and additional data requirements. Hydrodynamic models, which are based upon the conservation of mass and momentum, sometimes require special expertise to apply.

One might ask, do the benefits of linking the output from hydrodynamic models to water quality models justify

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the additional time, cost, and complexity? Additionally, one might ask should the linking be direct, i.e., the water quality computations and the hydrodynamics are performed at the same time interval in perhaps the same code, or can adequate accuracy be obtained through indirect linkage. Such linking involves applying the hydrodynamic and water quality models separately with the hydrodynamic output normally averaged and stored over some interval of time, e.g., a tidal cycle. The primary reason for indirect linkage is to reduce computational requirements. This paper attempts to address these questions by reviewing the experience at WES for water quality modeling of various types of surface waters, including reservoirs, streams, and estuaries.

Reservoirs

The first reservoir water quality models were one-dimensional (1D) along the vertical axis and averaged over the surface area for each layer. The hydrodynamics consist of vertical flows and eddy diffusivities. Vertical flows are determined from inflow and outflow boundary conditions and flow conservation for each layer. Inflow and outflow boundary conditions are determined from theoretically based relations for inflow density currents and outflow selective withdrawal mechanics. Vertical diffusivities are usually based on integral energy concepts and simplified, zero order turbulence closures. All reservoir models must compute heat exchange and the distribution of temperature, which affects water density and stratified flow hydraulics.

Two-dimensional (2D), laterally-averaged hydrodynamic and transport models began to appear around the middle of the 1970s. These models use continuity and density dependent momentum principles to compute longitudinal and vertical velocities. The 2D, laterally-averaged reservoir and estuarine model CE-QUAL-W2 (Environmental and Hydraulics Laboratories 1986) computes hydrodynamics and twenty water quality constituents. The hydrodynamics and water quality are directly linked and dynamically coupled (e.g., temperature, suspended solids, and salinity, or total dissolved solids, can affect density which affects the hydrodynamics). At one time there was an interest in indirectly linking the water quality model code, except for variables that affect water density, e.g., temperature. However, with the dramatic increases in computational power, computational requirements are not of concern (even for 80386 or better PCs), and interest in indirect linkage for this 2D model has diminished.

Although 1D and 2D models have been calibrated for DeGray Reservoir to match observations reasonably well, the mechanisms to achieve calibration were different for the two models (Martin and Wlosinski 1986). Metalimnetic dissolved oxygen (DO) minima were developed in the 1D model through settling and decomposition of detrital material. The minima in the 2D model occurred naturally, through the use of properly computed hydrodynamics, without forced calibration. In the 2D model, river inflow density currents, which flow along the thermocline during most of the stratification season, transported water through the metalimnion that was low in DO and high in biodegradable organic matter thus causing the minima (Martin 1988). The 2D model mechanism is considered to be correct for large reservoirs with river inflows, such as DeGray, which are often eutrophic near the inflow and oligotrophic at the downstream end.

Two-dimensional reservoir models actually require little more effort to apply than the 1D models. Bathymetric and geometric input do require more time to develop for 2D models than for 1D models, but the benefits of being able to more accurately simulate observed 2D phenomena far outweigh this additional effort.

Stream Environments

Most river/stream water quality issues can be adequately modeled with 1D longitudinal models. The exceptions are 2D jet/plume model studies used for near-field mixing zone analyses. One question that might be raised is whether it is necessary to use hydraulic routing models for developing advective transport versus using simpler methods, such as steady flow estimates (e.g., Manning equation with simple channel geometry or backwater computations) or hydrologic routing.

Most of the above mentioned methods for describing hydraulic conditions have been successfully used for riverine water quality model studies (e.g., Hamlin-Tillman and Haake 1990). The primary factor for selecting a particular method is whether steady flow can be assumed or not. The water quality issues for a study of the Chattahoochee River (Zimmerman and Dortch 1988) could not have been satisfactorily addressed without the use of an unsteady flow model.

The growth in computer power and the availability of hydraulic routing models (i.e., solution of the Saint Venant equations for conservation of mass and momentum) seem to have displaced much of the need for hydrologic routing methods for unsteady flow problems. Although hydraulic routing models require stream cross-section information, they are accurate for a wide range of flow conditions once the roughness is calibrated. Hydraulic routing models provide the most flexibility and accuracy, assuming cross-section information is available.

Estuarine and Coastal Environments

Most numerical water quality models of estuarine or coastal areas require a full 3D treatment of the water body. To provide accurate 3D flow fields in such areas for water quality models, numerical hydrodynamic models are a necessity. Currents are influenced by freshwater river inflow, density effects, wind, tides, and perhaps the earth's rotation (Coriolis effect) and large-scale ocean circulation. Short-period wind waves are often present at the surface and result in the generation of turbulence that can cause strong mixing in the water column, thus, impacting water quality. With the additional influences of the complex geometry and topography normally found in estuarine and coastal areas, the hydrodynamics of such environments is extremely complex. The major question to be answered in water quality model studies of such dynamic environments is can the hydrodynamic output, which is normally computed at time intervals of seconds to a few minutes, be processed, i.e., time averaged, in such a way that it can be indirectly linked to the water quality model while preserving the basic transport processes. Normally, water quality variables are slowly varying, e.g., hours to days. Thus, directly linking 3D water quality and hydrodynamic computations is unnecessary from a physical standpoint and leads to excessive CPU requirements.

During the recent development of a 3D hydrodynamic model of Chesapeake Bay by Johnson, et al. (1991), and a companion 3D water quality model by Cerco and Cole (1991), Dortch (1990) developed a procedure for computing 3D Lagrangian residual (i.e., tidally-averaged) circulation from the 3D hydrodynamics computed at a time interval of 5 minutes. A simple time average of the flow field over a tidal cycle produces Eulerian residual currents. However, the mass passing a fixed point does not depend solely on the mean velocity at that point but also depends on the gradient of the velocity at that point. As a first-order approximation, Dortch computed the Lagrangian residual currents as the sum of Eulerian residual velocities and Stokes' drift. The Stokes' drift approximates residual currents induced by the nonlinear interactions of the tidal currents and represents the net drift experienced by a particle passing through a spatially varying velocity in an oscillating flow. This procedure provides a practical means of making long-term 3D transport computations for weakly nonlinear tidal systems.

The importance of properly incorporating the transport properties of an estuarine or coastal water body into computations for a conservative substance such as salinity has been demonstrated (Dortch 1991). However, results from the Chesapeake Bay study indicate that the horizontal distribution of some constituents, e.g., DO, is primarily dependent upon the reaction kinetics or various sources/sinks for that constituent. Local sources/sinks, such as benthic fluxes, can be the dominate factor causing the longitudinal gradient in a constituent, and transport can have only a minor effect. For stratified systems, vertical transport, especially diffusion, must still be properly represented over the water column to achieve reasonable water quality results, even for constituents that are kinetic dominated. Therefore, a numerical hydrodynamic model is still required, although one may not have to be as concerned about the manner in which the output is processed in the indirect linking.

Conclusions

Other than for simple reservoir models, the most straightforward method for providing transport characteristics is through the application of a numerical hydrodynamic model. One might be able to provide such information from field data for 1D models applied to relatively steady flow in streams; however, for multi-dimensional models, the only practical means of providing information on the advective and diffusive transport of the water body is to apply a numerical hydrodynamic model. This is especially true in dynamic estuarine and coastal environments where a 3D representation is often required.

Successful water quality model applications have been conducted with rather crude estimates for hydraulic transport. The reason for this success is that kinetic processes can outweigh the effects of transport. However, with the technology and computer resources available today, it seems inappropriate to use crude hydraulic descriptions for water quality modeling. Furthermore, how does one know the relative importance of transport without first providing a reasonably accurate transport description. Realistic hydraulic simulations can be obtained at reasonable costs. The use of accurate hydraulics helps to remove some of the uncertainty associated with water quality modeling, which facilitates acceptance of results. For computationally demanding 2D and 3D studies, hydrodynamic information can be averaged over a larger interval of time in such a manner that the proper transport properties are preserved and computational requirements are reduced.

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