# CH3D-WASP: A LINKED HYDRODYNAMIC AND WATER QUALITY MODEL

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ABSTRACT: The CH3D-WASP model was developed to simulate water quality in estuaries for short-term periods ranging from minutes to days. CH3D (Johnson et al., 1991) is a three-dimensional hydrodynamic model for estuaries. WASP (Ambrose et al., 1991) is the EPA's water quality model for surface waters. Because CH3D is designed to simulate time-varying flow variations due to external forcings including tides, wind, geometric configuration and varying bottom depths, the model uses fine resolutions in grid cell (meters) and time step (seconds-minutes). WASP, however, is a box-model that uses "box" cells (kilometers) and a much larger time step (hours-days). In order to link the hydrodynamic transport in CH3D with the biological/chemical kinetics of WASP, an effort was taken in linking CH3D with WASP. The linked CH3D-WASP model simulates water quality variations at the same spatial and temporal resolutions as those for the hydrodynamic model, CH3D. First, the eutrophication kinetic modules in WASP were identified, separated, and modulized. The modulized eutrophication subroutines, which provide sink/source terms for the transport equation, were linked to CH3D. To test the linkage accuracy, two model runs were executed: one was for a two-dimensional case and the other for a three-dimensional case. For the two-dimensional case, simulation results of CH3D-WASP and WASP were compared for ammonia, carbonaceous BOD, and DO. Results from both models were almost identical, within the significant digits. For the three-dimensional case with grid dimensions of 11 (x) x 7 (y) x 5 (z), results of nitrification from scenarios with boundary conditions and initial-value conditions and combinations were reasonable, as predicted. The test scenarios demonstrated that the linked CH3D-WASP model is capable of water quality simulation at fine resolutions in both space and time.
KEY TERMS: hydrodynamic; water quality; eutrophication; CH3D; WASP.

## INTRODUCTION

Estuaries are biologically productive bodies of water. They are important as the spawning and nursery grounds for many coastal fish and invertebrates. Thus, estuaries support commercial and recreational fishing and shell-fishing. Many are valuable for recreational boating and bathing, and are prized aesthetic resources. Many estuaries flush municipal and industrial wastewater out to sea. The various uses of an estuary place conflicting demands and burdens on water quality (Ambrose and Martin, 1990). Mathematical models serve as an aid in assessing the effects of these conflicting demands and in developing protective management strategies (Martin and McCutcheon, 1999).

The movement of tides into and out of estuaries such as Sinclair and Dyes Inlets in Washington, the associated density effects created by the incursion of salinity, is of particular importance in describing the water quality of such bodies of water. Estimating the time and spatial behavior of water quality in estuaries is complicated by the effects of tidal motion. The upstream and downstream currents produce substantial variations of water quality at certain points in the estuary and the calculation of such variation is indeed a complicated problem. CH3D model was selected to simulate hydrodynamic flow at the Sinclair and Dyes Inlets. CH3D model is focused on flow modeling within estuaries, not water quality modeling. So WASP, US EPA's water quality model, is to be linked to CH3D for simulating water quality at Sinclair and Dyes Inlets in Washington.

The WASP-CH3D linkage was developed to simulate chemical/biological process at Sinclair and Dyes Inlets in Washington. The background of this study is that WASP is a well-accepted model for simulating water quality in estuaries, eutrophication model is needed to simulate nutrient TMDLs in Sinclair and Dyes Inlets, and CH3D model

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is a calibrated three-dimensional transport model to set up for Sinclair and Dyes Inlets. The benefit of this study is that eutrophication for Sinclair and Dyes Inlets for a short-term period can be calculated, extracted eutrophication module (EEUTRO) will be isolated as a stand-alone program, and EEUTRO will be simply linked with CH3D as a subroutine. The scope of this study is as follows: The eutrophication part from WASP was separated. The screen option subroutines in WASP were deleted. The common blocks for transport and eutrophication in WASP were modified and separated. The subroutines for transport and eutrophication modules in WASP were separated physically. To test successful separation of EEUTRO from WASP, the model runs for CH3D-WASP were executed for two- and three-dimensional cases.

## EXTRACTION OF EUTROPHICATION MODULE FROM WASP

WASP program is composed of main program and many subroutines. The subroutines can be categorized as “Screen option,” “Input,” “Process,” and “Utility” subroutines. Separating the eutrophication module from WASP is one of the keys for this study. The separated EUTRO module (EEUTRO) is a stand-alone program and finally is linked with CH3D. The procedure for CH3D-WASP linkage development follows ICM-TOXI development procedure. ICM-TOXI was developed by Waterways Experiment Station (WES). The procedures for extracting of eutrophication module from WASP to link with CH3D are as follows:

1. Comment out the WISP option subroutines: WASP program includes the User Shell (WISP). The subroutines for the User Shell (WISP) were commented out.
2. Modifying the COMMON blocks for transport and eutrophication: Data in WASP (EUTRO) are shared among the subroutines primarily through the WASP COMMON blocks. The common blocks for WASP (EUTRO) were modified for transport and eutrophication COMMON blocks.
3. Regrouping the subroutines of WASP (EUTRO) program for transport and eutrophication modules: WASP (EUTRO) is a modular program. Its many subroutines are grouped into the functional categories of “input,” “process,” “output,” and “utility”.

## CH3D-WASP PROGRAM

Current in coastal, estuarine and lake waters can be quite complex as they respond to tides, winds, density gradients, water quality, and flows and are also affected by complicated basin geometry and bathymetry. CH3D-WASP is designed to solve the following system of governing equations along with initial and boundary conditions, which describes flow, transport and eutrophication in estuaries. The basic assumptions of the CH3D-WASP model are: (1) hydrostatic pressure distribution, (2) Boussinesque approximation, and (3) eddy-viscosity concept is employed. The basic equations for an incompressible fluid in a right-handed Cartesian coordinate system (x,y,z) are:

$$\partial u/\partial x + \partial v/\partial y + \partial w/\partial z = 0 \tag{1}$$

$$\frac{\partial u}{\partial t}+\frac{\partial u^2}{\partial x}+\frac{\partial uv}{\partial y}+\frac{\partial uw}{\partial z}= fv-\frac{1}{\rho_0}\frac{\partial p}{\partial x}+\frac{\partial}{\partial x}\left(A_H\frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(A_H\frac{\partial u}{\partial y}\right)+\frac{\partial}{\partial z}\left(A_V\frac{\partial u}{\partial z}\right) \tag{2}$$

$$\frac{\partial v}{\partial t}+\frac{\partial uv}{\partial x}+\frac{\partial v^2}{\partial y}+\frac{\partial vw}{\partial z}= -fu-\frac{1}{\rho_0}\frac{\partial p}{\partial y}+\frac{\partial}{\partial x}\left(A_H\frac{\partial v}{\partial x}\right)+\frac{\partial}{\partial y}\left(A_H\frac{\partial v}{\partial y}\right)+\frac{\partial}{\partial z}\left(A_V\frac{\partial v}{\partial z}\right) \tag{3}$$

$$\partial p/\partial z = -\rho g \tag{4}$$

$$\frac{\partial T}{\partial t}+\frac{\partial uT}{\partial x}+\frac{\partial vT}{\partial y}+\frac{\partial wT}{\partial z}=\frac{\partial}{\partial x}\left(K_H\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_H\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(A_V\frac{\partial T}{\partial z}\right) \tag{5}$$

$$\frac{\partial S}{\partial t}+\frac{\partial uS}{\partial x}+\frac{\partial vS}{\partial y}+\frac{\partial wS}{\partial z}=\frac{\partial}{\partial x}\left(D_H\frac{\partial S}{\partial x}\right)+\frac{\partial}{\partial y}\left(D_H\frac{\partial S}{\partial y}\right)+\frac{\partial}{\partial z}\left(D_V\frac{\partial S}{\partial z}\right) \tag{6}$$

$$\frac{\partial C_i}{\partial t}+\frac{\partial uC_i}{\partial x}+\frac{\partial vC_i}{\partial y}+\frac{\partial wC_i}{\partial z}=\frac{\partial}{\partial x}\left(E_H\frac{\partial C_i}{\partial x}\right)+\frac{\partial}{\partial y}\left(E_H\frac{\partial C_i}{\partial y}\right)+\frac{\partial}{\partial z}\left(E_V\frac{\partial C_i}{\partial z}\right)\pm SS_i \tag{7}$$

$$\rho = \rho(T,S,C_i) \tag{8}$$

where *(u,v,w)* are velocities in *(x,y,z)* directions, *f* is the Coriolis parameter defined as $2\Omega\sin\phi$ where $\Omega$ is the rotational speed of the earth, and $\phi$ is the latitude, $\rho$ is density, p is pressure, *T* is temperature, *S* is salinity, $C_i$ is pollutants concentration, ($A_H$, $K_H$, $D_H$, $E_H$) are horizontal turbulent eddy coefficients, ($A_V$, $K_V$, $D_V$, $E_V$) are vertical turbulent eddy viscosities, and $SS_i$ (where *i*=1~8) is source/sink term for pollutants due to eutrophication.

The CH3D-WASP model was developed to simulate water quality in estuaries for short-term periods ranging from minutes to days. CH3D (Johnson et al., 1991) is a three-dimensional hydrodynamic model for estuaries. WASP (Ambrose et al., 1991) is the EPA's water quality model for surface waters. Because CH3D is designed to simulate time-varying flow variations due to external forcings including tides, wind, geometric configuration and varying bottom depths, the model uses fine resolutions in grid cell (meters) and time step (seconds-minutes). WASP, however, is a box-model that uses "box" cells (kilometers) and a much larger time step (hours-days). In order to link the hydrodynamic transport in CH3D with the biological/chemical kinetics of WASP, an effort was taken in linking CH3D with WASP. The linked CH3D-WASP model simulates water quality variations at the same spatial and temporal resolutions as those for the hydrodynamic model, CH3D. CH3D-WASP consists of a MAIN program and thirty (30) subroutines. The eutrophication kinetic modules in WASP were identified, separated, and modulized. The modulized eutrophication subroutines, which provide sink/source terms for the transport equation, were linked to CH3D. To test the linkage accuracy, two model runs were executed: one was for a two-dimensional case and the other for a three-dimensional case.

## Test Runs for CH3D-WASP Model

The purpose of model test runs is to check the physical separation of eutrophication module (EEUTRO) from the original WASP program. To test the linkage accuracy, two model runs were executed: one was for a two-dimensional case and the other for a three-dimensional case. For the two-dimensional case, simulation results of CH3D-WASP and WASP were compared for ammonia, DO, and carbonaceous BOD. For the three-dimensional case with grid dimensions of 11 (x) x 7 (y) x 5 (z), nitrification from scenarios with boundary conditions and initial-value conditions and combinations was adopted to have test runs.

### Test runs for two-dimensional case

5 (x) x 4 (y) grids shown in Figure 1 were selected to test CH3D-WASP linkage for two-dimensional case. In Figure 1, three flows such as F1, F2, and F3 were set, and the flow rate of F2 and F3 was the same. Steady-state flow, that means no variation of the velocities with time, was selected to compare the simulation results of the original WASP with those of CH3D-WASP. In the x-direction, grids are spaced at $\Delta x$ = 1Km. In the y-direction, grids are spaced at $\Delta y$ = 1Km

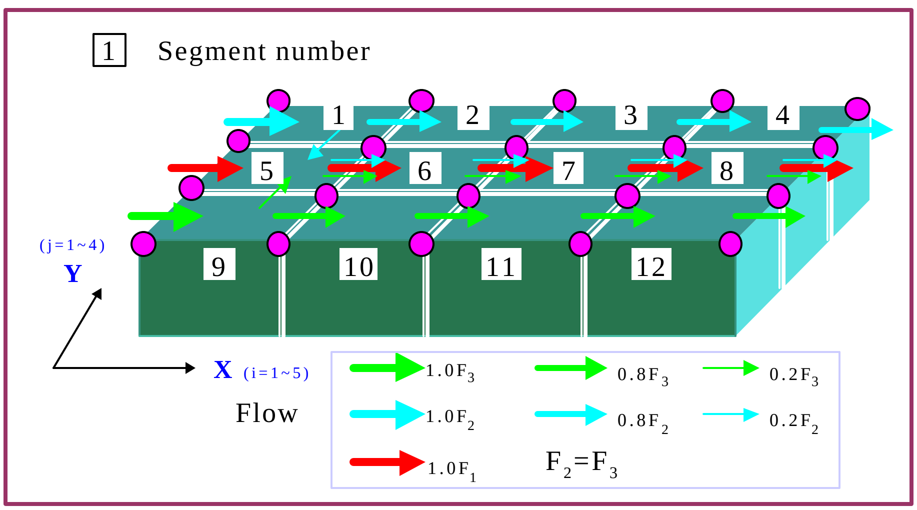


Figure 1. Two-Dimensional Grids for Test Runs

The concentrations of ammonia, carbonaceous BOD (CBOD), and DO comparing simulation results for WASP and CH3D-WASP are listed in Table 1. For the two-dimensional case, simulation results of CH3D-WASP and WASP were compared for ammonia, DO, and carbonaceous BOD. Results from both models were almost identical, within the significant digits as shown in Table 1.

Table 1. Concentrations of Ammonia, DO, and CBOD for Two-Dimensional Case Test Runs

| State Variables | CH3D-WASP/ WASP | Time (Days) | Concentrations at Segment Number 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Ammonia | CH3D-WASP | 1.0 | 6.71 | 2.30 | 0.50 | 0.06 | 8.73 | 6.86 | 4.08 | 1.69 | 6.71 | 2.30 | 0.50 | 0.06 |
| | WASP | 1.0 | 6.71 | 2.30 | 0.50 | 0.06 | 8.73 | 6.86 | 4.08 | 1.69 | 6.71 | 2.30 | 0.50 | 0.06 |
| | CH3D-WASP | 3.0 | 9.51 | 7.26 | 4.28 | 1.94 | 9.86 | 9.74 | 9.49 | 8.94 | 9.51 | 7.26 | 4.28 | 1.94 |
| | WASP | 3.0 | 9.51 | 7.26 | 4.28 | 1.94 | 9.86 | 9.74 | 9.49 | 8.94 | 9.51 | 7.26 | 4.28 | 1.94 |
| | CH3D-WASP | 7.0 | 9.99 | 9.98 | 9.16 | 7.87 | 10.0 | 9.99 | 9.99 | 9.98 | 9.99 | 9.98 | 9.16 | 7.87 |
| | WASP | 7.0 | 9.99 | 9.98 | 9.16 | 7.87 | 10.0 | 9.99 | 9.99 | 9.98 | 9.99 | 9.98 | 9.16 | 7.87 |
| DO | CH3D-WASP | 1.0 | 6.59 | 5.14 | 4.40 | 4.21 | 7.15 | 6.92 | 6.14 | 5.25 | 6.59 | 5.14 | 4.40 | 4.21 |
| | WASP | 1.0 | 6.59 | 5.14 | 4.40 | 4.21 | 7.15 | 6.92 | 6.14 | 5.25 | 6.59 | 5.14 | 4.40 | 4.21 |
| | CH3D-WASP | 3.0 | 7.93 | 8.62 | 8.86 | 8.83 | 7.62 | 8.05 | 8.46 | 8.83 | 7.93 | 8.62 | 8.86 | 8.83 |
| | WASP | 3.0 | 7.93 | 8.62 | 8.86 | 8.83 | 7.62 | 8.05 | 8.46 | 8.83 | 7.93 | 8.63 | 8.86 | 8.83 |
| | CH3D-WASP | 7.0 | 7.98 | 9.04 | 9.98 | 10.8 | 7.63 | 8.08 | 8.50 | 8.91 | 7.98 | 9.04 | 9.98 | 10.8 |
| | WASP | 7.0 | 7.98 | 9.04 | 9.98 | 10.8 | 7.63 | 8.08 | 8.50 | 8.91 | 7.98 | 9.05 | 9.99 | 10.8 |
| CBOD | CH3D-WASP | 1.0 | 3.67 | 1.24 | 2.56 | 0.03 | 4.84 | 3.66 | 2.17 | 0.92 | 3.67 | 1.24 | 2.56 | 0.03 |
| | WASP | 1.0 | 3.67 | 1.24 | 2.56 | 0.03 | 4.84 | 3.66 | 2.17 | 0.92 | 3.67 | 1.23 | 2.56 | 0.03 |
| | CH3D-WASP | 3.0 | 4.76 | 3.21 | 1.77 | 0.78 | 5.27 | 4.78 | 4.30 | 3.79 | 4.76 | 3.21 | 1.77 | 0.78 |
| | WASP | 3.0 | 4.76 | 3.21 | 1.77 | 0.78 | 5.27 | 4.78 | 4.30 | 3.79 | 4.76 | 3.20 | 1.76 | 0.78 |
| | CH3D-WASP | 7.0 | 4.87 | 3.78 | 2.88 | 2.11 | 5.30 | 4.83 | 4.41 | 4.02 | 4.87 | 3.78 | 2.88 | 2.11 |
| | WASP | 7.0 | 4.87 | 3.78 | 2.88 | 2.11 | 5.30 | 4.83 | 4.41 | 4.02 | 4.87 | 3.76 | 2.86 | 2.09 |

Test runs for three-dimensional case

A three-dimensional case is selected to test the CH3D-WASP linkage accuracy. The grids are composed of 11 (x) x 7 (y) x 5 (z) as shown in Figure 2. There are two kinds of grid cells; one represents for land and the other for water. At grid cells for land, the water isn't flowing. The region consists of 10 Km in x-direction, 6 Km in y-direction, and 15 m in z-direction. In the x-direction, grids are spaced at $\Delta x$ = 1Km. In the y-direction, grids are spaced at $\Delta y$ = 1Km. There are five (5) layers in z-direction, so the thickness of each layer is 3 m. The tidal boundary was located at the right-hand side of grids domain. In the simulation, the time step was five (5) minutes and the ending time was 34 days.

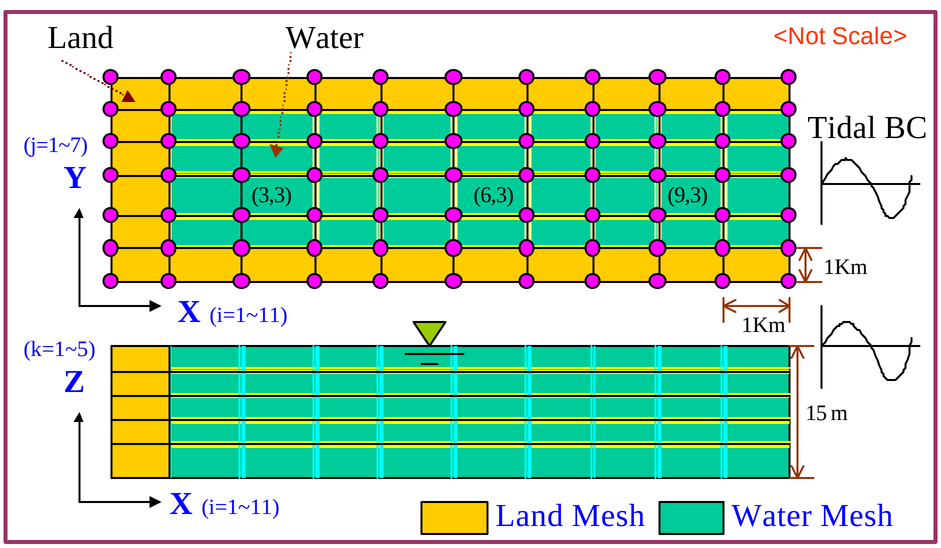


Figure 2. Three-Dimensional Grids for Test Run

The complex eutrophication can't test of checking the success of CH3D-WASP linkage. So the nitrification scenario was applied to CH3D-WASP model to test the linkage accuracy, because this is so simple process that is only affected to ammonia and nitrate. Grid cells such as (3,3), (6,3), and (9,3) as shown in Figure 2 were selected to check the concentrations of eight-state variables ($NH_3$, $NO_3$, $OPO_4$, Phytoplankton, CBOD, DO, ON, and OP) due to several physical/chemical processes that can affect the transport and interaction among the nutrients, phytoplankton, carbonaceous material, and dissolved oxygen in the aquatic environment. The concentrations of ammonia and nitrate due to nitrification are shown in Figure 3 through Figure 4 with initial and boundary conditions.

For the first scenario, the concentrations of ammonia and nitrate due to nitrification were illustrated in Figure 3 and 4. In the simulation, the initial condition of ammonia and nitrate was 0.1 mg/l and 0.01 mg/l, and the boundary condition of ammonia and nitrate was 0.1 mg/l and 0.01 mg/l respectively. In Figure 3, the ammonia concentration at the (9,3) grid cell varied around 0.1 mg/l because the boundary condition was 0.1 mg/l, and the concentration was also oscillated due to tidal effects near the right-hand side boundary of the domain. The concentration of ammonia at the (3,3) grid cell was decreased from 0.1 mg/l to 0.05 mg/l due to nitrification at the 31 days, and the concentration was increased after 31 days. The concentration of ammonia at the (3,3) grid cell was a little oscillated because the grid cell was 7 Km far from the tidal boundary condition. For Figure 4, the concentration of nitrate at the (3,3) grid cell was increased from 0.01 mg/l at the initial condition to 0.06 mg/l due to nitrification, and decreased after 31 days. The concentration of nitrate at the (9,3) grid cell was oscillated near 0.01 mg/l due to the boundary condition and tidal effect.

For the second scenario, the concentrations of ammonia and nitrate for initial condition were 0.1 mg/l and 0.0 mg/l respectively, and the ammonia and nitrate for boundary condition were 0.0 mg/l and 0.1 mg/l respectively. The concentration of ammonia at the (9,3) grid cell was decreased near 0.0 mg/l within 0.5 days because the boundary condition was 0.0 mg/l. The concentration at the (3,3) grid cell was decreased due to nitrification, and 0.04 mg/l at the time 31-day. The concentration of nitrate at the (3,3) grid cell was increased near 0.1 mg/l within 0.5 days due to the boundary condition. The concentration of nitrate at the (9,3) grid cell was increased due to nitrification, and 0.06 mg/l at the time 31-day. The simulation results of ammonia and nitrate due to nitrification were very reasonable because the value of ammonia concentration decrease from nitrification was the same as that of nitrate concentration increase at a certain time step.

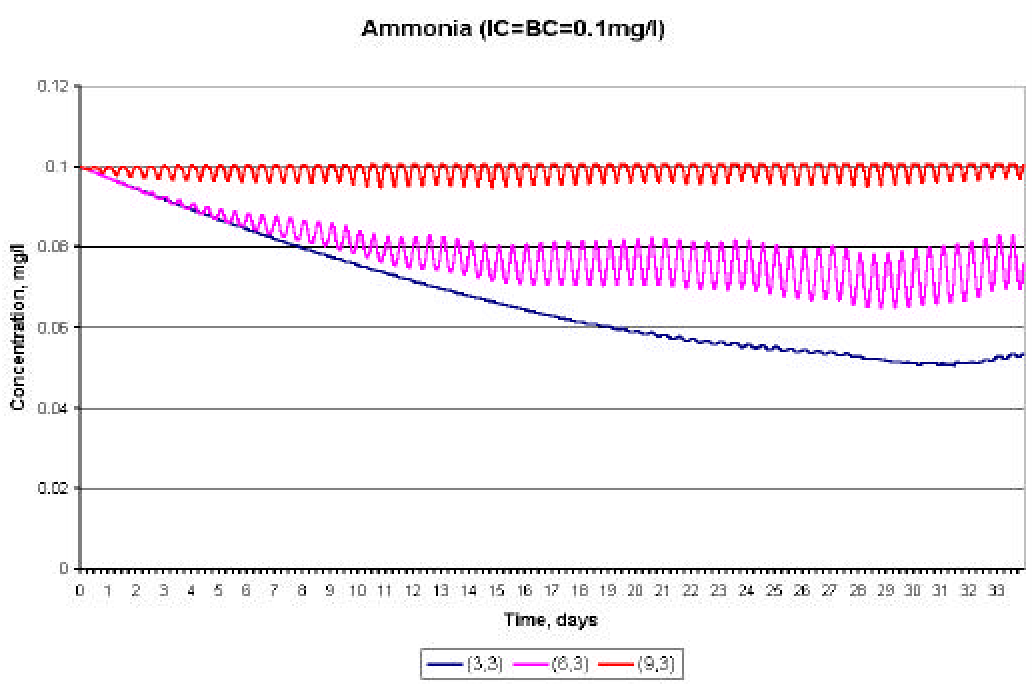


Figure 3. Concentration of Ammonia due to nitrification (IC=0.1mg/l, BC at Tidal Boundary=0.1 mg/l); (3,3), (6,3), and (9,3) are located at 7 km, 4 km, and 1 km from the tidal boundary condition

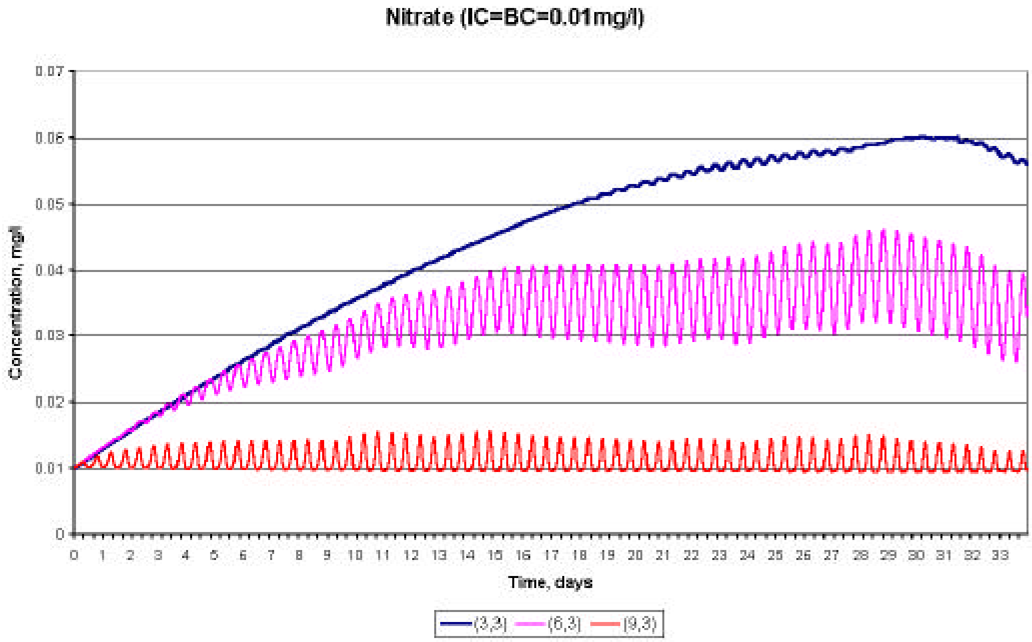


Figure 4. Concentration of Nitrate due to nitrification (IC=0.01mg/l, BC at Tidal Boundary=0.01 mg/l); (3,3), (6,3), and (9,3) are located at 7 km, 4 km, and 1 km from the tidal boundary condition

## CONCLUSION

In conclusion, the eutrophication kinetic modules in WASP were identified, separated, and modulized. The modulized eutrophication subroutines, which provide sink/source terms for the transport equation, were linked to CH3D. To test the linkage accuracy, two model runs for two- and three-dimensional cases were executed. For the two-dimensional case, simulation results of CH3D-WASP and WASP were compared for ammonia, carbonaceous BOD, and DO. Results from both models were almost identical, within the significant digits. For three-dimensional case, the results of nitrification from scenarios with boundary conditions and initial-value conditions and combinations were reasonable, as predicted. The test scenarios demonstrated that the linked CH3D-WASP model is capable of water quality simulation at fine resolutions in both space and time.

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