Kor. J. Env. Hlth., Vol. 31, No. 6, pp 489~497(2005)

2-Dimensional Model Development for Water Quality Prediction

Do Hyeon Paik†

Department of Health & Environment of Seonam University

(Received Nov. 10, 2005/Accepted Dec. 10, 2005)

Abstract : A numerical method for the mathematical water modeling in 2-dimensional flow has been developed. The model based on a split operator technique, in which, the advection term is calculated using the upwind scheme. The diffusion term is one- dimensionalized and calculated using Crank-Nicholson's implicit finite difference scheme to reduce the numerical errors from large time steps and variable spacings. It also provides a relatively simple and economic method for more accurate simulation of pollutant dispersion. Water depths and flow velocities in the Boreyong reservoir during the normal water periods were predicted by numerical experiments with a 2-dimensional flow model so as to provide current field data for the study of advection and diffusion of pollutants. Developed 2-dimensional water quality model is applied to Boreyong reservoir to simulate a spatial and periodical changes of water quality.

Keywords : numerical method, 2 dimensional water quality modeling, water quality

Introducton

In modeling the transport and dispersion of water pollutant in a stream or river, there are a wide ranges of models available. when modelling the impact of water pollution emission from non-point sources during precipitation or the water quality during unsteady water quality accident, however, it is strongly recommended to water level and velocity from continuity and momentum equations and the water quality by applying dispersion equation afterwards.

As most of water flow in river or stream is dominated by one dimensional flow, one-dimensional model requiring small account of input and computational time is acceptable. In case of reservoir or weir, however, two-dimensional flow is strong enough to consider, which requires 2-dimensional model subsequently.

It is well knows that hydraulic water quality model requires a large amount of input but produces various output data including water level, velocity, water quality, etc.

In this study, we describe the method in detail of developed 2-dimensional water quality model and present example on Boreyong reservoir as estuary dam (Park, 1997).

†Corresponding author : Department of Health & Environment of Seonam University
Tel. 82-63-620-0124, Fax. 82-63-620-0013
E-mail : pdh315@hanmail.net

Theoretical Background

Module for 2-dimensional Flow

The 2-dimensional flow model adapts Heaps model assuming depth-averaged flow. The fundamental equations are derived from continuity and momentum equations.

In this method, two equations are employed : the continuity equation derived from 3-dimensional incompressible fluid with mass conservation assumption and the 3-dimensional Reynolds equation with momentum conservation in turbulent flow.

The two equations are primarily integrated over the water depth and the term for dispersion is erased secondary, which produce next three equations

$$\frac{\partial \xi}{\partial t} + \frac{\partial (hU)}{\partial x} + \frac{\partial (hV)}{\partial y} = 0 \tag{1}$$

$$\frac{\partial U}{\partial t} + U\frac{\partial U}{\partial x} + V\frac{\partial U}{\partial y} - 2\omega(\sin\phi)V + \frac{fU\sqrt{U^2+V^2}}{8H} + g\frac{\partial \xi}{\partial x} = 0 \tag{2}$$

$$\frac{\partial V}{\partial t} + U\frac{\partial V}{\partial x} + V\frac{\partial V}{\partial y} + 2\omega(\sin\phi)U + \frac{fV\sqrt{U^2+V^2}}{8H} + g\frac{\partial \xi}{\partial y} = 0 \tag{3}$$

Where,

t : time

x : Horizontal Cartesian coordinate (x)
y : Horizontal Cartesian coordinate (y)
ξ : Water level height over the sea level
h : Averaged water depth
H : Total water depth ($h + \xi$)
g : gravity acceleration
U, V : depth-averaged current velocity in x, y direction
f : Darcy-Weisbach's bottom friction coefficient) = $8\tau_b/(\rho U^2)$
ω : angular velocity of earth rotation,
ϕ : latitude of calculation point.

In these equations applied, the momentum conservation factor is assumed to be '1' as the vertical variation of water velocity is ignorable and the vertical directional component in momentum equation is also ignored.

2-dimensional Module for Water Quality

The water quality in water body is affected by the transport/dispersion, source & sink of water pollutants which is subjected to the model development in this study.

1. Governing Equations

The 2-dimensional in this study counts the transport/dipersion of water pollutant and the spatial and time serial data for water quality, as follows

$$\frac{\partial C}{\partial t}+U\frac{\partial C}{\partial x}+V\frac{\partial C}{\partial y}=\frac{1}{H}\frac{\partial}{\partial x}\left(Hk_{11}\frac{\partial C}{\partial x}\right)+\frac{1}{H}\frac{\partial}{\partial x}\left(Hk_{12}\frac{\partial C}{\partial y}\right)+\frac{1}{H}\frac{\partial}{\partial y}\left(Hk_{12}\frac{\partial C}{\partial x}\right)+\frac{1}{H}\frac{\partial}{\partial y}\left(Hk_{22}\frac{\partial C}{\partial y}\right) \quad (4)$$

where,

x, y : Horizontal Cartesian coordinate
t : time
$H(x, y, t)$: Depth
$C(x, y, t)$: depth-averaged pollutant concentration
$U(x, y, t)$, $V(x, y, t)$: depth-averaged current velocity in x, y, direction
k_{11}, k_{12}, k_{22}: components of diffusion tensor (K)

The directional component of the dispersion coefficient k is calculated by the process from the coordinate in the streamline direction to the coordinate in the x-y cartesian.

Each component can be obtained by considering the normal component to the streamline direction i.e., flow direction, as follows.

$$\begin{aligned} k_{11} &= \varepsilon\xi\cos^2\theta + \varepsilon\eta\sin^2\theta \\ k_{12} &= (\varepsilon\xi - \varepsilon\eta)\cos\theta\sin\theta \\ k_{22} &= \varepsilon\xi\sin^2\theta + \varepsilon\eta\cos^2\theta \end{aligned} \quad (5)$$

where,

$\varepsilon\xi$, $\varepsilon\eta$: longitudinal and transverse diffusivities
θ : Th angle (positive counter-clockwise) of the ξ-axis from the x-axis

$\varepsilon\xi$ and $\varepsilon\eta$ are achieved by Eldar equation using the characteristics of mean flow

$$\begin{aligned} \varepsilon\xi &= e_L\, u*\, H \\ \varepsilon\eta &= e_T\, u*\, H \end{aligned} \quad (6)$$

In which e_L and e_T are dimensionless coefficients whose laboratory values determined by Elder are 5.93 and 0.23 respectively, and $u*$ is the local shear velocity. H is a water depth.

2. Model for Numerical Analysis

In Conventional numerical methods, numerical affenuation or irregular fluctuation are accured which applying identical numerical methods to different mathematical characteristics such as advection term and dispersion term, which is a common limitation to release. Therefore the complex flow containing the transport/dispersion of water pollutant is separated into advection and dispersion terms, Then different methods are introduced separately.

The advection-dispersion equation (4) can be splitted into two equations which considering the physical characteristics. Primarily,

$$\frac{\partial C}{\partial t}+U\frac{\partial C}{\partial x}+V\frac{\partial C}{\partial y}=0 \quad (7)$$

which is the equation for pure advection in two dimensions

$$H\frac{\partial C}{\partial t}=\frac{\partial}{\partial x}\left(Hk_{11}\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial x}\left(Hk_{12}\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial y}\left(Hk_{12}\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(Hk_{22}\frac{\partial C}{\partial y}\right) \quad (8)$$

which is the equation for pure dispersion in two dimensions.

While in equation (4) advection and dispersion are occurred simultaneously physically, in this study the advection and dispersion terms are separated to apply optimal numerical method. For the time interval Δt, the computation for the advection term in Eq. (7) is carried out firstly. then the dispersion term is calculated in turn. This procedure is commonly called by split operation.

• Numerical method for advection

There are several numerical methods for advection but the methods commonly have the problems such as unstability in computation, numerical damping, fluctuation by phase shift. In this study, up-wind scheme, which is commonly applied for the numerical analysis for advection is employed.

The up-wind scheme is the explicit finite difference scheme. When the scheme is differentiated over time Eq. (5) is obtained.

$$\frac{\partial C}{\partial t} \simeq \frac{C_i^{n+1} - C_i^n}{\Delta t} \tag{9}$$

When the differentiated over space for the flow direction, eq. (10) is obtained.

$$\frac{\partial C}{\partial x} \simeq \frac{C_i^n - C_{i-1}^n}{\Delta x} \tag{10}$$

When Crount number (Cr), defined by $u\Delta t/\Delta x$, is less than 1 and closes to 1, it lead an acceptable solution.

• Numerical method for dispersion

Eq. (8) is separated into the one dimensional dispersion equation.

$$H\frac{\partial C}{\partial t} = \frac{\partial}{\partial z}\left(Hk\frac{\partial C}{\partial z}\right) + \frac{\partial}{\partial z}\left(Hk_{12}\frac{\partial C}{\partial w}\right) \tag{11}$$

where $z = x$ or y, $w = y$ or x, $k = k_{11}$ or k_{22}

The dispersion of x-direction is computed by applying Eq. (11) along the line with constant y value. The dispersion of y-direction is computed Eq. (11) along the line with constant x value. To obtain the numerical solution of Eq. (11), the equation is differentiated using Crank-Nicolson method, and the solution is obtained using double-sweep method. the differentiated equation is as follows.

$$H_i\frac{C_i^{n+1} - C_i^n}{\Delta t} =$$
$$\frac{2\theta}{(\Delta z_{i-1} + \Delta z_i)}\left[\frac{(HK)_i^+}{\Delta z_i}(C_{i+1}^{n+1} - C_i^{n+1}) - \frac{(HK)_i^-}{\Delta z_{i-1}}(C_i^{n+1} - C_{i-1}^{n+1})\right]$$
$$+\frac{2(1-\theta)}{(\Delta z_{i-1} + \Delta z_i)}\left[\frac{(HK)_i^+}{\Delta z_i}(C_{i+1}^n - C_i^n) - \frac{(HK)_i^-}{\Delta z_{i-1}}(C_i^n - C_{i-1}^n)\right]$$
$$+\frac{2}{(\Delta z_{i-1} + \Delta z_i)}\left[\left(Hk_{12}\frac{\partial C}{\partial w}\right)_i^+ - \left(Hk_{12}\frac{\partial C}{\partial w}\right)_i^-\right] \tag{12}$$

in which,

$$H_i^+ = \frac{H_{i+1} + H_i}{2}$$

$$H_i^- = \frac{H_i + H_{i-1}}{2}$$

To the adaptation of Eq. (12) allows to manage dynamic mesh, to count the physical characteristics of advection term numerically, to pursue proper computation with acceptable error. The concentration of water pollutants in every inerts are required as the boundary condition and the

Table 1. Differential equations for water quality model

State Variables	Terms
Dissolved oxygen	$\frac{\partial O}{\partial t} = K_2(O^* - O) + (\alpha_3\mu - \alpha_4\rho)A - K_1L$ $\frac{K_4}{d} - \alpha_5\beta_1N - \alpha_6\beta_2N$
Carbonaceous BOD	$\frac{\partial L}{\partial t} = -K_1L - K_3L$
Organic Nitrogen	$\frac{\partial N_4}{\partial t} = \alpha_1\rho A - \beta_3N_4 - \alpha_4N_4$
Ammonia Nitrogen	$\frac{\partial N_1}{\partial t} = \beta_3N_4 - \beta_1N_1 + \frac{\sigma_4}{d} - F_1\alpha_1\mu A$
Nitrite Nitrogen	$\frac{\partial N_2}{\partial t} = \beta_1N_1 - \beta_2N_2$
Nitrate Nitrogen	$\frac{\partial N_3}{\partial t} = \beta_2N_2 - (1-F)\alpha_1\mu A$
Organic Phosphorus	$\frac{\partial P_1}{\partial t} = \alpha_2\rho A - \beta_4P_1 - \sigma_5P_1$
Dissolved Phosphorus	$\frac{\partial P_2}{\partial t} = \beta_4P_1 + \frac{\sigma_2}{d} - \alpha_2\mu A$
Chlorophyll_a	$\frac{\partial A}{\partial t} = \mu A + \rho A + \frac{\sigma_1}{d}A$

inner source or sink of water pollutant can be also considered.

3. Source & Sink of Water Pollutant

In the case of considering non-conservative water pollutant, following 9 state variables are considered typically. Each reaction model is refered from the water quality model for rivers QUAL2E and CE-QUAL-W2 and modified in parts.

• Numerical method for the Source & Sink term for Water Pollutant

To compute term for sink and source, Runge-kutta method is introduced. Although the source/ sink of pollutant is expressed in partial differential equation for **, It is an ordinary differential equation in time domain. the fourth order of Runge-Kutta method, which is one of most popular models, is therefore adapted. Runge-Kutta method is typically beneficial to achieve the accuracy of high order of Taylor Series without the computation of high order differential equation. there are various forms of Runge-Kutta models and the conventional method is employed in this study (Steven C. Chapra, Raynold P. Canale, 1998).

$$Y_{i+1} = Y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h \quad (13)$$

where k_1, k_2, k_3, k_4 are as follows.

$$k_1 = f'(x_i, y_i)$$

$$k_2 = f'\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h\right)$$

$$k_3 = f'\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_2 h\right)$$

$$k_4 = f'(x_i + h, y_i + k_3 h)$$

4. Flow_chart for 2-dimensional water quality module

The model set up is coded using Fortran (77) and complied using Lahey Fortran (3.0). Fig. 1 shows the flow chart for the water quality module. As shown, the computation for water quality uses the mesh grid similar to flow grid and the depth data and sets the initial concentrations. Using the outputs from the flow model, with other variable,

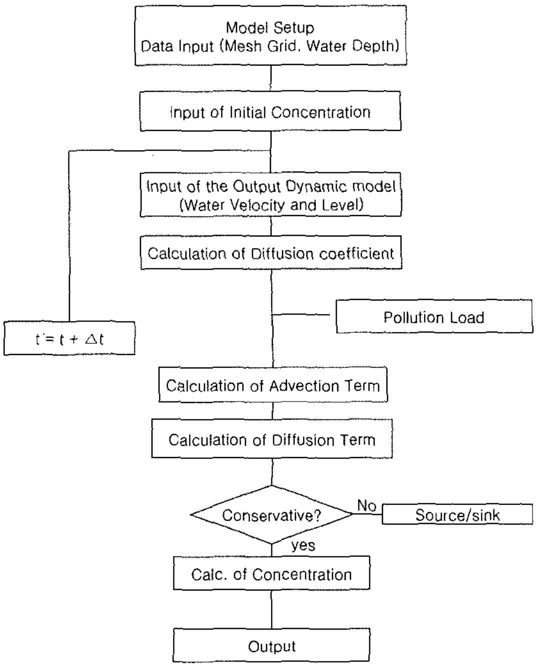

Fig. 1. Flow chart of 2-dimensional water quality module.

the advection and dispersion are computed. In case of non-conservative pollutant, the computation of source and sink is added.

Study Area

Boreyoung reservoir Basin, located in Chung

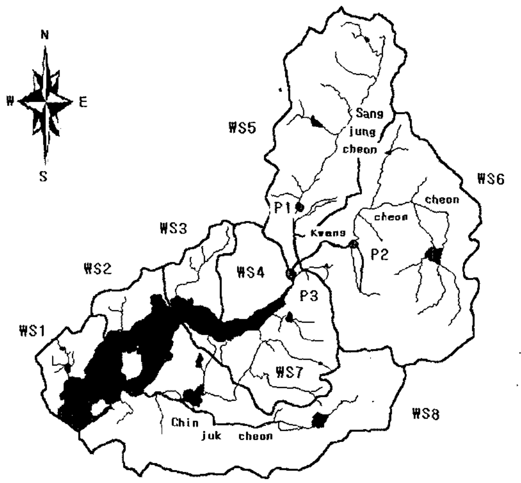

Fig. 2. Basin map of study area.

Cheong Province, is selected for this study as shown Fig. 2. The upper stream area is a typical agricultural area and the down stream area is a combined urban-agricultural area. In down-stream area there exists Boreyong Reservoir which was constructed by national project and has been in freshing. In the study area, there exist many livestock complex, but no waste water treatment plant or livestock waste water treatment pant is in operation. It in turn causes the negative effect on the water quality of the lake the large amount of water pollutant is discharged. It also implies the demand of the plan for the water quality management. As shown in Fig. 2, three streams (Sang Jung, Kwang Cheon, Jin Juk) are being flows into Boreyong reservoir.

Results and Discussion

Model Build

To simulate the water flow in the that area; Several steps are conducted as follows

① Determine the scope of computation
② Determine the size of grid
③ Input water depth
④ Define boundary condition

In this study, Base level is defined is averaged sea level.

① Determination of modeling area Boreyong Reservoir for the test area in numerical modeling

② Determination of the grid size

As the accuracy and precision of water depth have direct effect on the result of numerical model, accurate data for water depth will be used and the mesh grid with the high resolution will be generated. when the resolution of water depth is increased, however, the total amount of computation is also increased. It subsequently requires proper selection. the mesh grid in this numerical grid is consisted of 100 m-mesh grid and the target water

Table 2. Boundary and grid system of the model

Modeling Range	85 km × 39 km
No. of grid	85 × 39
Size of grid	100 m × 100 m
System od grid	cartesian coordinates
Used model	2-dimensional flow model

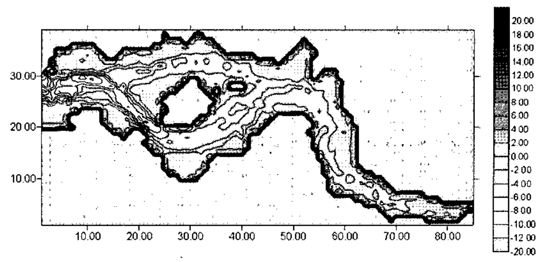

Fig. 3. Contour lines of Boryoung reservoir.

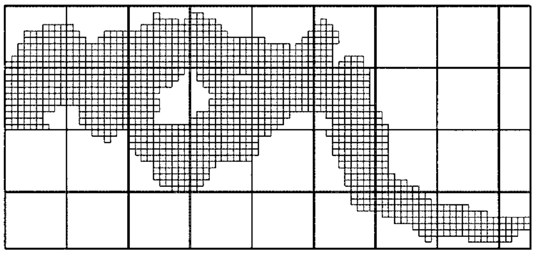

Fig. 4. Grid system of Boryoung reservoir.

body is consisted of 85 × 39 grid.

③ Input of water depth

Fig. 3 displays the contour for bottom level and Fig. 4 shows the map of mesh grid. when the regional variation in sea level is significant and occurs the hydraulic problem, modification without making any important change to hydraulic parameter such as cross_section area, etc.

④ Open Boundary Condition

The inflow from the Kwang Cheon stream is assumed to be 10 CMS. As Boreyong Reservoir does not have any significant reservation effect, the discharge rate might be the same as the inflow rate 10 CMS.

⑤ prediction test

The initial velocity are set to be "0" in all grid points and the water level are "0" m. as the numerical tests require a long-term and averaged values, it is assumed for Boreyong Reservoir to have constant average inflow. In the words, the flow for steady state condition is obtained.

Results of Model Application

The simulation for water quality is carried out using the integrated water quality model in may. 2001. As this model is able to simulating the

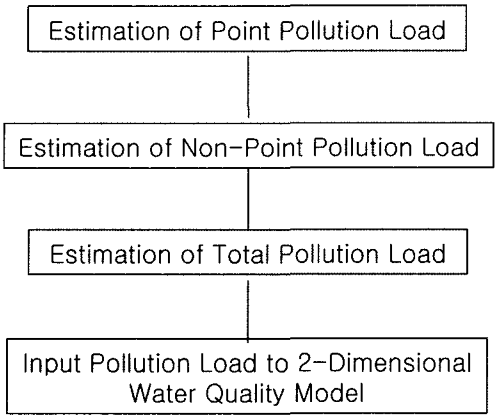

Fig. 5. Flow-chart of water quality Simulation.

variation of water quality in spatial/time-serial distribution, the water quality in Boreyong Reservoir is modeled during dry season and spatial/time-serial changes one also simulated for non-point pollution load during rainfall.

Firstly, the arrival rate is calculated based on the inflow load into Boreyong Reservoir from the pollution emission load and point pollution load is estimated. the point pollution load is used for model input after considering arrival rate. During rainfall, the results of SWMM simulation is used for model input as the non-point pollution load. In other words, utilizing the point and non-point pollution load as the input of developed water quality model, the influence of non-point pollution load can be estimated.

Fig. 6 display the hourly runoff flows and pollutant concentration in sub_basins for non-point pollution load.

Fig. 7-10 show the water velocity and concentration in reservoir after 3-8 hours from rainfall start. While the distribution of flow velocity shows a slight variation after 3 hours, the effective region is expanded after 8 hours. The distribution of BOD concentration also shows the significant impact by the non-point pollution load.

Conclusion

In this study, 2-dimensional water quality model is developed and applied and for the cases with large reservoir or estuary dam. The test area is located near Boryoung City and the water quality during rainfall is numerically simulated.

The Major findings are as follows.

1. The 2-D simulation of water flow employed Heaps model and the water quality in Boreyong Reservoir is simulated using the developed 2-dimensional water quality model.

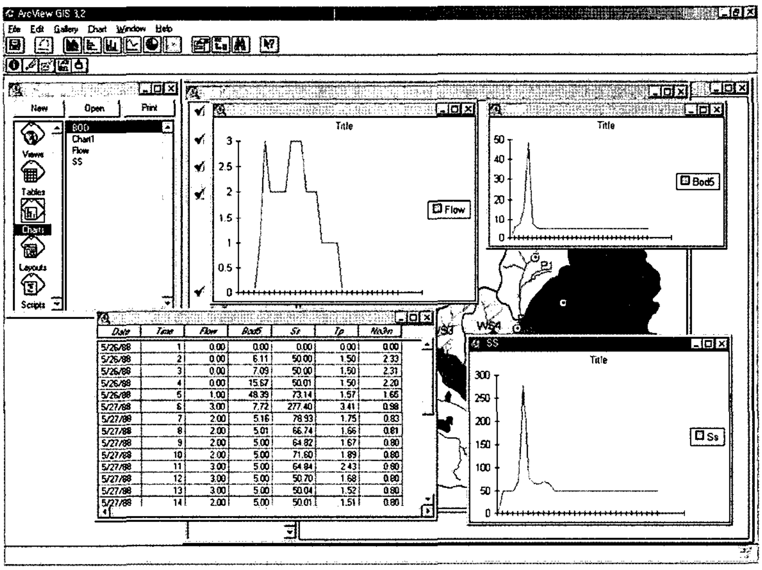

Fig. 6. Results of SWMM Simulation during rainfall event.

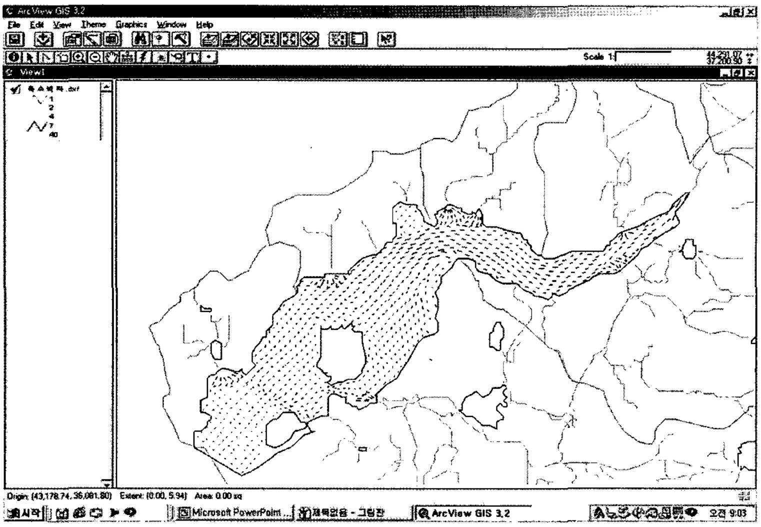

Fig. 7. Flow field during rainfall event (after 3 hours).

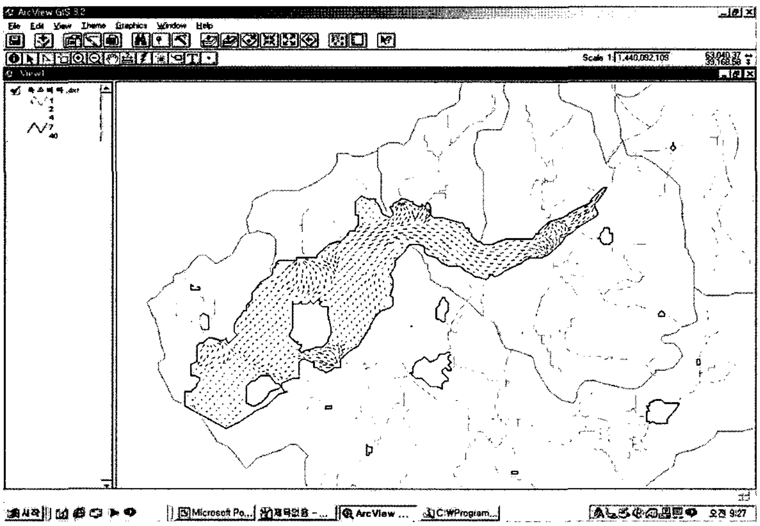

Fig. 8. Flow field during rainfall event (after 8 hours).

2. The Developed modeling system is based on a split operator technique, in which, the advection term is calculated using the upwind scheme, and the diffusion term is one- dimensionalized and calculated using Crank-Nicholson's implicit finite difference scheme to reduce the numerical errors from large time steps and variable spacings and a provide a relative simple and economic method for accurate simulation of pollutant dispersion.

3. After applying the 2-Dimensional water quality model to the Boreyong Reservoir, It is possible to simulate the effect of point and non-point pollution load simultaneously. The distribution of spatial/ time-time serial water quality is also achieved and detailed simulation for water quality is also available.

Acknowledgment

This study is supported by "Korea Science and Engineering Foundation". Therefore the writers

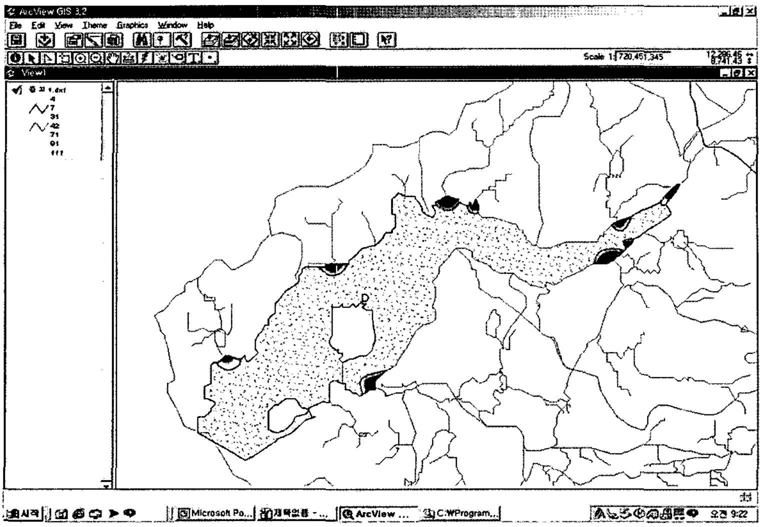

Fig. 9. BOD concentration field during rainfall event (after 3 hours).

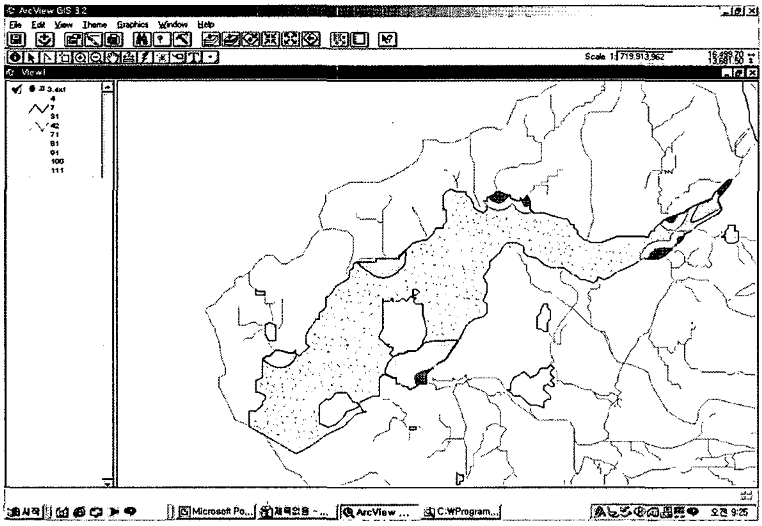

Fig. 10. BOD concentration field during rainfall event (after 8 hours).

are grateful for This support.

References

1. Park, I.B. : Numerical modeling of 2-dimensional advection and diffusion of pollutants. *Kookmin University*, **20**, 1997.
2. Lee, H.K., Paik, I.B., Oh, K.D., Paik, D.H., etc. : The study on the development of water quality models and decision support system for water quality management. *The Minister of Environment of Korea*. 1995.
3. CADLAND, Using GRID with ARC/INFO - Rev 6.1: Modeling Surface Hydrology, pp.18-1-18-23. 1993.
4. McAlister, E., Domburg, N., Edwards, T. and Ferrier, B. : Hydrological modelling of the River Ythan using ARC/INFO GRID, 1996.
5. Wurbs, R.A. : Computer models for water resources planning and management. U.S. Army Corps or Engineers, IWR Report 94-NDS-7, pp.97-112, 1994.
6. Holly, F.M., J.M. Usseglio_Pollatera, Dispersion Simulation in 2-dimensional Tidal Flow, *Journal of Hydraulic Engineering*, ASCE, **110**(7), 1984.

7. Benque, J.P., Cunge, J.A., Feuillet, J., Hauguel, A. and Holly, F.M. : New method for tidal current computation. *Journal of the Waterway, Port, Coastal and Ocean Division*, ASCE, **108**(WW3), 1983.
8. Kim, H.Y., Kim, J.Y., Hwang, D.H., Paik, D.H. and Lee, H.K. : Impact assessment of inflowing tributaries on water quality of youngsan lake WASP/EUTRO5 model. *Korean Journal of Environmental Health*, **26**(1), 15-23, 2000.
9. Hwang, K.L., Hwang, D.H., Paik, D.H. and Lee, H.K. : Study on allocation of pollution discharges by watersheds and administrative regions with pollution sources for the TMDL(Total Maximun Daily Load) in Tamjin river. *Korean Journal of Environmental Health*, **30**(5), 449-454, 2004.