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ITJ

ISSN 1812-5638

INFORMATION TECHNOLOGY JOURNAL

ANSInet
Asian Network for Scientific Information
308 Lasani Town, Sargodha Road, Faisalabad - Pakistan

Information Technology Journal 12 (20): 5424-5431, 2013
ISSN 1812-5638 / DOI: 10.3923/itj.2013.5424.5431

Simulation of Point Source Pollution Diffusion Using a Velocity Field-cellular Automata Coupled Method

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Abstract: To overcome the deficiencies of conventional diffusion algorithms based on Cellular Automata (CA), a point source diffusion algorithm that considers water flow is proposed in this study. The diffusion process has two parts: the point source pollution diffusion process and the movement of pollution driven by water flow. First, the turbulent diffusion coefficient is introduced into conventional CA algorithm based on diffusion theory and used to amend the pollutant exchange coefficient, while this paper also improves the correction coefficient based on this amended exchange coefficient, which makes the algorithm agree better with the diffusion law. Second, to overcome the deficiencies of conventional CA diffusion simulation algorithms for water flow, it proposes a method known as particle tracing that calculates the pollution in each cell based on the velocity field, which implements the pollution diffusion effect driven by the water flow. Finally, the improved algorithm was used to simulate point pollution diffusion in the Fengdu area of Chongqing city in China with good results.

Key words: Cellular automata, point source pollution, simulation, velocity field

INTRODUCTION

Point source pollution is one of the most important types of water pollution. To improve the operational efficiency of environmental protection departments and to reduce damage to the ecological environment by water pollution, it is necessary to simulate and predict the diffusion of point source pollution and provide scientific proof to regulators who engage in preventative management.

At present, the main method used to analyze water pollution diffusion is a numerical method, which must establish a mathematical model of pollution diffusion in the water, i.e., the water quality model. This method has been used successfully for analysis and simulation. Earlier water quality models focused on the construction of mathematical models based on statistics and were generally one-dimensional, such as the one-dimensional convection-dispersion model abstracted from water pollution diffusion (Van Mazijk, 2002). A multi-dimensional water quality model has been used widely by computer applications to provide an in-depth understanding of diffusion mechanisms. Giri *et al.* (2001) established a water quality model that simulated water pollution in a dynamic manne. At present, many researchers use numerical methods for point source pollution diffusion modeling and predictive analysis, while they are also combined with GIS to produce a visual tool that displays water pollution diffusion. For example, Wu *et al.* (2009) analyzed water pollution diffusion in a river using a two-dimensional (2D) numerical model combined with GIS visualization technology. The numerical accuracy is closely related to the mathematical model of water pollution diffusion but accurate mathematical models are usually very complex, which reduces the efficiency of actual calculations. Thus, it is difficult to meet the real-time requirements of point source pollution diffusion simulations based on large-scale three-dimensional water flow systems using an ordinary computer.

Cellular Automata (CA) was introduced as a new spatial analysis method in the field of GIS since1980s. CA is simple to use local features of the space field, which can simulate the evolution of complex problems, so they have attracted considerable interest from researchers. CA models are more suitable for simulating detailed physical processes compared with the water quality model (Bandman, 1999; Chopard and Droz, 2005). In addition, some researchers have used lattice gas automata models to simulate the diffusion of gases. These methods were based on statistical mechanics and could simulate fluids and gases. In general, current approaches are based on ordinary cellular evolution rules that integrate many factors into each cell and they abstract the basic data at

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a high level. Thus, the simulation results obtained using these methods are too rough for the problems of water pollution diffusion and cannot facilitate emergency decision-making by administrators. Thus, the problem of using CA to simulate and predict the diffusion of water pollution in complex water bodies remains difficult.

After point source pollution events, the pollutants float on the water surface and then spread quickly via diffusion, evaporation, dissolution, light degradation, biological degradation, absorption migration, transformation and other processes. The diffusion of pollutants in water has spatiotemporal features (Wang *et al*., 2009), so based on the traditional methods used to calculate differential or partial differential equations, this study considers the spatiotemporal distribution of water pollutants based on diffusion-migration, which combine with factors, such as the flow velocity in the water pollution diffusion field and the wind field and constructs a water pollution diffusion model with an improved CA method coupled with the flow velocity.

2D POINT POLLUTION DIFFUSION SIMULATION BASED ON TRADITIONAL CA

The theory of CA was proposed by Von Neumann and Burks (1966). In this model, space is segmented into a number of units, i.e., CA. Each cell or lattice is assigned a discrete numerical value that represents the state of the point. Time is discrete in this method, so each cell state is updated at the same time during each iteration. The cellular status is updated based on local rules and the next state of each cell depends only on the cell itself and its neighbors. There have been many studies of point source pollution diffusion algorithms based on CA. Karafyllidis (1997) proposed a general algorithm for point source pollution diffusion in calm water conditions and the main concepts of this method are described as follows.

The cellular neighborhood often uses a Moore model, where the central cell has eight neighbors, i.e., up, down, left, right, upper left, lower left, upper right and lower right, which including the cell itself makes a total of nine. Thus, the local evolution rule can be calculated as:

$$N_{i,j}^{t+1} = N_{i,j}^{t} + m\left[\left(N_{i,j+1}^{t} - N_{i,j}^{t}\right) + \left(N_{i+1,j}^{t} - N_{i,j}^{t}\right) + \left(N_{i,j-1}^{t} - N_{i,j}^{t}\right) + \left(N_{i-1,j}^{t} - N_{i,j}^{t}\right)\right] + md\left[\left(N_{i+1,j+1}^{t} - N_{i,j}^{t}\right) + \left(N_{i+1,j-1}^{t} - N_{i,j}^{t}\right) + \left(N_{i-1,j-1}^{t} - N_{i,j}^{t}\right) + \left(N_{i-1,j+1}^{t} - N_{i,j}^{t}\right)\right] \quad (1)$$

where, $N_{i,j}^{t}$ is the value of the cellular pollutant concentration of cell (i, j) in a 2D grid; m is one of four directions (i.e., north, south, east and west) for the pollutant transfer coefficient, which is related to the water depth, type of pollutant and the cellular step; d is one of the four oblique directions (northeast, southeast, southwest and northwest) for the correction coefficient. Equation 1 shows that the value of the central cell at the next step is the sum of the combined effect of the values of the eight cell directions and the current value of the central cell. In this method, lets d = 0.16 and m = 0.084 and the shape of diffusion phenomenon can be viewed as a circle. The aim of the algorithm is to simulate the shape of the point pollution diffusion, so it does not have a real physical meaning. Thus, the quantitative capacity of the algorithm is insufficient and it is more suitable for simulating the diffusion of insoluble pollutants. This method can only simulate the approximate shape of the diffusion of pollution.

Karafyllidis (1997) also considered the impact of water flow on diffusion and proposed diffusion rules with water flow, as follows:

$$N_{i,j}^{t+1} = N_{i,j}^{t} + m\left[(1 + C_{i,j}^{t})N_{i,j+1}^{t} - N_{i,j}^{t}\right] \quad (2)$$

In contrast to Eq. 1, this equation includes a water flow coefficient $C_{i,j}$, where $C_{i,j}^{t} = V_{i,j}^{t}/V_{max}$, $V_{i,j}^{t}$ is the flow velocity in cell (i, j) at time step t and N_{max} is the maximum flow velocity ever observed. This algorithm standardizes the migration of pollutants with flow using a coefficient but it does not reflect the pollution diffusion mechanism, which is driven by water flow, so the accuracy is poor.

POINT SOURCE POLLUTION DIFFUSION BASED ON COUPLED WITH THE FLOW FIELD

The water flow changes constantly in actual water systems. Therefore, this paper aims to establish an improved CA diffusion algorithm where the migration of pollutants is driven by a flow field. This method considers the effect of the flow field on the dispersion of the point source pollutant.

At the micro-level, the diffusion flux is equal to the sum of transport and diffusion transport, so the process used to model pollution diffusion in water has two parts, as shown in Figure 1. The first part is the diffusion of the point source pollution itself and the second part is the migration of the pollutant with the flow field. This calculation is repeated until the end condition is satisfied. Each part of this procedure is represented using a grid and the pollutant concentration in each cell needs to be calculated in the simulated region of the grid. The methods used to calculate the two parts are as follows.

Improvement of the transfer coefficient m and the correction coefficient d: Our CA algorithm is based on a

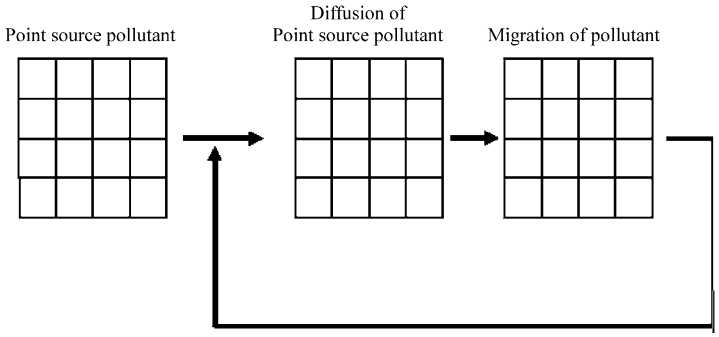

Fig. 1: Calculation process during each step

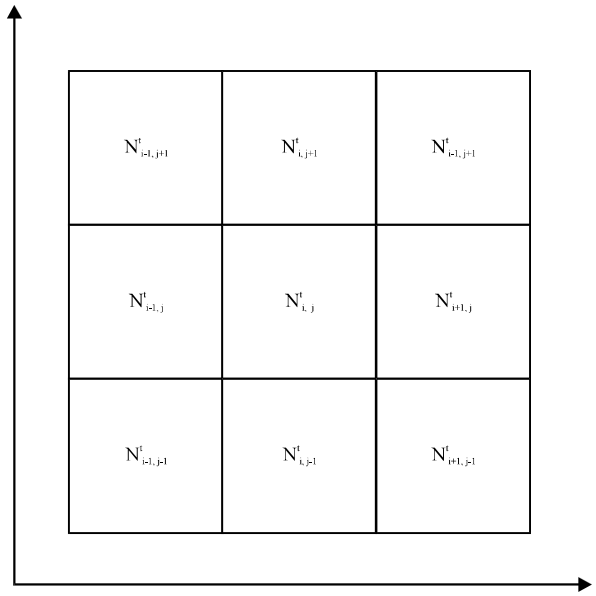

Fig. 2: Moore neighborhood model

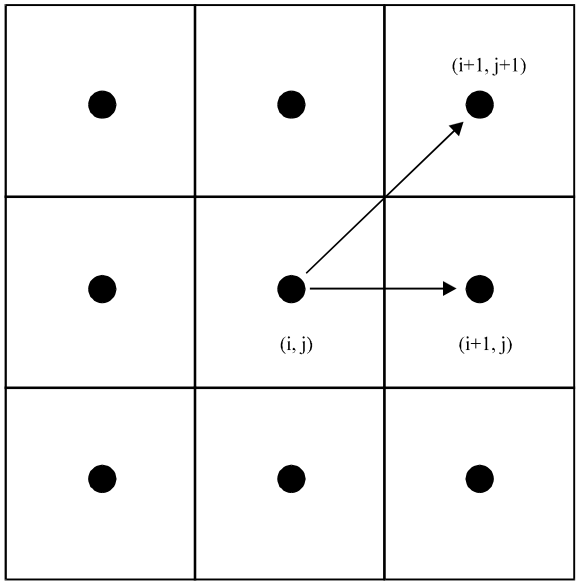

Fig. 3: Center point of CA

Moore neighborhood type, as shown in Fig. 2. During every operation, each cell is related only to the neighboring cells in eight directions. For each cell, we assume that the concentration value of the central point of the cell approximately represents the concentration of the entire cell, as shown in Fig. 3.

In a river, because of the difference in scale, turbulent spread is the main cause of pollutant migration, which often excludes the role of molecular diffusion. In the first step, water flow movement is not considered and turbulent flow in the water is regarded as homogeneous isotropic turbulence, so the horizontal and vertical turbulent diffusion coefficients are both E. Vertical refers to the flow direction of the river, whereas horizontal refers to a direction perpendicular to the direction of flow. The contaminant concentration per unit time in a certain direction through a certain area in calm water conditions is proportional to the concentration gradient in this direction, as follows:

$$q = -E\frac{\partial N}{\partial x} \tag{3}$$

where, q is the pollutant quality per unit time through unit area, N is the concentration of the pollutant and x is the concentration diffusion direction. According to Eq. 1, we can see that the rule for the spread of pollutants from the center cell to the right (which is the same for diffusion to the west, south and north) is:

$$q_N = m\left(N_{i+1,j} - N_{i,j}\right) = m\Delta N \tag{4}$$

where, q_N is the concentration at the interface between two cells, which is the pollutant concentration exchanged per unit time (Fig. 4).

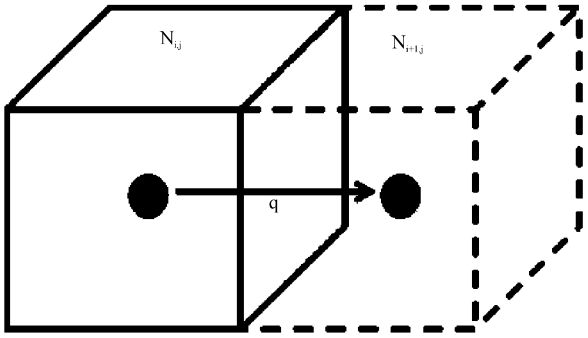

Fig. 4: Exchange of pollutants between two cells

Assuming that the cell length is a, the relation between q and q_N is q_N = (q*exchange area of the cellular interface)/volume of pollutants. Based on Eq. 3 and 4, m can be described as Eq. 5:

$$m = E/a^2 \quad (5)$$

In Eq. 5, E is the turbulent diffusion coefficient, the value of which varies with different water flows and it can be obtained based on empirical knowledge. After E has been determined, the value of the exchange coefficient m can be obtained. Thus, the coefficient of the cellular diffusion rules is associated with the actual pollutant diffusion pattern.

In addition, Eq. 2 shows that the contaminant concentration exchanged between two cells per unit time is inversely proportional to the distance between the two center points of the cells. Thus, this rule can be used to determine the coefficient d in Eq. 1 where the value is equal to the distance between a vertical or horizontal cell and the central cell divided by the distance between a diagonal cell and a central cell in the Moore neighborhood: $d = 1/\sqrt{2} = 0.707$.

The improved static water point source pollutant diffusion rules based on CA can be described as follows:

$$N_{i,j}^{t+1} = kN_{i,j}^{t} + \frac{E}{a^2}\left[\left(N_{i,j+1}^{t} - N_{i,j}^{t}\right) + \left(N_{i+1,j}^{t} - N_{i,j}^{t}\right) + \left(N_{i,j-1}^{t} - N_{i,j}^{t}\right) + \left(N_{i-1,j}^{t} - N_{i,j}^{t}\right)\right]$$
$$+0.707 \cdot \frac{E}{a^2}\left[\left(N_{i+1,j+1}^{t} - N_{i,j}^{t}\right) + \left(N_{i+1,j-1}^{t} - N_{i,j}^{t}\right) + \left(N_{i-1,j-1}^{t} - N_{i,j}^{t}\right) + \left(N_{i-1,j+1}^{t} - N_{i,j}^{t}\right)\right] \quad (6)$$

where, k is the self-purification coefficient, which is used to represent different types of pollutants, while it also can be used to express the soluble pollutant sedimentation, etc. and it is related to factors such as the pollutant type, temperature and water depth.

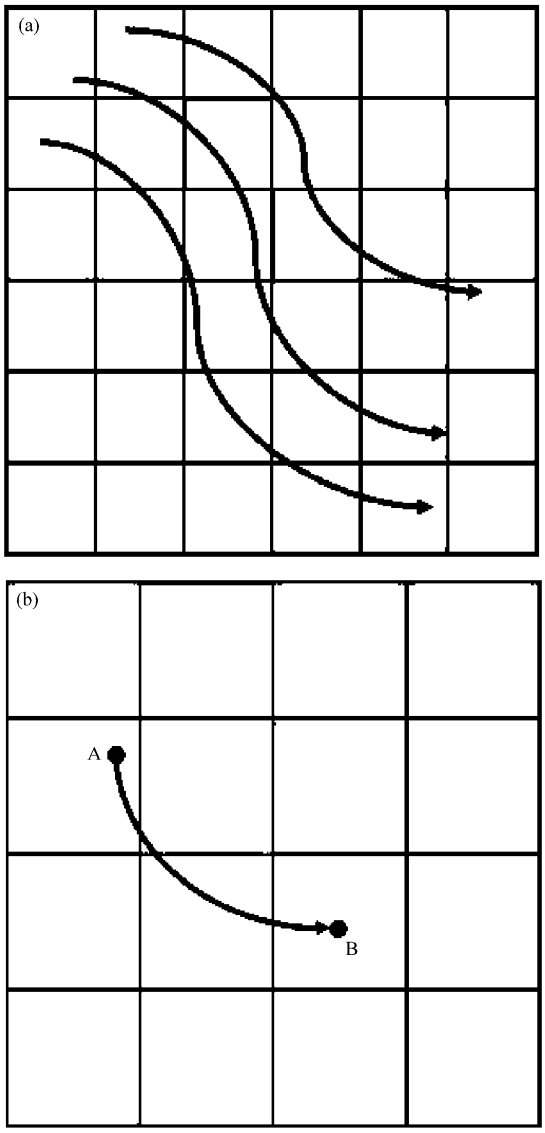

Fig. 5(a-b): Tracing the movements of particles in the velocity field, (a) Velocity field of water and (b) Movement of a particle

Pollution diffusion with the water flow: To simulate the contaminant flow motion, it is necessary to determine the movement trajectory and the concentration of pollutant. To calculate the concentration of each cell in the center after dt (the time per iteration), we propose a method called particle tracking that traces the pollutant diffusion path with the water flow.

If it assumes that each cell center has a particle, the trajectories of the particles can be determined using flow field information, as shown in Fig. 5a. In Fig. 5b, point B is the center of the cell where A flows after dt time. As mentioned above, the cellular concentration at the center

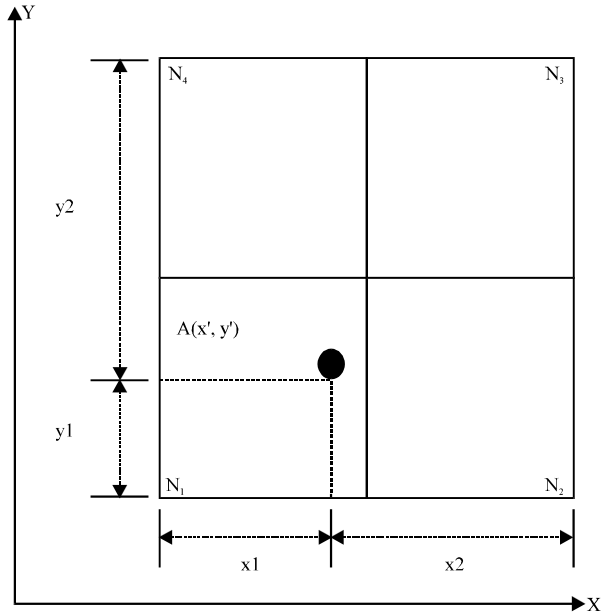

Fig. 6: Centroid interpolation method

is used to represent the overall cell concentration. Thus, the concentration at point B is the current cell that needs to be calculated.

The concentration at point B can be calculated using the backstepping method. As shown in Fig. 5b, before time step dt, when the water is not flowing, the pollutant is at point A and its concentration is the last calculated value by CA. Point A flows to point B after time dt. If dt is not a long time, the pollutant concentration at point B can be deemed to equal to point A approximately. Point A is not in the cell center, which means that it needs to calculate the concentration value at point A based on the neighboring four points using an interpolation method. The centroid interpolation method can be used for this 2D interpolation and the algorithm is as follows.

If the neighboring four nodes of the interpolated point A (x′, y′) are N_1, N_2, N_3 and N_4 and their concentration values are N_1 (x_i, y_j), N_2 (x_{i+1}, y_j), N_3 (x_{i+1}, y_{j+1}) and N_4 (x_i, y_{j+1}), as shown in Fig. 6, the increments of the four nodes in the x and y directions are (x = x1+x2) (y = y1+y2), where x1 and x2 are around the distance of x′ in the x direction and y1 and y2 are around the distance of y′ in the y direction. Based on the centroid principle, we assume that the weighting factors that define (x', y') for the four nodes are w_1, w_2, w_3 and w_4, which means that the 2D centroid interpolation formula can be written as Eq. 7:

$$A(x', y') = \frac{1}{\Delta x \Delta y}(x_2 y_2 \cdot N_1 + x_1 y_2 \cdot N_2 + x_1 y_1 \cdot N_3 + x_2 y_1 \cdot N_4) \quad (7)$$

Thus, we have established a point source water pollution diffusion algorithm coupled to a CA with flow movement but the simulation environment is limited to a specific water area such as rivers and lakes. Therefore, we still need to establish a suitable boundary condition.

Boundary treatment: If we assume that the simulation area is a river, the river flow velocity is relatively slower at the bank of the river than at the center of the river. In addition, it only has a longitudinal velocity component and not a horizontal velocity component on the boundary. Some pollutants may be accumulated because of the slow diffusion on the boundary. We can set the pollutant self-purification coefficient k depending on the actual situation to obtain a realistic effect.

However, the pollutant diffusion only occurs on one side when the pollution source is at the bank of the river, which means that the rules are slightly different. Thus, we need to process the CA separately along the bank of the river and we can use a one-dimensional cellular method to compute these types of grids.

Algorithm flow description: The basic implementation steps for the point source pollutant diffusion model established in the present study are as follows.

- Determine the simulation parameters and the mesh to simulate the river area. The main parameters required for the CA simulation are the time interval, cellular size, average depth of the river, etc. Draw an outline of the river using the river's DEM (Digital Elevation Model) data and remote sensing data
- Determine the location of the point source pollution and the type of pollutant. Depending on the environmental factors, calculate the self-purification coefficient of the pollutant. The water temperature data can be measured at different points and interpolated to satisfy the mesh grids. The local turbulent diffusion coefficient can be determined based on published data
- Collect information related to the flow field in the simulation area. The flow field was set as a uniform flow in the present study because of the limited data available. Next, we calculate the average flow velocity in the local area. An accurate velocity field can be obtained by solving the hydrodynamic equation for complex water systems
- Finally, we calculate the pollutant concentration in each cell at each time step. We calculate the color of each cell according to the layering principle set

EXAMPLES AND DISCUSSION

Study area: A Chemical Oxygen Demand (COD) pollution diffusion outlet at Xingyi Bridge in Fengdu county of Chongqing city was selected to test a non-point source pollutant diffusion simulation based on our method. First, the river was meshed using a grid, which represented the cells and a 2D cellular space was constructed. We assumed that X was the direction of flow. Therefore, the coordinate system XOY was established as shown in Fig. 7.

The simulation parameters were as follows: cellular edge length = 5 m, water level = 175 m, self-purification coefficient of the COD in water = 0.04 and the average flow rate was calculated using the Chezy formula. To establish a uniform flow pattern in the flow field, the computational time step Δt = 60 s. We simulated two types of pollution emissions: a sewage outlet in the middle of the river channel and another outlet on the bank of the river.

RESULTS AND DISCUSSION

Fig. 8a and 11 show the water pollution diffusion events where the outlet positions were in the middle and on the bank of the river channel, respectively, where the released COD was 1.5 tons.

Figure 8a shows the simulation of the drainage outlet in the center of the river and Fig. 8b shows the COD distribution curve in the diffusion direction, which agree with Dong's numerical solution of the diffusion equation flow (Dong, 2008).

Figure 9 shows that the contaminated zone has two characteristics. First, the contaminated zone extended

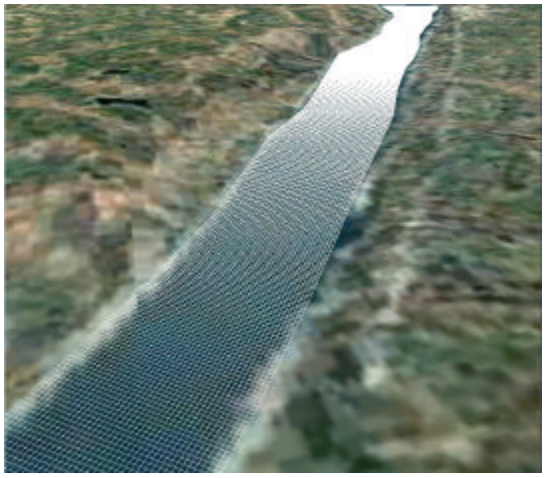

Fig. 7: Computational grid on the river

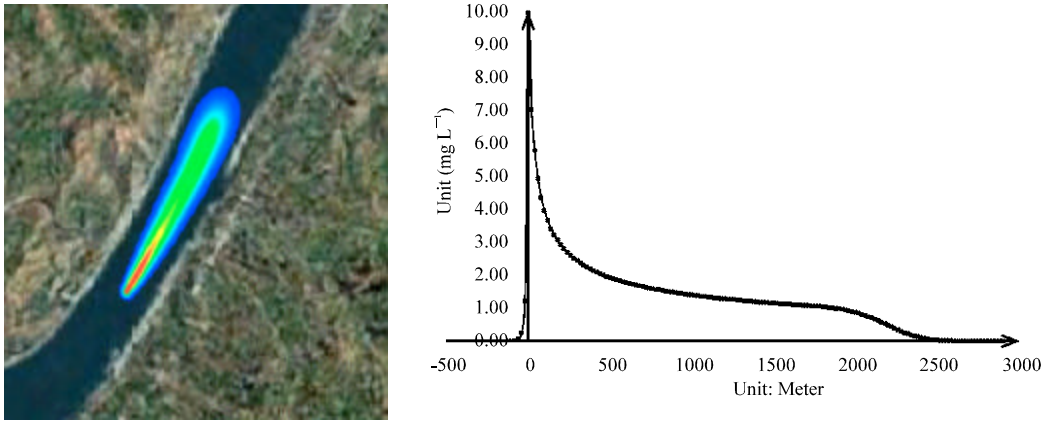

Fig. 8(a-b): Simulation for a sewage outfall in a river, (a) Simulation results within 2 h and (b) COD curve along the river

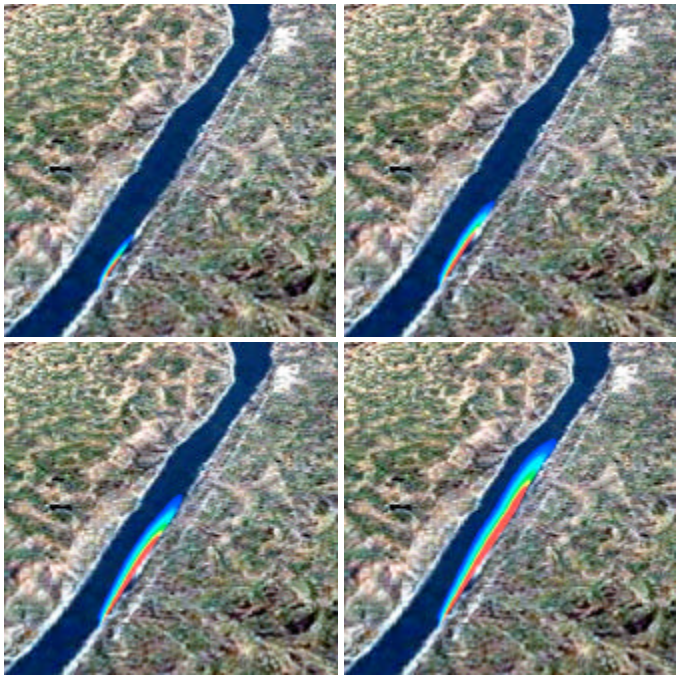

Fig. 9(a-d): Simulation for sewage outfall on the river bank, (a) Simulation results at 0.5 h, (b) Simulation results at 1 h, (c) Simulation results at 2 h and (d) Simulation results at 5 h

gradually in the flow direction and the concentration declined with distance from the pollutant outlet in a longitudinal direction. Second, the concentration declined with distance from the contaminant source in the transverse direction from the river bank. These results were consistent with the actual situation, which means that this method is also suitable for simulating pollution diffusion where the drainage outlet is on the bank of a river.

CONCLUSIONS

In this study, we established an improved point source water pollution diffusion model, which was coupled to CA with water flow information. The three main advantages of this approach were as follows. (1) We improved the transfer coefficient m and the correction coefficient d for a traditional point source diffusion algorithm based on CA by introducing a turbulent diffusion coefficient, which improved the numerical accuracy of the CA method and allowed the CA method to simulate the actual situation in a quantitative manner. (2) We introduced flow field information into the CA model, which allowed the cell pollution diffusion model to be applied to different waters, while the precision of the improved CA model was higher. (3) Instead of using conventional partial differential equations, we used a rapid algorithm based on CA with real-time properties to facilitate the large-scale 3D visual simulation of point source pollution events.

The model still has some limitations. First, actual river flows are very complex (such as larger rapids) and our model is not suitable for extremely complex flow field areas. Second, the concentration results calculated using our model still differed from the actual measured values. Therefore, we need to establish a more detailed model based on the actual data. In addition, we developed a 2D diffusion model that did not consider the diffusion of pollutants in a vertical direction. These significant points will be addressed in our future research. The rules used by the CA are vital for simulating important physical processes; hence, new CA rules will be required to simulate more complex natural phenomena. For some problems, however, there is no perfect rule in CA simulations. Thus, it takes a long time to explore the best way to simulate real phenomena using CA methods.

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