Numerical criteria for calculating the density diffusion in a water reservoir

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Abstract

In an earlier study, an attempt was made to ameliorate the concentration of oxygen in the lower layer of a reservoir by using a machine that supplies dissolved oxygen (DO). Field studies in a few water reservoirs have led to reports of a phenomenon in which the distance reached by the DO-rich water was more than 300 m (metres) in spite of the very low velocity of the water flow. In order to represent this phenomenon numerically, we proposed a velocity increase caused by the liquid density ρ, the gravity acceleration g and the time increment Δt. In this paper, we refer to call the velocity increase as the density diffusion, since the velocity increase seems to allow the area of DO diffusion to increase in the vertical direction. We would like to investigate the numerical criteria for calculating the density diffusion in a water reservoir using two-dimensional convective diffusion equations. Using the signs of the space division h (=Δs), the time increment k (=Δt), the diffusion parameter Γ (= D*k/(h)^2), and the Courant number C_r (=V*k/h), we discuss the order estimate for calculating the density diffusion.

Keywords: numerical criteria, density diffusion, meshless method, boundary element method, concentration in water reservoirs, observed concentration distribution in model simulation of water reservoir.

1 Introduction

When the DO concentration equals 100 mg/L (milligrams per litre) the liquid density ρ becomes 1.0001 Kg/L (kilograms per litre). To estimate the liquid density ρ of 1.0001 Kg/L in the numerical analysis, it is necessary to ensure that

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the space division h is less than $(0.0001)^{1/3}$ (=0.046) m in the calculation by using the method of the order of three-degree accuracy. If the order of two-degree accuracy is used, the space division h becomes less than $(0.0001)^{1/2}$ (=0.01) m. When diffusion parameter Γ, which is less than 0.288 in the calculation using the finite difference method (FDM), satisfies the order of four-degree accuracy ($O(h^4)$), the FDM can yield very accurate and convergent solutions when analysing the two-dimensional diffusion equation. To calculate the convection term, we use the FDM called the UTOPIA scheme or the QUICK scheme, which satisfies the order of three-degree accuracy ($O(h^3)$) (Leonard [2]). With respect to analysing the DO concentration by using the two-dimensional convective diffusion equation in the problem described above, we combine the FDM of the order of four-degree accuracy ($O(h^4)$) and the UTOPIA scheme or the QUICK scheme of the order of three-degree accuracy ($O(h^3)$). When the combined method above is adopted, the space division h should be less than $0.0001^{1/3}$ (=0.046) m for the estimation of the liquid density ρ of 1.0001 Kg/L. Next, we tried to upgrade the order of the accuracy of the meshless method, the BEM, and the finite element method (FEM). The upgrade was performed by introducing the radial basis functions of the Gaussians or the multiquadric to the meshless method, the special fundamental solution to the BEM, and the upwind shape function to the FEM. The newly developed methods, the meshless methods, the BEM, and the FEM, were tested to analyse the problem described above, and the order of the accuracy of these methods was analysed numerically. The calculated solutions obtained by using these methods were compared with the observed results in our model simulation, and the effectiveness and accuracy of the alternative numerical methods were estimated.

2 Governing equations

Convective-diffusion Equation (1) governs the diffusion of the concentration of oxygen in a water reservoir in the vertical (x_1, x_2) plane, as illustrated in Fig. 1,

$$C_{,t} + u_1 \cdot C_{,1} + u'_2 \cdot C_{,2} - D_1 \cdot C_{,11} - D_2 \cdot C_{,22} = 0 \qquad (1)$$

where C is the concentration of dissolved oxygen (DO), $C_{,t}$ is the time derivative of C, u_1 and u'_2 are the velocities of the x_1 and x_2 directions, respectively, and D_1 and D_2 are the diffusion coefficients of the x_1 and x_2 directions, respectively. Here, $C_{,1}$ and $C_{,2}$ describe the derivatives of C differentiated with respect to x_1 and x_2, respectively, and $C_{,11}$ and $C_{,22}$ are the derivatives of C differentiated twice with respect to x_1 and x_2, respectively. The velocity u'_2, which is shown in the above Equation (1), is defined as written in Equation (2),

$${}_{t+\Delta t}u'_2 = {}_t u_2 + (1 - \rho_{DO} / \rho_0)\rho g \Delta t = {}_t u_2 + \omega g \Delta t \quad \text{in the finite difference scheme} \qquad (2)$$

where ${}_{t+\Delta t}u'_2$ and ${}_{t}u_2$ are the velocities at time (t+Δt) and time (t) in the vertical direction, respectively. The second term (ωgΔt) of the right-hand side of Equation (2) means that the DO concentration increases the velocity of the vertical direction, and ω describes the density of the liquid that dissolves DO. Here, the velocity increase is caused by the liquid density ρ, the gravity acceleration g, and the time increment Δt. We refer to the velocity increase as the density diffusion, since the velocity increase seems to allow the area of DO diffusion to increase in the vertical direction, as described above, and expect that the velocity increase in the convective diffusion can be used as a device or evidence to explain the phenomenon in which the distance reached by the DO-rich water was more than 300 metres in spite of the very low velocity of the water flow Here, the density ρ is connected to the DO concentration C, as written in Equation (3), where ρ_0 and ρ_{DO} describe the densities of pure water and dissolved oxygen, respectively.

$$\rho = \rho_0 + C \cdot 10^{-6}(1 - \rho_{DO}/\rho_0) \qquad (3)$$

3 Numerical methods for calculating the density diffusion

We applied the meshless method, the FDM, the FEM and the BEM to analyse the density diffusion in the unsteady state in a water area, as shown in Fig. 1.

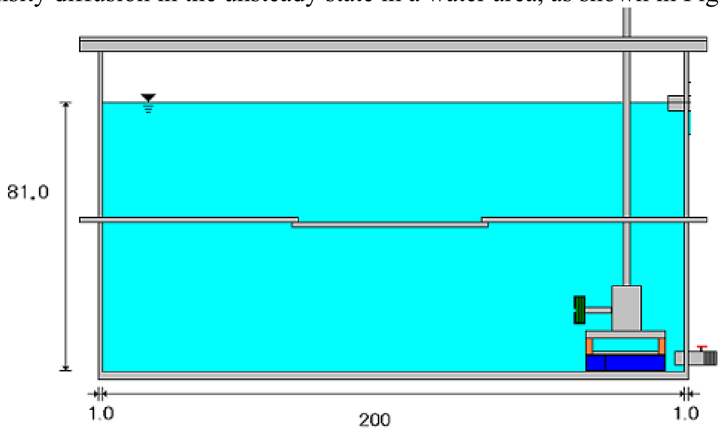

Figure 1: Analytical domain and a DO-supplying machine in a constructed model of a water reservoir.

3.1 Meshless method formulation for concentration analysis

The concentration in the steady state is expressed as Equation (4) with Equation (5) (Sakamoto et al. [1]),

$$C = \gamma_j X j \;\;,\;\; Xj = (r^2+c^2)^{-1/2} \;\;\text{or}\;\; Xj = \exp(-c\, r^2) \qquad (4)$$

$$\left\{\left(\underline{u}_1 \frac{\partial X_j}{\partial x_1} + \underline{u}_2 \frac{\partial X_j}{\partial x_2}\right) - (D_1 \frac{\partial^2 X_j}{\partial x_1{}^2} + D_2 \frac{\partial^2 X_j}{\partial x_2{}^2})\right\}\gamma_j = 0 \tag{5}$$

where r equals $\{(x-x_j)+(y-y_j)\}^{1/2}$ and c is the constant. The transient convective-diffusion equation is then rewritten as follows

$$C_{,t} + L(C) = 0 \tag{6}$$

where $C_{,t}$ is the time derivative of C and L(C) has the terms of convection and diffusion in the steady state. Applying the finite difference scheme, Equation (6) yields

$$(C^{t+\Delta t} - C^t)/\Delta t + \{L^{t+\Delta t}(C) + L^t(C)\}/2 = 0 \tag{7}$$

$$C^{t+\Delta t} + L^{t+\Delta t}(C)\cdot\Delta t/2 = C^t - L^t(C)\cdot\Delta t/2 \tag{8}$$

where $C^{t+\Delta t}$ and C^t are the concentrations at time (t+Δt) and time (t), respectively, and $L^{t+\Delta t}$ and L^t are the terms of convection and diffusion at time (t+Δt) and time(t), respectively. Finally, using Equations (3), (4), and (8), the meshless method can be used to analyse the DO concentration in the unsteady state using the global expansion function Xj (= $(r^2+c^2)^{-1/2}$ or $\exp(-c\ r^2)$) of the mesh-free RBF collocation method (Divo et al. [3]) or the radial basis functions of the Gaussians (Powell [4]).

3.2 Finite difference method for convective-diffusion analysis

To analyse the DO concentration by using the two-dimensional convective - diffusion equation, we combine the finite difference scheme of the order of four-degree accuracy ($O(h^4)$) for the diffusion terms and the UTOPIA scheme of the order of three-degree accuracy ($O(h^3)$) for the convective terms (Leonard [2]). The weighted finite difference method (WFDM) (Kanoh et al. [5]) is also applied to convective-diffusion analysis.

3.3 Finite element method for convective-diffusion analysis

The upwind shape function (Kanoh and Kuroki [6]) and the ordinary shape function are tested to analyse the two-dimensional convective-diffusion problem using the FEM. The upwind finite element formulation is expected to yield a high order of accuracy to the computation of the problem, since the upwind weights of the exponential function give an exact solution to the one-dimensional convective -diffusion equation (Kanoh and Kuroki [6]). With respect to the analysis of the one-dimensional convective-diffusion equation, we propose that the analysis of the two-dimensional density diffusion be calculated by using the one-dimensional convective-diffusion analysis twice. The pure diffusion analysis can be perfectly calculated using the 7,500 elements (h=0.011m) with the ordinary shape function.

3.4 Boundary conditions and boundary discretisation

Both the boundary conditions and the boundary discretisation for the flow and concentration analyses have been previously proposed for the meshless method, the BEM, the FEM, the FDM, and the WFDM (Sakamoto et al. [1]).

4 Model simulation

We introduced a concept, described in the next subsection, in the simulation model constructed in our laboratory and obtained some observed velocity vectors and the distributions of the DO concentration in the model. In reference to the observed results, we tried to obtain some evidence to explain the phenomena that the distance reached by the DO-rich water was more than 300 metres in a reservoir in spite of the small velocity of the water flowing out. For this purpose, it was necessary to reproduce, in our model simulation, the density flow and convective diffusion of the DO concentration in the lower layer of a water reservoir at a depth of about 50 metres.

4.1 Simulation technique in the model

The concept introduced in our simulation model is described as follows: the density difference among 7 mg/L, 30 mg/L, and 100 mg/L in the DO concentration was changed to the density difference of the water temperature, since it was very difficult to make up the high concentration of DO of 100 mg/L in our model simulation at a depth of about 1.0 metres. Referring to Table 1, the density difference between 7 mg/L and 30 mg/L in DO was equal to the difference of the water temperature between 15.00°C and 14.87°C. Furthermore, the density difference between 7 mg/L and 100 mg/L in DO was equal to the difference of the water temperature between 15.00°C and 14.55°C. We iced the water that flowed out of the tank of the model and could easily control the difference of the water temperature among 15.00°C, 14.87°C, and 14.55°C. In this paper, the analogy between the differences in the water temperature and the DO concentration was proved by referring to the concentration distribution in the reservoir model visualised using a pigment and a VTR. The demonstration procedure is described as follows. First, we flowed out iced water at 14.87°C into water at 15.00°C with the same DO concentration. Secondly, we flowed out water with DO of 30 mg/L into water with DO of 7 mg/L with the same water temperature. Thirdly, we compared the VTR pictures of the movement of the area of the concentration distribution of both the differences of the water temperature and the differences of the DO concentration and observed that the VTR pictures of both movements were almost the same at every second. We consider that the analogy between the differences in the water temperature and the DO concentration can reproduce the horizontal direction of water flow and the convective diffusion of the DO of the water reservoir at a depth of about 50 metres in our model simulation. Here, 5 Kg/cm^2 (kilogram per square

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Table 1: Density difference between 100 mg/L and 30 mg/L in DO and that of the water temperature among 15.00, 14.87, and 14.55 (°C).

Place / Value	B water reservoir (waterdepth:50m)	Our model simulation (water depth:1m)
Maximum DO value (mg/L)	100	30
Water head (Kg/cm^2)	5.0	0.1
Value of ρ (using Equation (3): at 15°C)	0.999127+0.0001	0.999127+0.00003
Water temperature that corresponds to the above value of ρ (°C)	14.55 (=15.0-0.45)	14.87 (=15.0-0.13)

centimetre) corresponds to 0.5 MPa (megapascal) in the international system of units (SI).

5 Results and discussion

As described above, we introduced a concept in the simulation model constructed in our laboratory and were able to observe some velocity vectors and obtain the distributions of the DO concentration in the model. In reference to the observed results, we tried to obtain some evidence to explain the phenomena that the distance reached by the DO-rich water was more than 300 metres in a reservoir in spite of the small velocity of the water flowing out. The numerical results of the meshless method, the BEM, the FEM, and the WFDM are also discussed in this section in order to investigate the numerical criteria for calculating the density diffusion in a water reservoir using two-dimensional convective diffusion equations.

5.1 Observed values in a model around a DO-supplying machine

5.1.1 Flow velocity in a model

Figure 2(a) is an illustration of the velocity vectors of the temperature difference, -0.1, caused by a DO-supplying machine in a reservoir model visualised using a pigment (methylene blue), aluminium flakes, a strobe light, and a digital VTR. Figure 2(b) shows the velocity vectors of the DO concentration difference, 23 mg/L, in the reservoir model. We consider that the analogy between the differences of the water temperature and the DO concentration can be proved by using the observed velocity vectors, since both profiles of Fig. 2(a) and Fig. 2(b) seemed almost identical.

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5.1.2 Concentration distribution of DO in a model

Figure 3 is an illustration of the concentration distribution of the temperature difference, -0.1, caused by a DO-supplying machine in a reservoir model visualised using a pigment (methylene blue) and a VTR. We consider that the analogy between the differences of the water temperature and the DO concentration can also be proved by using the observed concentration distribution, since both profiles of the temperature difference (Fig. 3) and the DO-concentration difference seemed almost identical (the figure to illustrate the concentration distribution of the DO-concentration difference, 23 mg/L, in the reservoir model was omitted).

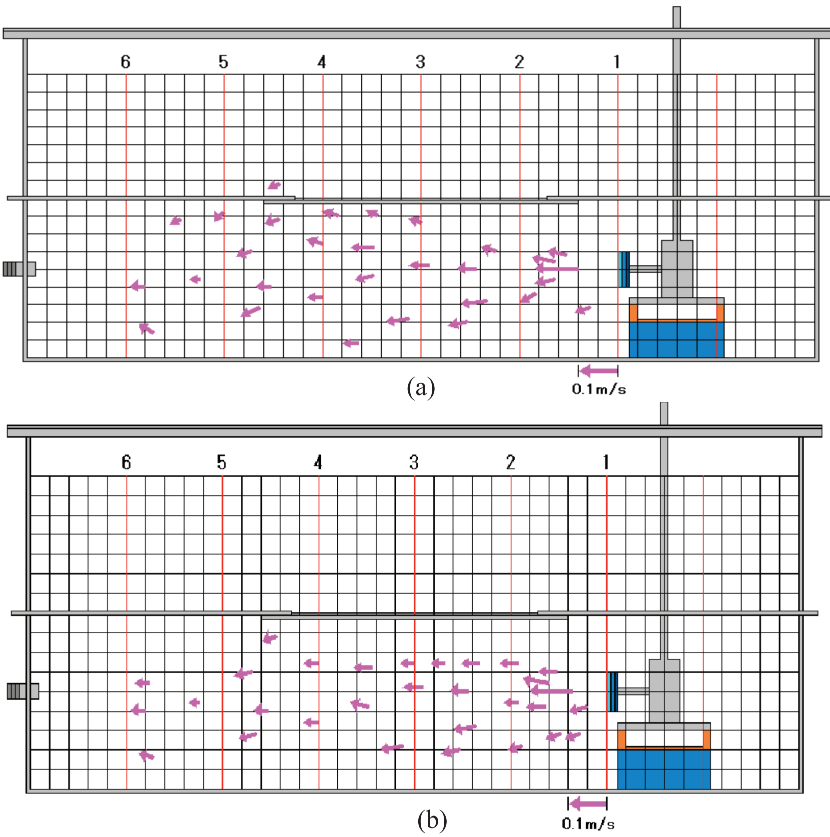


Figure 2: (a) Observed velocity (Temperature difference:-0.1). (b) Observed velocity vectors (DO difference: 23mg/L).

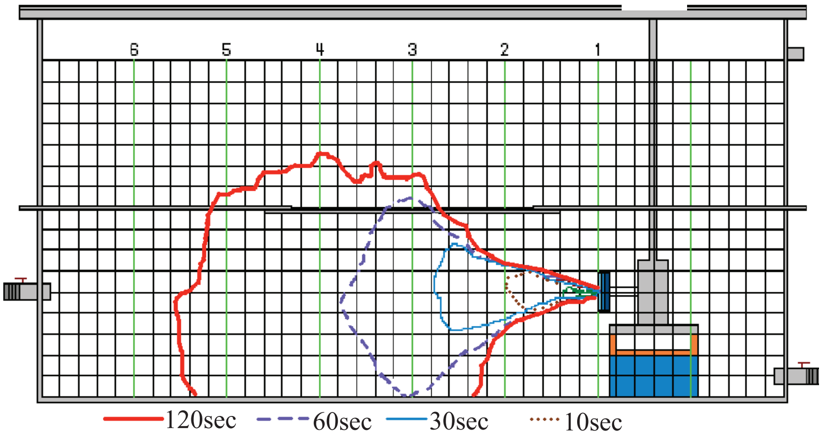


Figure 3: Observed areas of diffusion of pigment (temperature difference:-0.1).

5.2 Flow analysis in the model of a water reservoir

For computing the density diffusion, the velocity data are important and have significant influence on the calculated results. However, we would like to focus on the numerical criteria for calculating the density diffusion in this paper. The figures to illustrate the calculated velocity vectors were omitted, and discussions of flow analysis are limited to their influence for computing the density diffusion.

5.3 DO concentration analysis in the model of a water reservoir

5.3.1 Time required by the four numerical methods for the DO analysis

Table 2 shows the time required by the four numerical methods for analysing the DO concentration in the model. When the number of divisions of the analytical domain was 4,961, the FDM, the FEM, and the meshless method needed almost 1.1, 4.4, and 10.3 times the time required by the WFDM, respectively. For the purposes of saving time, the WFDM was the best; the FDM was second best; the FEM was the third best; and the meshless method was the poorest performer. We believe that the reason that the WFDM was the best, the FDM was the second best, and the FEM was the third best is that the WFDM and FDM can be easily applied to an explicit scheme and the coefficient matrix of the FEM is suitable for employing the skyline solver. On the other hand, for the purpose of saving the time and labour required for preparing the input data, the meshless methodwas the best, the FDM was thesecond best, the FEM was the third best and the BEM was the worst.

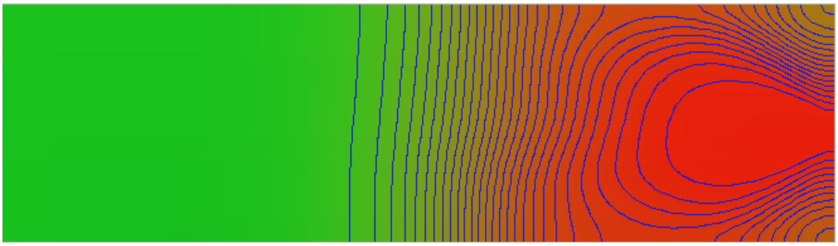
5.3.2 FEM calculation of the concentration distribution

Figures 4(a) and 4(b) are illustrations of the concentration distribution calculated using the FEM with the ordinary shape function, in which the number of

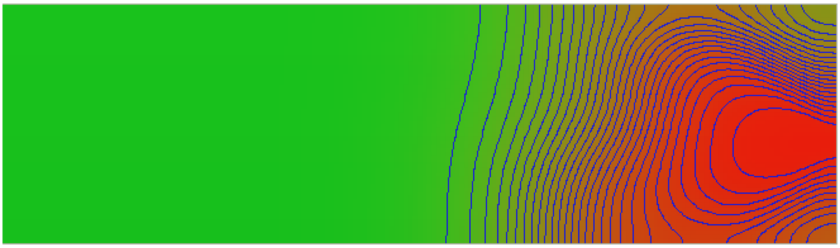
Table 2: The time required by the four methods for analysing the unsteady convective diffusion of DO for 240 seconds in a model of a water reservoir.

Relative computational time / Numerical method	Number of divisions: 4,961	Time increment: Δt (sec)
WFDM	1.00	0.005
FDM	1.10	0.005
FEM	4.40	0.1
Meshless method	10.3	5.0

divisions in the FEM is 4,800 and 10, 800, respectively. Here, the two values of λ and ν are 1,000.0 and 0.0001 m^2/sec, respectively. Comparing Fig. 4(a) (in which the adopted number of divisions is 4,800) with Fig. 4(b) (in which the adopted number of divisions is 10, 800), it was noted that the increase of the number of divisions made the areas of the DO distribution wider in the vertical direction in the FEM analysis. With respect to the influence of flow analysis for computing the density diffusion, it is important to use an appropriate value of ν in the FEM flow analysis. The value of ν changed the velocity-vector



(a)



(b)

Figure 4: DO-concentration distribution calculated using the FEM with (a) 4,800 elements (4,961 points) [t=240sec]; (b) 10, 800 elements (11,041 points) [t=240sec].

distribution so significant that it was necessary to adopt the optimum value of ν. We believe that the upwind shape function may make it possible to set the optimum value of ν in the FEM flow analysis.

5.3.3 Meshless calculation of the concentration distribution

Figure 5 is an illustration of the concentration distribution calculated using the meshless method, in which the term of the velocity increase (ωgΔt) is adopted, the number of divisions in the meshless method is 4,800, and the value of ν is 0.0001 m^2/sec. Referring to Figs. 4(a) and 5, the solutions of the meshless method showed the same tendency as those of the FEM in this problem. We considered that the convergence and accuracy of the FE, the FD, the BE, and the meshless methods for this problem were satisfactory (the figures to illustrate the concentration distribution calculated using the FEM with the upwind shape function and the BE method have been omitted).

Figure 5: DO-concentration distribution using the meshless method with 4,961 points [t=240sec].

5.3.4 FDM calculation of the concentration distribution

Fig. 6 is an illustration of the concentration distribution calculated using the FDM, in which the finite difference scheme of the order of four-degree accuracy ($O(h^4)$) for the diffusion terms and the UTOPIA scheme of the order of three-degree accuracy ($O(h^3)$) for the convective terms are combined. Here, the numbers of divisions in the FDM are 4,800 and 8,800 and the value of ν is 0.0038 m^2/sec. We believe that the convergence and accuracy of the FDM for

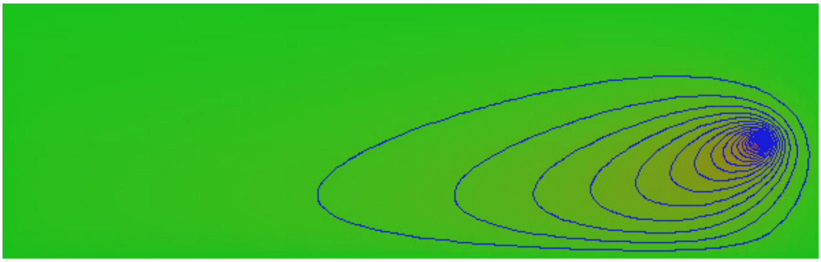


Figure 6: DO-concentration distribution using the FDM with 4,961 points [t=60sec].

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this problem were satisfactory. The term (ωgΔt) of the density diffusion seemed to make the areas of the diffusion wider in the vertical and flowing-out directions and the speed of the convective diffusion higher than those in the analyses of the FDM when this density diffusion was not applied.

6 Conclusion

In summary, (1) in this paper, the velocity increase was defined as the density diffusion that was caused by the water density ρ, the gravity acceleration g, and the time increment Δt; (2) the meshless method, the BEM, the FEM, the FDM, and the WFDM were developed and applied to the analysis of the density diffusion; (3) introducing the radial basis functions of the Gaussians or the multiquadric to the meshless method, the special fundamental solution to the BEM and the upwind shape function to the FEM, we tried to upgrade the order of the accuracy these methods; (4) the finite difference scheme of the order of four-degree accuracy ($O(h^4)$) for the diffusion terms and the UTOPIA scheme of the order of three-degree accuracy ($O(h^3)$) for the convective terms were successfully combined for the FDM;(5) the density diffusion could make the areas of the diffusion wider in the vertical and outflow directions and make the speed of the convective diffusion be higher than in the analyses of these methods when this velocity increase was not applied; (6) the stability and convergence of the five kinds of analysis using these newly developed methods seemed satisfactory; (7) the analogy between the differences of the water temperature and the DO concentration could be proved by using both the observed concentration distribution and the visualised velocity vectors in our model simulation; (8) these developments and ideas described above were investigated, and the numerical criteria for calculating the density diffusion in a water reservoir using the two-dimensional convective diffusion equations was discussed.

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