Devised numerical criteria for calculating the density diffusion in a water reservoir

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Abstract

In an earlier study to numerically represent the phenomenon described below, we proposed the density diffusion caused by the liquid density $\rho$, the gravity acceleration $g$, and the time increment $\Delta t$. During field studies, an attempt was made to ameliorate the concentration of oxygen in the lower layer of a few water reservoirs by using a machine that supplies dissolved oxygen (DO), which led to reports of a phenomenon in which the distance reached by the DO-rich water was more than 300 metres despite the very low velocity of the water flow. In this report, we investigate the numerical criteria for calculating the density diffusion in a water reservoir by using two-dimensional convective-diffusion equations. Using the signs of the space division $h$ (= $\Delta s$), the time increment $k$ (= $\Delta t$), the diffusion parameter $\Gamma$ (= $D*k/(h)^2$), and the Curant number $C_r$ (= $V*k/h$), we discuss the order estimate for calculating the density diffusion.

1 Introduction

If the DO concentration equals 100 mg/L (milligrams per litre), the liquid density ($\rho$) becomes 1.0001 Kg/L (kilograms per litre). To analyse the two-dimensional convective-diffusion equation in the problem described above, we combine the finite difference scheme of the order of four-degree accuracy (O($h^4$)) for the diffusion term and the UTOPIA scheme of the order of three-degree accuracy (O($h^3$)) for the convection term. When the above combined method is adopted, the space division $h$ should be less than 0.0001\textsuperscript{1/3} (= 0.046) m for the estimation of the liquid density $\rho$ of 1.0001 Kg/L. If the methods of the order of two-degree accuracy are used, the space division $h$ becomes less than 0.0001\textsuperscript{1/2} (= 0.01) m. The weighted finite difference method (WFDM) is newly investigated to
introduce the scheme of the order of three-degree accuracy \( (O(h^3)) \) for both the diffusion and the convection terms to calculate the density diffusion. The WFDM and the FDM may greatly reduce the CPU time for problem analysis (when comparing with the meshless and the BE methods) since the schemes of both methods are expressed explicitly. We tried to upgrade the convergence and the stability or the order of the accuracy of the finite element method (FEM), the meshless method, and the boundary element method (BEM) by introducing the upwind shape function to the FEM, the various basis functions to the meshless method, and the especial fundamental solution to the BEM. It is expected that the fundamental solution of the BEM (Kanoh et al. [2]) may yield accurate and convergent solutions in the analysis of the two-dimensional convective-diffusion equation since the fundamental solution includes the velocity term. The newly developed meshless, BE, and FE methods are used, and the order of the accuracy of each method is investigated numerically. The solutions calculated by these methods are compared with the observed results in our model simulation, and the effect and accuracy of the alternative numerical methods are estimated.

2 Governing equations

Equations (1), (2), and (3) govern the diffusion of the concentration of oxygen in a water reservoir in the vertical \((x_1, x_2)\) plane, as illustrated in Fig. 1,

\[
C_t + u_1 \cdot C_{x_1} + u_2' \cdot C_{x_2} - D_1 \cdot C_{x_1} - D_2 \cdot C_{x_2} = 0
\]  

\(\text{Equation (1)}\)

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, \(C_{x_1}\) and \(C_{x_2}\) describe the derivatives of \(C\) differentiated with respect to \(x_1\) and \(x_2\), respectively, and \(C_{x_1} x_{x_1}\) and \(C_{x_2} x_{x_2}\) 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),

\[
t_+ \Delta t u_2' = t u_2 + (1 - \rho_{DO} / \rho_0) \rho g \Delta t = t u_2 + \omega g \Delta t
\]  

\(\text{in the finite difference scheme expression} \quad \text{(2)}\)

where \(t_+ \Delta t u_2'\) and \(t u_2\) are the velocities at time \((t+\Delta t)\) and time \(t\) in the vertical direction, respectively. The second term \((\omega g \Delta t)\) of the right-hand side of Equation (2) means that the DO concentration increases the velocity of the vertical direction, and \(\omega\) describes the density of the liquid that dissolves DO. The velocity increase is caused by the liquid density \(\rho\), the gravity acceleration \(g\), and the time increment \(\Delta t\). 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 \( \rho \) is connected to the DO concentration \( C \), as written in Equation (3), where \( \rho_0 \) and \( \rho_{DO} \) describe the densities of pure water and dissolved oxygen, respectively.

\[ \rho = \rho_0 + C \cdot 10^{-6} (1 - \rho_{DO} / \rho_0) \]  

(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.

![Analytical domain and a DO-supplying machine in a constructed model of a water reservoir.](image)

**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]),

\[ C = \gamma_j X_j , \quad X_j = (r^2+c^2)^{-1/2} \text{ or } X_j = \exp(-c r^2) \text{ or } X_j = 1/\log(r^2+c^2)^{1/2} \]  

(4)

\[ \left\{ \left( \frac{\partial X_j}{\partial x_1} + \frac{\partial X_j}{\partial x_2} \right) - \left( D_1 \frac{\partial^2 X_j}{\partial x_1^2} + D_2 \frac{\partial^2 X_j}{\partial x_2^2} \right) \right\} \gamma_j = 0 \]  

(5)

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

\[ C_{st} + L(C) = 0 \]  

(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

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

where $C^{t+\Delta t}$ and $C^t$ are the concentrations at time $(t+\Delta t)$ and time $(t)$, respectively, and $L^{t+\Delta t}$ and $L^t$ are the terms of convection and diffusion at time $(t+\Delta t)$ 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 $X_j = (r^2 + c^2)^{-1/2}$ or $\exp(-c r^2)$ or $1/\log((r^2 + c^2)^{1/2})$ of the mesh-free RBF collocation method (Devo et al. [3]) or the radial basis functions of the Gaussians (Powell [6]).

### 3.2 Finite difference and weighted finite difference methods for convective-diffusion analysis

With respect to the analysis of the one-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 [4]). To analyse the DO concentration by using the two-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 weighted finite difference scheme of the order of three-degree accuracy ($O(h^3)$) for both the diffusion and the convective terms is proposed and applied to the calculation of the two-dimensional density diffusion by using also the one-dimensional convective-diffusion analysis twice. The WFDM and FDM can be expressed explicitly.

### 3.3 Finite element method for convective-diffusion analysis

The upwind shape function of the Ptrov-Galerkin weighting (ZienKiewicz and Taylor [3]) is tested to analyse the two-dimensional density diffusion using the FEM. To reduce the CPU time of the FEM, the technique of the skyline solver and the conjugate gradient method are combined and applied to our upwind FEM.

### 3.4 Boundary element method for convective-diffusion analysis

Using the ordinary fundamental solution, our BEM does not yield any advantage for calculating the density diffusion over the FE, the FD and the meshless methods. Namely, the convection terms should be treated on the right hand side of our BEM, where the solution cost is significantly larger due to the full and
non-symmetry of the coefficient matrices. On the other hand, since the especial fundamental solution of the BEM (Kanoh et al. [2]) is expected to yield accurate and convergent solutions in the analysis of the two-dimensional convective-diffusion equation, we need to mathematically integrate the fundamental solution in the time domain.

4 Model simulation

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 (Sakamoto, et al. [1]). Using the analogy, we 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. In reference to the observed some velocity vectors and the distributions of the DO concentration in the model, 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.

5 Results and discussion

As described above, we introduced a concept in the simulation model developed 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 produce 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 Concentration distribution of DO in a model

Figure 2 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. 2) 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).
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

The table 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 9,075, the WFDM, the FDM, and the meshless method needed almost 18.3, 27.5, and 495 times the time required by the upwind FEM, respectively. For the purposes of saving time, the upwind FEM was the best; the WFDM was second best; the FDM was third best; and the meshless method was the poorest performer. We believe that the reason that the upwind FEM was the best, the WFDM was second best, and the FDM was third best is that the coefficient matrix of the upwind FEM was developed to be suitable for employing both the skyline solver and the conjugate gradient method, and the WFDM and FDM can be easily applied to an explicit scheme.
Table 1: 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.

<table>
<thead>
<tr>
<th>Numerical method</th>
<th>Number of divisions:</th>
<th>Time increment: Δt (sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>FDM</td>
<td>0.0005</td>
<td>27.5</td>
</tr>
<tr>
<td>WFDM</td>
<td>18.3</td>
<td>5.0</td>
</tr>
<tr>
<td>FDM</td>
<td>27.5</td>
<td>0.0005</td>
</tr>
<tr>
<td>Meshless method</td>
<td>495</td>
<td>9,075</td>
</tr>
</tbody>
</table>

5.3.2 FEM calculation of the concentration distribution

Figures 3(a) and 3(b) are illustrations of the concentration distribution calculated using the FEM with the upwind shape function, in which the duration of convective-diffusion of DO is 120 and 240 sec, respectively. Figure 4 shows the concentration distribution calculated using the FEM, in which the number of divisions in the FEM 9,075. Comparing Fig. 3(b) (in which the adopted number of divisions is 4,800 and the space division (h) is 0.013 m) with Fig. 4 (in which the adopted number of divisions is 9,075 and the space division (h) is 0.010 m), it was noted that the both space divisions (h=0.013 and 0.010 m) made the areas of the DO distribution wide in the vertical direction and the effect of the density diffusion conspicuous in the upwind FEM analysis where the concentration of the flowing-out DO was 100 mg/L. Now, we discuss the order estimate for calculating the density diffusion with the upwind FEM, where the DO concentration equals 100 mg/L and the liquid density (ρ) becomes 1.0001 Kg/L. As described above, when the methods of the order of three-degree accuracy are used, the space division h should be less than 0.0001\(^{1/3}\) (≈ 0.046) m, and in case the methods of the order of two-degree accuracy are used, the space division h becomes less than 0.0001\(^{1/2}\) (≈ 0.010) m for the estimation of the liquid density ρ of 1.0001 Kg/L. We consider that the upwind FEM has the order of 2.14 degree accuracy (O(h\(^{2.14}\))) in the density diffusion analysis. The reason is that 0.013 to the 2.14 power is less than 0.0001 (0.013\(^{2.14}\)= 0.000097 < 0.0001). With respect to the influence of flow analysis for computing the density diffusion, the upwind shape function could make it possible to set the optimum value of ν and obtain the stable velocity distribution in the FEM flow analysis.

5.3.3 Meshless calculation of the concentration distribution

Figures 5(a), 5(b), and 5(c) are illustrations of the concentration distribution calculated using the meshless method, in which the term of the velocity increase (ogΔt) is adopted, the number of divisions in the meshless method is 4,800 or 9,075. Here, we investigated the convergence and the accuracy of three kinds of the global expansion function Xj, \((r^2+c^2)^{-1/2}\) or \(\exp(-c r^2)\) or \(1/\log((r^2+c^2)^{1/2})\), and
Figure 3: (a) DO-concentration distribution calculated using the upwind FEM with 4,800 elements (4,961 points, h=0.013m) [t=120 sec]. (b) [t=240sec].

Figure 4: DO-concentration distribution calculated using the upwind FEM with 9,075 elements (9,296 points, h=0.010m) [t=240sec].

adopted the logarithm type of the mesh-free RBF collocation method because of the convenience of determining the appropriate value of c in the function Xj and the convergence of it. Comparing Fig. 5(a) (in which the adopted space division (h) is 0.013 m) with Fig. 5(b) (in which the adopted space division (h) is 0.010 m), it was noted that the former space division (h=0.013) made the areas of the DO distribution slightly wide, but the latter space division (h=0.010 m) made it wider in the vertical direction. Furthermore, the effect of the density diffusion was conspicuous in the meshless method analysis where the concentration of the
Figure 5: (a) DO-concentration distribution using the meshless method with 4,961 points (h=0.013m) where the flowing–out DO is 100 mg/L [t=240sec]. (b) DO-concentration distribution using the meshless method with 9,296 points (h=0.010m) where the flowing–out DO is 100 mg/L [t=240sec]. (c) DO-concentration distribution using the meshless method with 4,961 points (h=0.013m) where the flowing–out DO is 120 mg/L [t=240sec].

flowing-out DO was 100 mg/L. Figure 5(c) shows that the larger space division (h=0.013 m) could make it wider in the vertical direction, and the effect of the density diffusion was conspicuous in the meshless method analysis when the concentration of the flowing-out DO was 120 mg/L. We consider that our meshless method has the order of 2.1 degree accuracy (O(h^{2.1})) in the density diffusion analysis. The reason for this is that 0.013 to the two point first power is
less than 0.00012 (0.013^{2.10} = 0.000115 < 0.000120). Namely, the combination of the order of 2.1 degree accuracy (O(h^{2.1})) and the larger space division (h=0.013 m) in our meshless method can yield the value of 0.000115 that is less than 0.000120, which is caused by the concentration of the flowing-out DO 120 mg/L.

5.3.4 FDM calculation of the concentration distribution

Figure 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 number of divisions in the FDM is 4,800. The term (\omega g \Delta t) 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. We conclude that the FDM satisfied the order of three-degree accuracy (O(h^3)).

![Figure 6: DO-concentration distribution calculated using the FDM with 4,961 points (h=0.013m) where the flowing–out DO is 100 mg/L [t=240sec].](image)

5.3.5 BEM calculation of the concentration distribution

Using the ordinary fundamental solution of our BEM, we could not reproduce the density difference of the high DO concentration (80 or 100 mg/L) of the water reservoirs with the space division (h) of 0.013 m. We concluded that the convergence and accuracy of the upwind FE, the FD, the WFD, the BE, and the meshless methods for this problem were satisfactory (the figures to illustrate the concentration distribution calculated using the WFD and the BE methods have been omitted).

6 Conclusion

In summary, (1) in this study, the meshless method, the BEM, the FEM, the FDM, and the WFDM were developed and applied to the analysis of the density diffusion that was caused by the water density \( \rho \), the gravity acceleration \( g \), and the time increment \( \Delta t \); (2) 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 upgraded the order of the accuracy of these methods; (3) using the technique of the ADI method, 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; (4) the weighted finite difference scheme of the order of three-degree accuracy \(O(h^3)\) for both the diffusion terms and the convective terms was defined; (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 higher than it was 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 degrees of accuracy of the four methods (the meshless, the FE, the FD, and the WFD methods) were upgraded sufficiently to calculate the density diffusion in case the space division \((h)\) was 0.0133 or 0.01 m; (8) the technique of the skyline solver and the conjugate gradient method were applied to our upwind FEM, and the CPU time of the FEM was greatly reduced; (9) the analogy between the differences of the water temperature and the DO concentration was used to reproduce the density-difference of the high DO concentration (80 or 100 mg/L) of the water reservoirs in our model simulation; and (10) the 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 equation were discussed.

**References**


