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OPI: DTIC-TID
BOUNDARY CONDITIONS OF SEDIMENT SURFACES VIEWED FROM DO BEHAVIOR

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ABSTRACT

In measurement of dissolved oxygen (DO) stratifications, the lowest point is chosen usually at a depth of 0.5 m above the sediment surface. DO concentrations in the overlying water just above the sediment are rarely measured. Therefore, the DO behavior in the sediment-water interface is not well known. In order to investigate DO behavior, column tests on DO were performed by use of special test apparatus. This paper deals with these test results and discusses the boundary conditions of sediment-water interface on DO behavior.

OUTLINE OF TESTS

The test column consists of two parts: the upper and lower sections. The latter is the column sampler itself, which has been used for sampling undisturbed sediment. Both tubes are connected by a ring coupling in the laboratory (Figures 1 and 2).

The connected test column is then provided with water jackets at its circumference and erected in an isothermal tank. In order to emerge from a thermal stratification in summer lake water, the overlying water column is heated by three isothermal tanks with different temperatures. Since we had to measure DO concentrations of very thin layers, we have paid close attention to water sampling and analysis.
The sampling tube (Figure 3) has a diameter of 6 mm, a horizontal length of 170 mm, and 8 holes of 0.5 mm. In the 1980 tests, 4 tubes were inserted at heights of 1, 10, 40, and 70 cm above sediment, and in the 1981 tests, 6 tubes at heights of 1, 4, 7, 10, 40, and 70 cm, respectively. The 15-ml water samples were taken gently so that the Reynolds' numbers did not exceed 100. Samples were put into the special DO meter, which was designed for this test (Figure 4). This meter has a small stirrer for medical use and is capable of measuring very small quantities of water.

The sediment samples were taken from Lake Nakanoumi and one of its inflowing rivers.

THERMAL STRATIFICATION

Quantities of heat flowing into and out of a segment of the water column may be expressed as shown in Figure 5.
As equilibrium equation for the heat quantities is represented as follows:

\[ \frac{\partial T}{\partial t} = \frac{k}{C_p} \frac{\partial^2 T}{\partial z^2} - \rho_T \frac{\partial p}{\partial z} - \rho_w \frac{\partial T}{\partial z} \]  

(1)

where

* T = water temperature °C
* t = time after incubation of tests, days
Figure 4. DO meter

Figure 5. Induction of thermal stratification

\[ w = \text{descending flow velocity due to water temperature difference, cm/sec} \]

\[ Cp = \text{specific heat of water, cal/} ^\circ \text{C/cm}^3 \]

\[ k = \text{thermal conductivity, cal/cm/sec/} ^\circ \text{C} \]

\[ \rho = \text{water density, g/cm}^3 \]

\[ z = \text{height of water column} \]

The solution of Equation 1 is obtained in the following series function:

\[ \frac{T}{T_0} = 1 + \frac{W}{4D^2} z^2 - \frac{7}{24} b^3 \omega_T z^3 \]  

(2)
where

\[ T_0 = \text{water temperature at } z = 0 \]

\[ \rho_{20} = \text{water density at } 20^\circ\text{C} \]

\[ \rho = \rho_{20} (1 - \alpha T) \text{ is assumed} \]  

(3)

\[ \beta = \frac{\alpha \rho_{20} C_p}{k} \]  

(4)

\[ D = \text{thermal diffusivity, cm}^2/\text{sec} \]

Here we calculate

\[ \beta = \frac{\alpha \rho_{20} C_p}{k} = \frac{2.55 \times 10^{-4} \times 0.9982 \times 1}{1.42} = 1.793 \times 10^{-4} \frac{\text{sec}}{^\circ\text{C cm}^2} \]

The observed water temperatures are distributed as shown in Figure 6. These are represented in Figure 7 in terms of the ratio of \( T/T_0 \).
Figure 7. Ratio of $T/T_o$

Putting the test results $T/T_o = 1.092$ at $z = 40$ cm (1981) into Equation 2, we can calculate the values of $w$:

$$1.092 = 1 + \frac{w^2}{D^2} \frac{40^2}{4} - \frac{7}{24} (1.793 \times 10^{-4})^3 \times w^3 \times 21.7^3 \times 40^3$$

$$0.092 = 400 \frac{w^2}{D^2} - 1.0995 \times 10^{-5} w^3$$

Neglecting the second term in the right side, we get

$$\frac{w^2}{D^2} = \frac{0.092}{400} = 2.3 \times 10^{-4}$$

$$\frac{w}{D} = 1.517 \times 10^{-2} \text{ cm}^{-1}$$

Similarly for $T/T_o = 1.1085$ at $z = 30$ cm (1980)

$$\frac{w}{D} = 2.195 \times 10^{-2} \text{ cm}^{-1}$$
Taking \( D = 1.5 \times 10^{-3} \text{ cm}^2/\text{sec} \), we get

\[
w = 1.517 \times 10^{-2} \times 1.5 \times 10^{-3} = 2.276 \times 10^{-5} \text{ cm/sec (1981)}
\]

\[
w = 2.195 \times 10^{-2} \times 1.5 \times 10^{-3} = 3.287 \times 10^{-5} \text{ cm/sec (1980)}
\]

From the water temperature profiles it is found that the descending velocity \( (w) \) due to temperature differences at greater differences is about one and a half times as large as at lower differences. (This means that the value of \( w \) is proportional to temperature difference. The larger temperature difference, the bigger \( w \).)

**VARIANCE OF DO AGAINST TIME**

As indicated earlier, sediment samples were taken from Lake Nakanoumi and one of its inflowing rivers. Tap water was used as overlying water.

The relationships between DO concentration profiles and time transfer are shown in Figures 8 and 9.

![Figure 8. DO stratification](image)
As the figures show, the initial DO profile is a nearly vertical line, located almost entirely in the portion overlying the sediment 10 cm above the interface. DO concentrations decrease rapidly and approach within 10 cm above the interface. We can see clearly that DO concentrations decrease gradually according to time and reach a final distribution shifted to the left in these figures. Their reduction is strong at the lower layers and weak in the upper layers (Figure 10).

DO STRATIFICATION

From our test results, we have learned that we should consider DO stratification in two parts. The first part is the distribution due to thermal stratification occurring in the portion of the water column above the water layer immediately overlying the sediment. The second part is the distribution due to sediment oxygen demand and occurring in the layer immediately overlying the sediment.
Figure 10. Change of DO against time

DO DISTRIBUTION DUE TO THERMAL STRATIFICATION

An equilibrium equation of dissolved oxygen is represented as follows:

$$\frac{\partial c_1}{\partial t} = w \frac{\partial c_1}{\partial z} - K \frac{\partial^2 c_1}{\partial z^2}$$  \hspace{1cm} (5)

where

c_1 = DO concentration, mg/l

w = descending velocity due to thermal stratification, cm/sec

K = diffusion coefficient of dissolved oxygen in the vertical direction, cm²/sec

z = length of water column, cm

t = time, sec

We assume that the solution of Equation 5 is a separate function of temperature (T) at time (t) and z as follows:
Then putting

\[ T(t) = T(t) S(z) \]  \hspace{1cm} (6)

\[
\frac{T'(t)}{T} = \frac{W \frac{\partial S}{\partial z} + K \frac{\partial^2 S}{\partial z^2}}{S(z)} = -n^2
\]

We get

\[ T' = -n^2 T \]  \hspace{1cm} (7)

\[ K \frac{\partial^2 S}{\partial z^2} - W \frac{\partial S}{\partial z} + n^2 S = 0 \] \hspace{1cm} (8)

From Equation 7

\[ T = Ce^{-n^2t} \]  \hspace{1cm} (9)

Equation 8 is rewritten as follows:

\[
\frac{\partial^2 S}{\partial z^2} - \frac{W}{K} \frac{\partial S}{\partial z} + \frac{n^2}{K} S = 0
\]  \hspace{1cm} (10)

\[
(D^2 - \frac{W}{K} D + \frac{n^2}{K}) S = 0
\]

\[
m^2 - \frac{W}{K} m + \frac{n^2}{K} = 0
\]

\[
m = \frac{W}{2K} \pm \sqrt{\frac{W^2}{4K^2} - \frac{n^2}{K}}
\]

\[
= \frac{W}{2K} \left(1 \pm \sqrt{1 - \frac{4nK}{w^2}}\right)
\]

Thereupon

\[ S(Z) = C_1 e^{m_1 Z} + C_2 e^{m_2 Z} \]
Finally

$$c_1 = e^{-n^2t} \left( c_1 e^{m_1z} + c_2 e^{m_2z} \right)$$  \hspace{1cm} (11)

At the water surface ($z = H$ where $H$ = total length of water column), the following condition is composed of

$$wC - K \frac{\partial C}{\partial z} = 0$$  \hspace{1cm} (12)

$$w e^{-n^2t} \left( c_1 e^{m_1H} + c_2 e^{m_2H} \right) - Ke^{-n^2t} \left( c_1 m_1 e^{m_1H} + c_2 m_2 e^{m_2H} \right) = 0$$

$$\left( w + m_1K \right) e^{m_1H} C_1 + \left( W + m_2K \right) e^{m_2H} C_2 = 0$$

$$C_2 = \frac{w + m_1K}{w + m_2K} e^{(m_1 - m_2)H} C_1$$

Then we get

$$c_1 = e^{-n^2t} C_1 \left[ \frac{e^{m_1z}}{w + m_1K} + \frac{w + m_1K}{w + m_2K} e^{(m_1 - m_2)H} \right]$$  \hspace{1cm} (13)

This is an equation on DO variance in an unsteady flow.

In a steady flow, the following solution is obtained from the equation:

$$\frac{\partial^2 c_1}{\partial z^2} - K \frac{\partial^2 c_1}{\partial z^2} = 0$$

$$c_1 = C_1 \frac{w}{K} e^{Kz}$$  \hspace{1cm} (14)

The curve of Equation 13 or 14 is connected to the curve of the deoxygenating zone, which is dealt with in the next section. Consequently, the arbitrary constant $C_1$ is determined by it. Then,
\[ |c_1|_{z=h} = |c_2|_{z=h} \]  

\[ c_1 \frac{K}{w} e^{\frac{w}{K} h} = c_0 \frac{\sin(\sqrt{\frac{r}{K}} + a)}{\sin a} \]  

\[ c_1 = c_0 \frac{w}{K} e^{\frac{w}{K} h} \frac{\sin(\sqrt{\frac{r}{K}} h + a)}{\sin a} \]  

DISTRIBUTION DUE TO THE DEOXYGENATION OF SEDIMENT

The test results showed that the water temperature in the water just above the sediment \((z < 10 \text{ cm})\) is constant (Figure 11). This means that there is no descending velocity due to thermal stratification. The variance of DO concentrations at this portion is represented as follows:

\[ \partial c_2 \partial t = -K \frac{\partial^2 c_2}{\partial z^2} - \lambda c_2 \]  

where

\[ c_2 = \text{DO concentration, mg/l} \]

\[ K = \text{diffusion coefficient of dissolved oxygen, cm}^2/\text{sec} \]

\[ \lambda = \text{deoxygenating rate, sec} \]
The solution of Equation 18 is obtained as follows:

\[
c_2 = e^{-n^2t} \left( c_1 e^{i \sqrt{\frac{\lambda-n^2}{K}} z} + c_2 e^{-i \sqrt{\frac{\lambda-n^2}{K}} z} \right)
\]

(18)

\[= e^{-n^2t} A \sin \left( \sqrt{\frac{\lambda-n^2}{K}} z + a \right)\]

since \( C = C_0 \) at \( t = 0, z = 0 \), we get

\[A = \frac{C_0}{\sin a}\]

Equation 18 becomes

\[c_2 = C_0 e^{-n^2t} \frac{\sin \left( \sqrt{\frac{\lambda-n^2}{K}} z + a \right)}{\sin a}\]

(19)

This is an equation of DO variance at the deoxygenating zone in an unsteady flow. In a steady flow, it becomes as follows:

\[c_1 = C_0 \frac{\sin \left( \sqrt{\frac{\lambda}{K}} z + a \right)}{\sin a}\]

(20)

\[\lambda = \frac{11.5 - 0.2}{11.5 \times 3 \times 24 \times 3600} = 3.73 \times 10^{-5} \text{ sec}^{-1}\]

(21)

Putting the data together:

\[z = 70 \text{ cm}; \ c_1 = 8.8 \text{ mg/l} \ (t = 0)\]

\[z = 10 \text{ cm}; \ c_1 = 7.6 \text{ mg/l} \ (t = 0)\]

We get

\[\frac{W}{K} = 0.00244\]
Since $w$ is already known (page 7), then we obtain

$$K = 1.345 \times 10^{-2} \text{cm}^2/\text{sec}$$

From the observed data,

$t = 0$, $C_2 = 11.5 \text{mg/}l$, and $t = 3$ days; $C_2 = 0.2 \text{mg/}l$,

we get

$$\sqrt{\frac{a}{K}} = 0.0527 \text{cm/sec}$$

$$a_0 = 0.025 \text{rad}$$

$$C_0 = 1.22 \text{mg/}l$$

Figure 12 shows the DO profile in the deoxygenating zone.

Figure 12. DO profile in deoxygenating zone

BOUNDARY CONDITIONS ON DO AT SEDIMENT SURFACE

As the test results show, we could reemerge DO stratifications in the laboratory. These behaviors were analyzed theoretically in the preceding chapter.
Owing to the DO stratification, the diffusion of dissolved oxygen travels from the upper layers to the lower ones, that is, from higher concentrations to lower ones. The quantities which reach from the top to the sediment surface are \(-K \frac{\partial c}{\partial z}\) per unit area and per unit time. On the other side, some quantities of oxygen are consumed by sediment during deoxygenation, as far as it is polluted.

These two quantities should be in equilibrium (Figure 13). Then we get the equation if we represent sediment oxygen demand (SOD) as \(O_2\).

![Figure 13. Equilibrium at sediment surface](image)

\[
O_2 - K \frac{\partial c}{\partial z} = 0 \quad (22)
\]

\[
O_2 = K \left| e^{-n^2 t} c_0 \sqrt{\frac{\lambda - n^2}{K}} \left( \cos \frac{\lambda - n^2}{K} z + a \right) \right|_{z=0}
\]

\[
= c_0 \sqrt{K(\lambda - n^2)} \cot a \cdot e^{-n^2 t} \quad (23)
\]

This is a fundamental equation of SOD. From this, we can say that SOD behaves exponentially against time (Figure 14).
Figure 14. Sediment oxygen demand behavior against time

The total consumption of oxygen (Figure 15) is obtained by a planimeter. If we represent it mathematically, it becomes

\[ Q = \frac{1}{AH} \left[ \int_{0}^{H} c(t = 0) \, dz - \int_{0}^{H} c(t) \, dz \right] \]

In Table 1, the measured and calculated values of SOD in one sample are indicated. The calculated values are obtained from the assumption that \( n^2 = 0.11 \).

<table>
<thead>
<tr>
<th>t</th>
<th>SOD</th>
<th>( \frac{O_2}{O_2(0)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>400</td>
<td>1.0</td>
</tr>
<tr>
<td>2</td>
<td>320</td>
<td>0.8</td>
</tr>
<tr>
<td>4</td>
<td>250</td>
<td>0.625</td>
</tr>
<tr>
<td>6</td>
<td>210</td>
<td>0.525</td>
</tr>
<tr>
<td>8</td>
<td>150</td>
<td>0.375</td>
</tr>
</tbody>
</table>
We can see from Figure 16 that there is a good agreement between observed and calculated values of SOD.

CONCLUSIONS

The DO stratifications that are often observed in lakes and other water areas are well known to pollution investigators. However, there are very few data regarding DO behavior on the sediment surface. From our test results, we can say that the sediment surface is always subject to an anoxic condition owing to its oxygen demand.

From our tests, we have learned that any DO stratification consists of two parts, that is, one due to thermal stratification and one due to the oxygen demand of the sediment. It was also found that the latter has a small height \( z \leq 10 \text{ cm} \).

In winter, no thermal stratification occurs. Consequently, the DO profile becomes a vertical straight line in most of the water column. In this case, it can incorrectly be considered to extend to the sediment surface.

The line bends at a large angle at the junction with the deoxygenating zone (Figure 17).

DO stratification generated in summer reveals an exponential profile represented by

\[ c_1 = C_1 \frac{K}{w} e^{Kz} \]
This curve is pulled to lower concentrations (to the left in the figure) at its lower end by the curve of the deoxygenating zone.

In our tests, we studied SOD behavior from both observation and theoretical considerations. We found that such DO behavior on the boundary layer of the sediment has a great effect upon the release mechanism of nutrients. However, this problem was not within the scope of this paper.