UNISENSE
ENABLING MICROSCALE RESEARCH

Calculations of Oxygen Consumption Rate Using SensorTrace Profiling

Abstract

In this note, you can learn how to use SensorTrace Profiling to quantify the consumption rate of oxygen as well as the oxygen exchange rate across the water - sediment interface, from a high resolution oxygen profile, measured with a MicroProfiling System.

As an example, we use an oxygen microprofile made in an organic rich sediment core collected at less than 30 cm water depth in the brackish Limfjorden in Denmark.

The software uses a one-dimensional mass conservation equation for the model calculation.

Before starting the analysis, we estimated the oxygen diffusion coefficient in all zones of the sediment and defined the boundary conditions. The model shows the rate distribution and compares the calculated profile with the actual measured profile.

Using a stepwise optimization, the rate distribution is redefined until the calculated profile does not deviate from the measured profile within a statistical margin.

We use the sum of squared error (SSE) and the p-value together with the modeled graph to estimate the best fit for the rate calculations. Using SensorTrace Profiling we found that the maximum oxygen consumption rate in the sediment from Limfjorden was 1.25 nmol cm^{-3} s^{-1} and the integrated oxygen flux across the water - sediment interface, 0.056 nmol cm^{-2} s^{-1}. These are comparable to rates found in similar environments (Glud, N. R. 2008, Epping et al 1999).

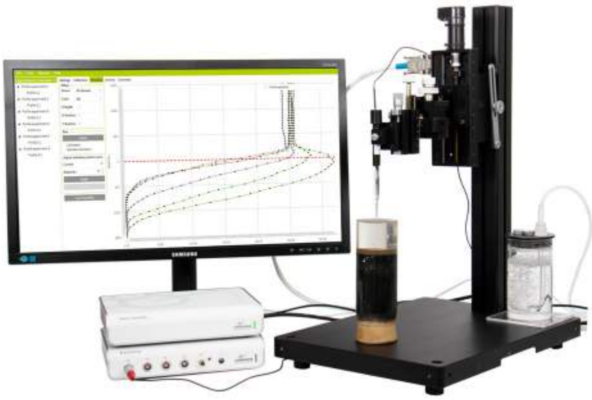
If you download SensorTrace Profiling, you can use the oxygen profile in this note for practice. You can find it in the folder 'Unisense Data' under 'Demo Experiments'.

Material & Method

We collected sediment cores by hand at Aggersund, Limfjorden, Denmark in August 2015 at a water depth of about 30 cm and brought them to the Unisense lab. We placed the sediment core in a container with brackish water (15 ‰ salinity), which we collected at the same location as the sediment. We stored the sample at in-situ temperature, about 20 °C.

We flushed the water with air using an aquarium pump and a bubble stone to ensure a good circulation and to establish a well-defined Diffusive Boundary Layer (DBL) just above the sediment-water interface (figure 2 and 3). We made the oxygen microprofiles using a motorized MicroProfiling System and an oxygen microsensor with a tip size of 50 µm (OX-50).

We used SensorTrace Profiling for sensor calibration, motor control, and data collection. The oxygen concentration was measured in units of µmol/L. Data was collected with 50 µm step size, 3 seconds wait and 1 second measuring time.



Assumptions

The software uses a one-dimensional mass conservation equation (Boudreau, 1984) for the rate calculations. The model assumes steady-state conditions where transport of oxygen occurs by diffusion, and it neglects effects of e.g. burial, groundwater flow, and wave actions. Temperature and salinity should be stable – preferably similar to the in-situ conditions.

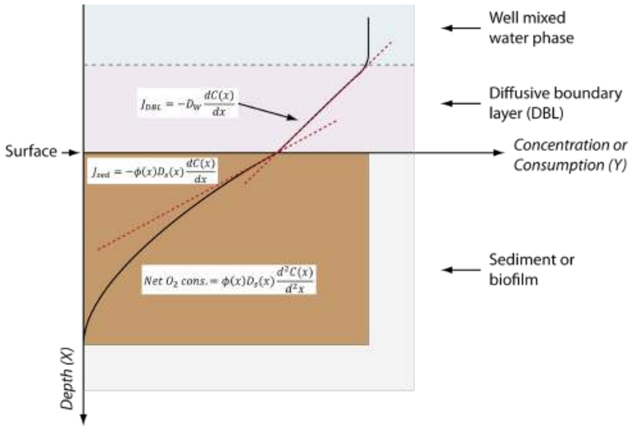


Figure 1: A typical oxygen profile in sediments with a well-mixed water phase above and a diffusive boundary layer right above the sediment surface. When the profile is a straight line, as in the Diffusive Boundary Layer, there is no net production or consumption, just a diffusive transport. Fluxes are calculated using Fick's first law of diffusion. Curvature of the profile, as below the surface in this profile, indicates consumption. The brown area is a bar graph showing the oxygen consumption rate per unit volume of sediment, calculated using Fick's second law of diffusion.

Sediment water interface

You can adjust the 0-line of the profile in the Visualization window of SensorTrace Profiling. The water - sediment is typically set to 0 µm depth. You can then use the profile with the adjusted 0-line in the Activity window.

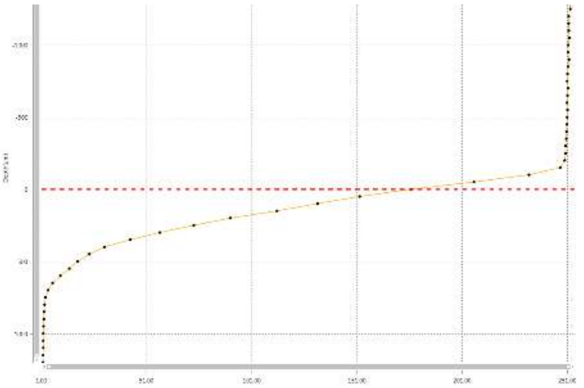


Figure 3: Oxygen microprofile in a sediment. Use the red line to adjust the water – sediment interface.

The interface – 0 µm depth – can sometimes be found from the oxygen profile, because the oxygen diffusion in water (D_0) is typically higher than the oxygen diffusion in the sediment (D_s), which shows as a change in the slope at the water – sediment interface. The sediment surface is at the bottom of the DBL, where the oxygen profile changes direction.

Activity

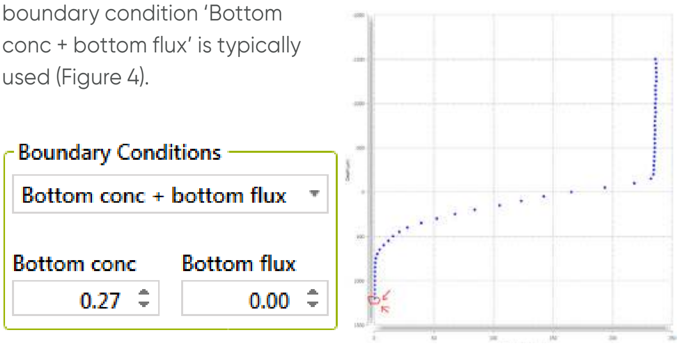
In the Activity window, SensorTrace Profiling calculates the consumption and production rates from the oxygen microprofile by using the one-dimensional mass conservation model. Before making the calculations, you have to provide the model with various information;

a. A profile
b. Boundary conditions
c. Depth interval and zones
d. Diffusion coefficient of oxygen (D_s and D_0) at the different depths
e. Porosity for the Ds determination

Below you can find examples of information that you can put into the model.

Profile: First, select the sensor that was used to measure the profile, then select the profile.

Boundary conditions: To constrain the model, two independent boundary values are needed for the analysis. In the program, you can select between 5 different pairs of boundary conditions, e.g. for oxygen profiles where the end concentration and flux deepest in the profile typically are 0 (as in the examples used here), the boundary condition 'Bottom conc + bottom flux' is typically used (Figure 4).

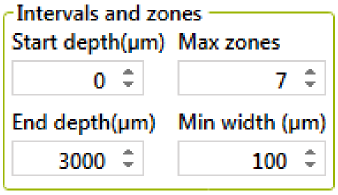


Boundary Conditions
Bottom conc + bottom flux
Bottom conc: 0.27
Bottom flux: 0.00

Figure 4: Boundary condition:
Boundary condition "Bottom conc + bottom flux"

In the sediment from Limfjorden, we start with 'Bottom conc + bottom flux' boundary condition with the values at 0.27 µM for Bottom concentration and 0 for Bottom flux.

Interval and zones: Here you define the area of the profile you want to model. It is most appropriate to calculate rates in the depth interval where a consumption or production of oxygen takes place. In the model sediments, we start at the water - sediment interface (0 µm) and end where all oxygen is consumed at the bottom of the profile.



Intervals and zones
Start depth(µm): 0
Max zones: 7
End depth(µm): 3000
Min width (µm): 100

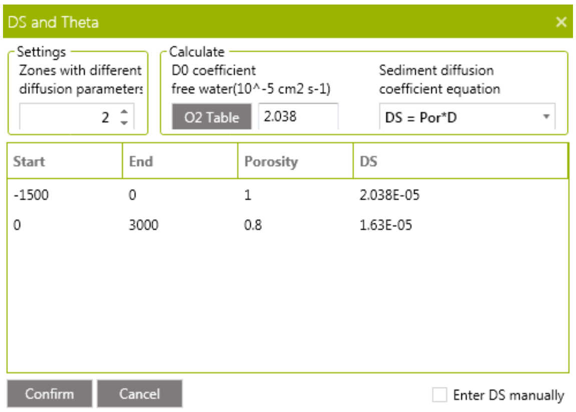
Figure 5: Settings for 'Intervals and zones'

Max zones refers to how many volume-specific rate calculations the model should list (maximum 10 zones). The volume-specific rate is calculated from the profile using Fick's second law of diffusion based on two or more measuring points. The appropriate number of zones can be estimated from the shape of the profile. Start by selecting a high number of zones e.g. 7. After the Analysis, the model highlights the most favorable number of zones based on the statistical values, SSE and p-value.

The minimum width of the zones should be at least twice the resolution of the profile. In our model profile, the resolution was 50 µm, so the minimum width should be at least 100 µm.

Diffusion rate of oxygen: In the D_s and Theta window of SensorTrace Profiling, the diffusion rates of oxygen in water (D_0) and sediment (D_s) are defined. D_0 is given in the oxygen diffusion table and is dependent on salinity and temperature. Enter the same temperature and salinity as measured when you made the profile.

D_s is dependent on D_0 and porosity of the sediment (ϕ). The software lists three emperical formulas found in the literature, for the D_s calculations. The formula $D_s = D_0 \times \phi$ is often used in sediment with a high porosity – like a biofilm, microbial mat, and soft silty sediments. The formula $D_s = D_0 \times \phi 2$ is typically used in sediments with lower porosity like sandy/silty sediment and compact mud. The formula $D_s = D_0/(1+3 \times (1 - \phi))$ has been used in all kinds of sediments. You can also manually add your own D_s value.



Settings
Zones with different diffusion parameters: 2

Calculate
D0 coefficient free water(10^-5 cm2 s-1): 2.038
Sediment diffusion coefficient equation: DS = Por*D

Start	End	Porosity	DS
-1500	0	1	2.038E-05
0	3000	0.8	1.63E-05

☐ Enter DS manually

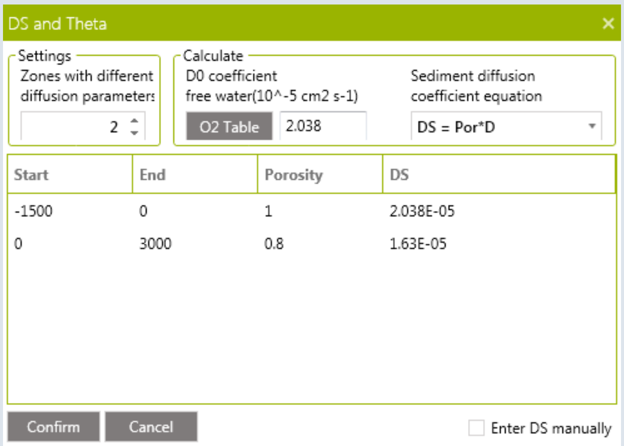
Figure 6: Settings for 'Intervals and zones'

In the sediment from Limfjorden the overlying water had a bottom tem perature of 20 °C and a salinity of 15 ‰ which gives a D_0 of 2.038 10^{-5} cm^2 s^{-1}.
Ds is calculated based on $D_s = D_0 \times \phi$, because the sediment had a relative high porosity, of 0.8, giving a D_s of 1.63 10^{-5} cm^2 s^{-1}.

Porosity: Porosity is the ratio between the volume of void space (like water) and the total volume of your sample. The porosity of the sediment is often determined as water content. If the porosity varies with depth, increase the number of zones and define the diffusion conditions for each depth interval. In the sediment from Limfjorden, we define D_s in two zones; one in the water column where $D_s = D_0$ = 2.038 10^{-5} cm^2 s^{-1} and one in the sediment where D_s = 1.63 10^{-5} cm^{-2} s^{-1}.

Summary of settings

Below you find the summary of all the settings we have defined in the Activity window before running the model the first time.



Settings
Zones with different diffusion parameters: 2

Calculate
D0 coefficient free water(10^-5 cm2 s-1): 2.038
Sediment diffusion coefficient equation: DS = Por*D

Start	End	Porosity	DS
-1500	0	1	2.038E-05
0	3000	0.8	1.63E-05

☐ Enter DS manually

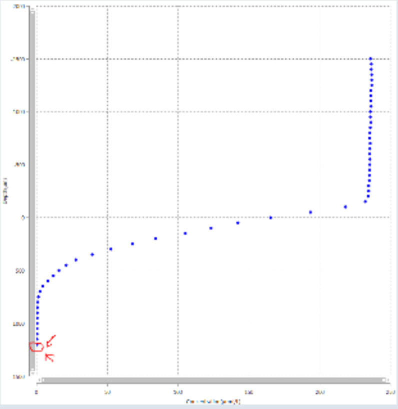
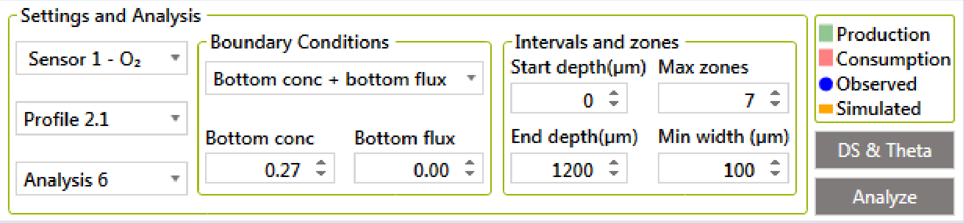


Figure 7: Oxygen microprofile and D_s calculations



Settings and Analysis
Sensor 1 - O_2
Profile 2.1
Analysis 6

Boundary Conditions
Bottom conc + bottom flux
Bottom conc: 0.27
Bottom flux: 0.00

Intervals and zones
Start depth(µm): 0
Max zones: 7
End depth(µm): 1200
Min width (µm): 100

🟩 Production
🟥 Consumption
● Observed
🟧 Simulated

Figure 8: Activity setting

When you have entered all the above information click **Analyze**.
After the first analysis, inspect the results and change settings to see if a better analysis can be made.

Results

The results of the model calculation are listed in the Statistics table and the Profile figure.
When you receive the results from the model it is important to verify if the results are scientifically correct. Below we will give you some factors you should give special attention to:

1. The yellow modeled profile
2. The volume based rate calculations
3. Zone number and statistics
4. Integrated production and consumption rates

A model is good if the yellow modeled profile is placed on top of the measured values at all depths. The green and red bars show the volume specific rate in the different depth zones.

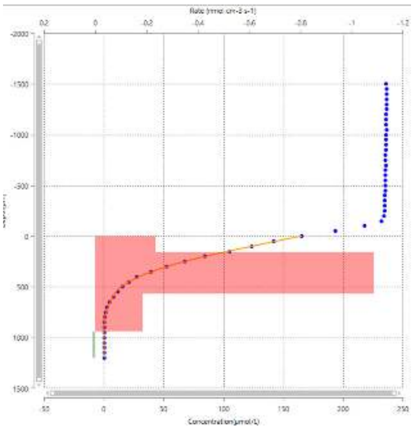
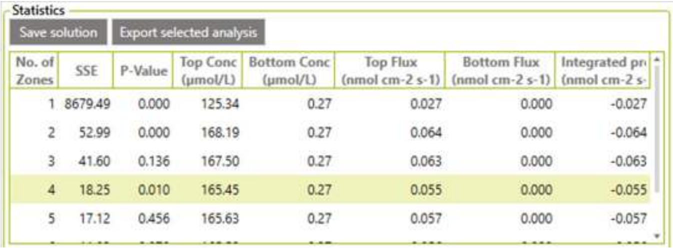


Figure 9: Modeled profile and specific oxygen consumption and production rates after 1st analysis

In the statistics table (figure 10), the model highlights the row with the optimal number of zones based on the statistics. The SSE indicates how well the measured and modeled profiles fit - the lower the SSE value the better. The P-Value may be used for selection of the best number of zones. The P-Value for n zones indicates whether increasing the number of zones from n - 1 to n resulted in a significantly improved fit.

Often $P < 0.05$ is used as the criterion. In Figure 10, going from 3 to 4 zones gave a significantly better fit ($P = 0.010$), whereas going from 4 to 5 zones did not ($P = 0.456$). . In the table you also find the calculated oxygen flux and the integrated oxygen consumption or production rates.


Statistics

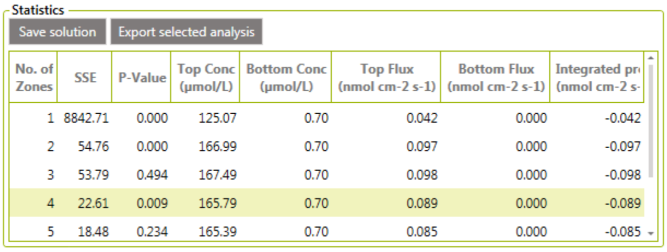
No. of Zones	SSE	P-Value	Top Conc (µmol/L)	Bottom Conc (µmol/L)	Top Flux (nmol cm-2 s-1)	Bottom Flux (nmol cm-2 s-1)	Integrated pr (nmol cm-2 s-
1	8679.49	0.000	125.34	0.27	0.027	0.000	-0.027
2	52.99	0.000	168.19	0.27	0.064	0.000	-0.064
3	41.60	0.136	167.50	0.27	0.063	0.000	-0.063
4	18.25	0.010	165.45	0.27	0.055	0.000	-0.055
5	17.12	0.456	165.63	0.27	0.057	0.000	-0.057

Figure 10: Statistics after 1st analysis

In our model system, 4 zones provides the best statistical values and an integrated oxygen consumption rate of 0.055 nmol cm^{-2} s^{-1}.

However, from the figure, we can see that the integrated rate was based on an oxygen production rate at the bottom of the profile, which scientifically is very unlikely and due to variation in data. To avoid this, we changed the depth interval to maximum depth of 850 µm. At 850 µm, the bottom oxygen concentration is 0.70 µM, which is used as the boundary conditions under 'Bottom concentration'.

Running **Analyze** with the new parameters gave the following result:


Statistics

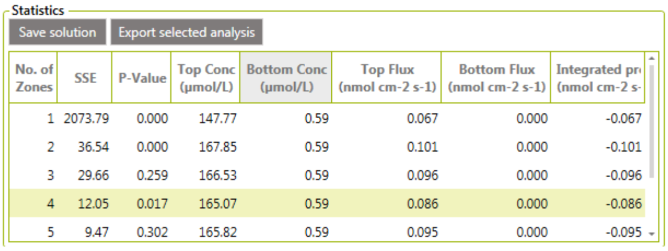
No. of Zones	SSE	P-Value	Top Conc (µmol/L)	Bottom Conc (µmol/L)	Top Flux (nmol cm-2 s-1)	Bottom Flux (nmol cm-2 s-1)	Integrated pr (nmol cm-2 s-
1	8842.71	0.000	125.07	0.70	0.042	0.000	-0.042
2	54.76	0.000	166.99	0.70	0.097	0.000	-0.097
3	53.79	0.494	167.49	0.70	0.098	0.000	-0.098
4	22.61	0.009	165.79	0.70	0.089	0.000	-0.089
5	18.48	0.234	165.39	0.70	0.085	0.000	-0.085

Figure 11: Statistics after 2nd analysis

Again the model suggests that 4 intervals result in the best solution (Figure 11). This provides an integrated oxygen consumption rate of 0.056 nmol cm^{-2} s^{-1}. The SSE value is lower than in the first analysis, whereas the P-value is a bit higher.

In an attempt to improve the fit we changed the boundary conditions because at a depth of 850 µm there is still oxygen and a small oxygen flux is expected in the sediment. Therefore, we changed the boundary conditions from 'Bottom conc + bottom flux' to 'Top conc + bottom conc' and made a third analysis. The result gave an optimal zone number of 3 and an integrated oxygen consumption rate of 0.056 nmol cm^{-2} s^{-1} (Figure 12 and 13). The statistical values were now better than the previous solutions with an SSE value of 7.81 and a P-value of 0.001.

After trying to change other parameters (see also 'Play around' below), we decided to use the data from the 3rd analysis as our final result. We recommend to make similar calculations for minimum two more profiles from the same location.


Statistics

No. of Zones	SSE	P-Value	Top Conc (µmol/L)	Bottom Conc (µmol/L)	Top Flux (nmol cm-2 s-1)	Bottom Flux (nmol cm-2 s-1)	Integrated pr (nmol cm-2 s-
1	2073.79	0.000	147.77	0.59	0.067	0.000	-0.067
2	36.54	0.000	167.85	0.59	0.101	0.000	-0.101
3	29.66	0.259	166.53	0.59	0.096	0.000	-0.096
4	12.05	0.017	165.07	0.59	0.086	0.000	-0.086
5	9.47	0.302	165.82	0.59	0.095	0.000	-0.095

Figure 11: Statistics after 3rd analysis

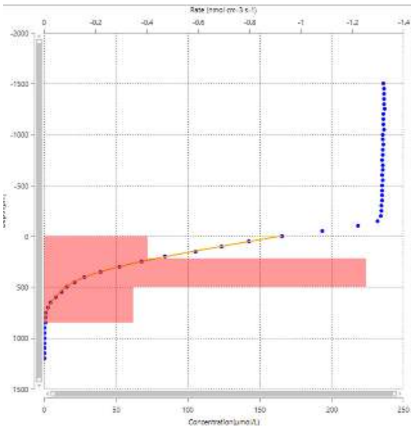


Figure 13: Modeled profile and specific oxygen consumption rates after 3rd analysis

Play around

The quality of the model depends on the input data. Some input data are associated with relatively high uncertainty – e.g. the porosity. In order to get a feel for how sensitive the fit and the calculated rates are to the input data, we recommend to play around with the different input information - e.g.:

1. Boundary conditions
2. Depth interval
3. The oxygen diffusion rate - e.g. by changing the temperature and salinity
4. Change the formula for the D_s calculation
5. Porosity

In our model a change of 2-3 °C or 2-3 ‰ in the calculation of D_0 did not give an important change in our results, and neither did a change in the formula from $D_s = D_0 \times \phi$ to $D_s = D_0 \times \phi 2$ or changing the porosity from 0.8 to 0.85.

Final result

Using the SensorTrace Profiling software on a high-resolution oxygen profile made in an organic rich sediment core from Limfjorden in Denmark, we found that the oxygen penetration was approximately 950 μm and the integrated oxygen consumption rate was 0.057 nmol cm^{-2} s^{-1}. The highest specific oxygen consumption rate, 1.25 nmol cm^{-3} s^{-1}, was found at approx. 200 μm to 500 μm sediment depth.

These oxygen consumption rates are similar to the rate found in similar organic rich sediments (e.g. Glud, 2008, Epping et al 1999).

Other solutes: The consumption and production rate of solutes like H_2S, H_2, and N_2O can also be calculated in SensorTrace Profiling from high resolution profiles.

The general procedure for other solutes is the same as for oxygen, although the inputs may vary depending on the profile. For example, the sulfide concentration is often 0 at the surface of the sediment and high at the bottom, therefore the boundary condition 'top conc and top flux' of 0 is often used. The Diffusion coefficient (D_0) for other gasses than oxygen can be calculated from the oxygen table "Seawater and Gases Table" found www.unisense.com under Knowledge/Technical Information, by multiplying the table values with a constant specific for the different solutes: for H_2S multiply by 0.7573, for H_2 with 1.9470 and for N_2O with 1.0049 (for more information see "Seawater and Gases Table").

References: Boudreau, B.P. 1984, On the equivalence of nonlocal and radial-diffusion models for porewater irrigation.
J. Mar. Res. 42: 731-735

Epping et al 1999, Photosynthesis and dynamics of oxygen consumption in a microbial mat calculated from transient oxygen microprofiles. *Limnology and Oceanography. 44(8): 1936-1948.*

Glud, N. R. 2008. Oxygen dynamics of marine sediments.
Marine Biology Research 4: 243-289.

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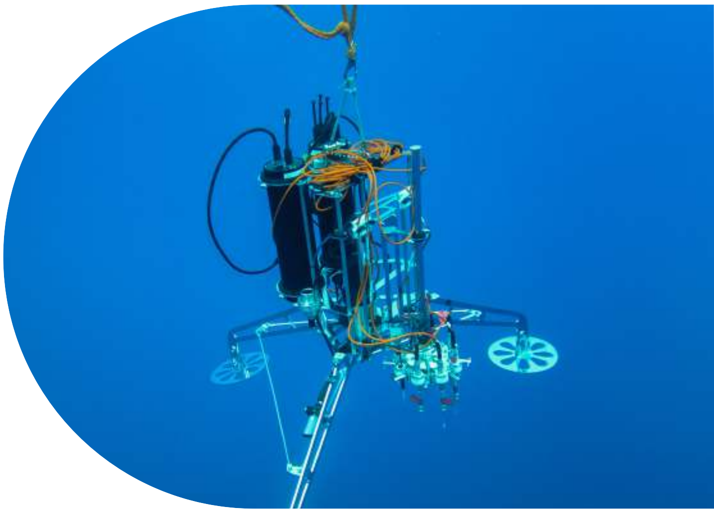

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