UNISENSE

# Calculations of oxygen consumption rate using SensorTrace Profiling


## Abstract

This note will explain 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 Unisense MicroProfiling System.
As an example we will 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 made estimates for 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.
Sum of squared error (SSE) and the *p*-value together with the modeled graph are used 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$^{-1}$, which are comparable to rates found in similar environments (Glud, N. R. 2008, Epping et al 1999).

The oxygen profile used in this note is available in the 'Unisense Data' folder under 'Demo Experiments' and you can use it for practice purposes.


## Material and Method

Sediment cores were collected by hand at Aggersund, Limfjorden, Denmark in August 2015 at a water depth of about 30 cm and brought to the Unisense lab. Here the sediment core was placed into a container with brackish water (15 ‰ salinity) collected at the same location as the sediment, and stored at *in-situ* temperature, about 20 °C.
The water was flushed with air using an aquarium pump and a bubble stone making sure that there was a good circulation and that a well defined Diffusive Boundary Layer (DBL) was established just above the sediment-water interface (figure 2 and 3).

Oxygen microprofiles were made by using a motorized MicroProfiling System and an oxygen microsensor with a tip size of 50 µm (OX-50). SensorTrace Profiling was used 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.

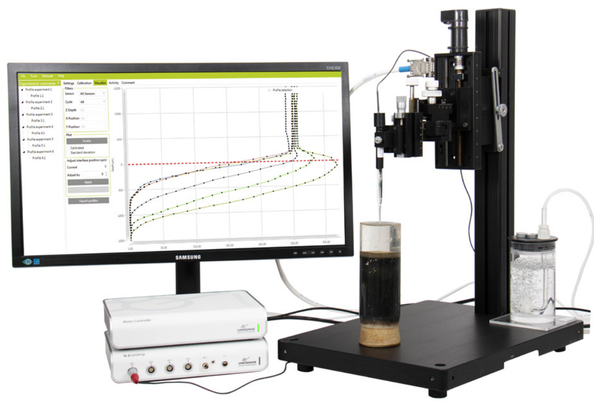


*Figure 1: Typical MicroProfiling set-up in the laboratory*

## 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 is occurring 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.

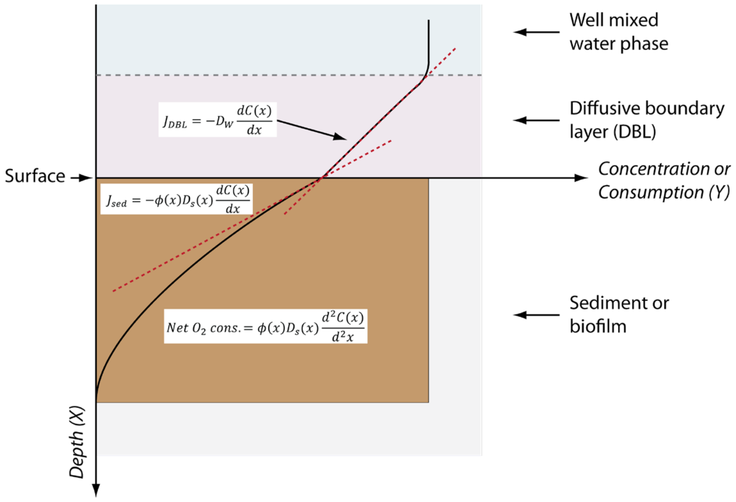


*Figure 2: A typical oxygen profile in sediments with a well-mixed water phase above and a diffusive boundary layer right above the sediment surface. When the profile is a straight line, as in the Diffusive Boundary Layer, there is no net production or consumption, just a diffusive transport. Fluxes 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

In the Visualization window of SensorTrace Profiling the 0-line of the profile can be adjusted. The water - sediment is typically set to 0 µm depth. The profile with the adjusted 0-line can be used in the Activity window.

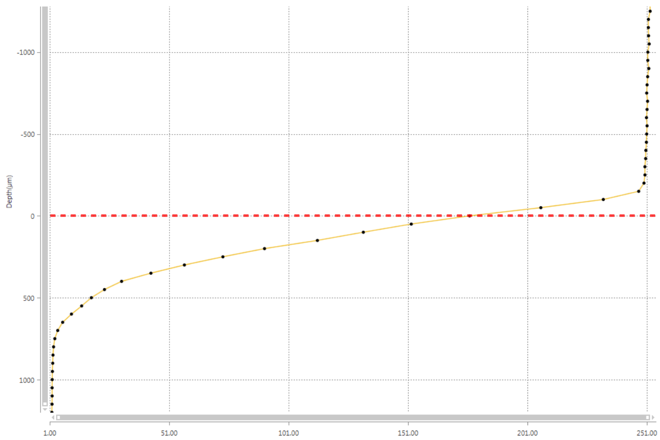


*Figure 3: Oxygen microprofile in a sediment. Use the red line to adjust the water – sediment interface.*

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

## Activity

In the Activity window of SensorTrace Profiling the consumption and production rates are calculated from the oxygen microprofile by using the one-dimensional mass conservation model. Before making the calculations the model needs various information that you have to provide:

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 $D_s$ determination

Below we will give examples of information that can be provided 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).

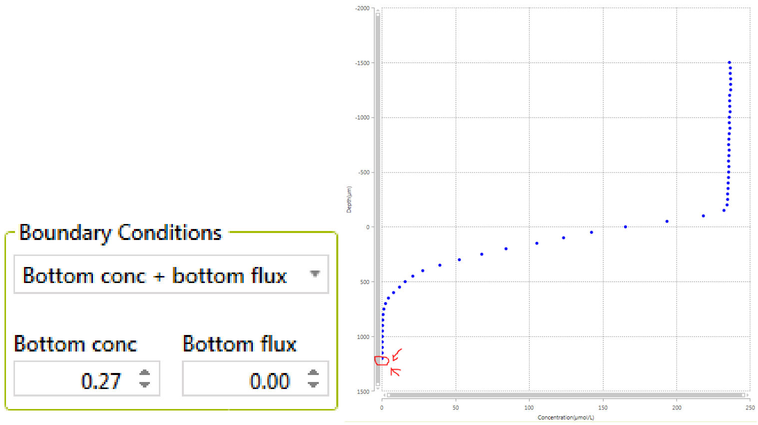


*Figure 4 Boundary condition: Boundary condition "Bottom conc + bottom flux"*

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 deep down in the profile.

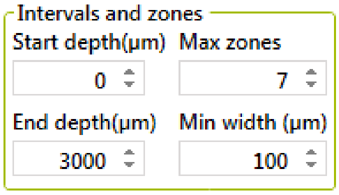


*Figure 5 Settings for 'Intervals and zones'*

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.

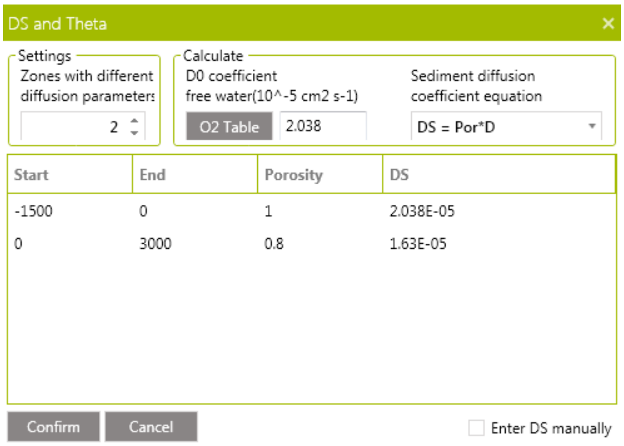


*Figure 6: Settings for 'Intervals and zones'*

## Diffusion rate of oxygen

In the Ds 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 ($\phi$). 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.
In the sediment from Limfjorden the overlying water had a bottom temperature of 20 °C and a salinity of 15 ‰ which gives a $D_0$ of 2.038 $10^{-5}$ $cm^2$ $s^{-1}$. $D_s$ 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** 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.


*Figure 7: Oxygen microprofile and $D_s$ calculations*

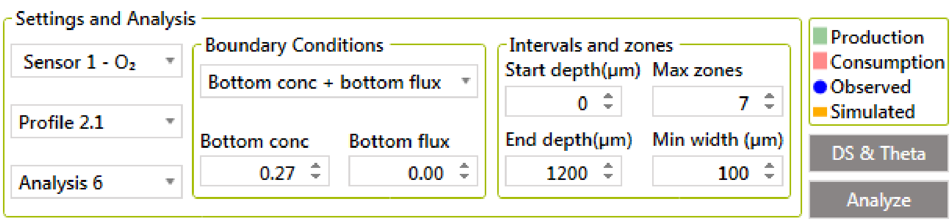


*Figure 8: Activity setting*

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.

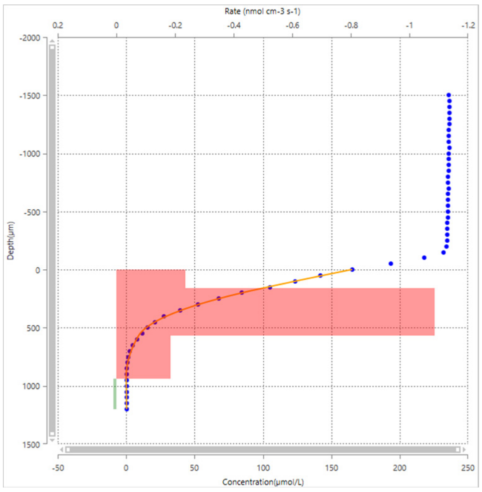


*Figure 9: Modeled profile and specific oxygen consumption and production rates after 1st analysis*

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

Save solution | Export selected analysis

| 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 gives 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, the depth interval was changed 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 these new parameters gave the following result:

Statistics

Save solution | Export selected analysis

| 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 | 1284.13 | 0.000 | 152.07 | 0.70 | 0.046 | 0.000 | -0.046 |
| 2 | 36.47 | 0.000 | 168.25 | 0.70 | 0.065 | 0.000 | -0.065 |
| 3 | 17.75 | 0.028 | 166.04 | 0.70 | 0.060 | 0.000 | -0.060 |
| 4 | 9.21 | 0.048 | 165.33 | 0.70 | 0.056 | 0.000 | -0.056 |
| 5 | 7.99 | 0.429 | 165.39 | 0.70 | 0.057 | 0.000 | -0.057 |

*Figure 11: Statistics after 2nd analysis*

Again the model suggests that 4 intervals result in the best solution (Figure 11), giving an integrated oxygen consumption rate of 0.056 nmol cm$^{-2}$ s$^{-1}$. The SSE values 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 a SSE value of 7.81 and a P-value of 0.001.

After trying to change other parameters (see also 'Play around' section) 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

Save solution | Export selected analysis

| 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 | 188.28 | 0.000 | 165.31 | 0.70 | 0.059 | -0.009 | -0.068 |
| 2 | 47.46 | 0.003 | 165.31 | 0.70 | 0.063 | -0.001 | -0.064 |
| 3 | 7.81 | 0.001 | 165.31 | 0.70 | 0.056 | -0.001 | -0.057 |
| 4 | 5.34 | 0.151 | 165.31 | 0.70 | 0.060 | -0.001 | -0.061 |
| 5 | 4.65 | 0.433 | 165.31 | 0.70 | 0.061 | -0.001 | -0.062 |

*Figure 12: Statistics after 3rd analysis*

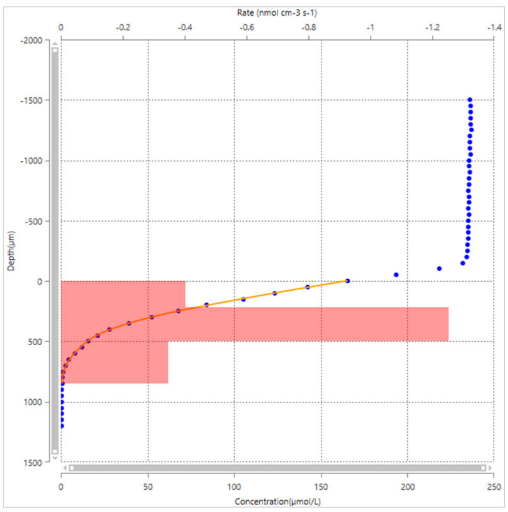


*Figure 13: Modeled profile and specific oxygen consumption rates after 3rd analysis*


## Play around

The quality of the model depends on the input data. Some input data are associated with relative 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 Ds 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, 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 support, 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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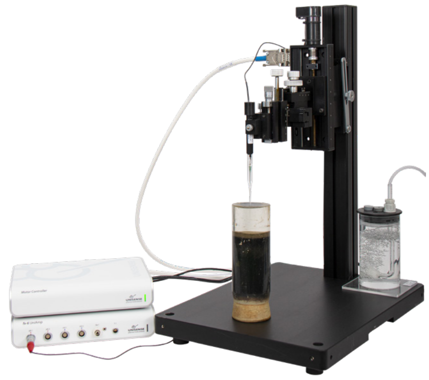

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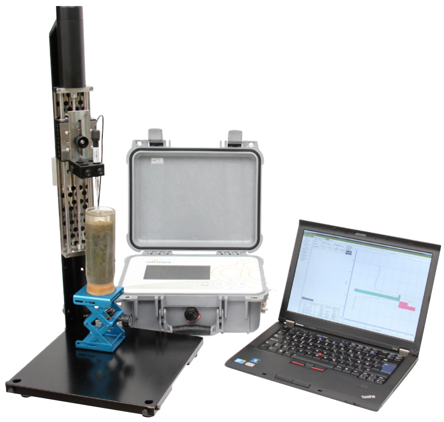

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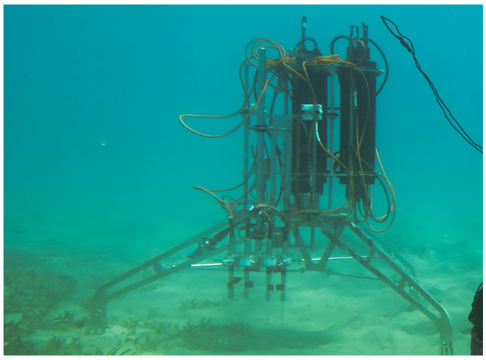

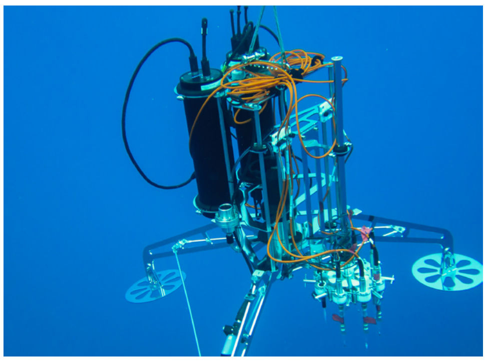

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