UNISENSE

O_2 N_2O H_2 NO H_2S Redox Temp Opto pH EP

The Microsensor Company

Demonstration of Activity Calculation - Software

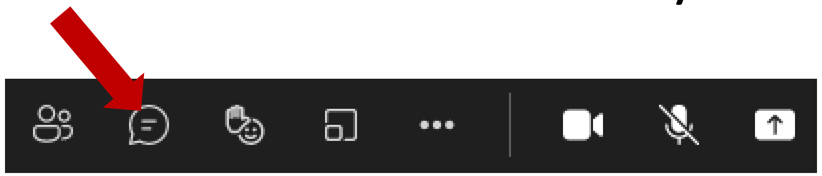
February 2022
Tage Dalsgaard

UNISENSE

A few rules before we get started

1. Please turn off your microphone

2. Questions: During lecture please use chat.
   After lecture you can unmute and ask.



Very application-specific questions may be better answered in a private session afterwards.

You will get access to all the presentations as PDF´s + recordings shortly after the workshop.

Online Biogeochemistry Workshop

Wednesday 23 February
14:30-15:30 CET - Introduction to Microsensors
15:45-16:45 CET - Lab-based Studies

Thursday 24 February
14:30-15:30 CET - Field Studies
15:45-16:30 CET - Demonstration of Field Microprofiling System
16:45-17:30 CET - Demonstration of Activity Calculation - Software

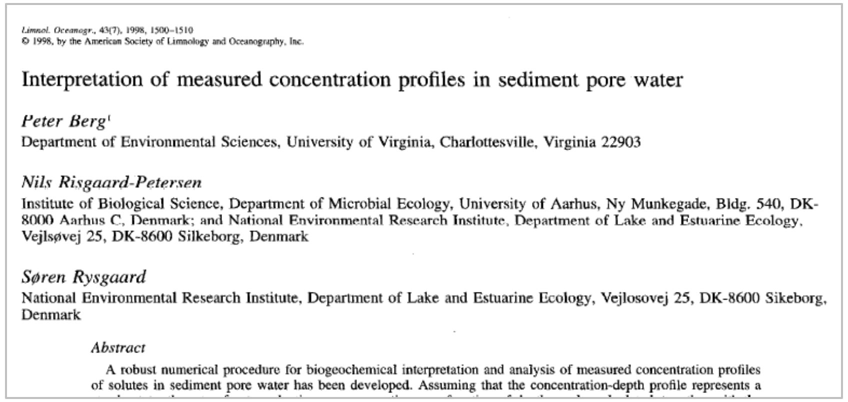
UNISENSE

Profile analysis

Calculation of production and consumption rates from microprofiles

Based on the method from:

Berg, P., N. Risgaard-Petersen, and S. Rysgaard. 1998. Interpretation of measured concentration profiles in sediment pore water. Limnol. Oceanogr. 43: 1500–1510.



Limnol. Oceanogr., 43(7), 1998, 1500–1510

Interpretation of measured concentration profiles in sediment pore water

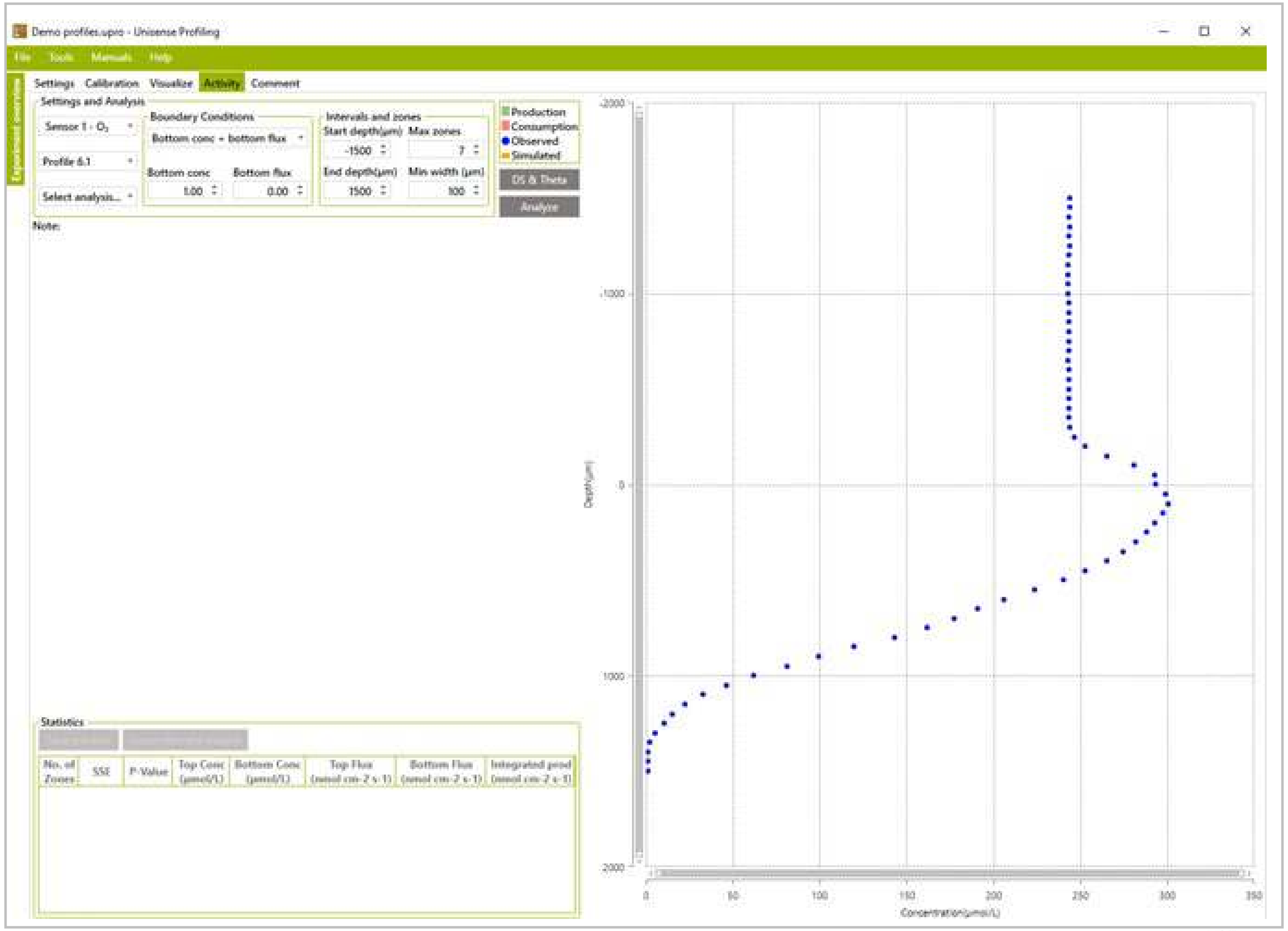
Peter Berg[1]
Department of Environmental Sciences, University of Virginia, Charlottesville, Virginia 22903

Nils Risgaard-Petersen
Institute of Biological Science, Department of Microbial Ecology, University of Aarhus, Ny Munkegade, Bldg. 540, DK-8000 Aarhus C, Denmark; and National Environmental Research Institute, Department of Lake and Estuarine Ecology, Vejlsøvej 25, DK-8600 Silkeborg, Denmark

Søren Rysgaard
National Environmental Research Institute, Department of Lake and Estuarine Ecology, Vejlosovej 25, DK-8600 Sikeborg, Denmark

Abstract

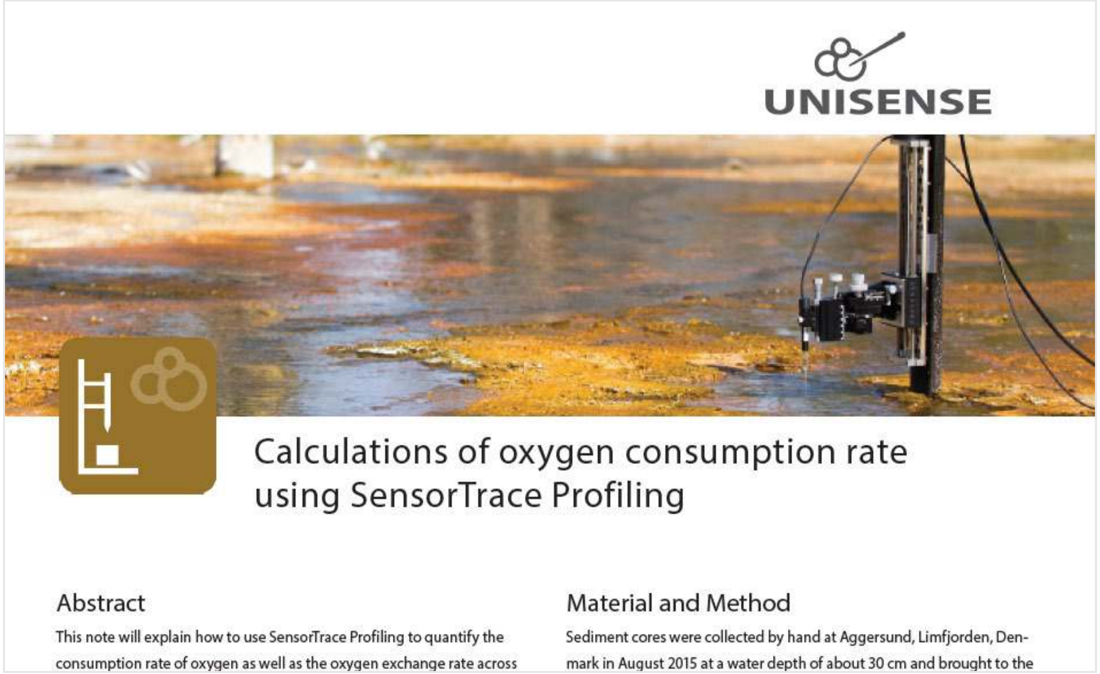
A robust numerical procedure for biogeochemical interpretation and analysis of measured concentration profiles of solutes in sediment pore water has been developed. Assuming that the concentration-depth profile represents a



Demo profiles

Demonstration profiles installed with *SensorTrace Suite*

- ProfilingDemo.upro – Read only
    - \Documents\Unisense Data\Demo Experiments
- Profiling application note
    - Unisense.com



UNISENSE

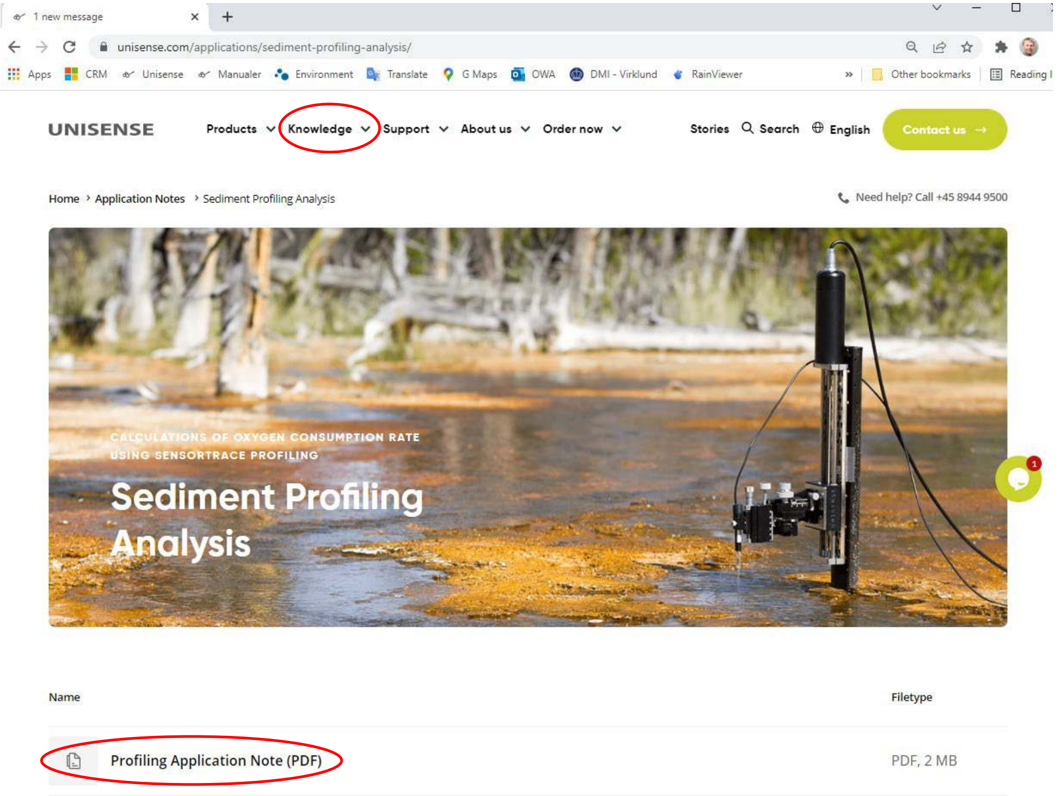
Calculations of oxygen consumption rate using SensorTrace Profiling

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

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

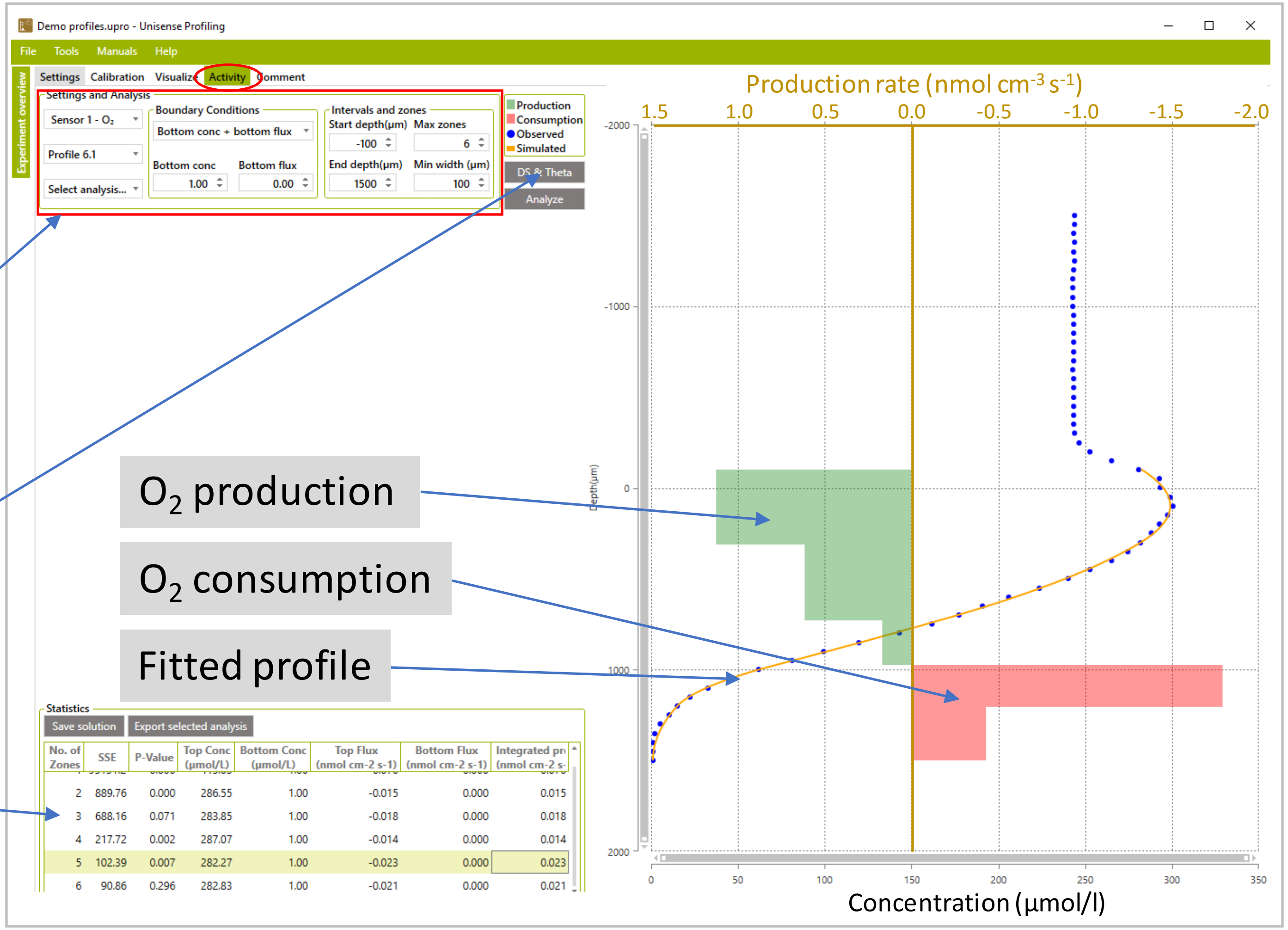
Profile analysis

Calculation of production and consumption rates from microprofiles

Select profile, depth range and boundary conditions

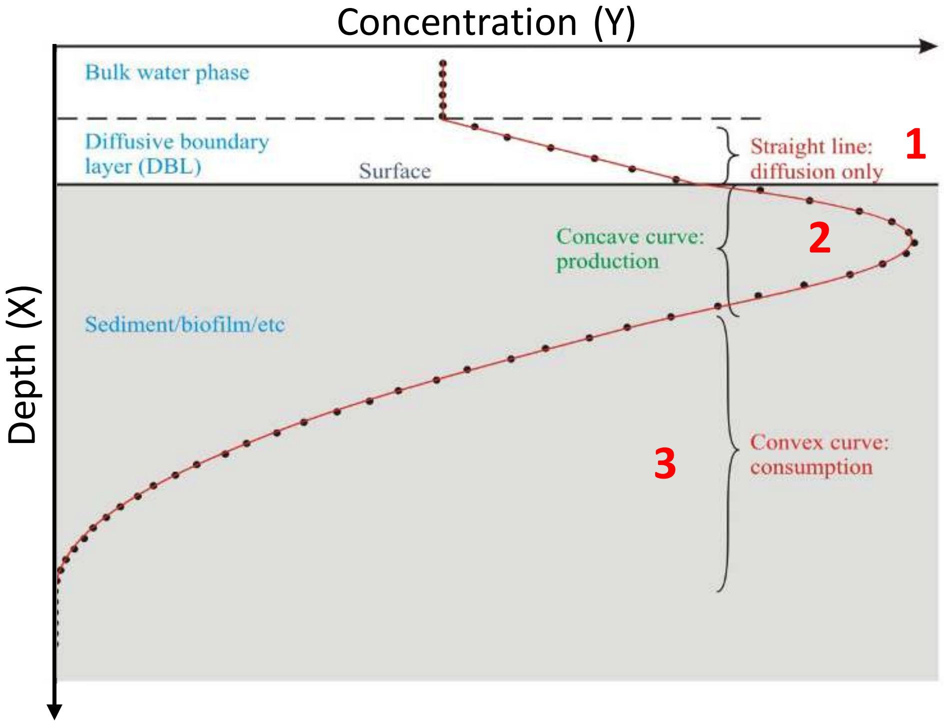
Specify diffusion coefficient and porosity

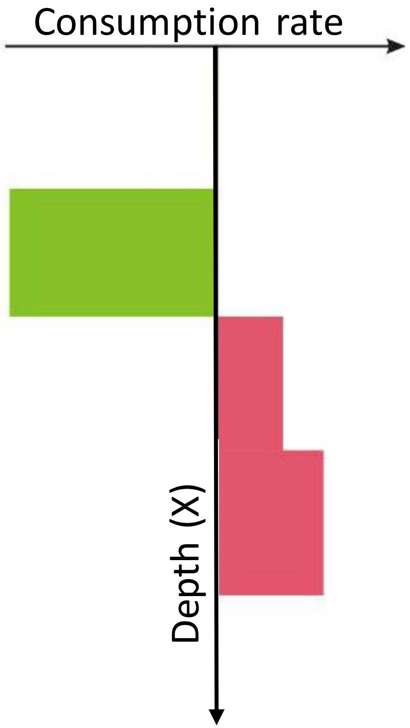
Output with rates and statistic parameters



Microprofiles - Theory

Example:
Biofilm with O_2 production in top layer, O_2 consumption below



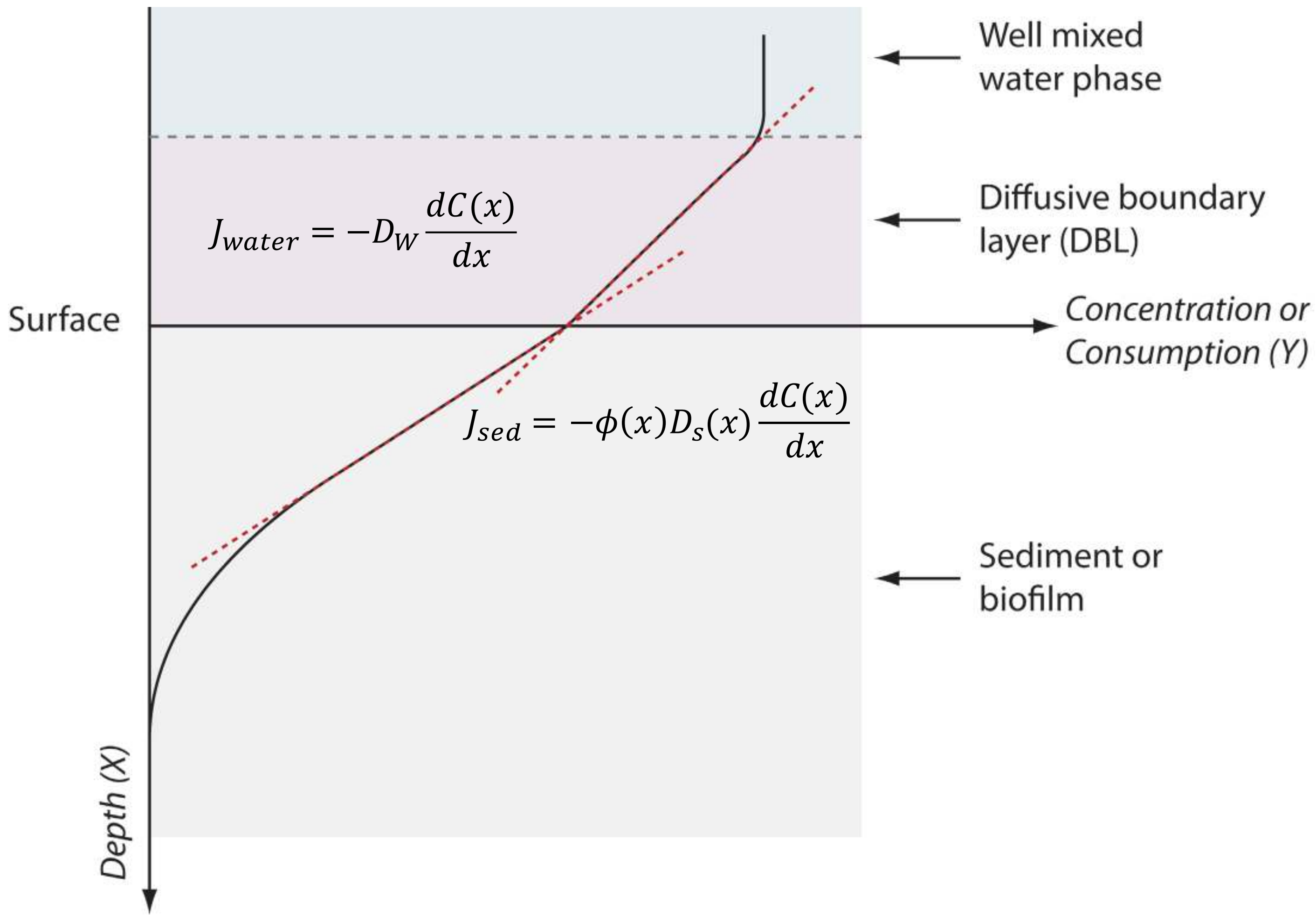


Qualitative information from profiles

1. Straight line: No net consumption or production – only diffusional transport.
2. Concave: Net production (e.g. O_2 production by photosynthesis, H_2S production by sulphate reduction)
3. Convex: Net consumption (e.g. Respiration, oxidation of reduced compounds)

Microprofiles - Theory

1-dimensional system – Steady state



Quantitative Information from microprofiles

1. **C(x) - Concentration**: Penetration depth, overlapping zones
2. **dC(x)/dx – Flux:** Into sediment, within sediment

D_w = Diffusion coefficient in water

$\phi(x)$ = Porosity

$D_s(x)$ = Diffusivity

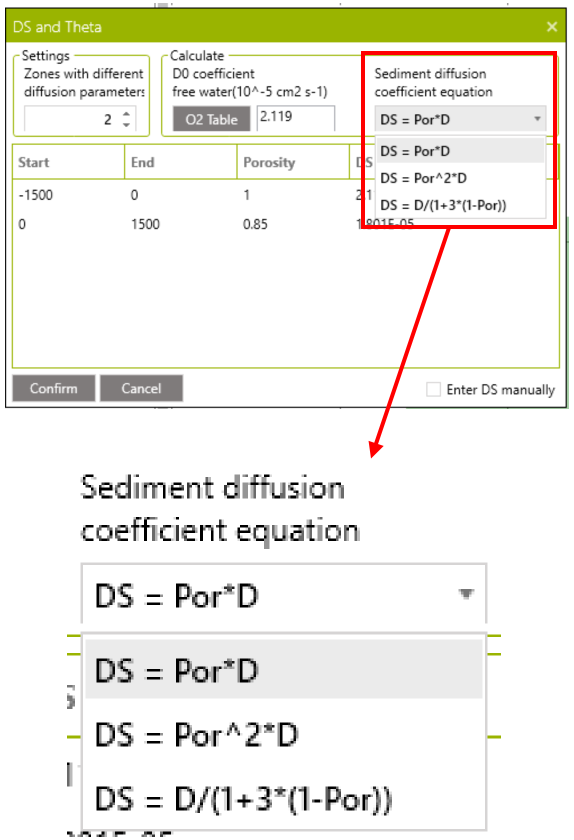
$D_s(x)$ = $D_w \times \phi(x)$ (simplest form)

UNISENSE

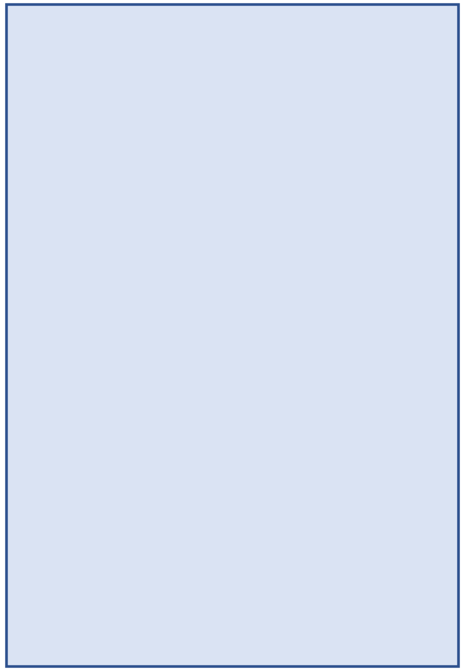
Diffusion in pure water and sediment

$$J_w = -D_W \frac{dC(x)}{dx}$$

$$J_{sed} = -\phi(x) D_s(x) \frac{dC(x)}{dx}$$

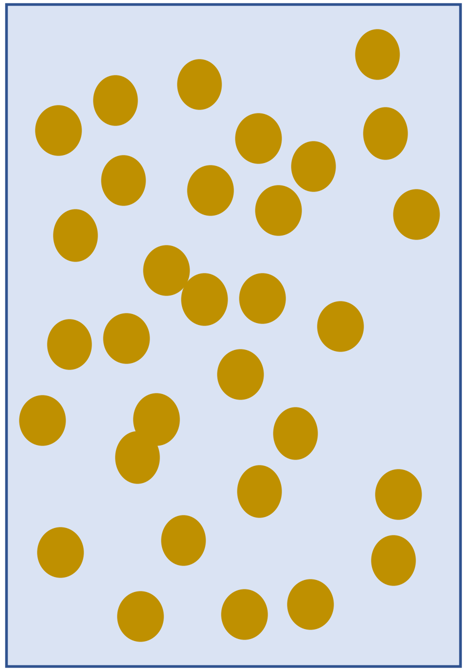


Pure water



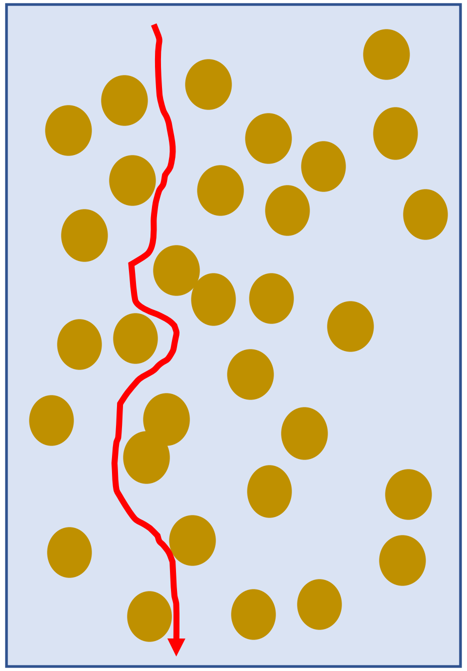
100% space for diffusion
Random movement

Porosity



Example:
Porosity = 0.8 =>
80% space for diffusion

Tortuosity

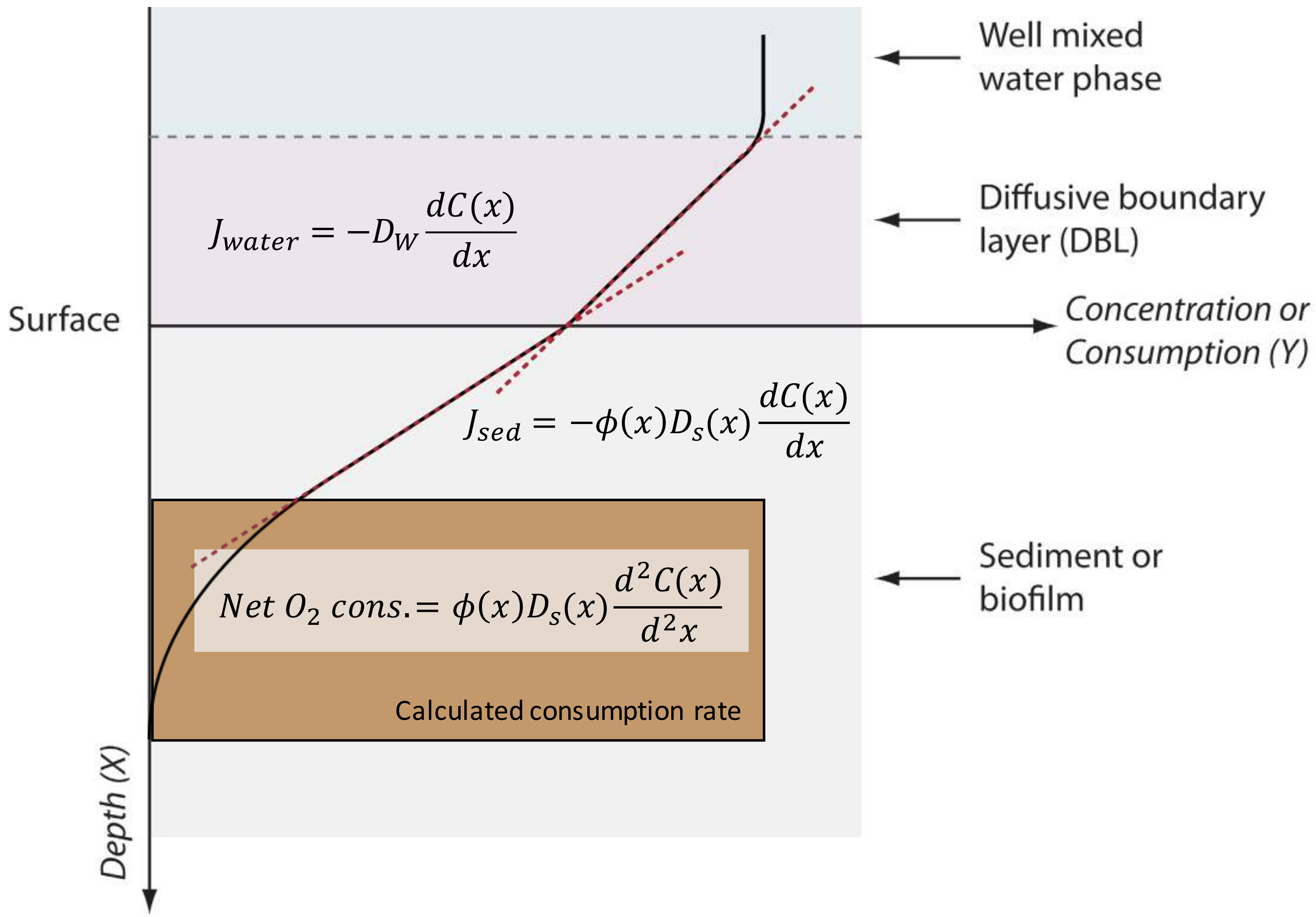


Longer diffusion path
Ds (x) = Dw × Porosity

UNISENSE

Microprofiles - Theory

1-dimensional system – Steady state



Quantitative Information from microprofiles

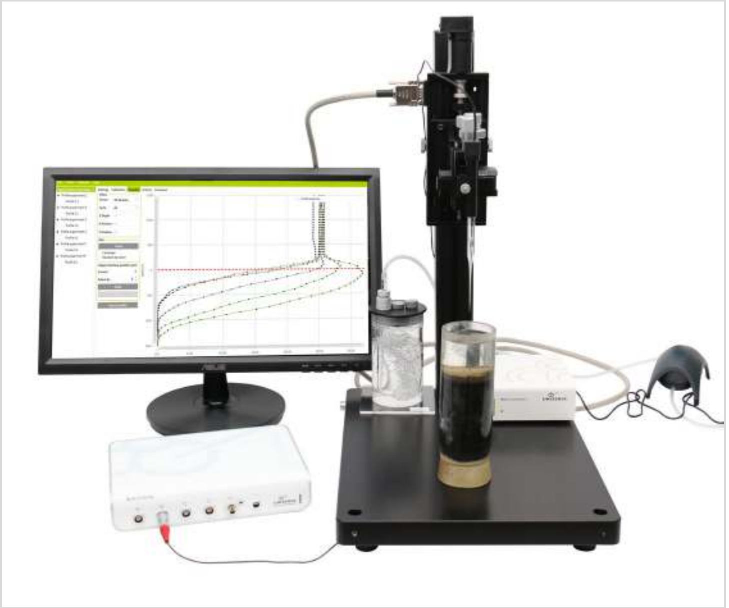
1. **C(x) - Concentration**: Penetration depth, overlapping zones
2. **dC(x)/dx – Flux:** Into sediment, within sediment
3. **$d^2C(x)/dx^2$ – Production and consumption:** Activity distribution within the sediment

D_w = Diffusion coefficient in water
$\phi(x)$ = Porosity
$D_s(x)$ = Diffusivity
$D_s(x)$ = $D_w \times \phi(x)$ (simplest form)

UNISENSE

Microprofiles from different instruments

Lab Microprofiling System

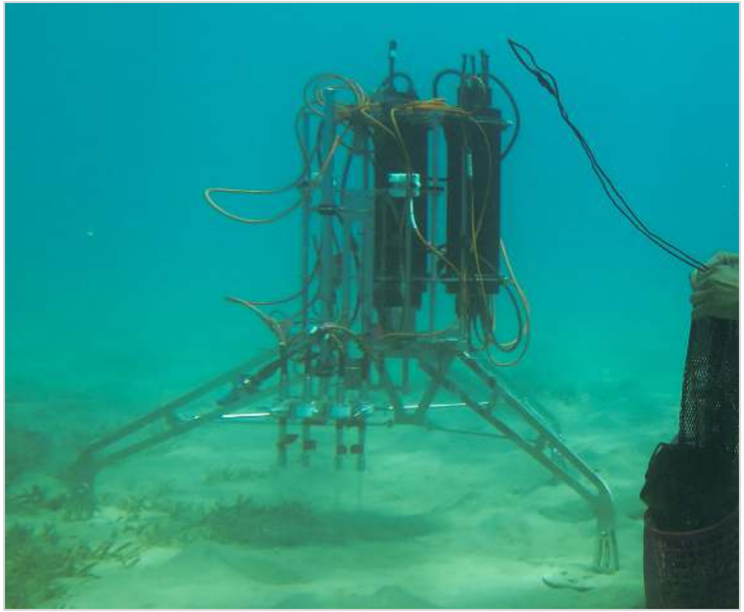


Lab conditions

Field Microprofiling System

Down to 10 m water depth

In situ Microprofiling System



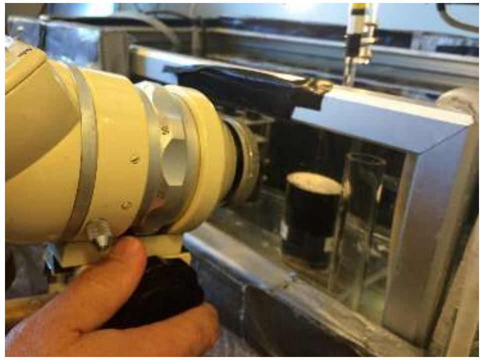
Down to 6000 m water depth

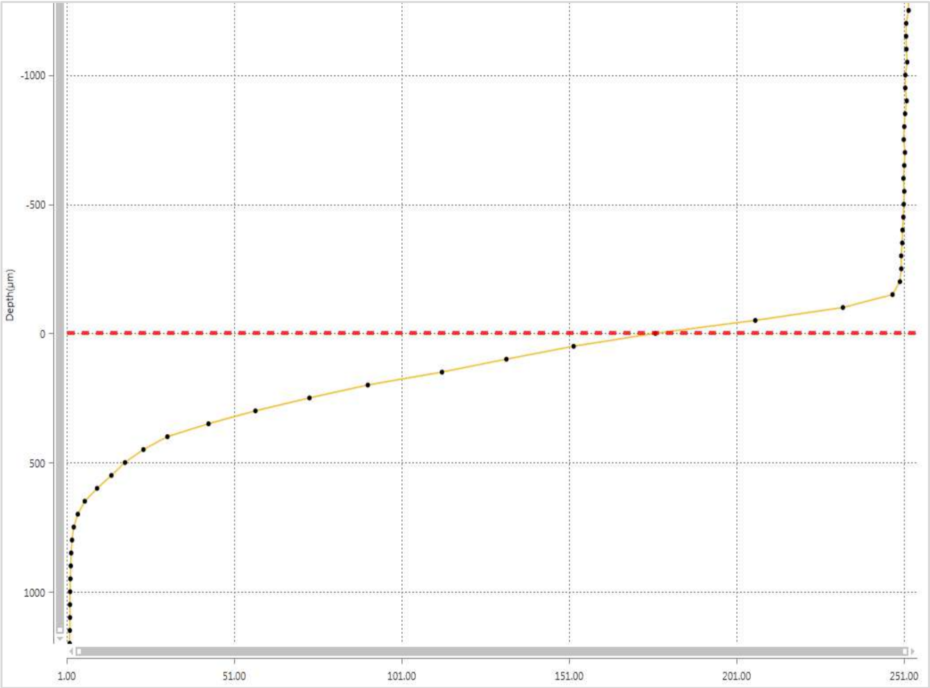
SensorTrace Profiling will record or import profiles from all system for analysis

UNISENSE

Find the sediment surface

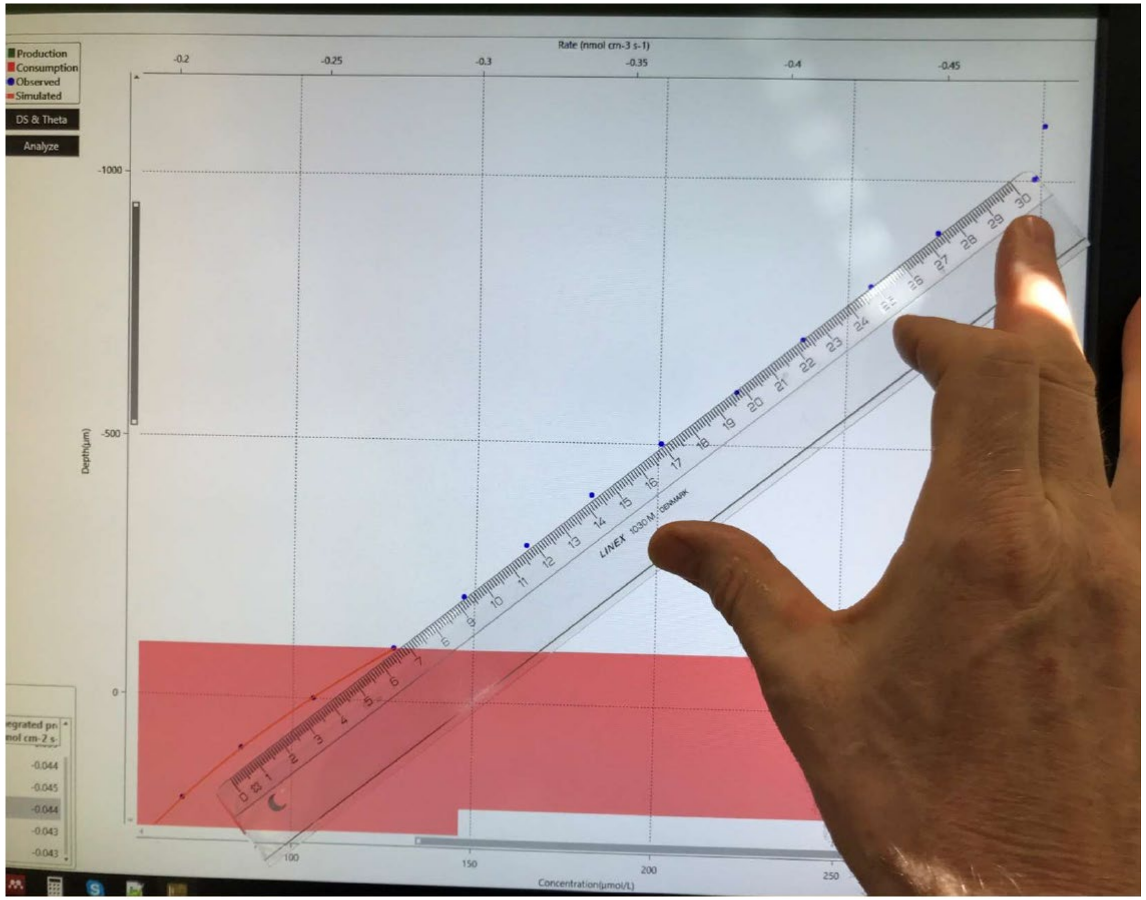
Stereo microscope while measuring





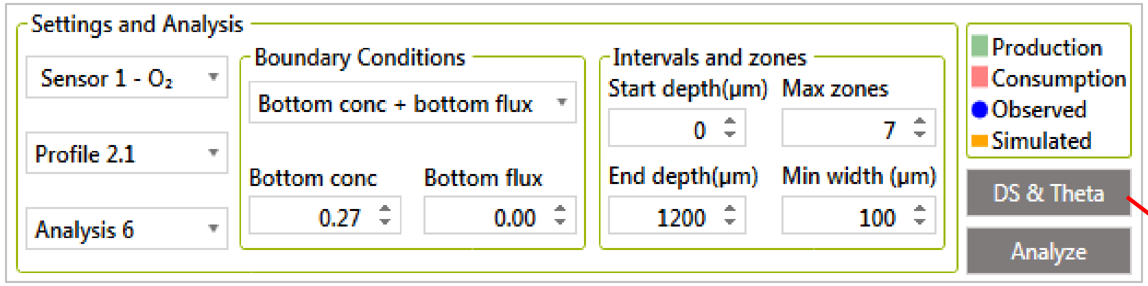
Find the sediment surface

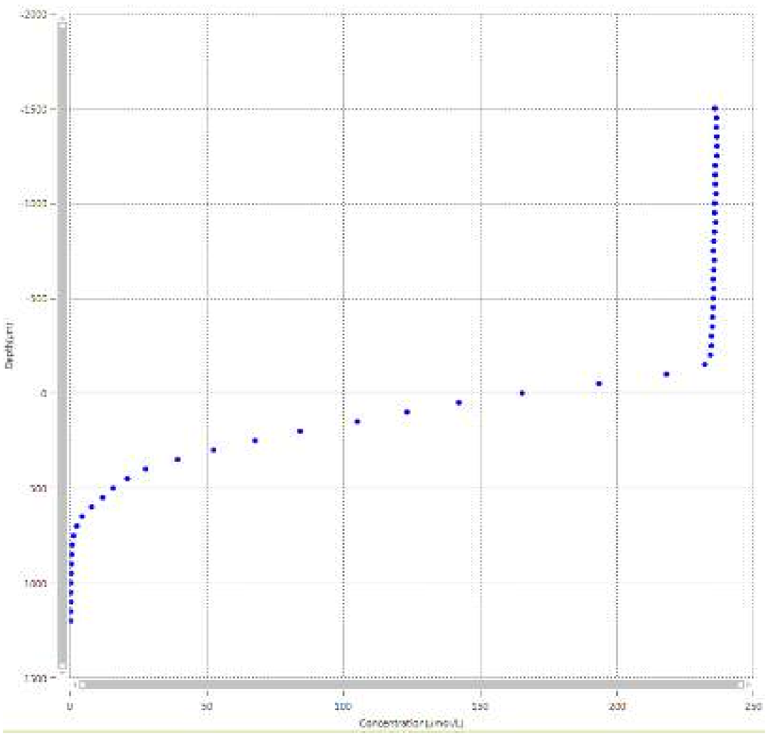
Locate surface after measuring

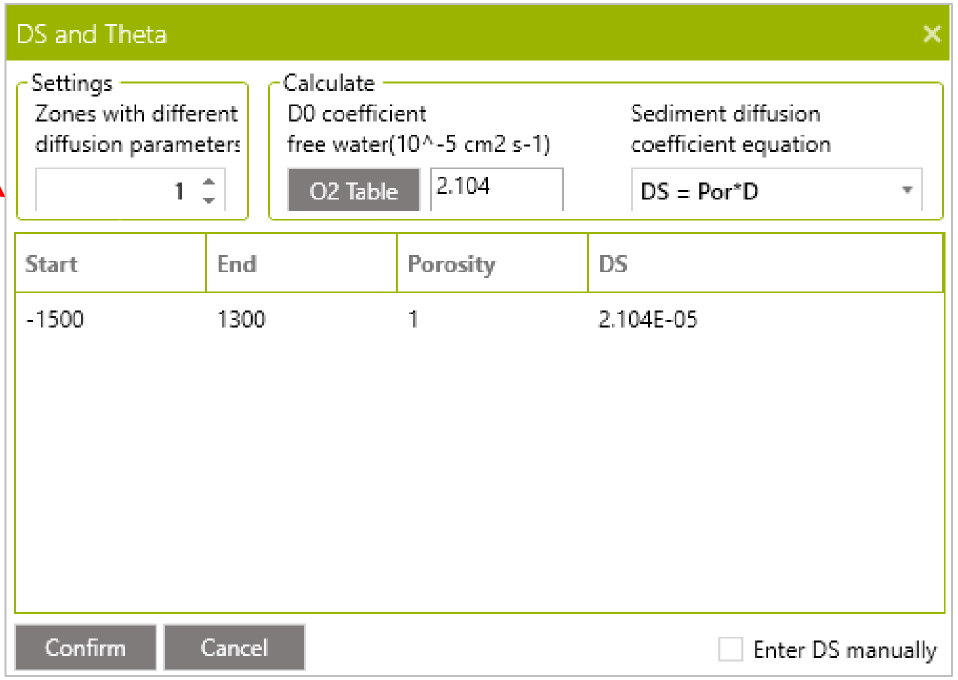


UNISENSE

Setting depth interval and boundary conditions

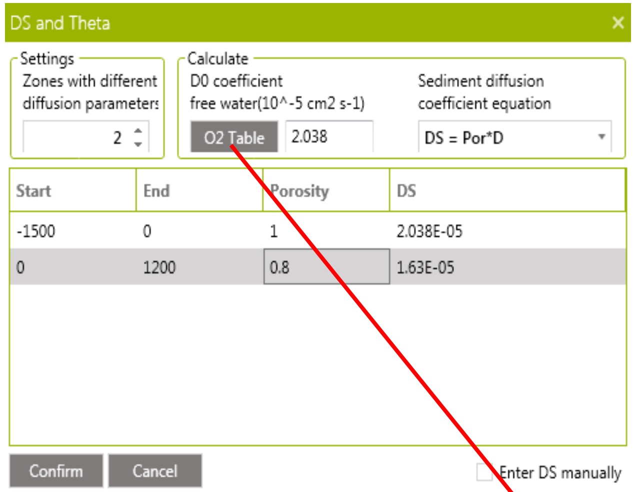


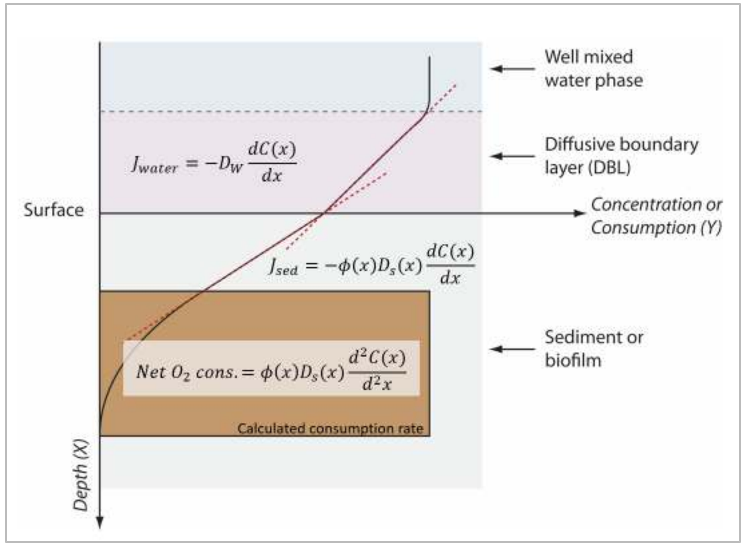




Diffusion coefficient

- Enter the diffusion coefficient for O_2 in water
- Depends on salinity and temperature
- As many depth intervals as you like



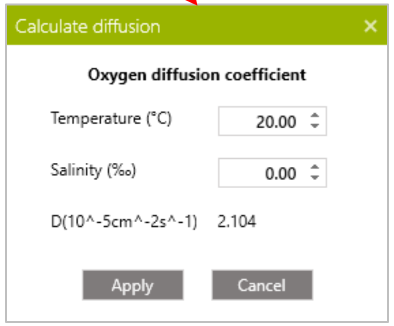


DATA-TABLE 1 *by Niels Ramsing & Jens Gundersen*

Diffusion coefficient for oxygen at different temperatures and salinities of seawater

Units: 10^-5 cm2 s-1

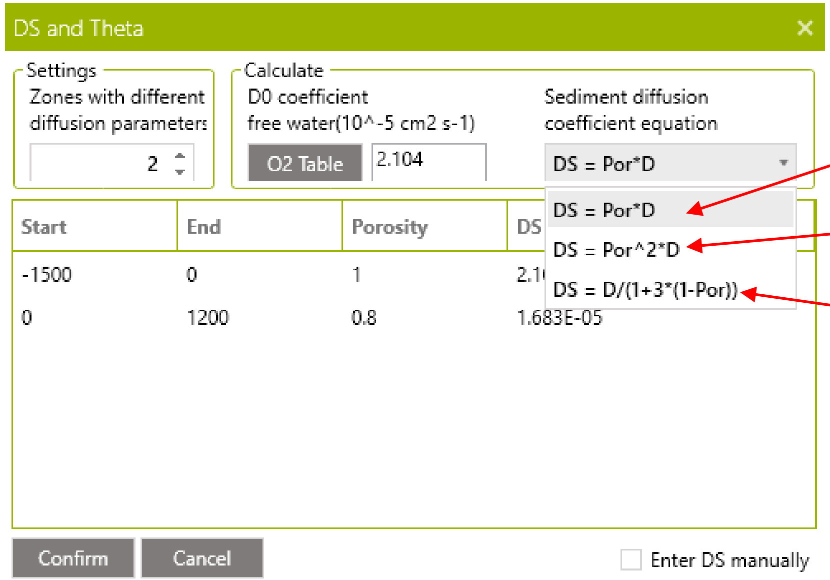
Salinity (‰)	Temperature (°C) 0.0	1.0	2.0	3.0	4.0	5.0	6.0	7.0	8.0	9.0	10.0	11.0	12.0	13.0	14.0	15.0	16.0
0.0	1.1041	1.1465	1.1899	1.2344	1.2798	1.3261	1.3734	1.4214	1.4702	1.5198	1.5700	1.6209	1.6723	1.7243	1.7769	1.8300	1.8836
1.0	1.1026	1.1448	1.1881	1.2324	1.2777	1.3239	1.3709	1.4188	1.4675	1.5169	1.5669	1.6176	1.6689	1.7208	1.7732	1.8261	1.8796
2.0	1.1011	1.1432	1.1863	1.2305	1.2756	1.3216	1.3685	1.4162	1.4647	1.5140	1.5639	1.6144	1.6656	1.7173	1.7695	1.8223	1.8756
3.0	1.0996	1.1415	1.1845	1.2285	1.2735	1.3193	1.3661	1.4137	1.4620	1.5111	1.5608	1.6112	1.6622	1.7137	1.7658	1.8185	1.8717
4.0	1.0981	1.1399	1.1827	1.2266	1.2714	1.3171	1.3637	1.4111	1.4593	1.5082	1.5578	1.6080	1.6588	1.7102	1.7622	1.8147	1.8677
5.0	1.0966	1.1382	1.1809	1.2246	1.2693	1.3148	1.3613	1.4085	1.4566	1.5053	1.5547	1.6048	1.6555	1.7068	1.7586	1.8109	1.8638
6.0	1.0950	1.1366	1.1792	1.2227	1.2672	1.3126	1.3589	1.4060	1.4539	1.5024	1.5517	1.6017	1.6522	1.7033	1.7550	1.8072	1.8599
7.0	1.0935	1.1350	1.1774	1.2208	1.2651	1.3104	1.3565	1.4034	1.4512	1.4996	1.5487	1.5985	1.6489	1.6998	1.7514	1.8034	1.8560
8.0	1.0921	1.1333	1.1756	1.2189	1.2631	1.3082	1.3541	1.4009	1.4485	1.4968	1.5457	1.5953	1.6456	1.6964	1.7478	1.7997	1.8522
9.0	1.0906	1.1317	1.1738	1.2169	1.2610	1.3060	1.3518	1.3984	1.4458	1.4939	1.5427	1.5922	1.6423	1.6930	1.7442	1.7960	1.8483
10.0	1.0891	1.1301	1.1721	1.2150	1.2589	1.3037	1.3494	1.3959	1.4431	1.4911	1.5398	1.5891	1.6390	1.6895	1.7406	1.7923	1.8445
11.0	1.0876	1.1285	1.1703	1.2131	1.2569	1.3015	1.3471	1.3934	1.4405	1.4883	1.5368	1.5860	1.6358	1.6861	1.7371	1.7886	1.8407
12.0	1.0861	1.1268	1.1686	1.2112	1.2549	1.2994	1.3447	1.3909	1.4378	1.4855	1.5339	1.5829	1.6325	1.6828	1.7336	1.7849	1.8369
13.0	1.0846	1.1252	1.1668	1.2093	1.2528	1.2972	1.3424	1.3884	1.4352	1.4827	1.5309	1.5798	1.6293	1.6794	1.7300	1.7813	1.8331
14.0	1.0832	1.1236	1.1651	1.2075	1.2508	1.2950	1.3401	1.3859	1.4326	1.4799	1.5280	1.5767	1.6261	1.6760	1.7265	1.7776	1.8293
15.0	1.0817	1.1220	1.1633	1.2056	1.2488	1.2928	1.3377	1.3835	1.4300	1.4772	1.5251	1.5737	1.6229	1.6727	1.7231	1.7740	1.8256
16.0	1.0802	1.1204	1.1616	1.2037	1.2467	1.2907	1.3354	1.3810	1.4274	1.4744	1.5222	1.5706	1.6197	1.6693	1.7196	1.7704	1.8218
17.0	1.0788	1.1188	1.1599	1.2018	1.2447	1.2885	1.3331	1.3786	1.4248	1.4717	1.5193	1.5676	1.6165	1.6660	1.7161	1.7668	1.8181



UNISENSE

Sediment diffusivity

- How should diffusivity be calculated?



Fine sand/mud with high porosity, biofilm

Compact mud, low porosity

All kinds of sediments

Now a demonstration of the software
ProfilingDemo.upro – Profile 6.1

Porosity measurement

- Core sediment slicing e.g. every 5 mm
- Weight loss after drying / specific density water

UNISENSE

Result – Statistics

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-
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
2	891.00	0.000	286.74	1.00	-0.015	0.000	0.015
3	688.98	0.071	284.07	1.00	-0.018	0.000	0.018
4	219.23	0.002	287.24	1.00	-0.014	0.000	0.014
5	102.52	0.007	282.56	1.00	-0.023	0.000	0.023
6	93.61	0.361	283.10	1.00	-0.021	0.000	0.021

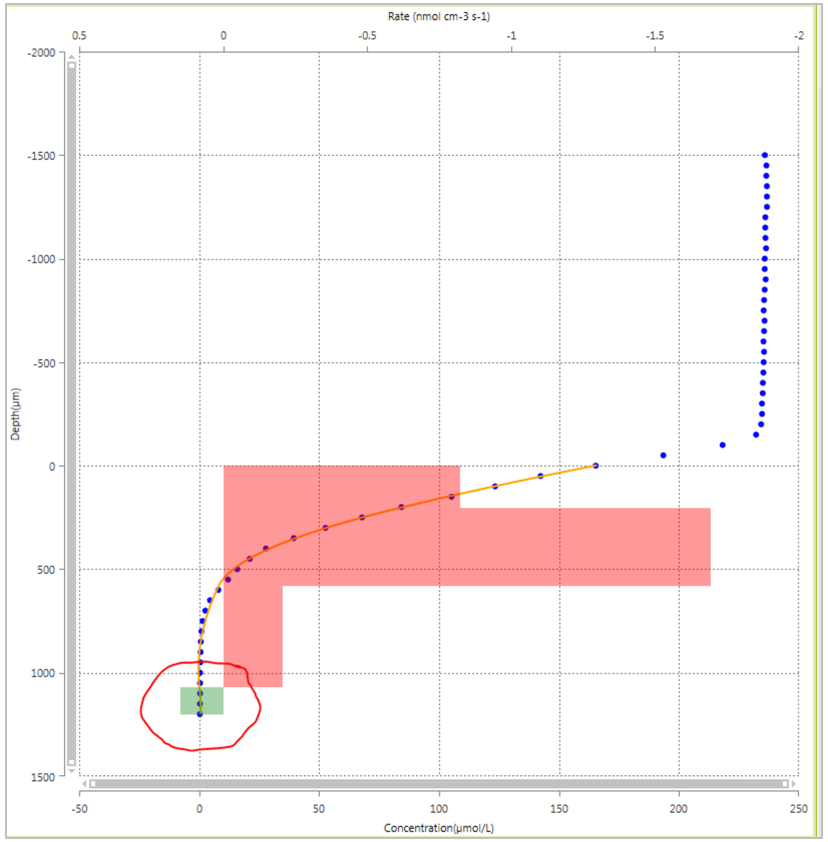
- Choose the right number of zones:
  - P: Did adding this zone improve the fit ($P < 0.05$)
  - SSE: Sum of squared errors
  - SSE and P-value should be as small as possible.
  - Look at the results and use common sense

Result – Avoid obvious errors

Statistics

Save solution | Export selected analysis

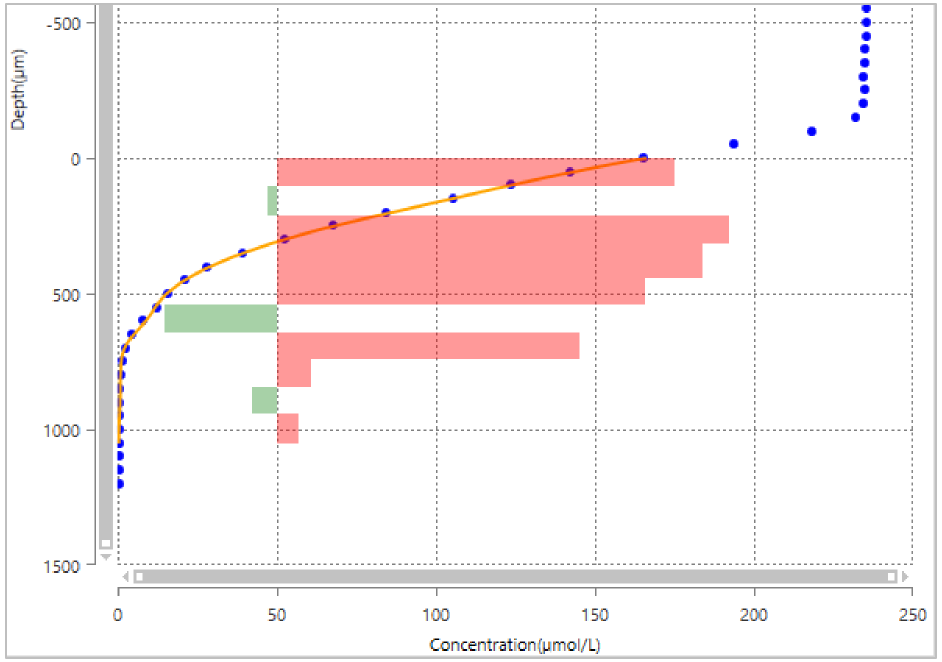
No. of Zones	SSE	P-Value	Top Conc (µmol/L)	Bottom Conc (µmol/L)	Top Flux (nmol cm-2 s-1)	Bottom Flux (nmol cm-2 s-1)	Integrated pr (nmol cm-2 s-
2	891.00	0.000	286.74	1.00	-0.015	0.000	0.015
3	688.98	0.071	284.07	1.00	-0.018	0.000	0.018
4	219.23	0.002	287.24	1.00	-0.014	0.000	0.014
5	102.52	0.007	282.56	1.00	-0.023	0.000	0.023
6	93.61	0.361	283.10	1.00	-0.021	0.000	0.021



- Production or consumption in zones where it is not possible
  - Analysis too deep into the anoxic zone
  - Maximum number of zones too high

UNISENSE

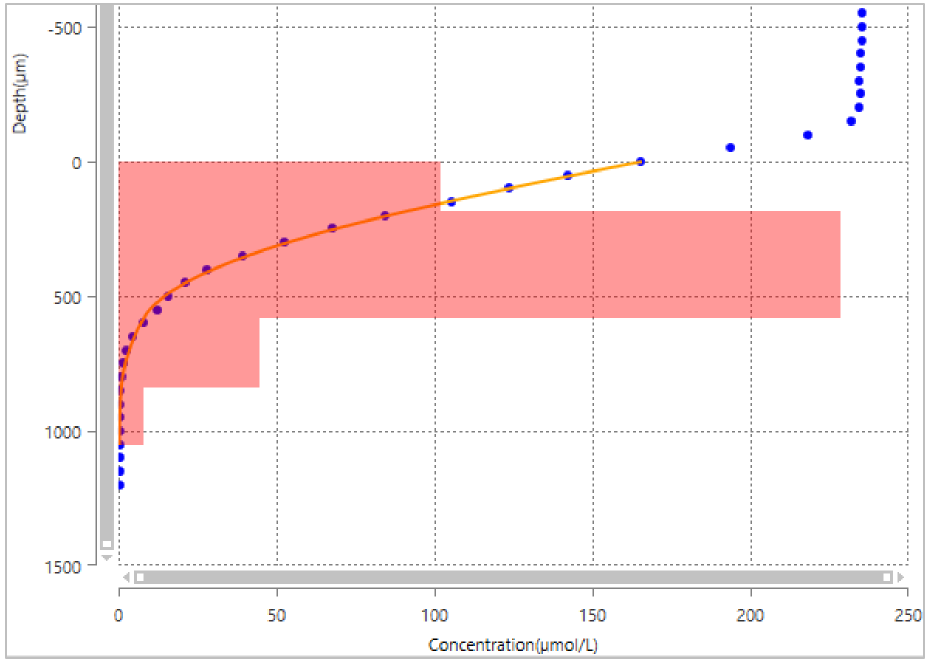
Results – Number of zones



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-
6	7.58	0.069	165.46	0.27	0.058	0.000	-0.058
7	6.07	0.347	165.50	0.27	0.058	0.000	-0.058
8	6.16	1.000	165.51	0.27	0.058	0.000	-0.058
9	5.10	0.457	166.02	0.27	0.064	0.000	-0.064
10	6.00	1.000	165.99	0.27	0.063	0.000	-0.063



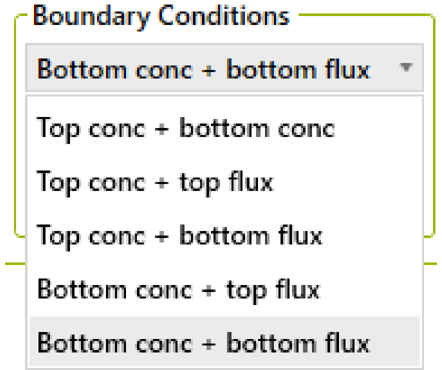
Statistics

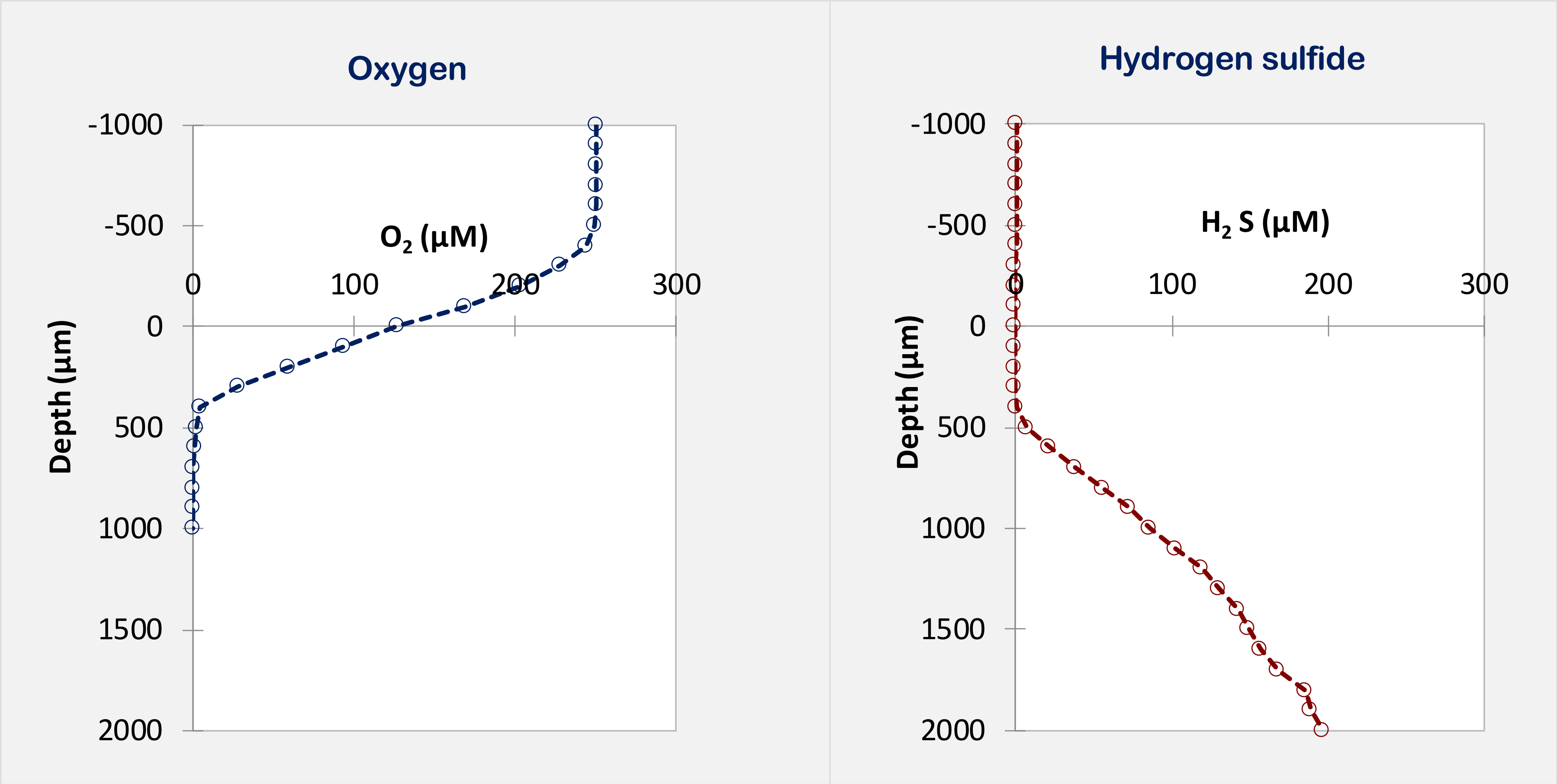
Save solution | Export selected analysis

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-
3	37.81	0.212	167.63	0.27	0.066	0.000	-0.066
4	20.13	0.030	165.59	0.27	0.059	0.000	-0.059
5	13.34	0.102	165.06	0.27	0.054	0.000	-0.054
6	7.58	0.069	165.46	0.27	0.058	0.000	-0.058
7	6.07	0.347	165.50	0.27	0.058	0.000	-0.058

UNISENSE

Other solutes than O_2





<u>Boundary conditions</u>

Bottom conc. = 0

Bottom flux = 0

<u>Boundary conditions</u>

Top conc. = 0

Top flux = 0

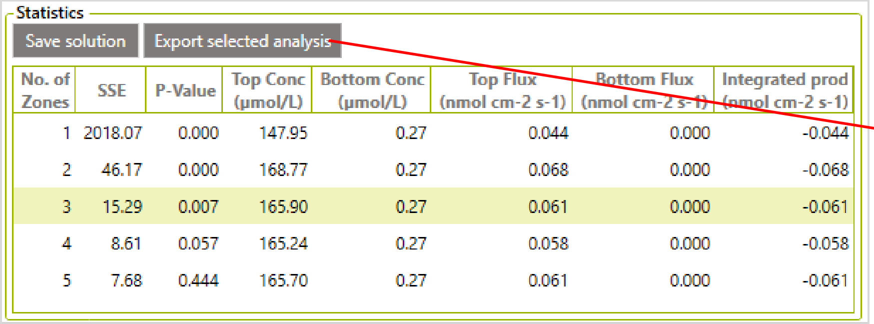
UNISENSE

Play arround

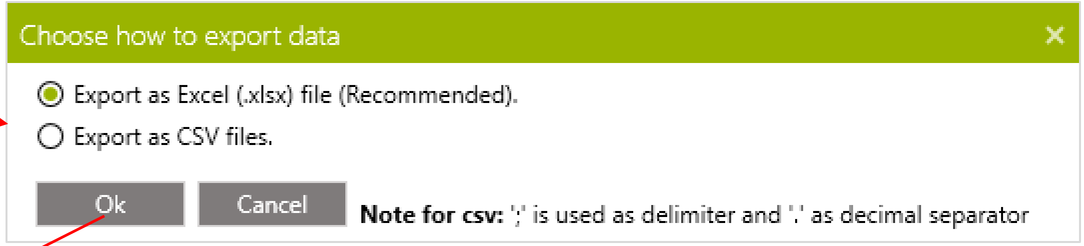
- Boundary conditions
- Depth interval
- The oxygen diffusion rate - e.g. by changing the temperature and salinity
- Change the formula for the Ds calculation
- Porosity

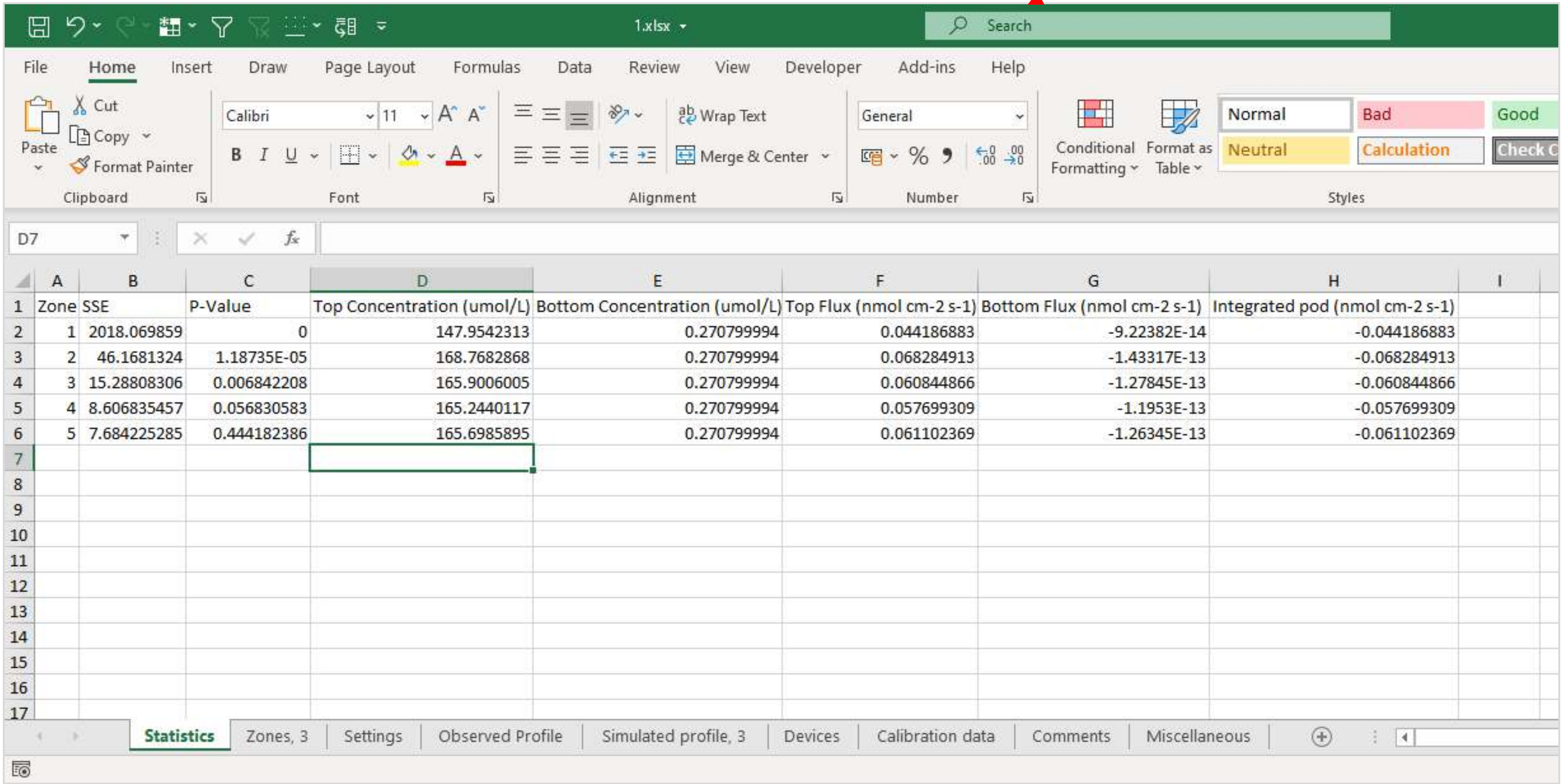
UNISENSE

Export data



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 prod (nmol cm-2 s-1)
1	2018.07	0.000	147.95	0.27	0.044	0.000	-0.044
2	46.17	0.000	168.77	0.27	0.068	0.000	-0.068
3	15.29	0.007	165.90	0.27	0.061	0.000	-0.061
4	8.61	0.057	165.24	0.27	0.058	0.000	-0.058
5	7.68	0.444	165.70	0.27	0.061	0.000	-0.061





Zone	SSE	P-Value	Top Concentration (umol/L)	Bottom Concentration (umol/L)	Top Flux (nmol cm-2 s-1)	Bottom Flux (nmol cm-2 s-1)	Integrated pod (nmol cm-2 s-1)
1	2018.069859	0	147.9542313	0.270799994	0.044186883	-9.22382E-14	-0.044186883
2	46.1681324	1.18735E-05	168.7682868	0.270799994	0.068284913	-1.43317E-13	-0.068284913
3	15.28808306	0.006842208	165.9006005	0.270799994	0.060844866	-1.27845E-13	-0.060844866
4	8.606835457	0.056830583	165.2440117	0.270799994	0.057699309	-1.1953E-13	-0.057699309
5	7.684225285	0.444182386	165.6985895	0.270799994	0.061102369	-1.26345E-13	-0.061102369

UNISENSE

Summary

SensorTrace Profiling – Activity calculations

- Calculate fluxes, consumption and production rates from high resolution concentration profiles.
- Fick's first and second law.
- Diffusivity and boundary conditions must be defined
- Use a stepwise optimization using the model-line and statistical values

UNISENSE

Time for questions !

Unisense Microsensor Academy:
https://www.unisense.com/support/knowledge

Contact us: sales@unisense.com