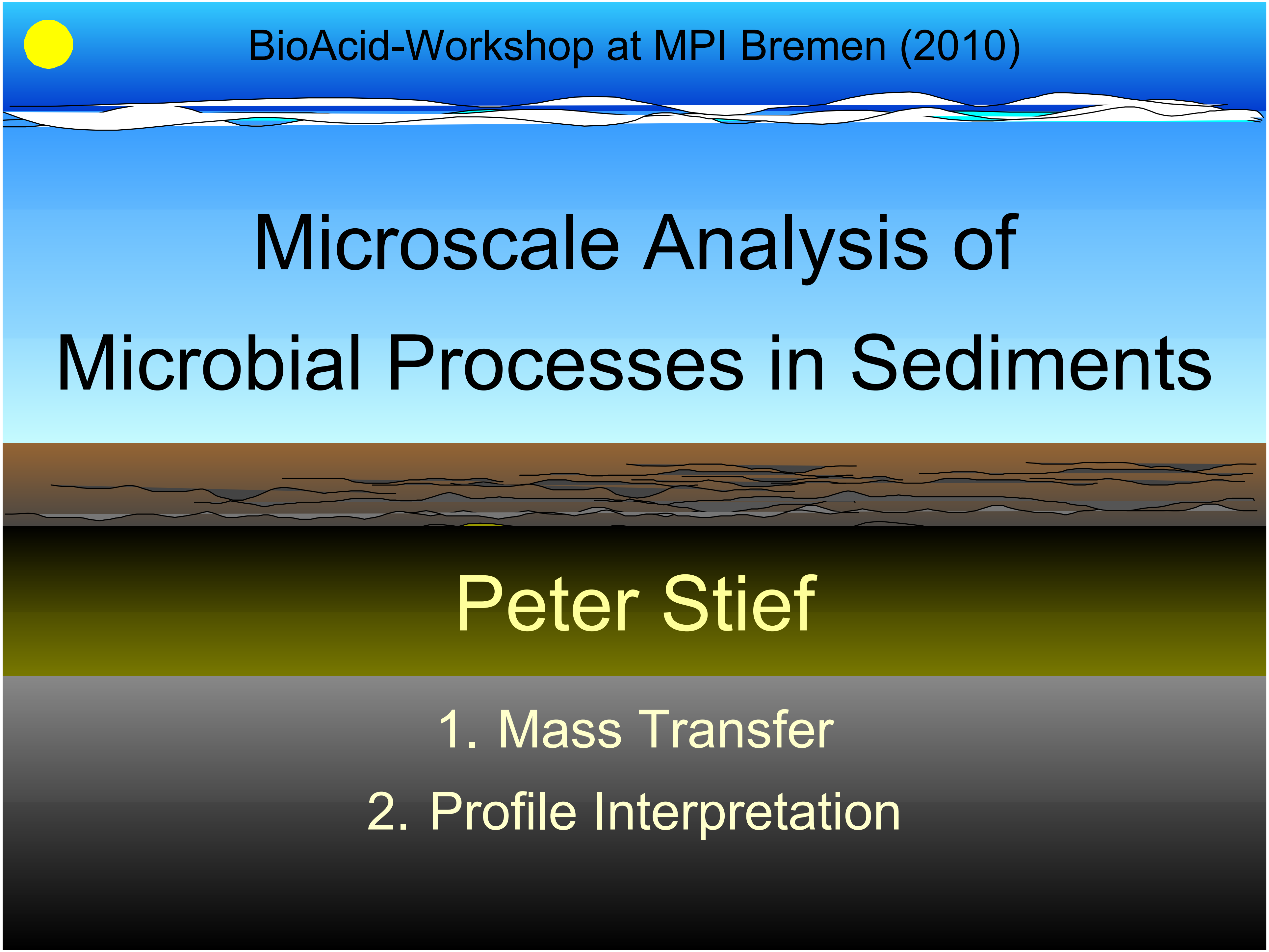


BioAcid-Workshop at MPI Bremen (2010)

Microscale Analysis of Microbial Processes in Sediments

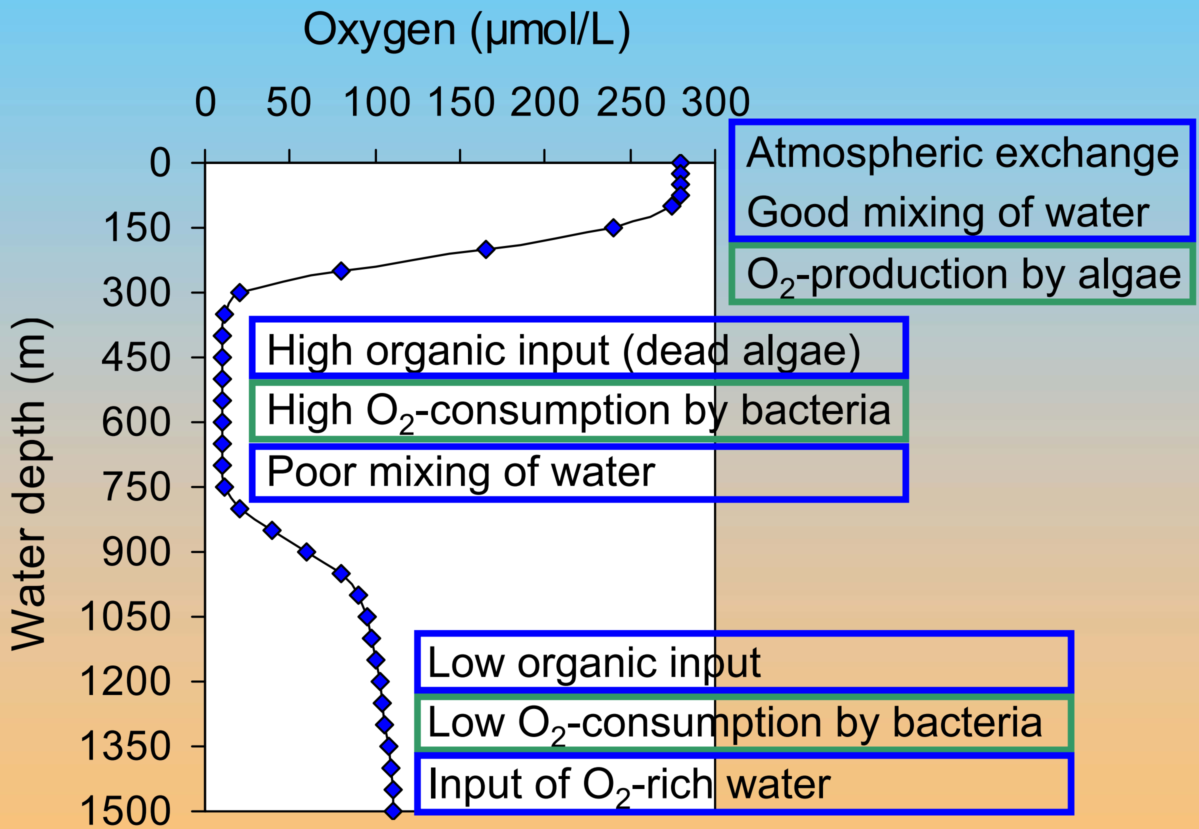
Peter Stief

1. Mass Transfer
2. Profile Interpretation

1. Mass Transfer

Large-scale concentration profiles

Oxygen minimum zones in the ocean



Atmospheric exchange

Good mixing of water

O_2-production by algae

High organic input (dead algae)

High O_2-consumption by bacteria

Poor mixing of water

Low organic input

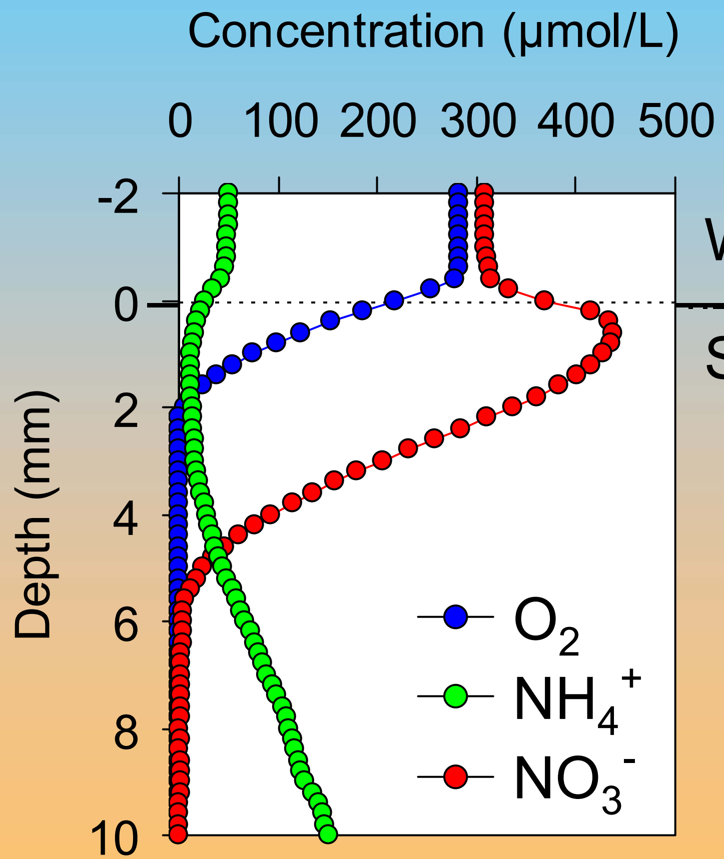
Low O_2-consumption by bacteria

Input of O_2-rich water

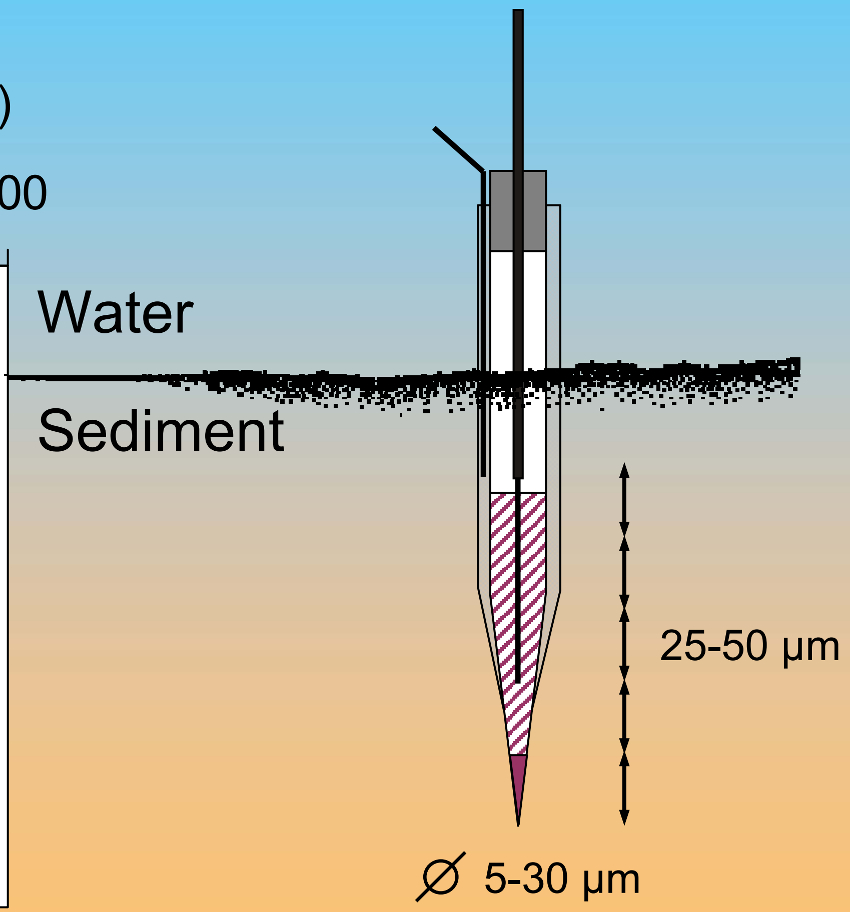
CTD: Vertical profiling of the water column
(Conductivity, Temperature, Depth)

Small-scale concentration profiles

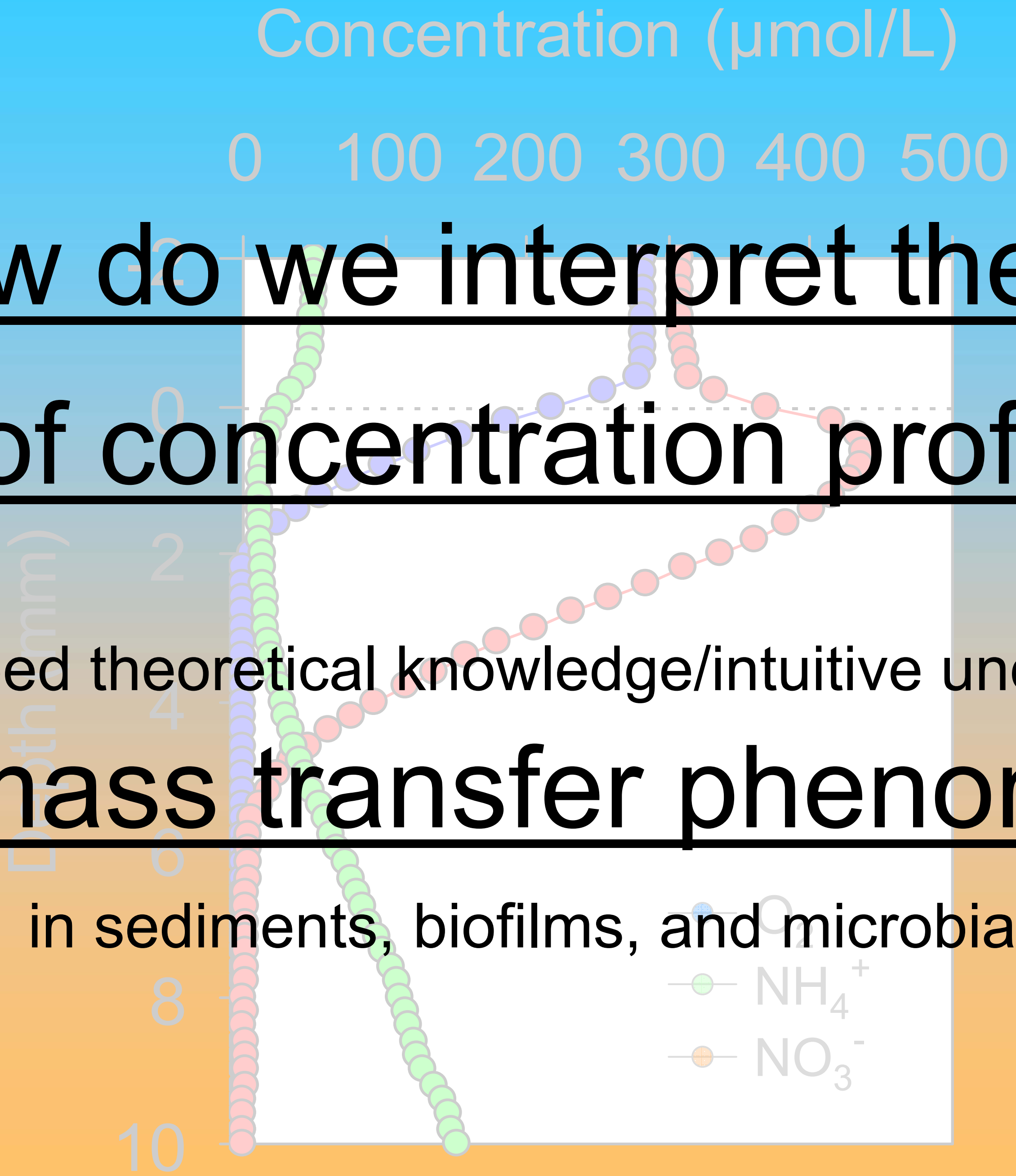
Microsensor measurements in sediment



Stief & De Beer (2006)



How do we interpret the shape of concentration profiles?



We need theoretical knowledge/intuitive understanding of

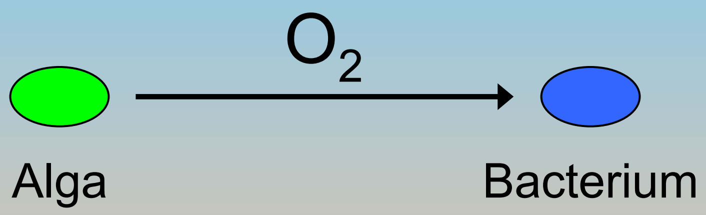
mass transfer phenomena

in sediments, biofilms, and microbial mats!

Importance of mass transfer

Interaction of microbes:

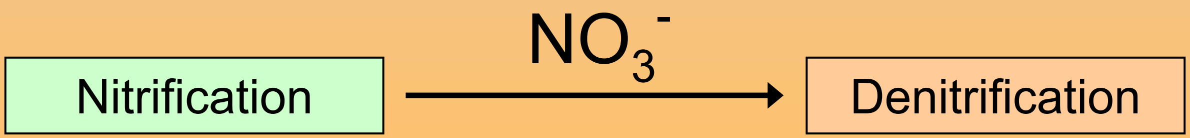
Mass transfer enables microbes to interact via exchange of solutes



Alga $\xrightarrow{O_2}$ Bacterium

Coupling of processes:

Mass transfer enables spatio-temporal coupling of biogeochemical processes



Nitrification $\xrightarrow{NO_3^-}$ Denitrification

Types of mass transfer

Diffusion:

Spontaneous movement of molecules in a medium directed by a concentration gradient
(in muddy sediment, biofilms, microbial mats)

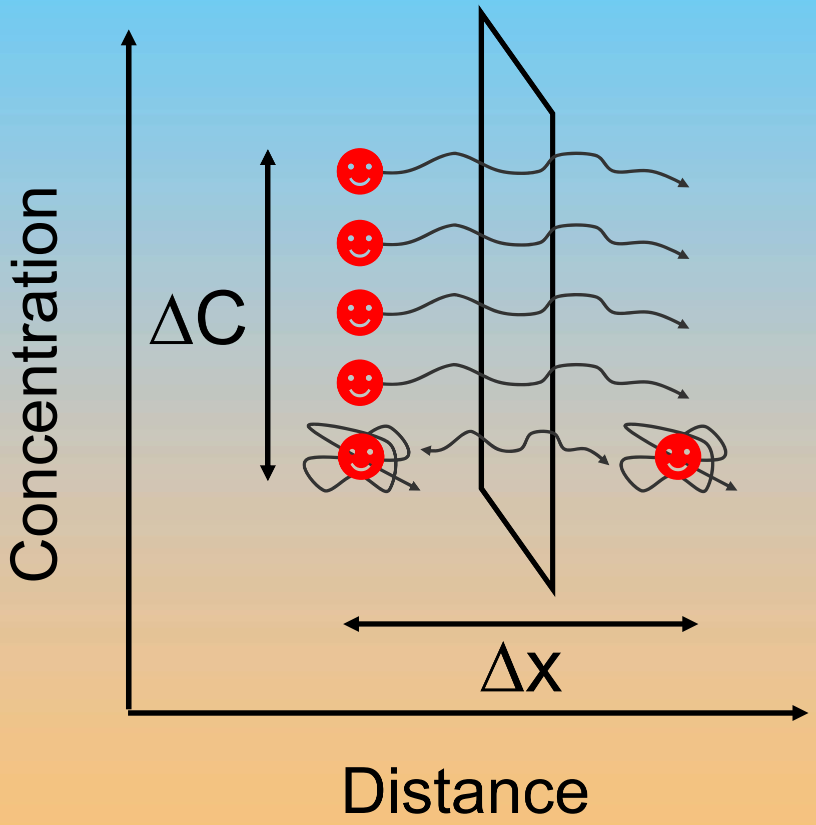
Advection:

Transport of molecules driven by movement of the medium
(in water column, sand, animal burrows, seeps)

Locomotion:

Self-powered movement by biological individuals

Diffusion



Concentration gradient:

= High degree of order

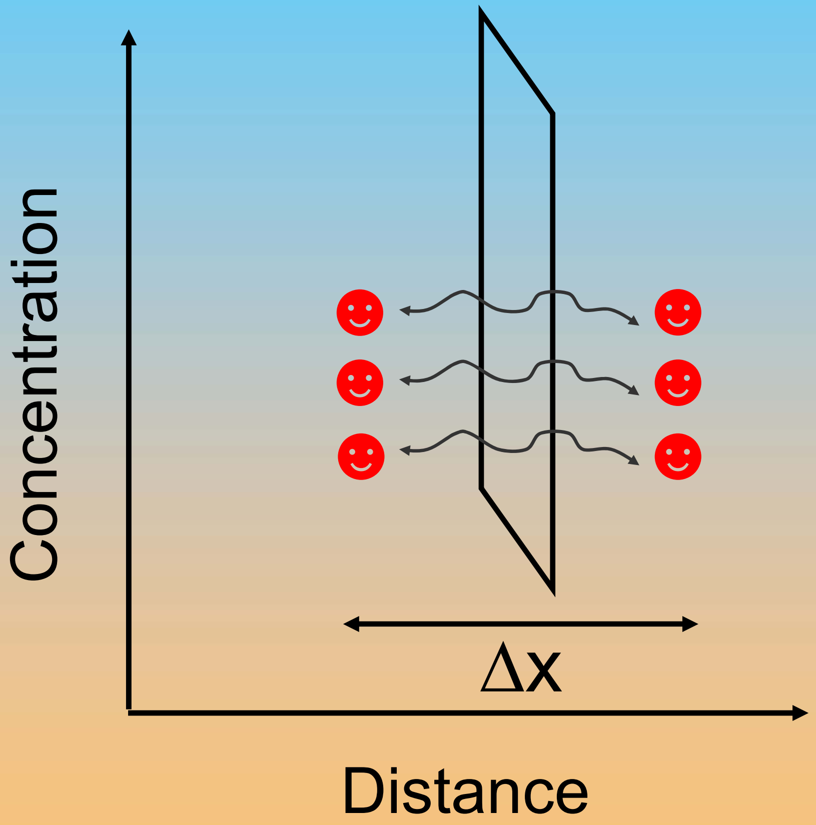
= Low entropy

→ Directed net motion

No concentration gradient:

→ Random „Brownian“ motion

Diffusion



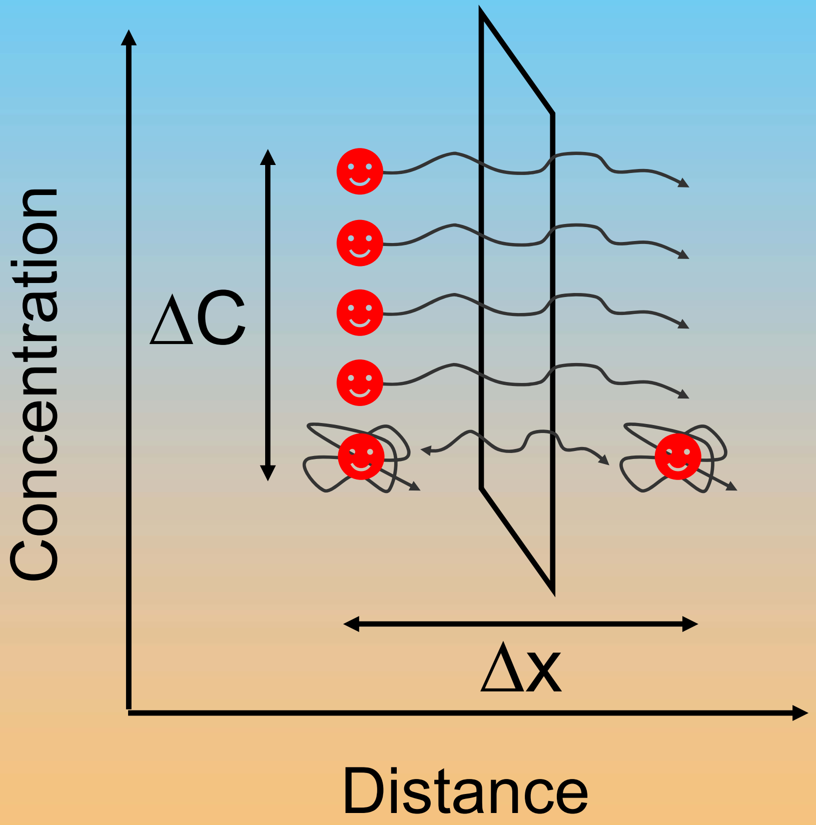
No concentration gradient:

= Low degree of order

= High entropy

→ No directed net motion

Diffusion



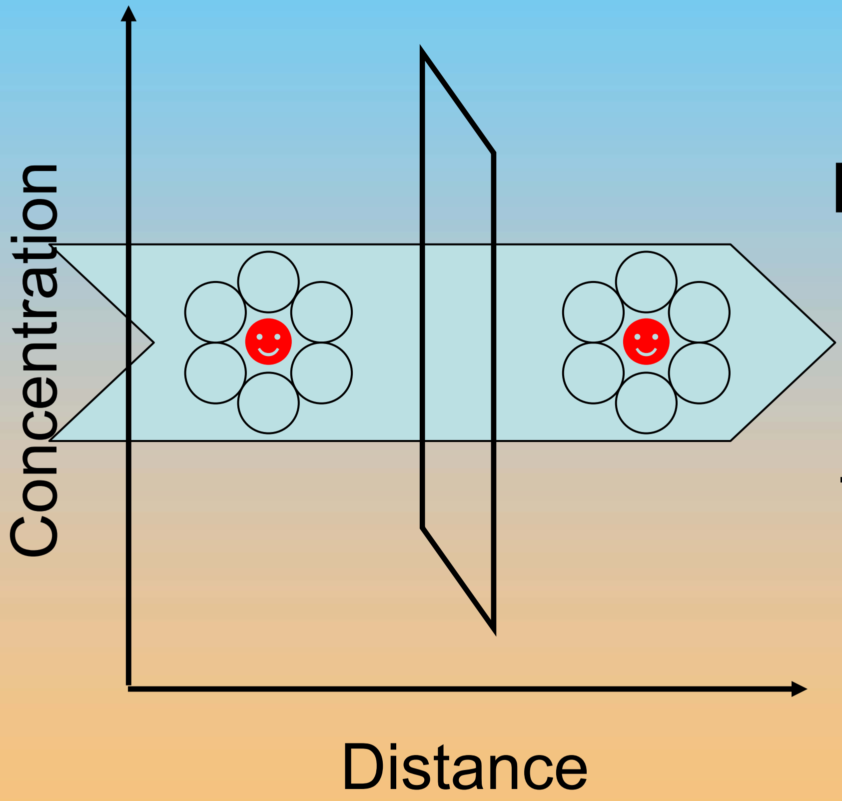
Directed net motion = Flux (J)

Quantification: Fick's law

$J = -D_0 \times \Delta C / \Delta x$

Units of J = mol m^{-2} s^{-1}

Advection



Directed net motion = Flux (J)

Quantification:

J = Concentration × Velocity

Units of J = mol m^{-2} s^{-1}

→ Efficient over long distances

Diffusion vs. Advection

Time it takes for an O_2 molecule to travel from Bremen to Bremerhaven in the Weser (60 km, 1 m s^{-1}, 15°C):

a) Advection: $t = 60\ \mathrm{km} / 1\ \mathrm{m/s} = 16.7\ \mathrm{h}$

b) Diffusion: $t = x^2 / (2 \times D_0) = 31.7$ billion years

Diffusion vs. Advection

Time it takes for an O_2 molecule to travel across the diffusive boundary layer (500 µm, 1 m s^{-1}, 15°C):

a) Advection: $t = 0.0005\ m / 1\ m/s = 0.5\ msec$

b) Diffusion: $t = x^2 / (2 \times D_0) = 70\ sec$

D_0 = Diffusion coefficient [$m^2\ s^{-1}$]

Depends on solute:

H_2: ~ $3\times10^{-9}\ m^2\ s^{-1}$

Glucose: ~ $0.3\times10^{-9}\ m^2\ s^{-1}$

Bacterial cell: ~ $0.01\times10^{-9}\ m^2\ s^{-1}$

Depends on medium:

High in gas: ~$10^{-5}\ m^2\ s^{-1}$

Lower in liquids: ~$10^{-9}\ m^2\ s^{-1}$

Very low in solids: ~$10^{-16}\ m^2\ s^{-1}$

Depends on temperature:

The higher T, the higher D_0

D_0 = Diffusion coefficient [$m^2\ s^{-1}$]

Temperature dependence of D_0:

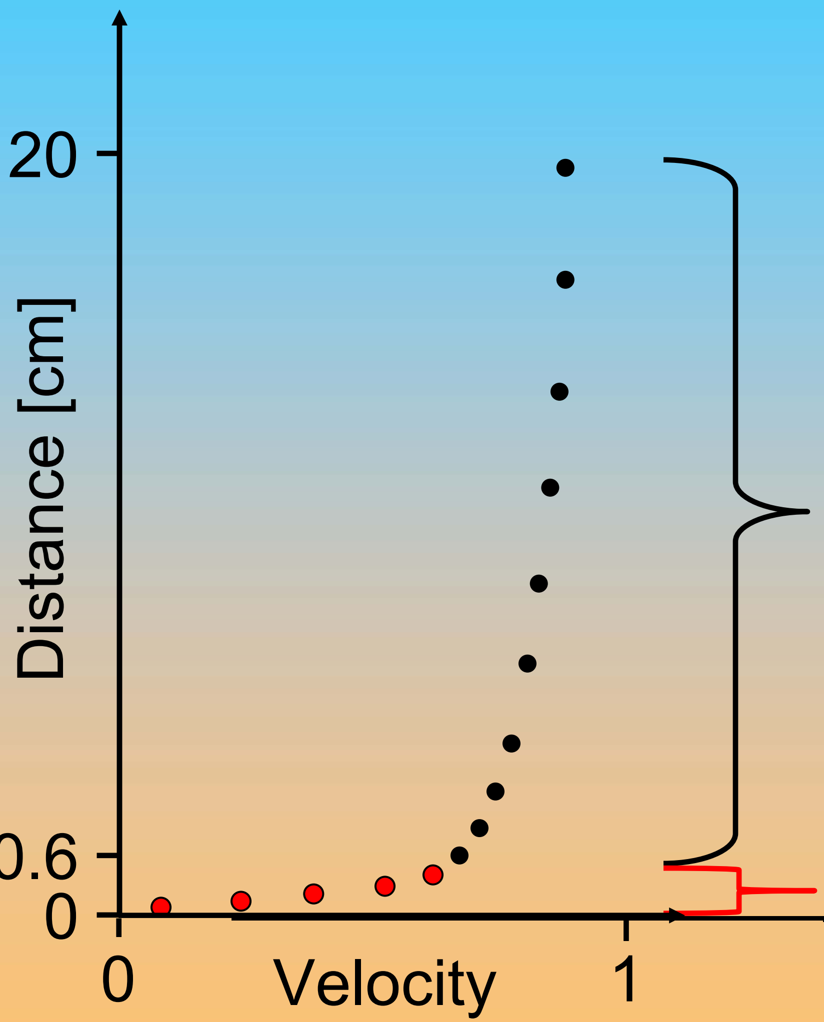
“The higher T, the higher D_0”

$$D_1 \times \nu_1 / T_1 = D_2 \times \nu_2 / T_2$$

$$D_2 = (D_1 \times \nu_1 \times T_2) / (T_1 \times \nu_2)$$

ν = Viscosity [$m^2\ s^{-1}$]

Diffusive boundary layer



Logarithmic layer:

Transfer of solutes

by turbulent flow

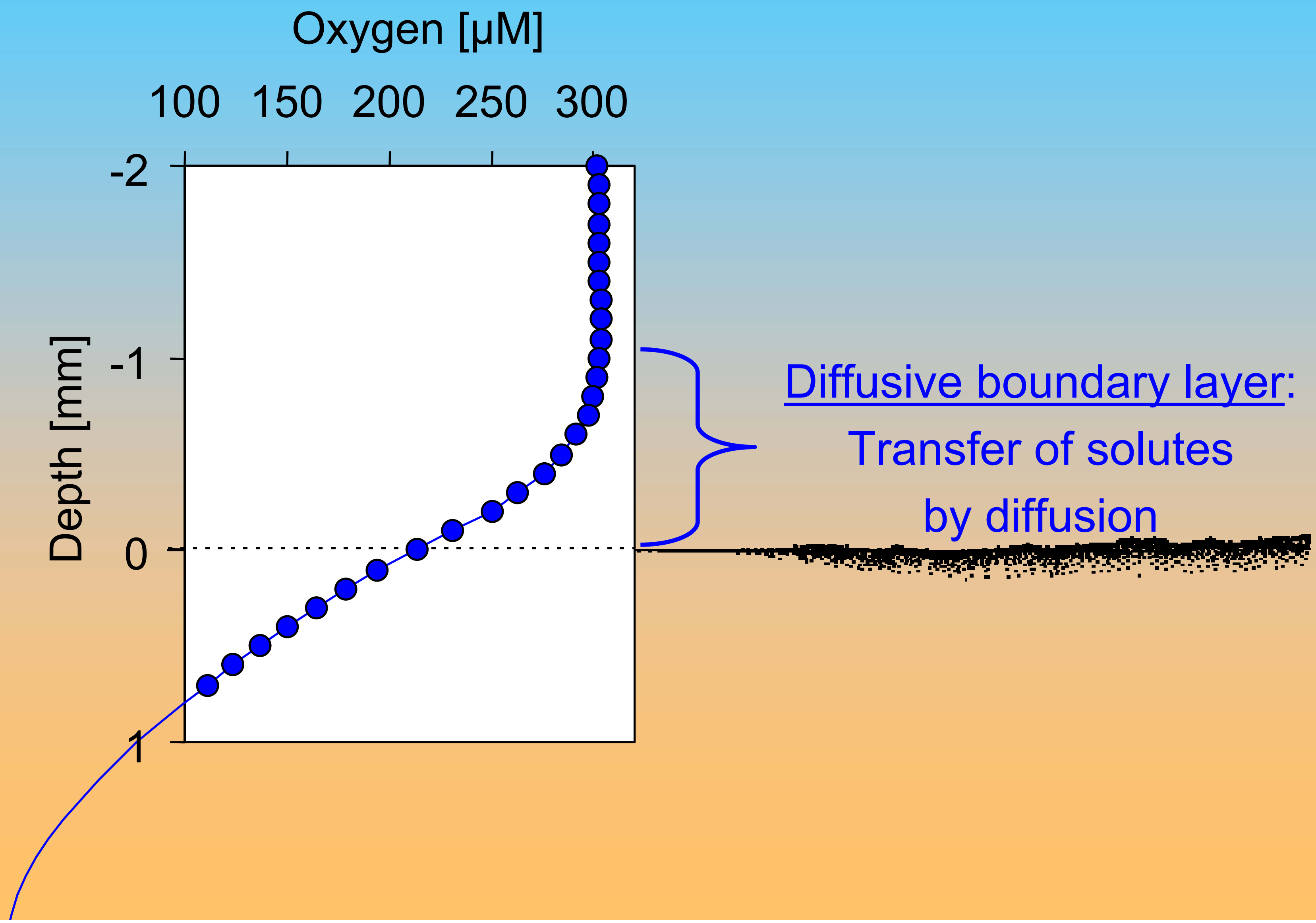
Viscous sublayer:

Transfer of solutes

by viscous flow

(Redrawn from Caldwell & Chriss 1979)

Diffusive boundary layer

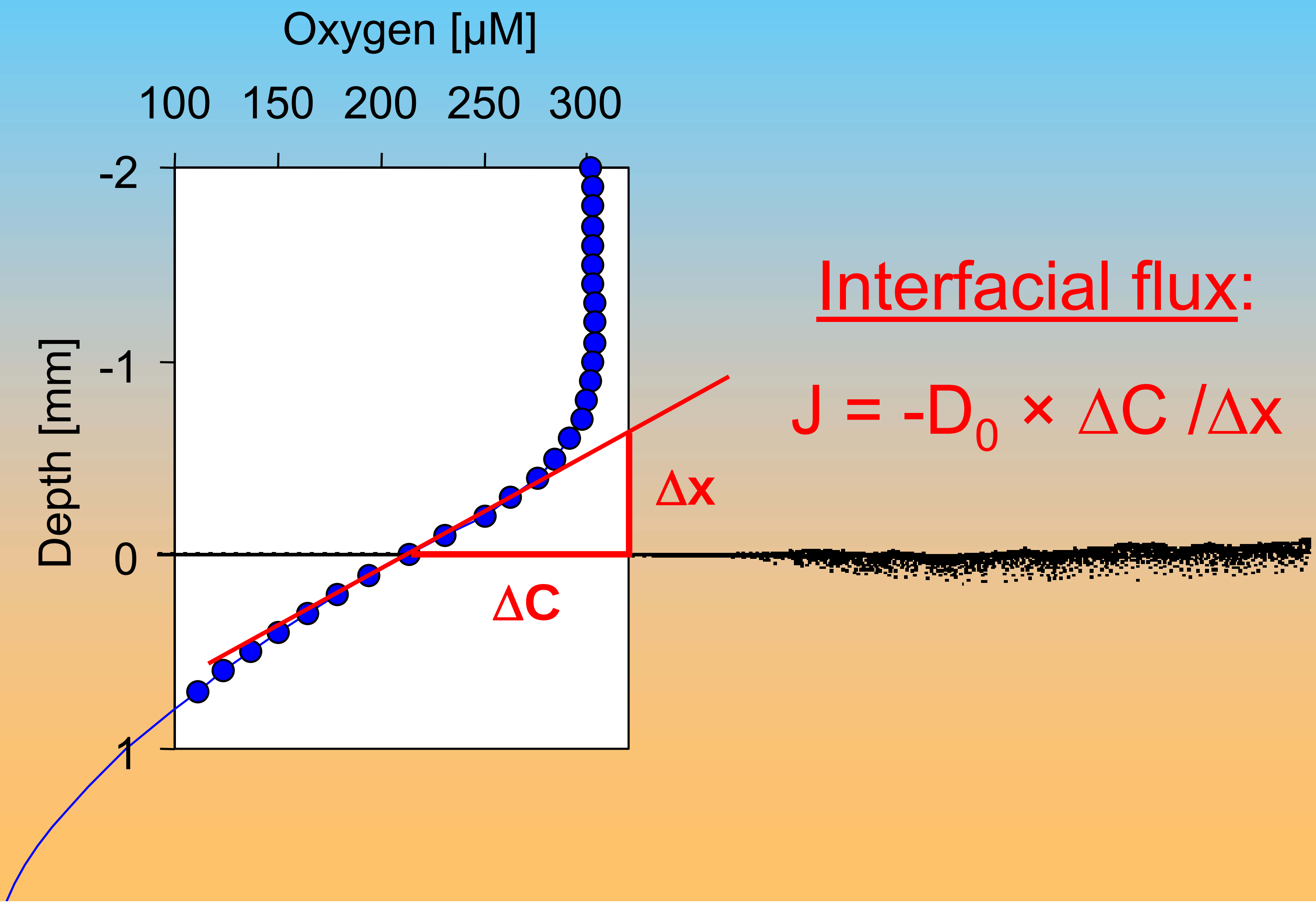


Diffusive boundary layer:
Transfer of solutes
by diffusion

Diffusive boundary layer

- Viscous film of water
- ~0.2-1.0 mm thick
- Mass transfer resistance
- Rate-limiting for solute reactions
- Allows measurement of interfacial flux

Diffusive boundary layer

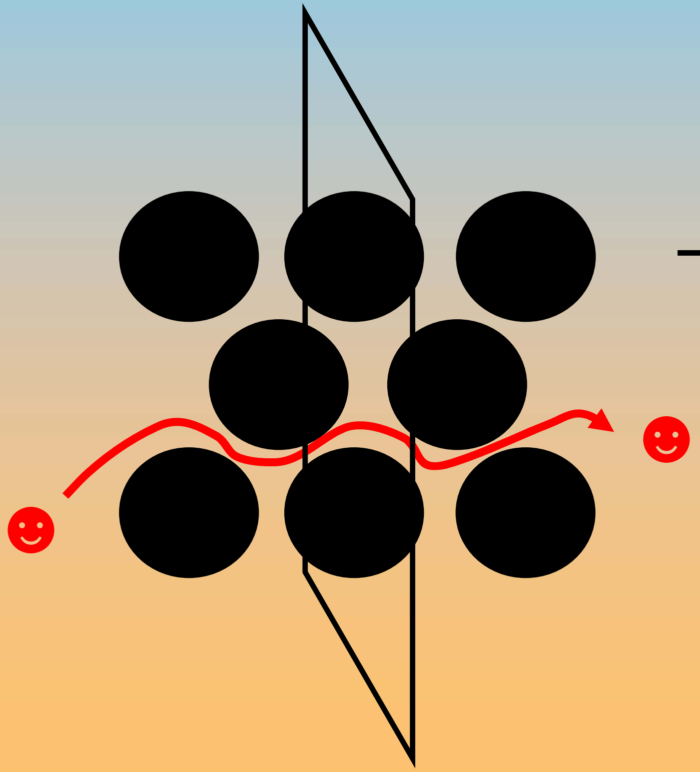


Interfacial flux:

$$J = -D_0 \times \Delta C / \Delta x$$

Diffusion in sediments

- Sediment = solids + water
- Diffusion only in porewater



→ Pathlength of diffusion longer

→ Area for diffusion smaller

→ $D_{sediment} < D_0$

D_{sed} = Sedimentary diffusion coefficient

$$D_{sed} \sim D_0 \times \varphi / \omega^2$$

φ = Porosity = Area reduction factor

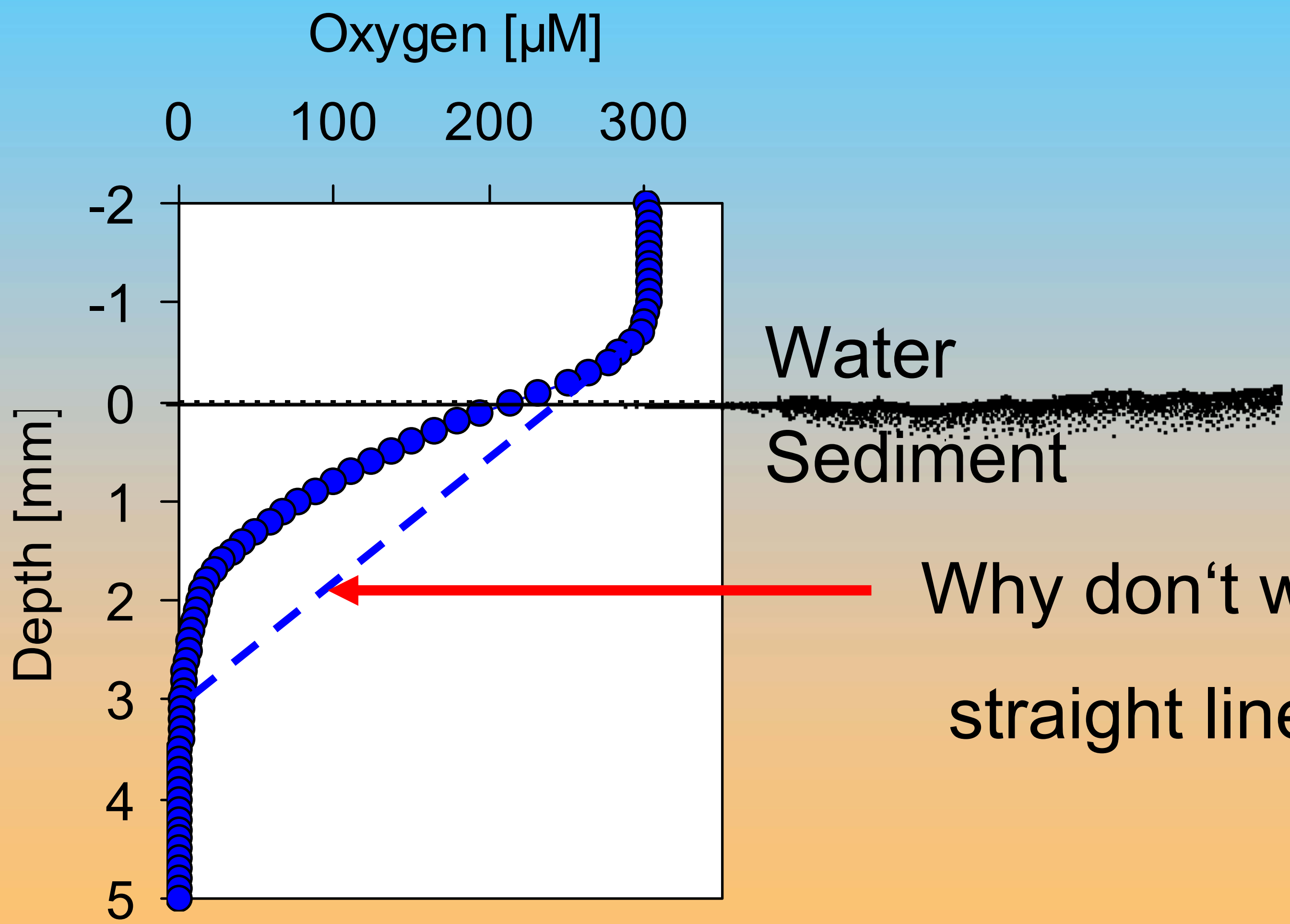
ω = Tortuosity, ω^2 = Pathlength elongation factor

Boudreau (1996): $\omega^2 = 1 - \ln(\varphi^2)$

$$D_{sed} \sim D_0 \times \varphi / (1 - \ln(\varphi^2))$$

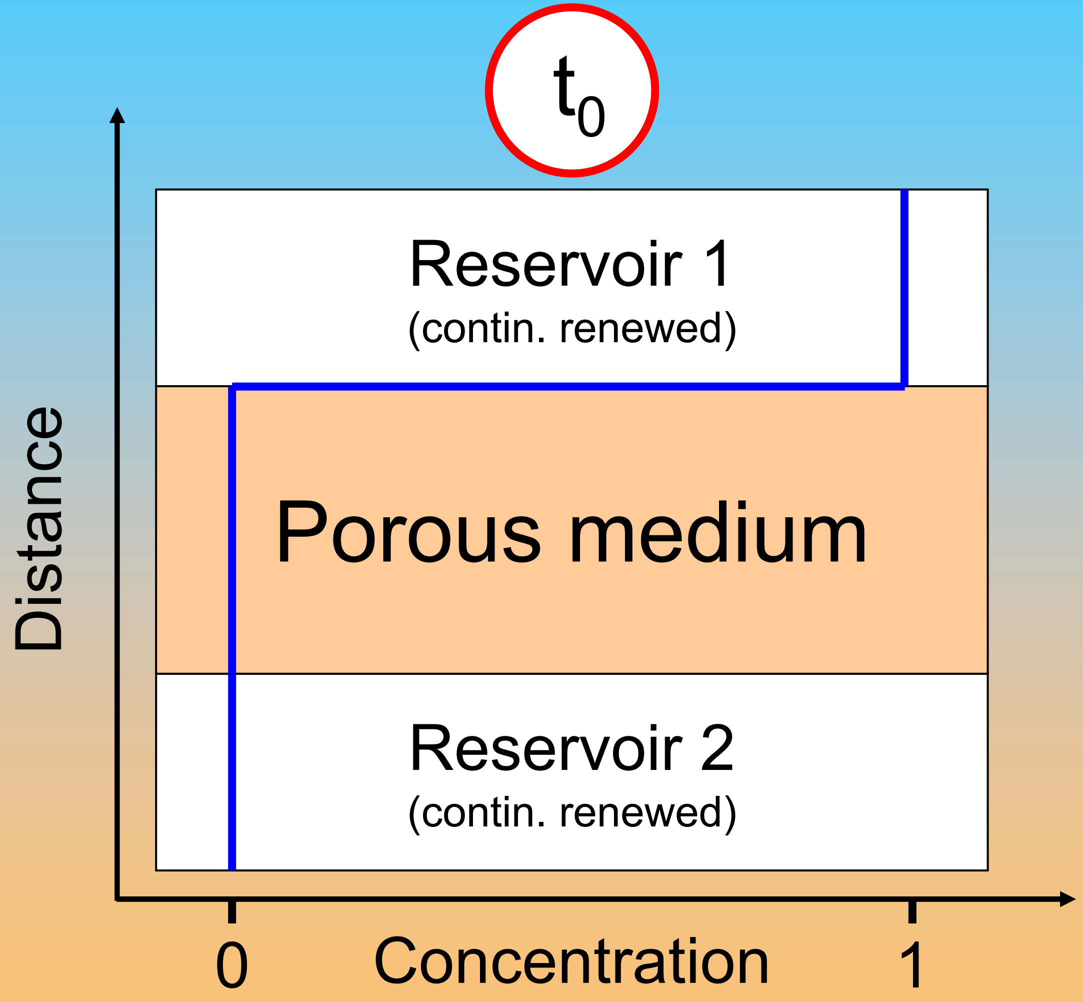
2. Profile Interpretation

Oxygen microsensor profile



Why don‘t we see a straight line here?

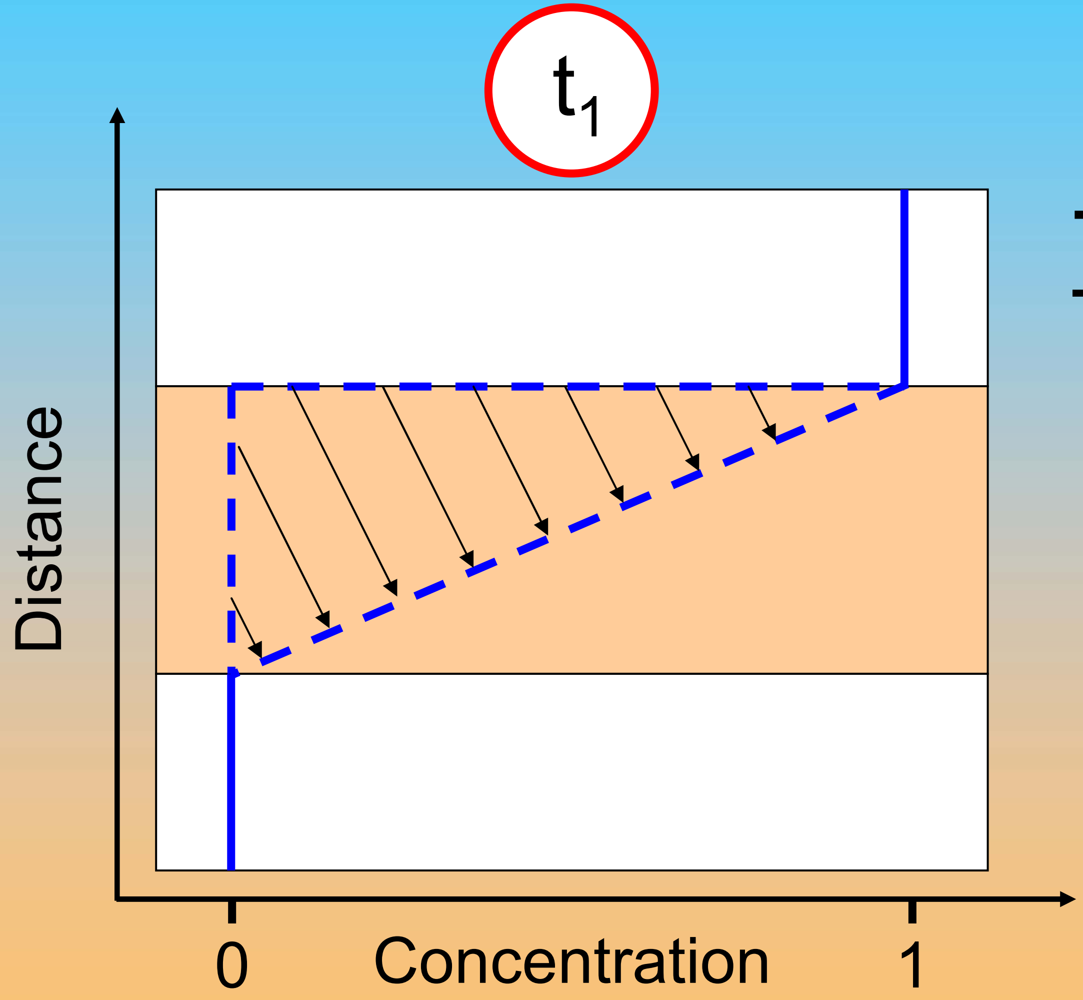
Profile interpretation: Box model



Start:

- Rectangular profile

Profile interpretation: Box model

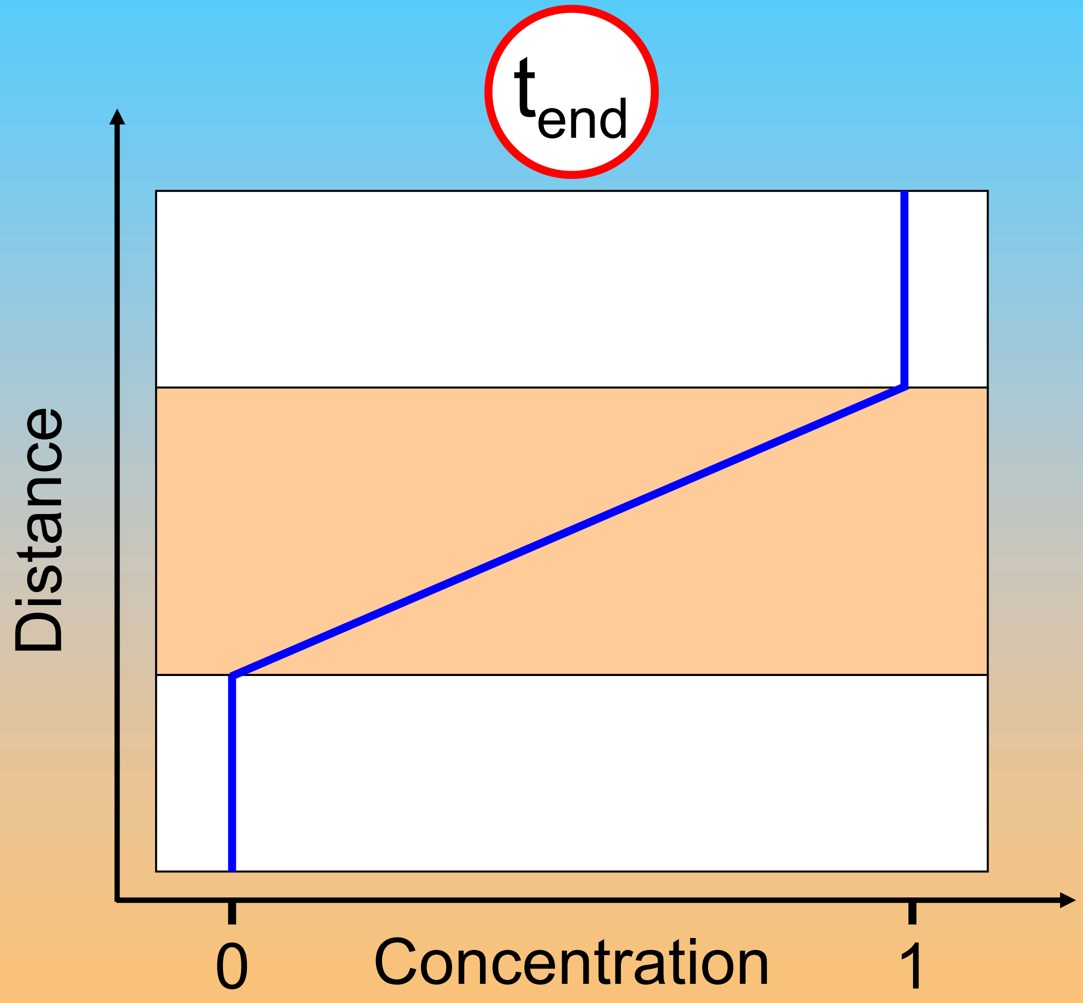


Transient state:

o Change of profile with time

o Driven by the continuous renewal of the reservoirs

Profile interpretation: Box model

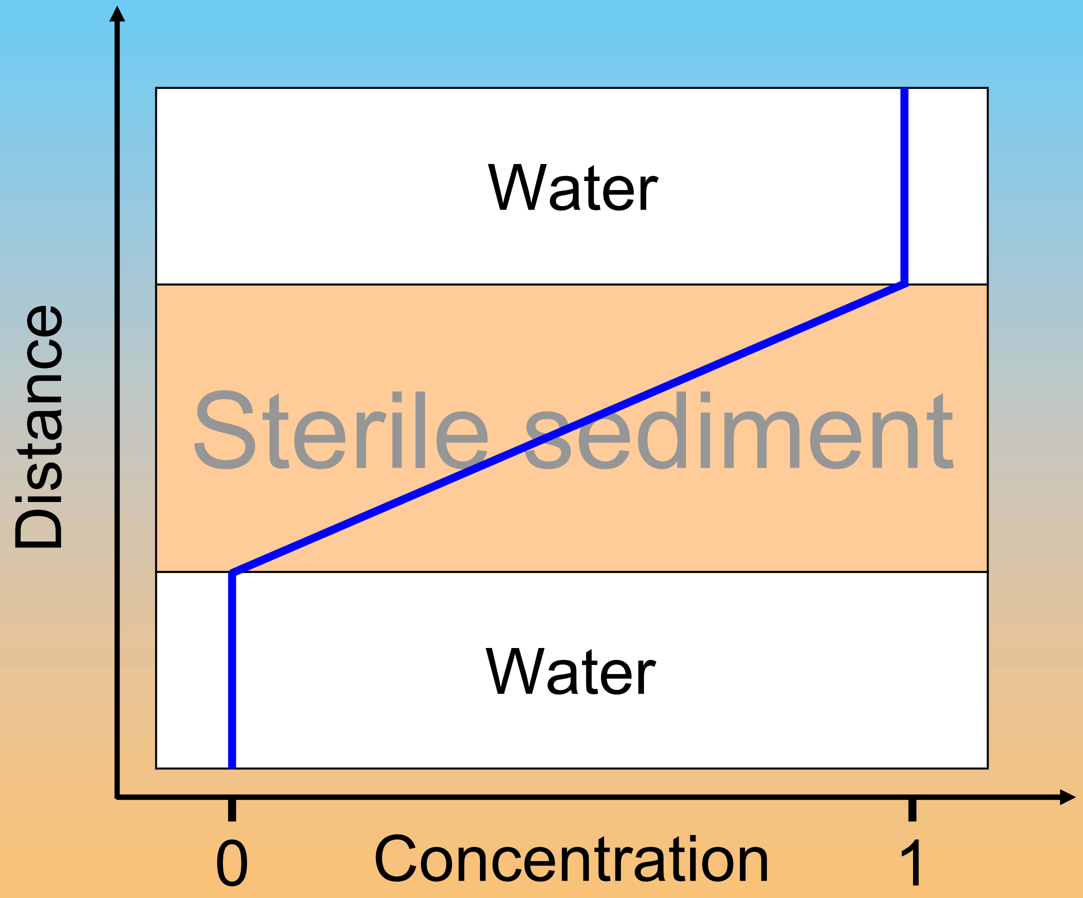


Steady state:

o No change of profile with time

o Maintained by continuous renewal of the reservoirs

Profile interpretation: Box model

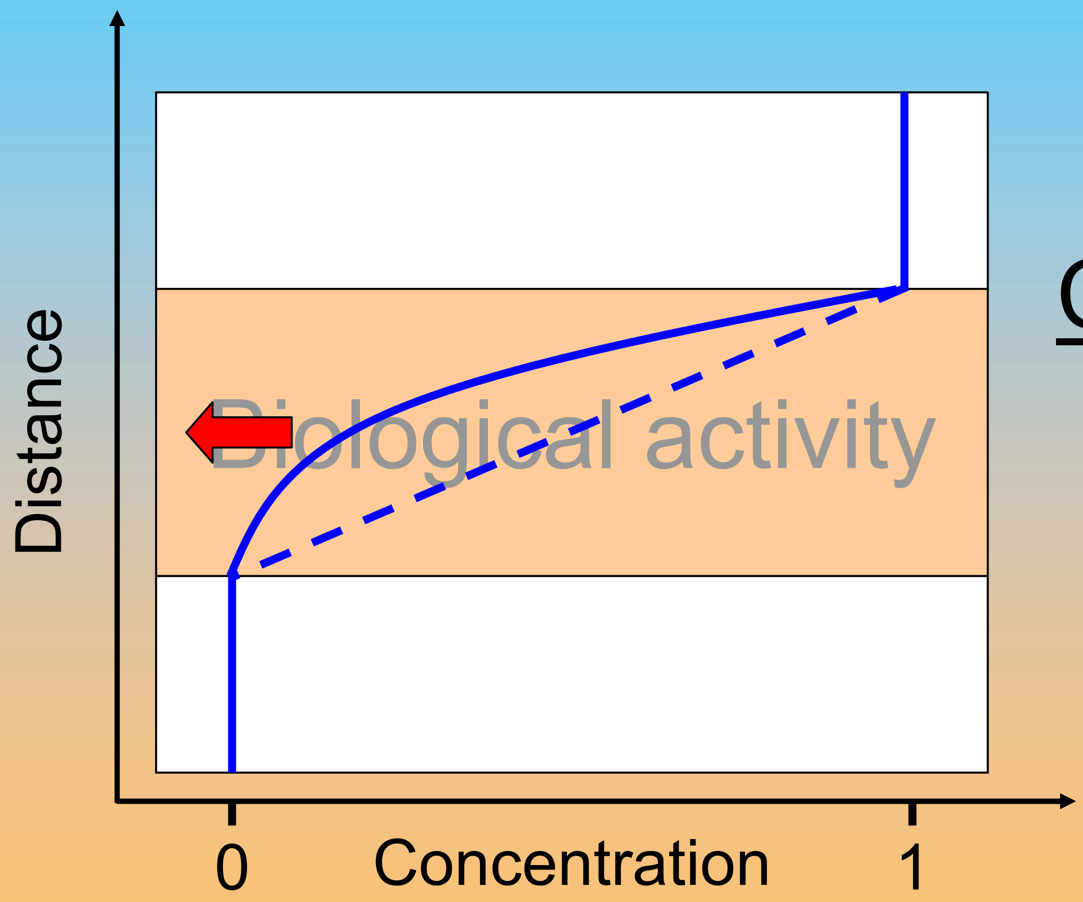


Steady state:

o No change of profile with time

o Maintained by continuous renewal of the reservoirs

Profile interpretation: Box model

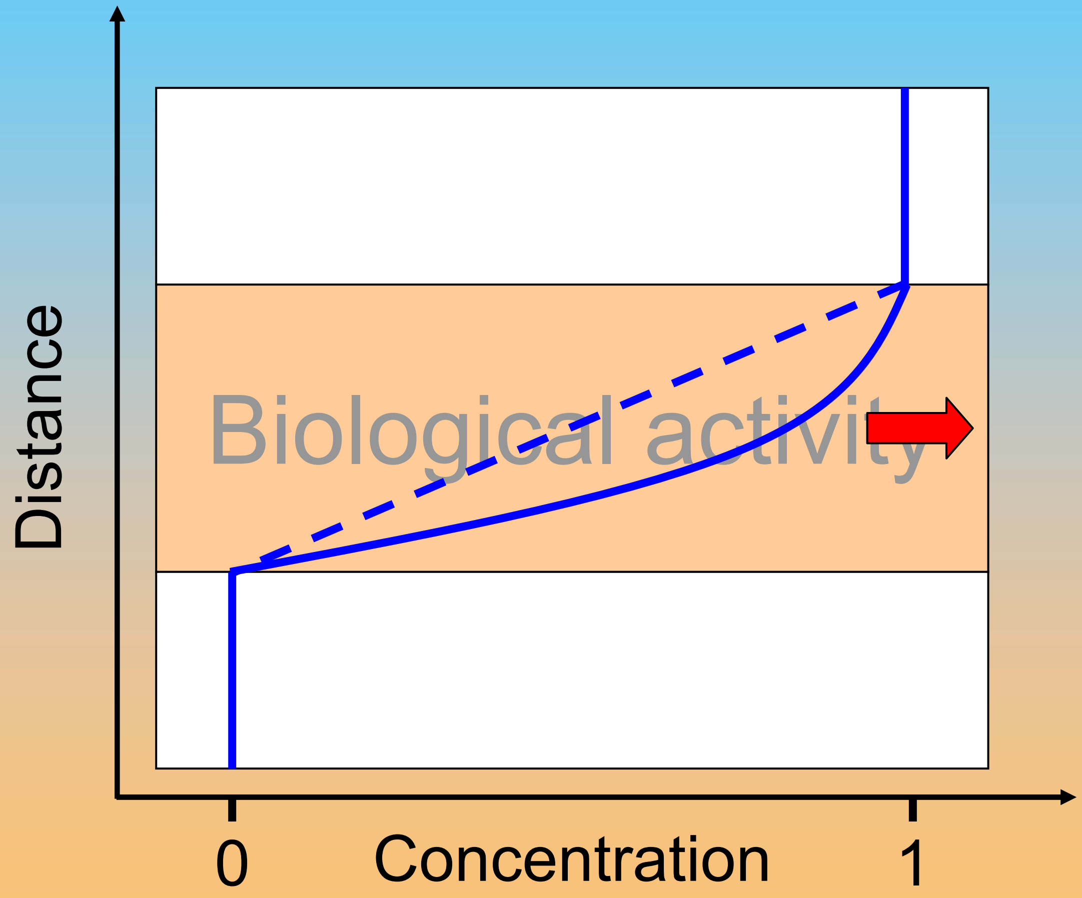


Concave shape:

$\text{Conc}_{\text{app}} < \text{Conc}_{\text{theor}}$

→ Consumption

Profile interpretation: Box model

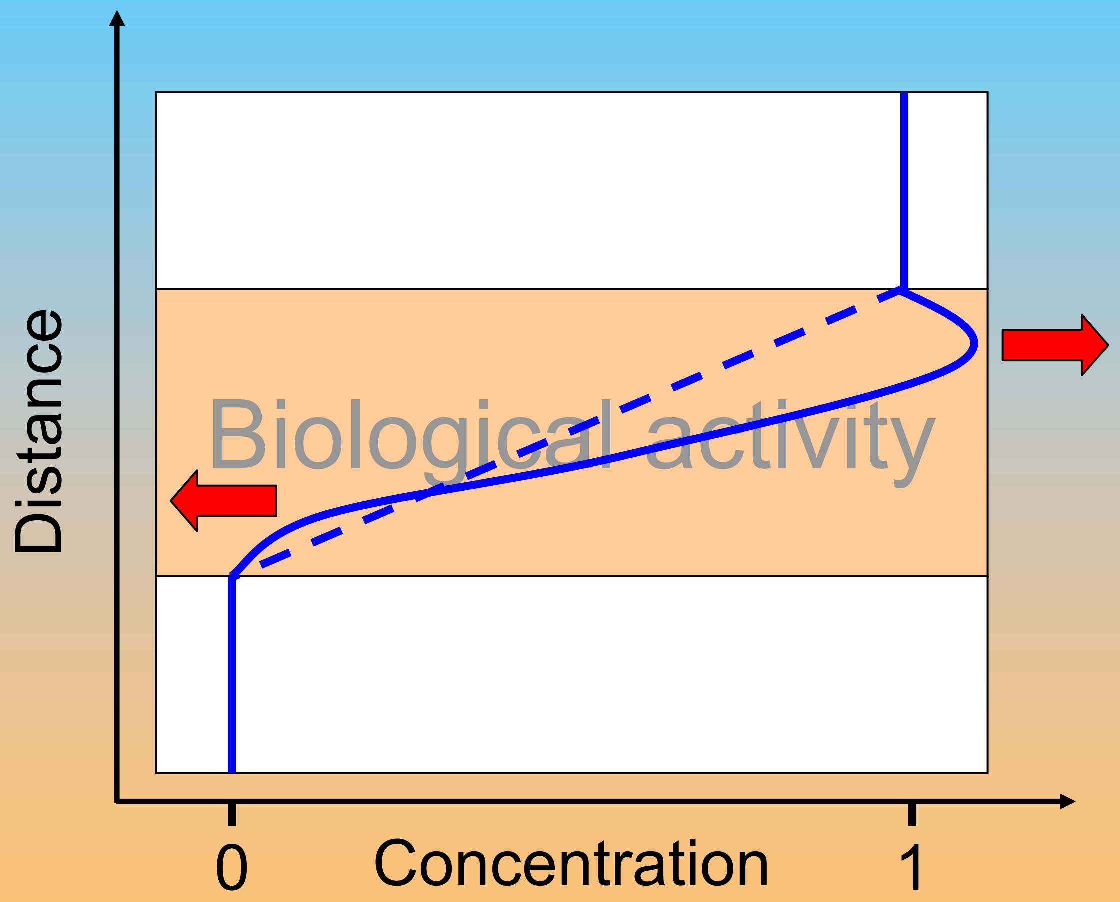


Convex shape:

$\mathrm{Conc}_{app} > \mathrm{Conc}_{theor}$

→ Production

Profile interpretation: Box model



→ Production

→ Consumption

Profile interpretation: Conditions

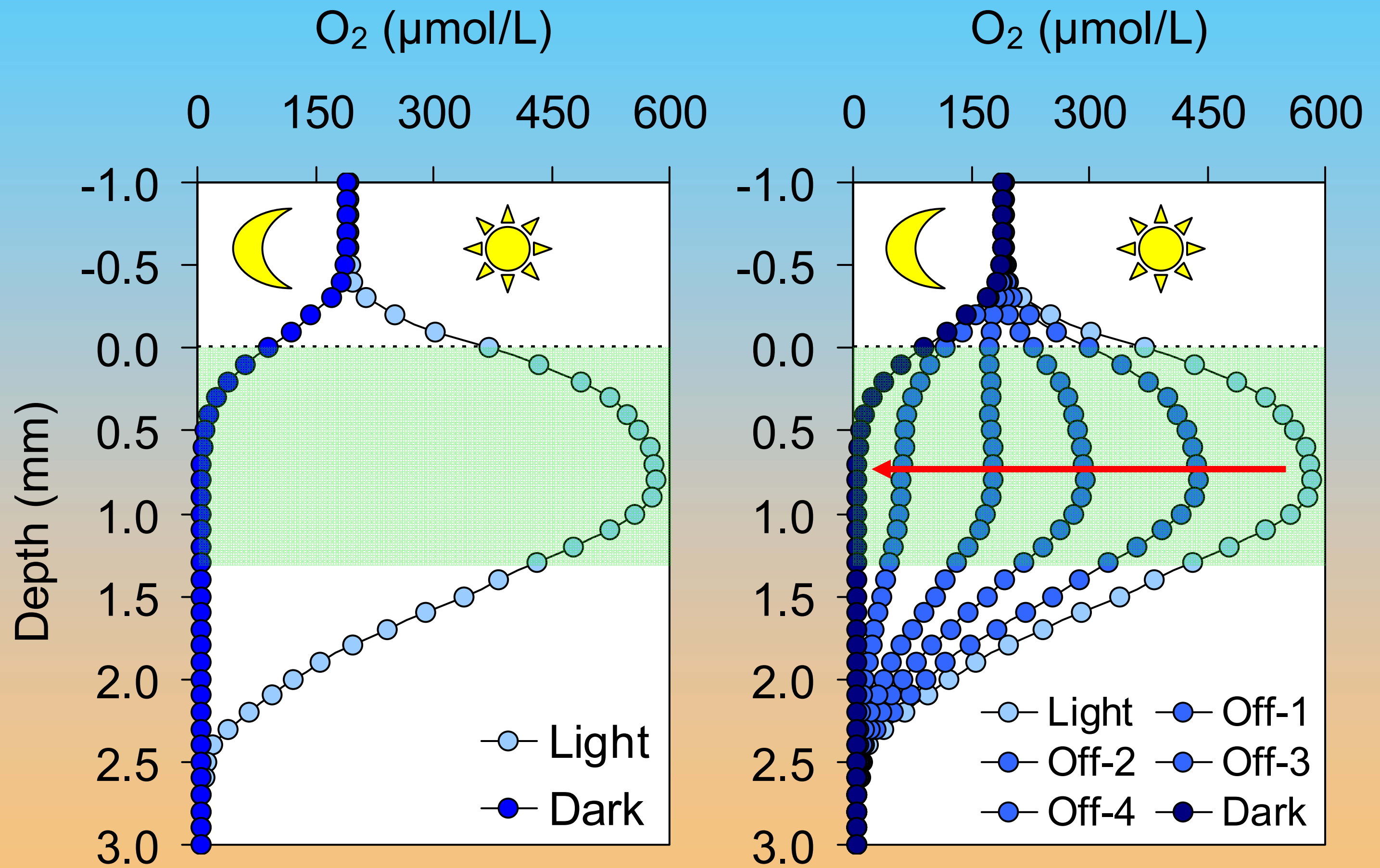
Diffusion is the only transport mode

- If advection plays a significant role,
  then different models for profile interpretation have to be used

Concentration profiles are in steady state

- No changes in shape are being observed with time
- Transport and conversion of a solute are in balance at every point

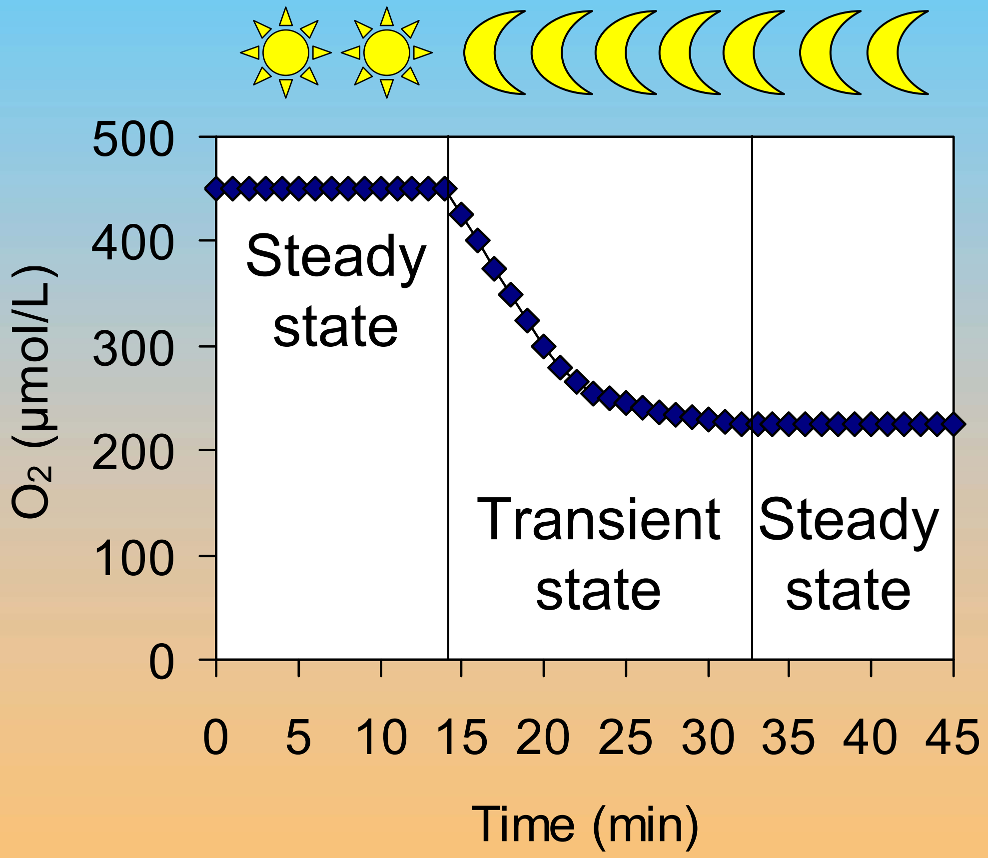
Profile interpretation: Conditions

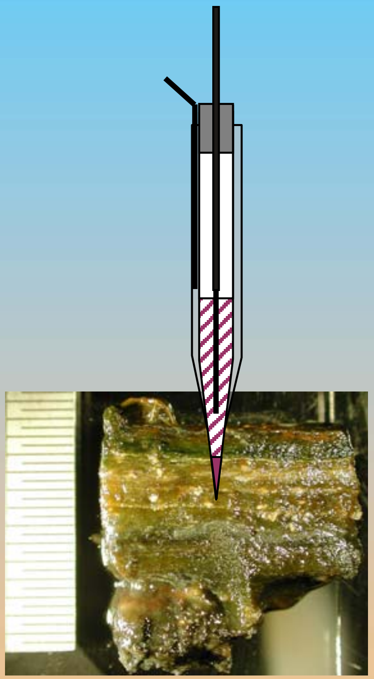


Steady state profiles

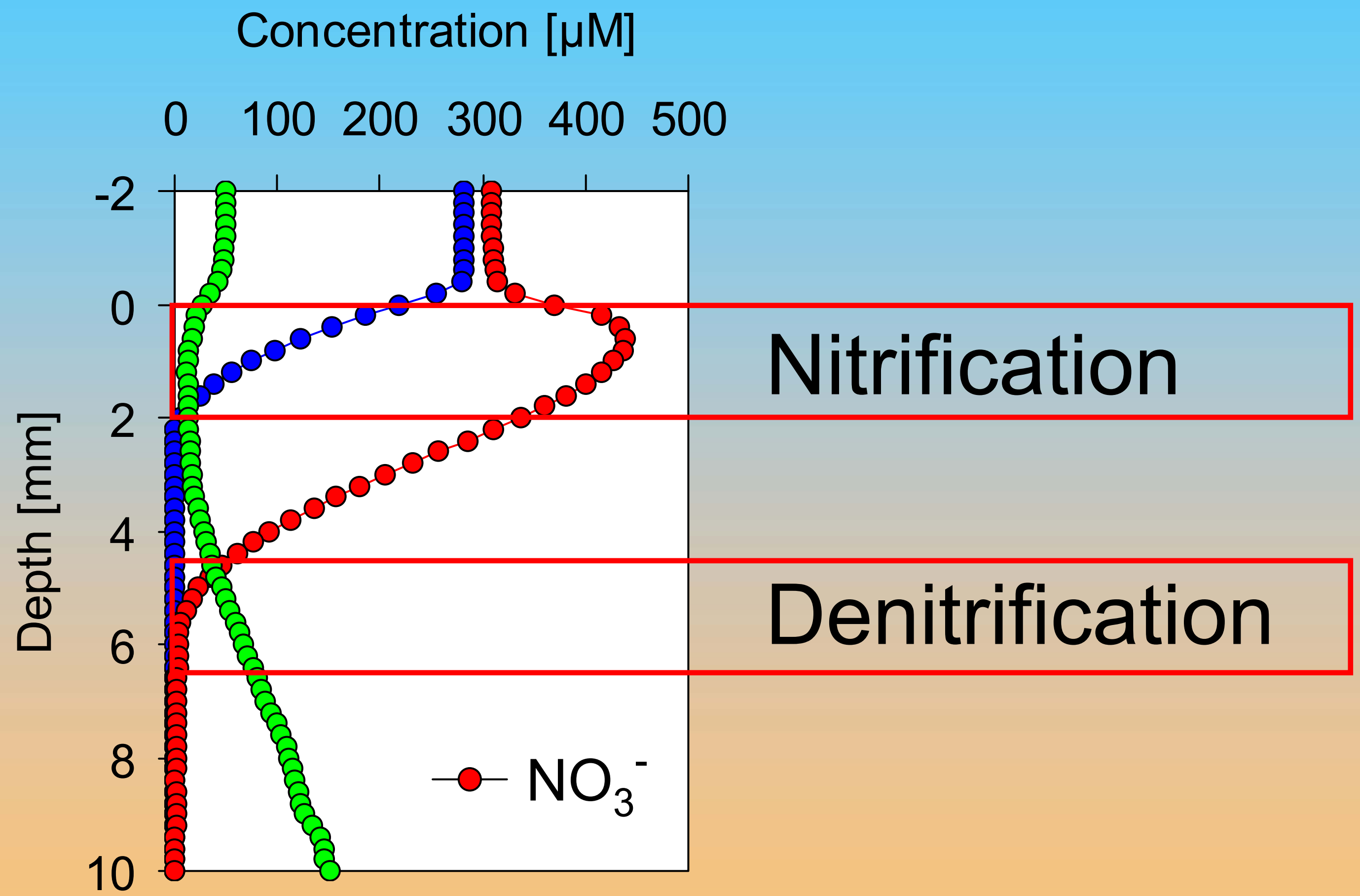
Transient state profiles

Profile interpretation: Conditions



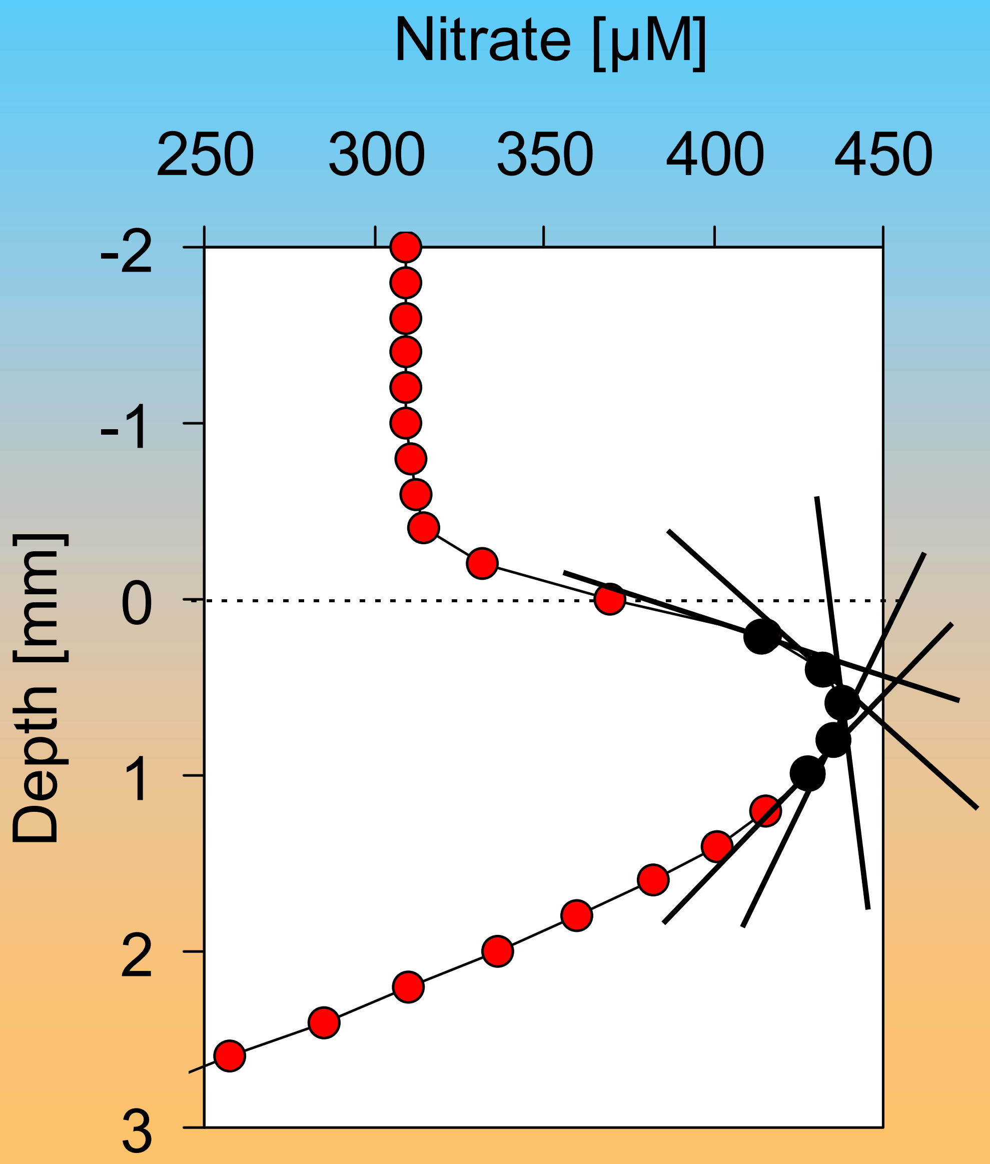


Rate calculation: (De)Nitrification



→ Quantification using a Diffusion-Reaction-Model

Rate calculation: Local flux

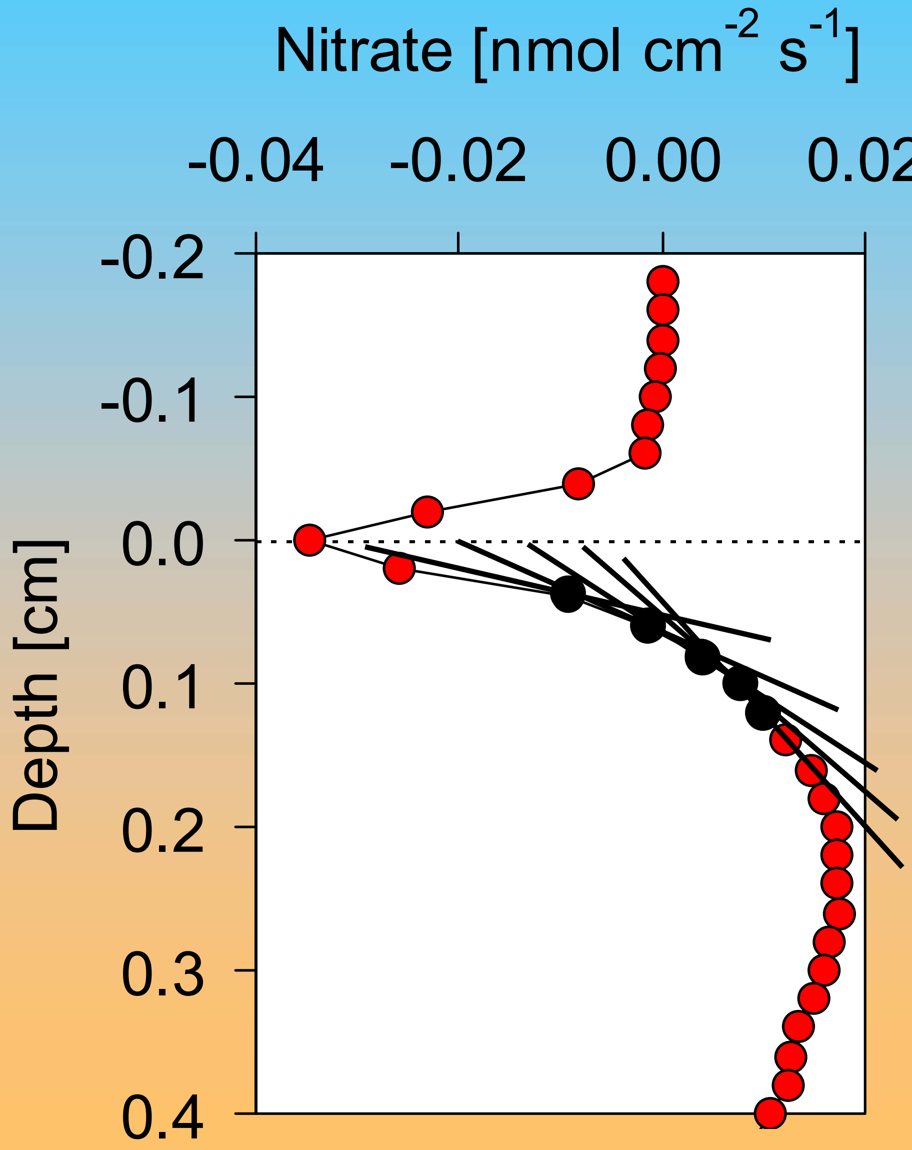


1st Derivative

Stepwise calculation of the tangent through each data point

Units = [nmol cm^{-2} s^{-1}]

Rate calculation: Local rate



2nd Derivative

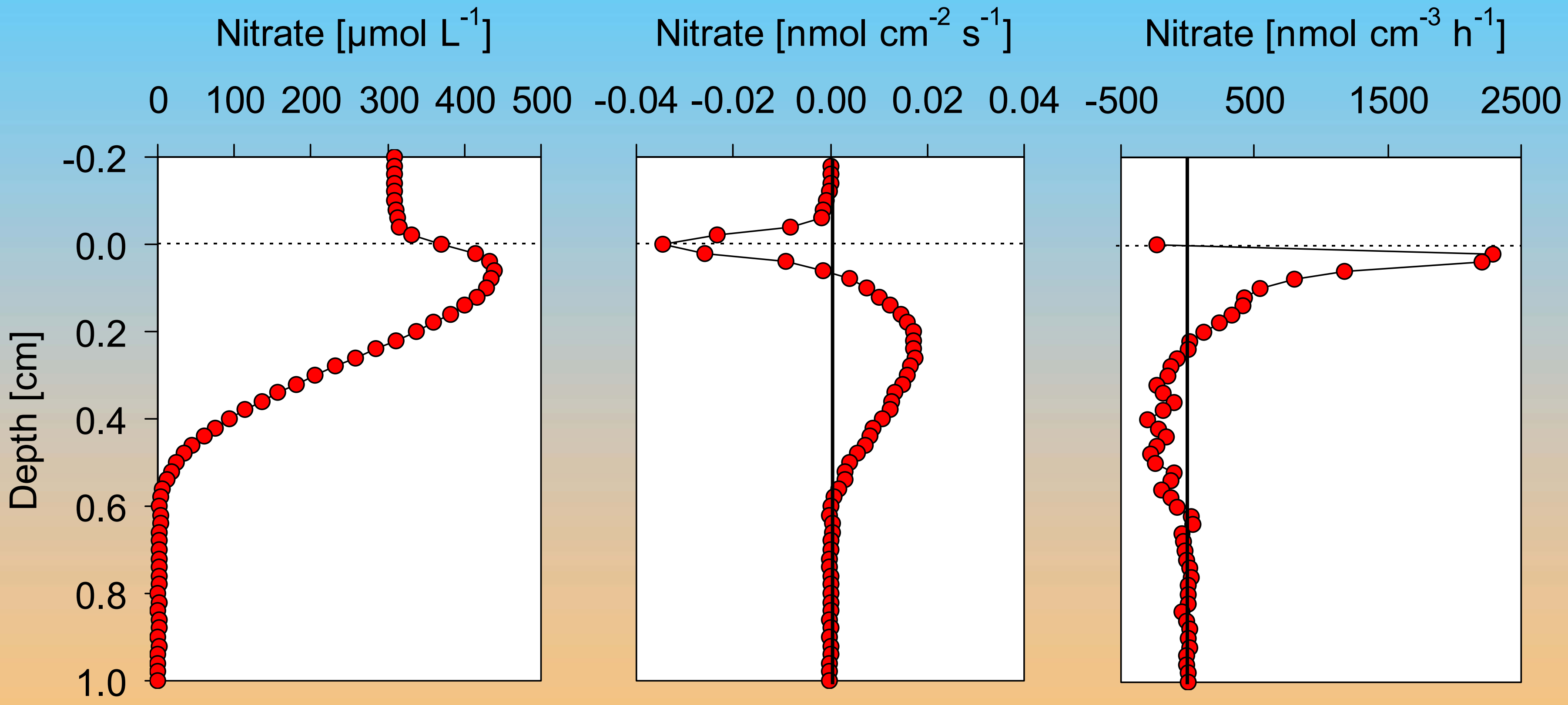
Stepwise calculation of

the tangent through

each local flux

Units = [nmol cm^{-3} s^{-1}]

Rate calculation: (De)Nitrification

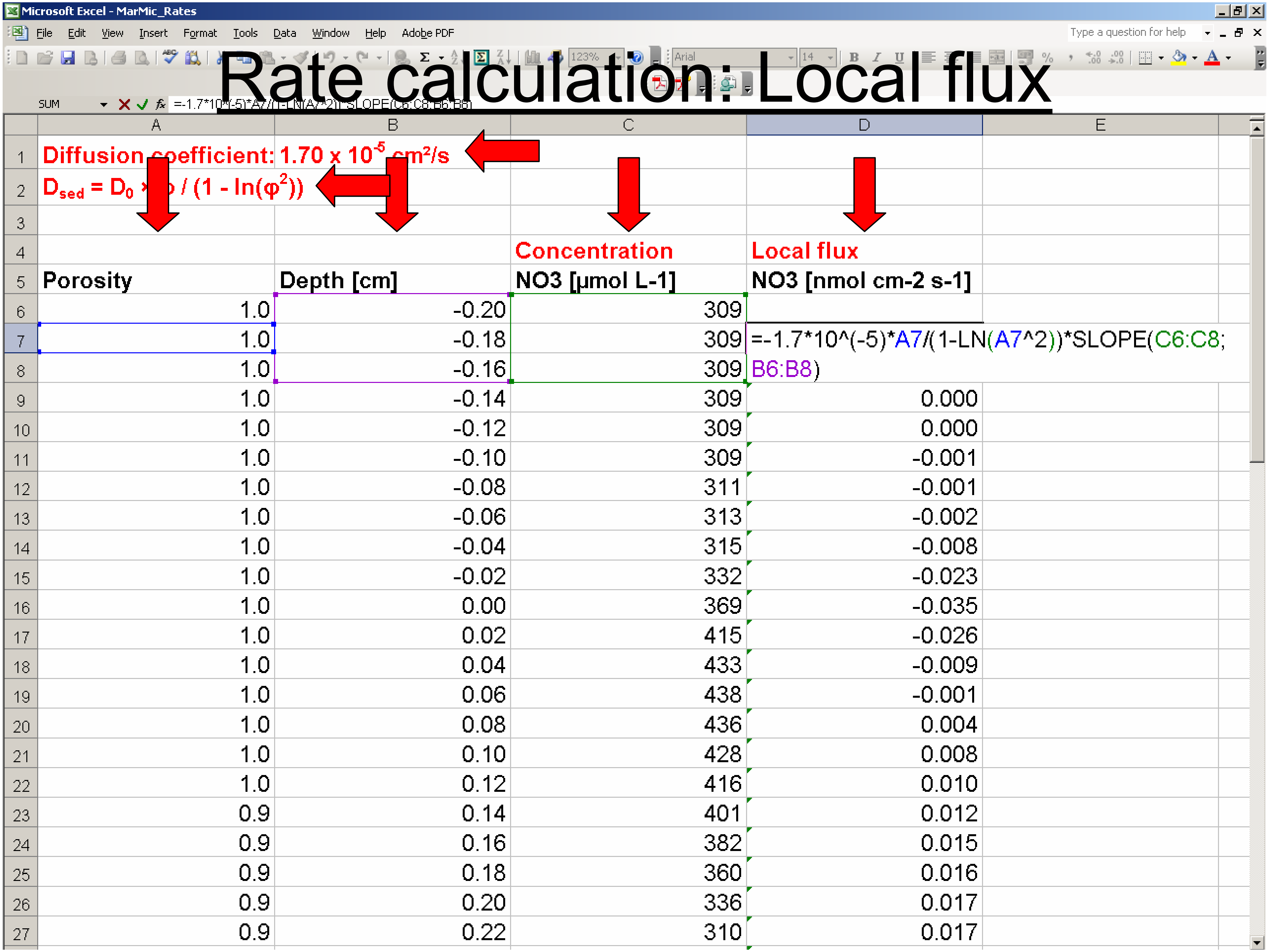


Concentration

Local flux

Local rate

Rate calculation: Local flux

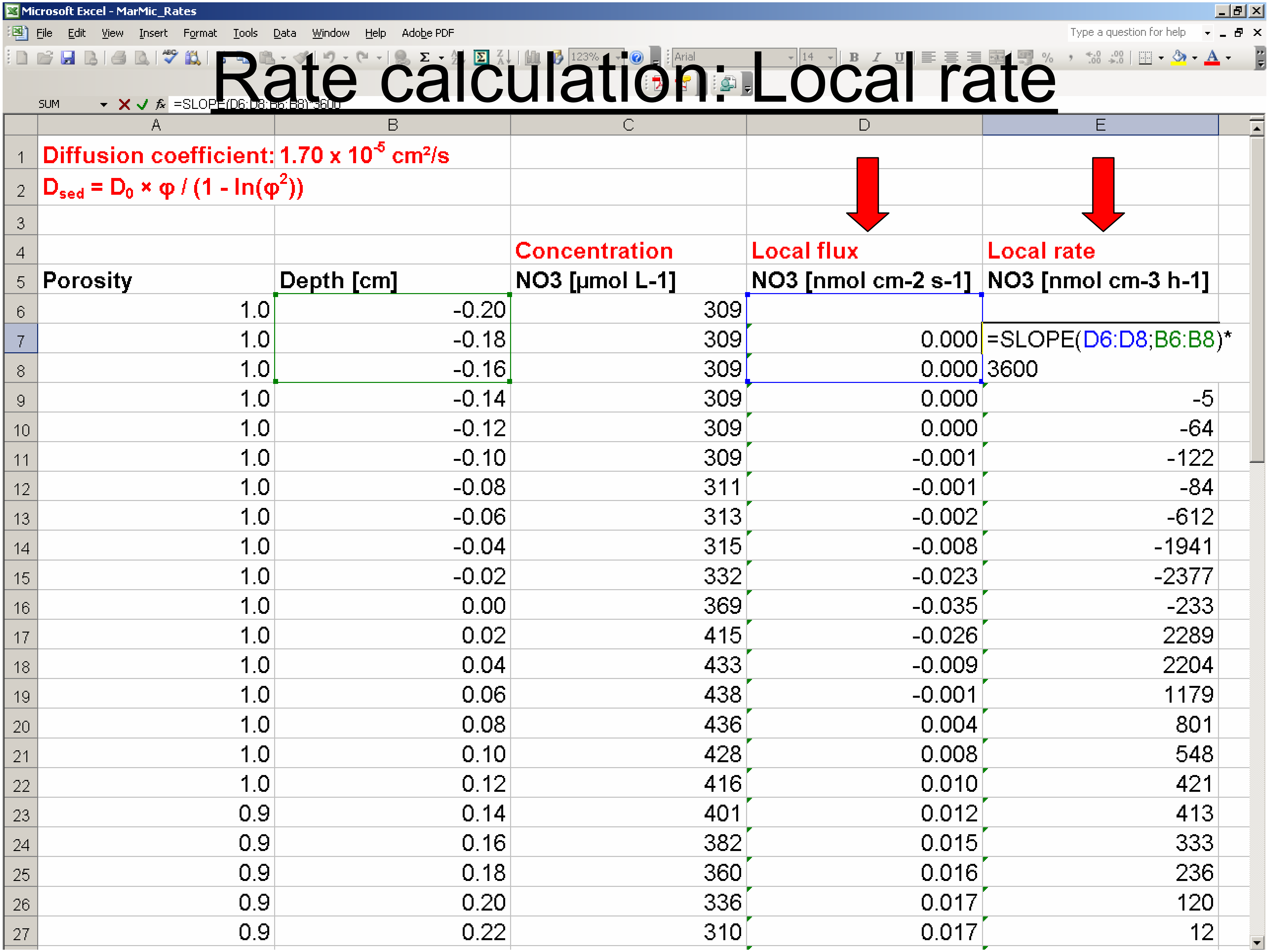


Diffusion coefficient: 1.70 x 10^{-5} cm²/s

$D_{sed} = D_0 \times \varphi / (1 - \ln(\varphi^2))$

	A	B	C	D
4			**Concentration**	**Local flux**
5	**Porosity**	**Depth [cm]**	**NO3 [µmol L-1]**	**NO3 [nmol cm-2 s-1]**
6	1.0	-0.20	309	
7	1.0	-0.18	309	=-1.7*10^(-5)*A7/(1-LN(A7^2))*SLOPE(C6:C8;B6:B8)
8	1.0	-0.16	309	
9	1.0	-0.14	309	0.000
10	1.0	-0.12	309	0.000
11	1.0	-0.10	309	-0.001
12	1.0	-0.08	311	-0.001
13	1.0	-0.06	313	-0.002
14	1.0	-0.04	315	-0.008
15	1.0	-0.02	332	-0.023
16	1.0	0.00	369	-0.035
17	1.0	0.02	415	-0.026
18	1.0	0.04	433	-0.009
19	1.0	0.06	438	-0.001
20	1.0	0.08	436	0.004
21	1.0	0.10	428	0.008
22	1.0	0.12	416	0.010
23	0.9	0.14	401	0.012
24	0.9	0.16	382	0.015
25	0.9	0.18	360	0.016
26	0.9	0.20	336	0.017
27	0.9	0.22	310	0.017

Rate calculation: Local rate



=SLOPE(D6:D8;B6:B8)*3600

	A	B	C	D	E
1	**Diffusion coefficient:**	**1.70 x 10^{-5} cm²/s**			
2	**$D_{sed} = D_0 \times \varphi / (1 - \ln(\varphi^2))$**				
3					
4			**Concentration**	**Local flux**	**Local rate**
5	**Porosity**	**Depth [cm]**	**NO3 [µmol L-1]**	**NO3 [nmol cm-2 s-1]**	**NO3 [nmol cm-3 h-1]**
6	1.0	-0.20	309		
7	1.0	-0.18	309	0.000	=SLOPE(D6:D8;B6:B8)*
8	1.0	-0.16	309	0.000	3600
9	1.0	-0.14	309	0.000	-5
10	1.0	-0.12	309	0.000	-64
11	1.0	-0.10	309	-0.001	-122
12	1.0	-0.08	311	-0.001	-84
13	1.0	-0.06	313	-0.002	-612
14	1.0	-0.04	315	-0.008	-1941
15	1.0	-0.02	332	-0.023	-2377
16	1.0	0.00	369	-0.035	-233
17	1.0	0.02	415	-0.026	2289
18	1.0	0.04	433	-0.009	2204
19	1.0	0.06	438	-0.001	1179
20	1.0	0.08	436	0.004	801
21	1.0	0.10	428	0.008	548
22	1.0	0.12	416	0.010	421
23	0.9	0.14	401	0.012	413
24	0.9	0.16	382	0.015	333
25	0.9	0.18	360	0.016	236
26	0.9	0.20	336	0.017	120
27	0.9	0.22	310	0.017	12

The End