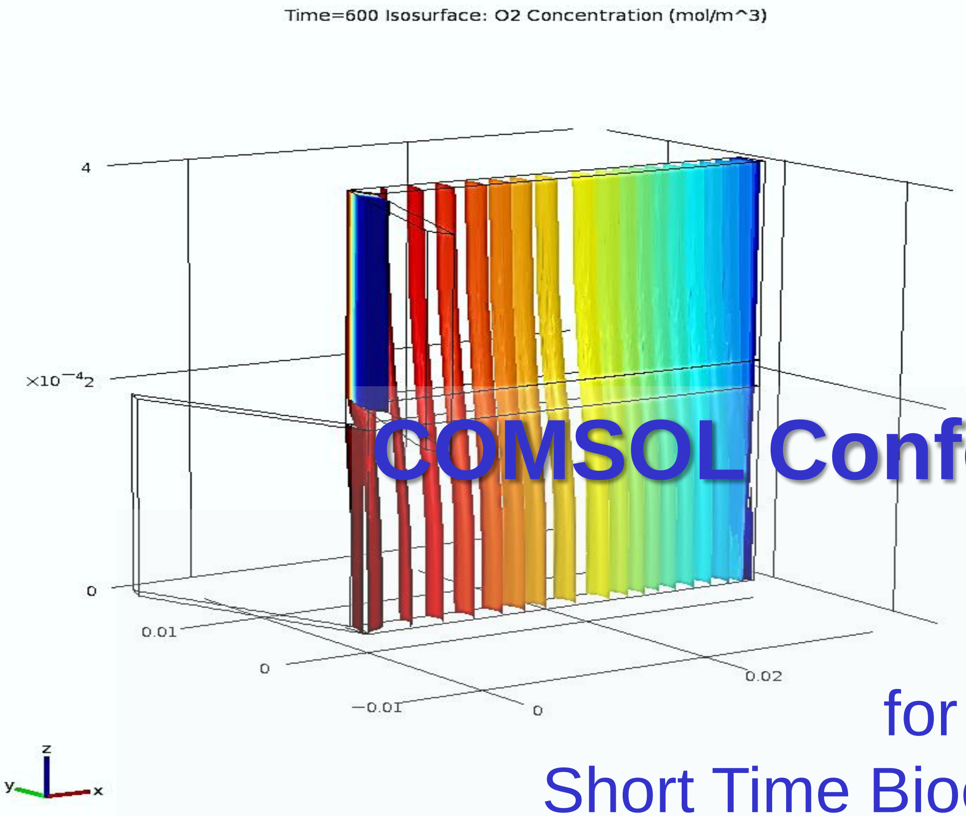

COMSOL Conference, Milan 2012

Modeling and Design of a Microfluidic Respirometer for Continuous Amperometric Short Time Biochemical Oxygen Demand (BOD_{st}) Analysis

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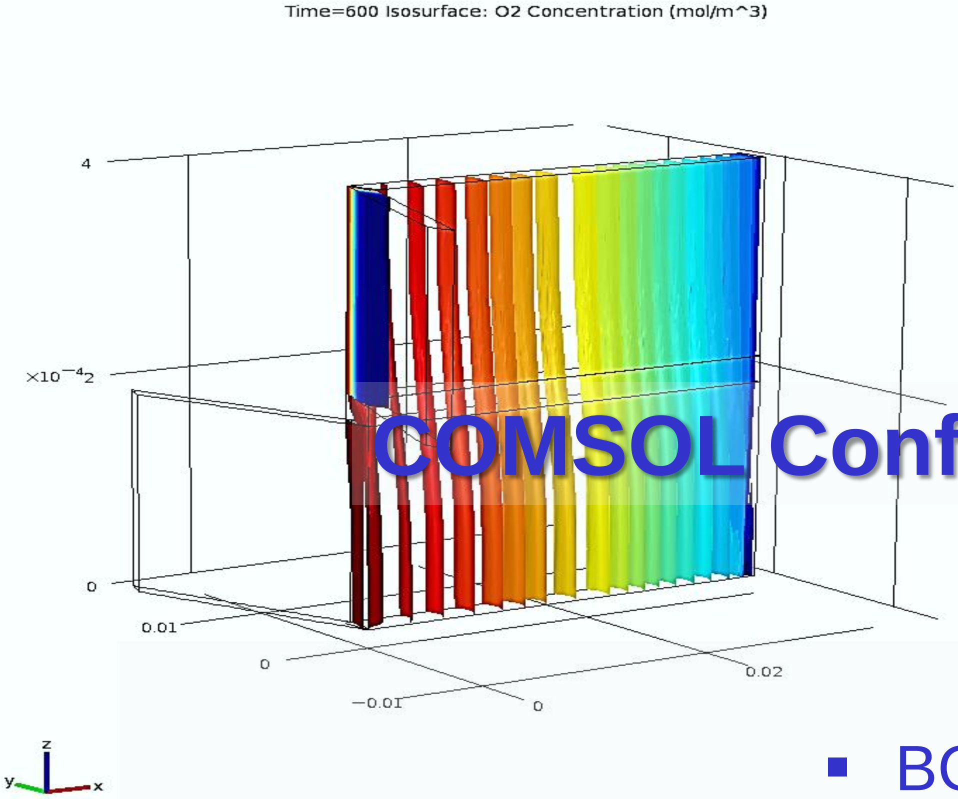
Excerpt from the Proceedings of the 2012 COMSOL Conference in Milan



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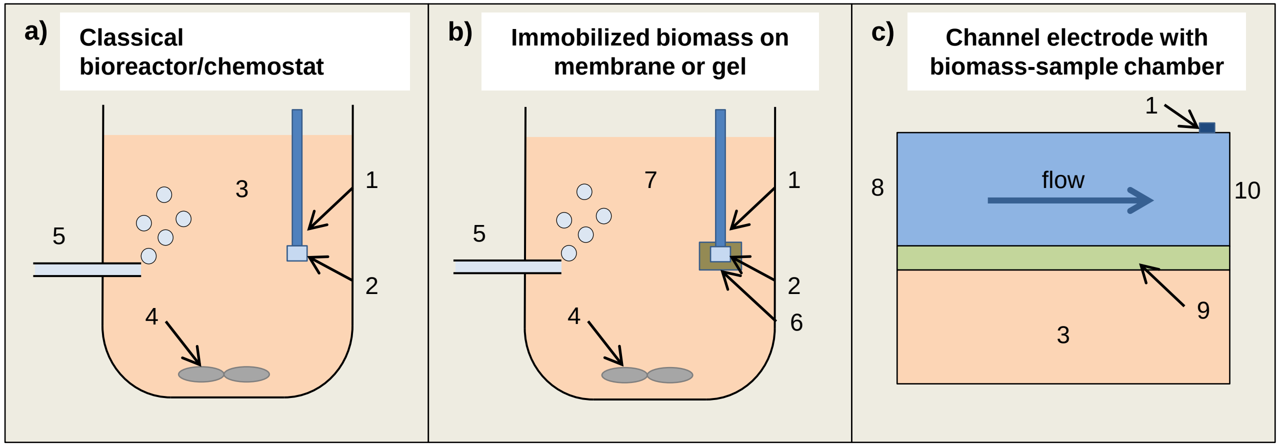
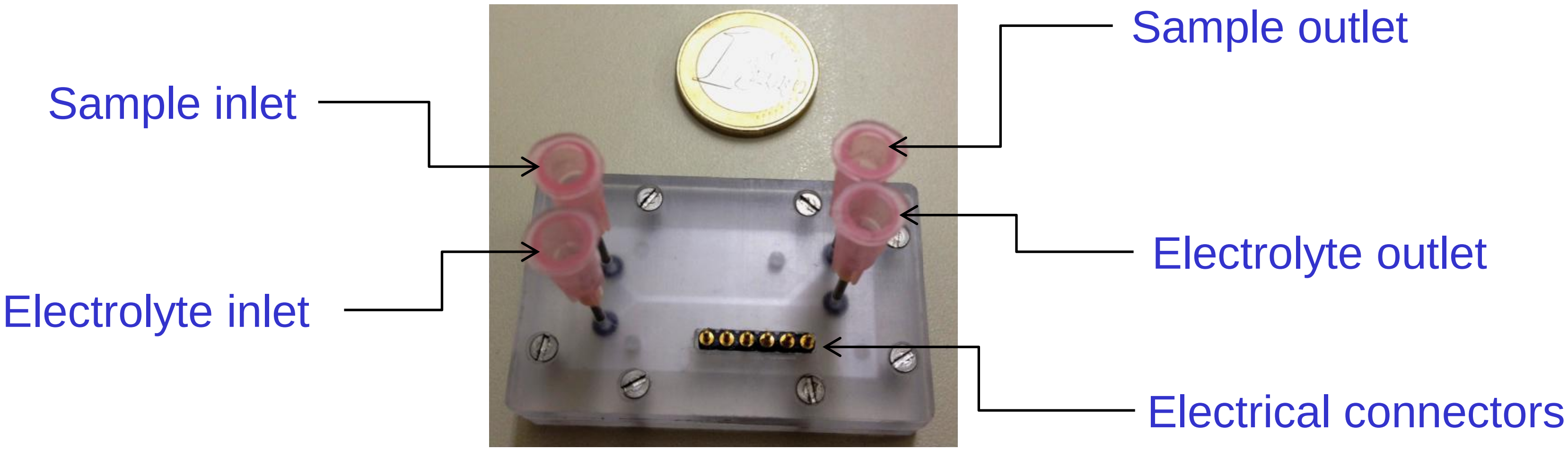
Index:

- BOD analysis considerations
- Design approach
- Simulations results
- Conclusions

Respirometer concept description:

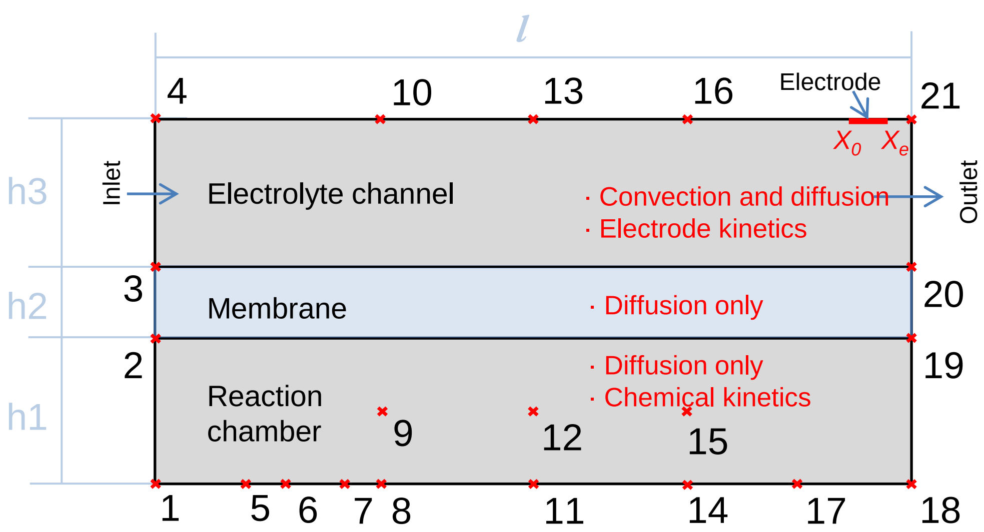




You can read the full article at: http://dx.doi.org/10.1016/j.bej.2012.04.014

Design approach:

- Simplified to a 2D model (not to scale)
- COMSOL modules:
  - Laminar flow
  - Diffusion and convection
  - Biochemical reaction
  - Electrode response (Bc and Intop)

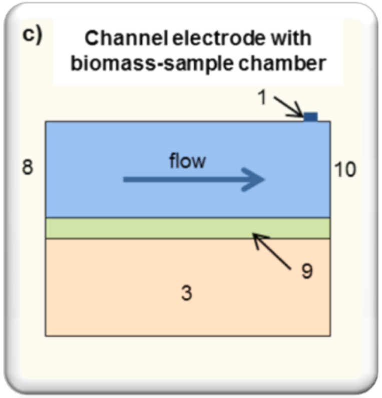


Parameters tested

- Thickness and materials of the membrane [25, 75 & 200 µm] [PTFE, PDMS] and channel length [120, 75 mm]
- Organics concentration [30,300,3000 mg/l BOD]
- Flow velocity [Flow x1 = 0.15 µl·min^{-1}][Flow x1, x2, x3, x4]
- O_2 sensor optimization

Fixed parameters

- Bacterial concentration [$1·10^9$ cfu/ml]
- Temperature and salinity [20 ºC; 5 g/kg]
- Simplified biochemical reaction [Glucose as only carbon source]



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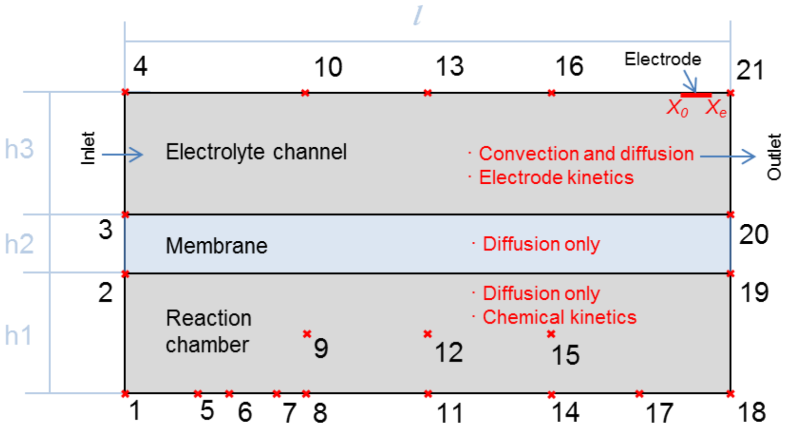
Model, mesh and solver:



1) Fluidics (stationary solver)

$$\rho(u\nabla)u - \eta\nabla^2 u + \nabla p = 0$$

$$\nabla \cdot u = 0$$

2) Chemical species (O_2 & Organics) diffusion, convection and biochemical reactions (transient solver)

$$\frac{\partial C_i}{\partial t} = D_i \nabla^2 C_i - u\nabla C_i \cdot R$$

$$\frac{dOrganics}{dt} = Bact_0 \cdot Organics \left\{ \frac{k_1(k_1 Organics + k_{-1})}{k_{-1} + k_2 O_2 + k_1 Organics} - k_1 \right\}$$

$$\frac{dO_2}{dt} = \frac{-k_1 k_2 Bact_0 \cdot Organics \cdot O_2}{k_{-1} + k_2 O_2 + k_1 Organics}$$

3) Electrochemical reaction (integration, transient solver)

$$O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$$

$$I = nFD_{O_2} w \int_0^{X_e} \left. \frac{\partial O_2}{\partial y} \right|_{y=0} dx$$

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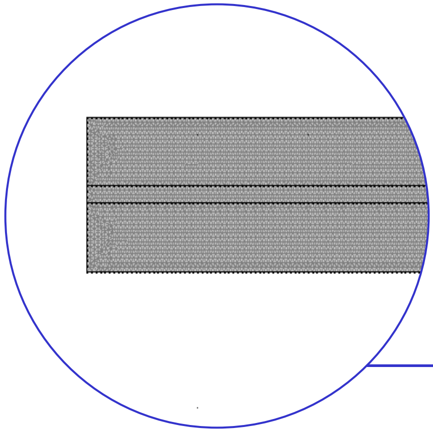
Model, mesh and solver:



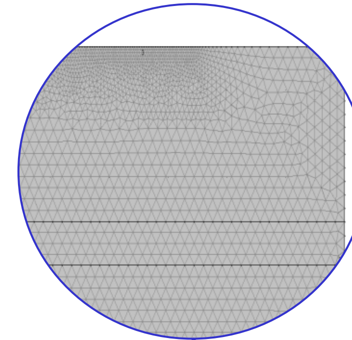
Mesh:

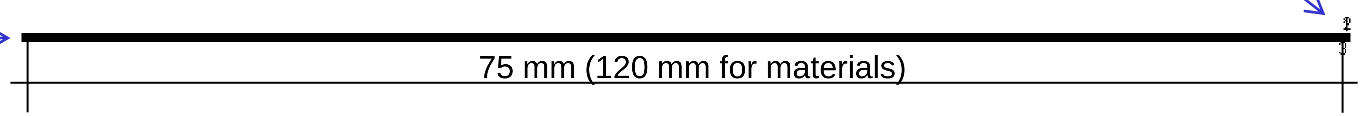
x: regular x-meshing

y: regular but ensuring 5 or more steps in the membrane

electrode: max elem. Size $2 \cdot 10^{-6}$m; min $2 \cdot 10^{-8}$m

Number of elements: From $1.4 \cdot 10^{5}$ to $4.5 \cdot 10^{5}$ depending on the model





Solver process:

Stationary solver for fluid flow
Var.: u, v & p
Solver: MUMPS
SD3

→

Time dependent solver for C&D and reaction (R)
Var.: O_2, BOD & R
Solver: MUMPS
Time: 0-8100 sec.
SD 1, 2 & 3

→

Integration of O_2 reduction on boundary 18·z (500μm)
Bc 18

Simulations were run in COMSOL Multiphysics 4.1 running on Linux OpenSuse on a SUN X2200 workstation (64 Gb RAM at 2.2 GHz clock speed dual Quad Core AMD Opteron 2354)

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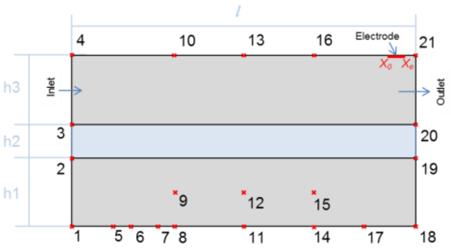
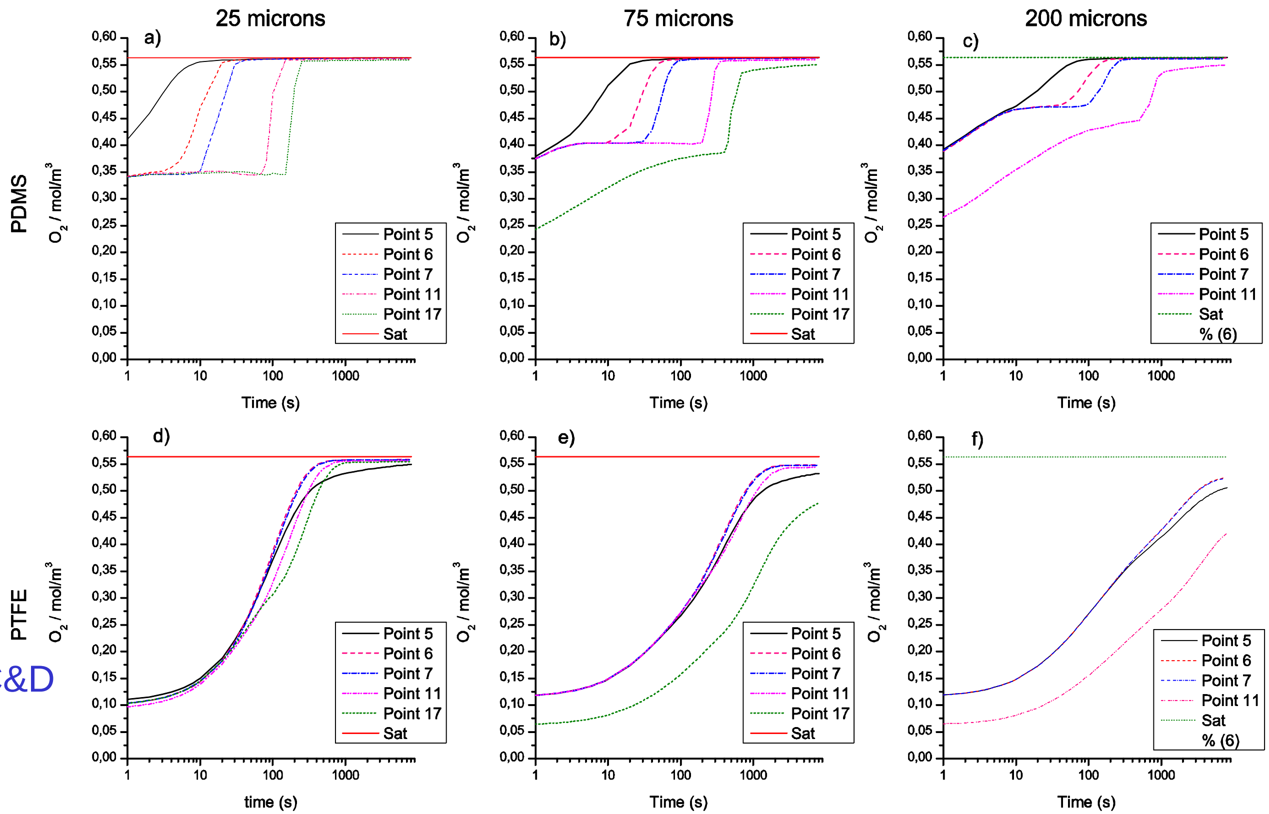
Analyzed parameters: Length (L) and membrane material

- Q 1: how long does it take for oxygen to reach saturation throughout?
- Q 2: How big is the effect of the material oxygen permeability?
- Q3: Is there an optimum channel length?



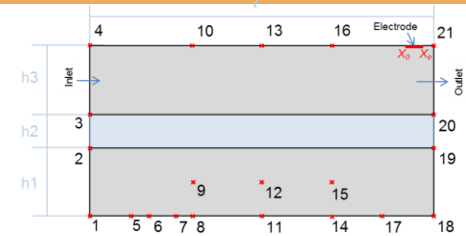


Models solved only for fluid flow and C&D
Not reaction considered
L = 120 mm

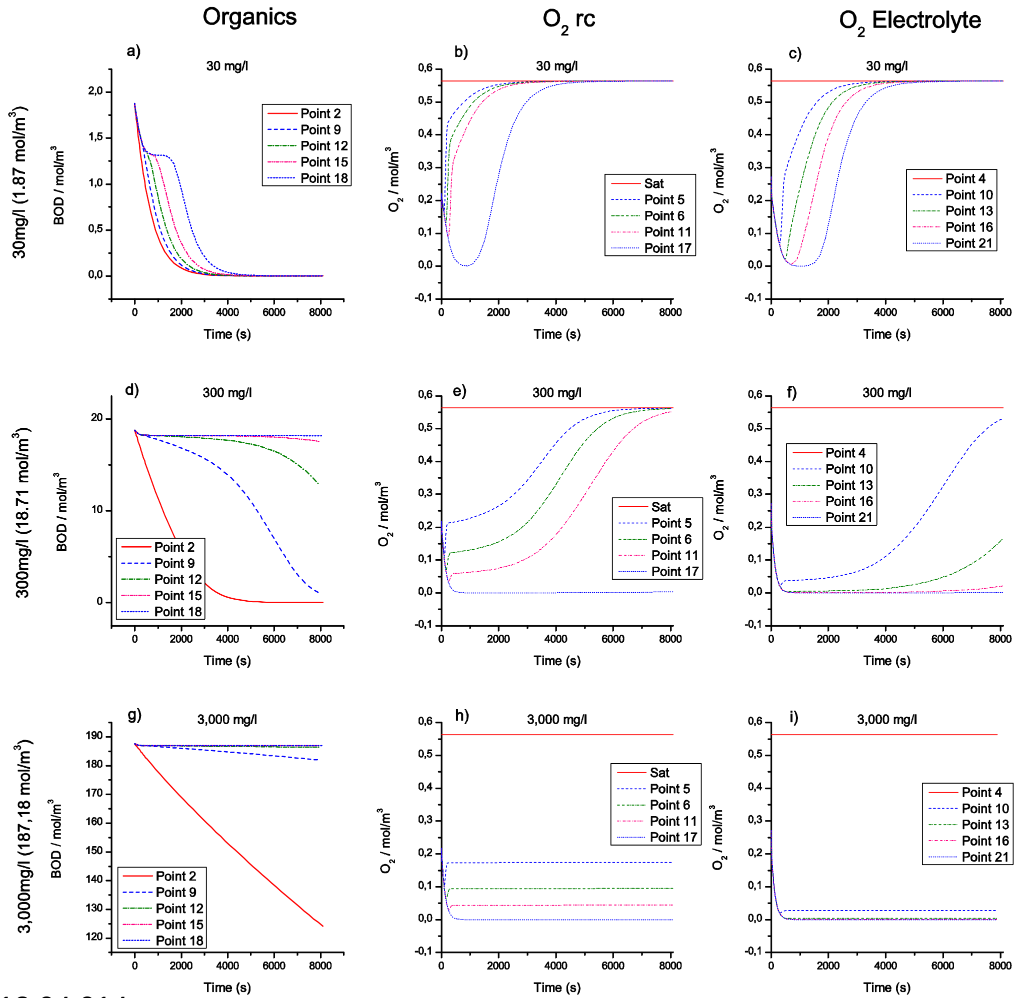
You can read the full article at: http://dx.doi.org/10.1016/j.bej.2012.04.014

Analyzed parameters: O2 & Organics

Time:
2,000 s → 33 min
4,000 s → 66 min
6,000 s → 100 min
8,000 s → 133 min



- Q1: How wide is the range of suitable organics concentrations?
- Q2: How much time do we need to have a result?
- Q3: How does channel length affect analysis time?

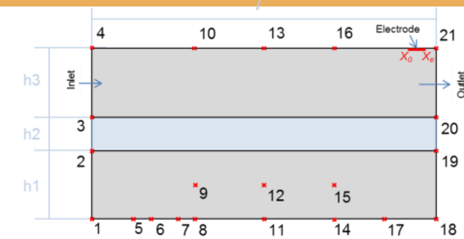


Models solved for fluid flow, C&D and biological consume of oxygen
L = 75 mm

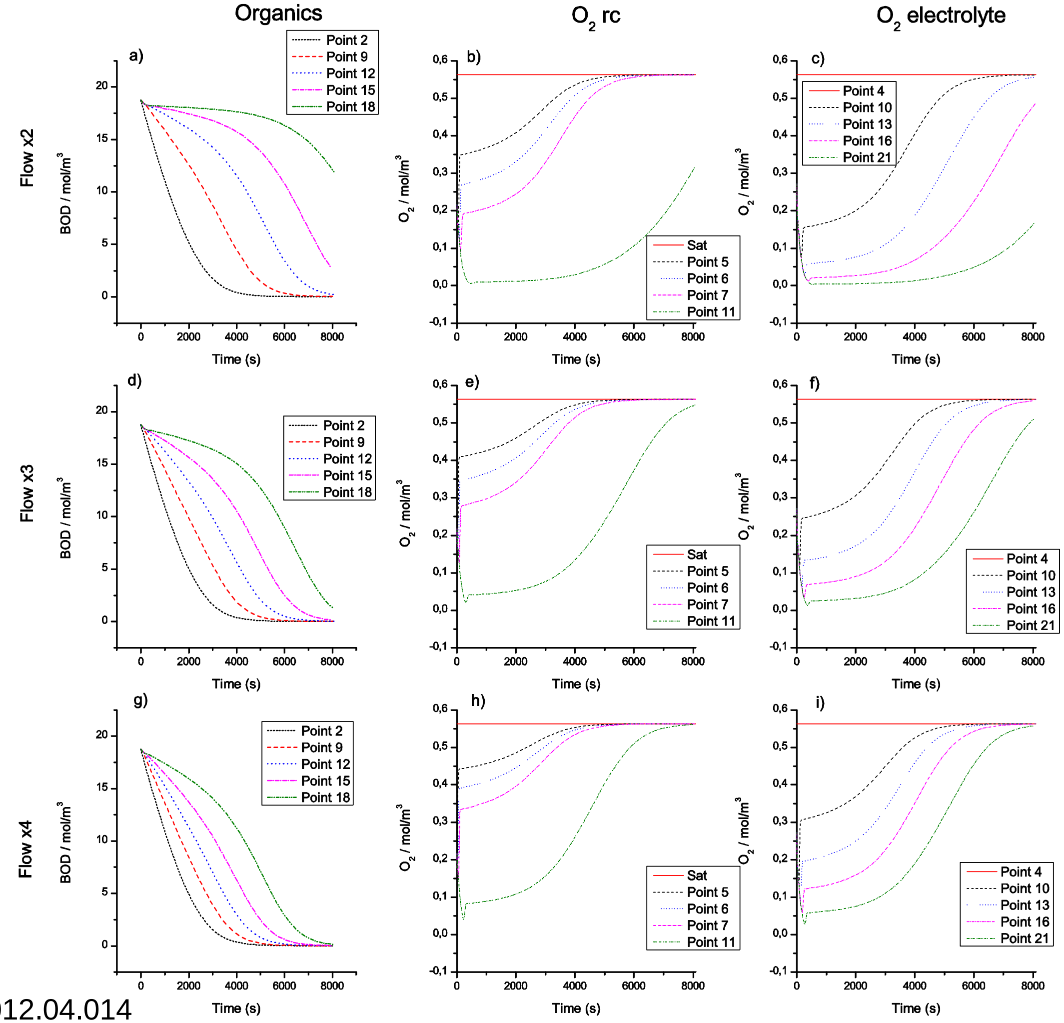
You can read the full article at: http://dx.doi.org/10.1016/j.bej.2012.04.014

Analyzed parameters: Flow velocity

Time:
2,000 s → 33 min
4,000 s → 66 min
6,000 s → 100 min
8,000 s → 133 min



- Q1: How does flow velocity affect reaction kinetics?
- Q2: How much versatility does flow give against different organics concentrations?
- Q3: Can it be modified to adapt the system to a wide range of organics?

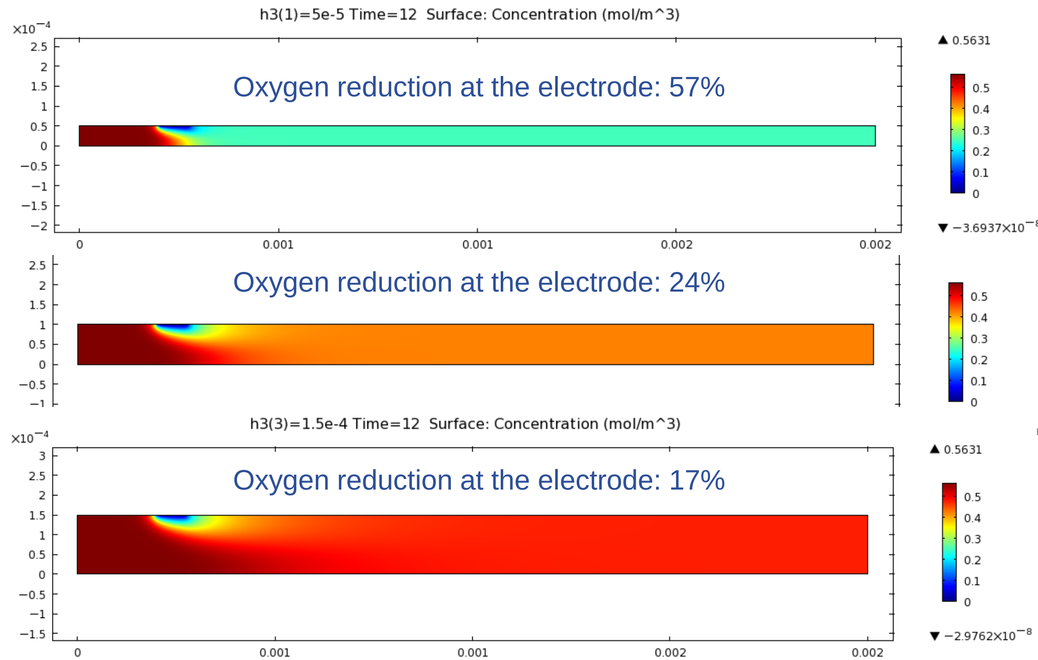


Models solved for fluid flow, C&D and biological consume of oxygen
L = 75 mm
Flow = 0.15 $\mu l \cdot min^{-1}$

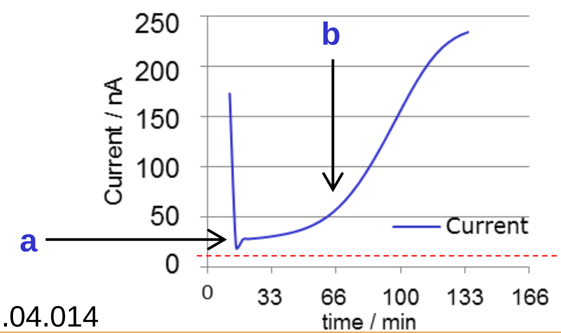
You can read the full article at: http://dx.doi.org/10.1016/j.bej.2012.04.014

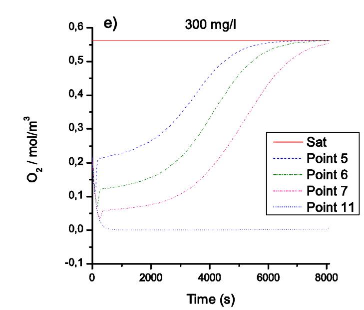
Analyzed parameters: Channel thickness and the electrode

- Q1: How does electrochemical measurement affect the oxygen concentration?
- Q2: Is it feasible to place more than one measuring electrode?
- Q3: What type of response can we expect and what are the key points?



$$O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$$





You can read the full article at: http://dx.doi.org/10.1016/j.bej.2012.04.014

Building the prototype: Main device specifications & constrains

- Greater control of oxygen concentration in the device.
  (this can be applied to a wide range of elements detectable by electrochemical technics)
- Best electrode protection in terms of electrode passivation due to organic compounds.
- Permits to work with small sample volumes (μl)
- Several factors permit to reduce analysis time (standard BOD requires 5 days):
  - Allows to use higher microorganisms concentrations ($1 \cdot 10^9$ to $1 \cdot 10^{11}$)
  - Micro-fabrication optimizes oxygen transport and no stirring is required.
  - Small sample in relation to microorganism concentration.
- Overall device of small size: a lab-on-a-chip system.
- Fast sampling and analysis (around 2 hours per analysis)
- Permits on-site analysis.

You can read the full article at: http://dx.doi.org/10.1016/j.bej.2012.04.014

Building the prototype: Benefits from the simulation and modeling approach

- Several approaches were tested; the model got more refined upon simulations results.
- This simplified model facilitates the development and data interpretation of an experimental system in terms of:
    - Modifying oxygen consumption velocity in complex or different composition samples.
    - Testing different microorganisms concentrations and mixtures.
    - Adapting the model to geometries that improve hydrodynamic performance.
- Simulations qualitatively explain possible complex responses before building the device.

You can read the full article at: http://dx.doi.org/10.1016/j.bej.2012.04.014

Thank You

Acknowledgements:

The authors acknowledge founding through projects:

- Microresp (PET2008-0165-01)
- Medra (TSI020100-2011-187)
- Bactotox (CTQ2009-14390-C02-01 & CTQ2009-14390-C02-02)
- Tragua (CSD2006-00044)

In addition Albert Torrents is funded by:

- FPU scholarship (AP2008-03848)

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