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

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Index:

- BOD analysis considerations
- Design approach
- Simulations results
- Conclusions
Respirometer concept description:

- Classical bioreactor/chemostat
- Immobilized biomass on membrane or gel
- Channel electrode with biomass-sample chamber

Sample outlet
Sample inlet
Electrolyte outlet
Electrolyte inlet
Electrical connectors

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]
- O₂ sensor optimization

Fixed parameters

- Bacterial concentration [1·10⁹ cfu/ml]
- Temperature and salinity [20 °C; 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\textsubscript{2} & Organics) diffusion, convection and biochemical reactions (transient solver)
\[ \frac{\partial C_i}{\partial t} = D_i \nabla^2 C_i - u \nabla C_i \cdot R \]
\[ \frac{d\text{Organics}}{dt} = B\text{act}_0 \cdot \text{Organics} \left\{ \frac{k_1 (k_1 \text{Organics} + k_{-1})}{k_{-1} + k_2 \text{O}_2 + k_1 \text{Organics}} - k_1 \right\} \]
\[ \frac{d\text{O}_2}{dt} = \frac{-k_1 k_2 B\text{act}_0 \cdot \text{Organics} \cdot \text{O}_2}{k_{-1} + k_2 \text{O}_2 + k_1 \text{Organics}} \]

3) Electrochemical reaction (integration, transient solver)
\[ \text{O}_2 + 4\text{H}^+ + 4e^- \rightarrow 2\text{H}_2\text{O} \]
\[ I = nFD_{\text{O}_2} w \int_0^{X_f} \left. \frac{\partial \text{O}_2}{\partial y} \right|_{y=0} \, dx \]

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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 $18 \cdot z$
  - (500 µm)
  - 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

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Analyzed parameters: O2 & Organics

- **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

\[ L = 75 \text{ mm} \]

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

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Analyzed parameters: Flow velocity

- **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

$L = 75 \text{ mm}$

Flow $= 0.15 \mu l\cdot \text{min}^{-1}$

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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?

\[ O_2 + 4H^+ + 4e^- \rightarrow 2H_2O \]

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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 (1·10⁹ to 1·10¹¹)
  - 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.

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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.

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Thank You

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