Computational Fluid dynamics of bioreactors with micro-aeration

James J Lischeske[1], Mohammad Rahimi[2], Hariswaran Sitaraman[2], and Jonathan J Stickel[3]

[1]National Bioenergy Center, [2]Computational Sciences Center, [3]Biosciences Center

Background

- Computational Fluid Dynamics (CFD) is an effective tool for testing reactor designs and configurations *in silico*, reducing risk in scale-up
- Traditionally, aerobic fermentation scaleup emphasizes total-reactor metrics, such as overall oxygen transfer rate, as that governs the overall rate of reaction
- New approaches in biological conversion of sugars to fuels, particularly with recombinant *S mobilis*, make use of the aerobic environment to influence product selectivity. Thus, a narrower (and often lower) range of oxygen concentrations may be required to generate the desired products
- CFD can characterize the distribution of oxygen in large-scale reactors, allowing us to evaluate the suitability of different design concepts

Model

Two-Phase Euler-Euler method -- OpenFOAM
(Rahimi et al, 2019)

Mass Conservation (per-phase; alpha is the volume-fraction of the gas phase):

$$\frac{\partial}{\partial t}(\alpha_i \rho_i) + \vec{\nabla} \cdot (\alpha_i \rho_i V_i) = 0;$$

Momentum equation (per-phase):

$$\frac{\partial}{\partial t}(\alpha_i \rho_i V_i) + \vec{\nabla} \cdot (\alpha_i \rho_i V_i V_i) = -\alpha_i \vec{\nabla} P + \alpha_i \rho_i g + \vec{\nabla} \cdot (\alpha_i \bar{R}_i) + F_i$$

F_i is a collection of interphase momentum transfer terms, including lift, drag, virtual-mass, wall-lubrication and turbulent-dispersion terms.

Chemical-species transport:

$$\frac{\partial}{\partial t}(\alpha_i \rho_i Y_{ij}) + \vec{\nabla} \cdot (\alpha_i \rho_i Y_{ij} V_i) = \vec{\nabla} \cdot (\alpha_i \rho_i \bar{D}_{ij} \vec{\nabla} Y_{ij}) + \dot{R}_{ij}^{\mathrm{MT}}$$

Oxygen transfer:

$$\mathrm{OTR} = k_{\mathrm{L}} a (C^*_{\mathrm{O_2}} - C_{\mathrm{O_2}})$$

Higbie (1964) penetration model:

$$k_{\mathrm{L}} = \sqrt{\frac{4D}{\pi} \frac{|\mathbf{u}_{\mathrm{slip}}|}{d_{\mathrm{b}}}}$$

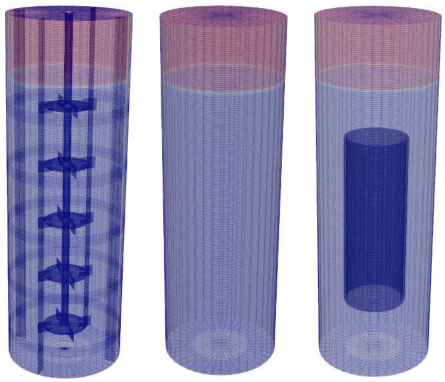
Oxygen uptake, assumed linear for low concentrations of oxygen:

$$\mathrm{OUR} = k_{\mathrm{O_2}} C_{\mathrm{O_2}} \alpha_{\mathrm{L}}$$

For each simulation, the liquid phase is initialized at a uniform oxygen concentration, with alpha at zero across the reactor (and 1 in the headspace). The gas-phase rises from a sparger in the bottom-center of the vessel.

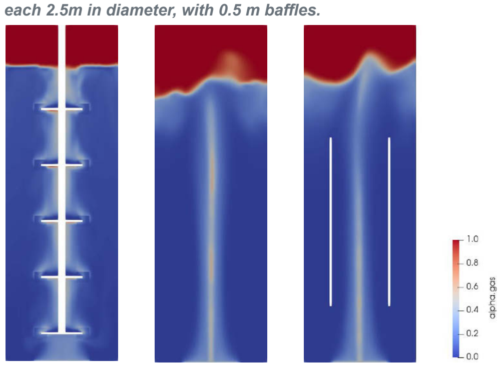
Rahimi, M., Sitaraman, H., Humbird, D., Stickel, J.J. (2018) Computational fluid dynamics study of full-scale aerobic bioreactors: Evaluation of gas-liquid mass transfer, oxygen uptake, and dynamic oxygen distribution. *Chem Eng Res Des*, **139**, 283-295.

CSTR | **Bubble Column (BC)** | **Airlift (AL)**

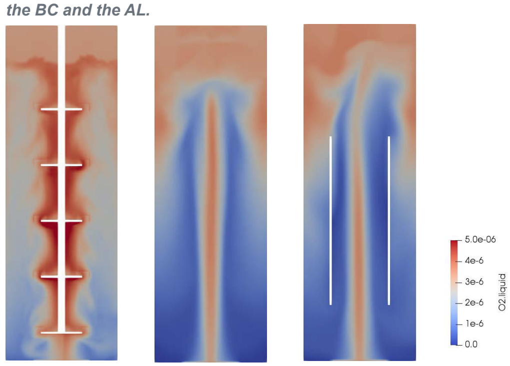


543k cells | ***180k cells*** | ***184k cells***

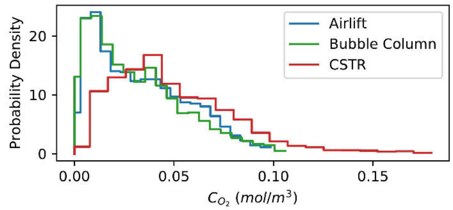
All are 500m[3] industrial scale reactors using the same geometry (5m D x 15m H). This is equivalent to the largest CSTRs in production. The CSTR uses five Rushton impellers, each 2.5m in diameter, with 0.5 m baffles.



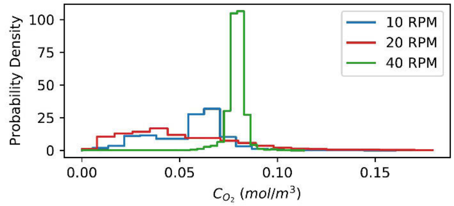
The gas-phase is concentrated in the center of the reactor (above). Oxygen concentration (below) is higher and more uniform in the CSTR (20 RPM); significant dead-zones exist in the BC and the AL.



Oxygen Distribution

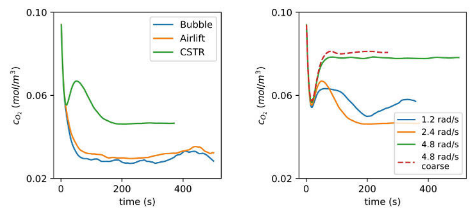


The airlift and bubble column reactors perform similarly (0.02 m/s), and they achieve lower oxygen concentrations relative to a 20 RPM CSTR.



Oxygen concentration is non-monotonic with mixing speed (superficial gas velocity of 0.02 m/s). However, very-high rotation rate (40 RPM) results in a higher oxygen concentration with a much tighter distribution. Achieving this rotational velocity (7 m/s tip speed) scale is both economically and technically infeasible in practice at this scale.

Time to Pseudo-Steady State



On the left, with superficial gas velocities of 0.02 m/s, the airlift and bubble column reactors again perform similarly, and they achieve lower mean oxygen concentrations relative to a 20 RPM CSTR.

On the right, CSTRs are compared at different rotation rates (superficial gas velocity of 0.02 m/s). Mean oxygen concentration is unstable at lower mixing speeds, requiring longer to achieve pseudo-steady state. However, very-high rotation rate (40 RPM) results in the simulation reaching steady state quickly.

Using a coarser mesh, the CSTR for the 40 RPM case gives similar qualitative results, though with some lose of fidelity.

Summary

- Oxygen concentration is highly heterogenous across all proposed reactor designs at 500 m[3] scale
- An extremely high mixing rate (tip speed of 7 m/s) is able to achieve a tight oxygen distribution, but this is likely to be uneconomical and technically infeasible
- Additional reactor concepts will be evaluated, such as pump-around loops and different CSTR impellers

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