Computational Fluid dynamics of bioreactors with micro-aeration

James J Lischkes1, Mohammad Rahimi2, Hariswaran Sitaraman2, and Jonathan J Stickel3
1National Bioenergy Center, 2Computational Sciences Center, 3Biosciences 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):
\[ \frac{\partial}{\partial t} \alpha_i (\rho_i V_i) + \nabla \cdot (\alpha_i \rho_i V_i V) = 0; \]

Momentum equation (per-phase):
\[ \frac{\partial}{\partial t} \alpha_i (\rho_i V_i) + \nabla \cdot (\alpha_i \rho_i V_i V_i) = -\alpha_i \nabla \rho + \alpha_i \rho \nabla + (\alpha_i \rho \frac{\nabla}{\rho \nabla} + F_i; \]

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

Chemical-species transport:
\[ \frac{\partial}{\partial t} (\alpha_i \rho_i Y_i) + \nabla \cdot (\alpha_i \rho_i Y_i V_i) = \nabla \cdot (\alpha_i \rho_i D_{ij} \nabla Y_i) + R_{MT}; \]

Oxygen transfer:
\[ OTR = k_{l,a} (C_{O_2} - C_{O_2}); \]

Higbie (1964) penetration model:
\[ k_{l,a} = \sqrt{\frac{4D_{ij}}{\pi \rho_{ij} \nabla}} \]

Oxygen uptake, assumed linear for low concentrations of oxygen:
\[ OUR = k_{O_2} C_{O_2} ; \]

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.

Summary

• Oxygen concentration is highly heterogeneous across all proposed reactor designs at 500 m³ 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.

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 loss of fidelity.