CFD Study of Full-Scale Aerobic Bioreactors
Evaluation of Dynamic $O_2$ Distribution, Gas-Liquid Mass Transfer and Reaction

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Computational Science at NREL

HPC projects at NREL include:
• Molecular dynamics of cellulosic enzymes
• Inverse design for energy materials
• Wind energy simulations

Mechanistic modeling of biochemical conversion of biomass:
• Pretreatment, enzymatic hydrolysis, aerobic bioreaction
• Continuum-scale predictive modeling
• Based on relevant physical and chemical principles, while remaining computational efficient
• Support process design, parameter optimization, and estimation of operating costs
• Team of chemical engineers and computational scientists

Peregrine is NREL’s flagship HPC capability:
• 1.19 PetaFLOPS
  • 31,104 Intel Xeon processors
  • 576 Intel Phi many-core co-processors
• 3 petabytes of mass storage
Industrial aerobic bioprocess

- NREL research is increasingly focused on advanced biofuels produced via aerobic microbial production pathways (e.g., oleaginous yeast).
- At “fuel-scale,” aerobic fermentation is the largest OPEX+CAPEX contributor in the process, even in extremely large bioreactors up to 1,000 m³.
- In order to improve economics through bioreactor and overall process design, we seek validation and improvement of the reactor design equations used in techno-economic analysis.
CFD of aerobic bioreactors

• We use CFD to confirm scale-up principles and optimize full-scale design
• Existing bioreactor CFD literature focuses on precise hydrodynamics of bubbly flows—no modeling of oxygen distribution
• We explicitly model O₂ mass transfer and consumption to study dissolved O₂ concentration distribution in bubble-column and airlift bioreactors
  o Bubble-columns are expected to have lower CAPEX and OPEX than stirred-tank bioreactors.
CFD Implementation

Numerical Approach

• Euler-Euler multiphase simulation in OpenFOAM
  o reactingTwoPhaseEulerFoam (OpenFOAM-3.0)
• Reynolds-averaged Navier-Stokes (RANS)
• $k$-$\varepsilon$ turbulence model

Multiphase assumptions

• Bubble diameter $<<$ reactor diameter
• Single bubble diameter (5 mm)

Gas-liquid mass transfer

• Oxygen transfer rate: $\text{OTR} = k_L a \left( C_{O_2}^* - C_{O_2} \right)$
• Mass transfer coefficient (Higbie): $k_L = \sqrt{\frac{4D u_{\text{slip}}}{\pi d_b}}$
• Specific interfacial area: $a = \frac{6}{d_b} \frac{\alpha_G}{1-\alpha_G}$
CFD model validation (small scale)

• Simulate lab-scale bubble column
  o 0.15 m diameter x 1.2 m height
  o Initial liquid height 0.75 m
  o 1,350 cells (45 x 30)
  o Air/water at 20 °C
  o Zero initial dissolved O₂ concentration

• Gas holdup and dissolved oxygen concentration analyzed
CFD model validation (small scale)

- Gas holdup is bound by theoretical calculation\(^1\) and design equation of Heijnen and van’t Riet\(^2\)
  \[\alpha_G = 0.6 v_{Gs}^{0.7}\]

- Rise in O\(_2\) concentration to saturation over time is fit to exponential
  \[C_{O_2} = C_{O_2}^* (1 - \exp(-k_L a t))\]

- Mass transfer coeff compares favorably to design equation of Heijnen and van’t Riet\(^2\)
  \[k_L a = 0.32 v_{Gs}^{0.7}\]

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1. Iordache and Muntean, 1981
2. Heijnen and van’t Riet, 1984
Oxygen uptake model

- Oxygen uptake rate (OUR, mmol/L-h) modeled with phenomenological O$_2$ sink function
- O$_2$ is removed from liquid phase at this rate
- Mimics real culture behavior
  
  Anaerobic $\rightarrow$ micro-aerobic $\rightarrow$ fully aerobic

\[
\text{OUR} = \begin{cases} 
0, & \text{if } C_{O_2} < C_{O_2}^{\text{min}} \\
\text{OUR}_{\text{max}} \left[ \frac{C_{O_2} - C_{O_2}^{\text{min}}}{C_{O_2}^{\text{max}} - C_{O_2}^{\text{min}}} \right], & \text{if } C_{O_2}^{\text{min}} \leq C_{O_2} < C_{O_2}^{\text{max}} \\
\text{OUR}_{\text{max}}, & \text{if } C_{O_2} \geq C_{O_2}^{\text{max}}
\end{cases}
\]
Gas-on/gas-off simulation

- Gas-on/gas-off experiment is performed in bench-scale bioreactors to determine operating parameters (OUR, cell growth rate, $k_La$)

1. $t=0$ s: Air introduced with $v_{Gs}=0.10$ m/s
2. $t=60$ s: Air turned off
3. $t=70$ s: $O_2$ sink function activated
4. $t=85$ s: Air reintroduced with $v_{Gs}=0.10$ m/s, sink function still active

\[
C_{O_2}^* = 0.310 \text{ mol/m}^3 \\
k_La = 0.064 \text{ s}^{-1} \\
\text{OUR} = 30.4 \text{ mol/m}^3 \cdot \text{h}
\]
Simulation of commercial-scale reactor

- Fully-coupled simulations
  - Two-phase flow
  - Interphase O₂ mass transfer
  - O₂ uptake model
- Probe for oxygen-depleted areas in full-size reactors
- Bubble column:
  - 5m diameter x 40m height
  - 25m initial liquid height
  - 25,000 cells (125x200)
- Draft-tube airlift
  - 3.5m draft tube in 5m column x 40m height
  - 25m initial liquid height
  - 38,000 cells (190x200)
Oxygen-limited regions

- Oxygen-limited defined as $C_{O_2} < C_{O_2}^{\text{max}}$ from sink function (0.05 mol/m$^3$)
- Operating $v_{Gs}$ constant (0.1 m/s), OUR increased
- $\text{OTR}_{\text{max}}$ taken as OUR where $O_2$-limited volume >20%

15% oxygen-limited volume in each
Maximum OTR simulation

- $\text{OTR}_{\text{max}}$ significantly larger in commercial-scale reactor
  - More oxygen transferred near reactor inlet where pressure is high
- Observed $\text{OTR}_{\text{max}}$ is in line with bubble column design heuristics
  - $\sim$100 mol/m$^3$-h at 0.14 m/s
- Additional data currently in production
Economic considerations

- Previously demonstrated that CFD validates the reactor design equations used in techno-economic analysis
- $\text{OTR}_{\text{max}} = f(v_{Gs})$ data from commercial-scale simulations gives $\text{O}_2$ delivery cost equivalent to design equations
- Additional $\text{OTR}_{\text{max}} = f(v_{Gs})$ results will supplement or replace the design equations
- CFD simulations will inform minimum superficial velocity and maximum reactor size

Aggregate (CAPEX+OPEX) $\text{O}_2$ delivery cost in bubble column as a function of OUR and reactor size
Summary

- Two-phase flow in bubble-column bioreactors was successfully simulated, including interphase O$_2$ mass transfer and consumption
- Gas holdup and O$_2$ mass transfer rates are consistent with typical bubble column design equations
- Oxygen-depleted regions occur at elevated oxygen uptake rates (OUR)
- By simulating multiple OUR levels, maximum oxygen transfer (OTR) rates were obtained for different superficial velocities of input air
- $OTR_{max}$ relationships can inform techno-economic analysis by indicating minimum superficial velocity and maximum reactor size
- Goal: validate CFD for standard reactors, then apply simulation techniques to novel geometries and operating spaces
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