Multiphase Reacting Flow Simulations and Optimization of Commercial-Scale Aerobic Bioreactors

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Introduction and Motivation

- Bioreactor: use microbial action for conversion
  - Pharmaceutical industry
  - Waste water treatment
  - Biofuels and molecules (Research at NREL)
    - Ethanol/Butane-diol/Methane

- Fermentation is a large cost contributor\(^1\)
  - Cost is important: low value products

- Improve economics through bioreactor design
  - More engineering than biology
  - Validated high-fidelity modeling
  - Scale-up/reactor-design optimization
  - Techno-economic analysis

Objectives

– Optimization and scale-up of bioreactors via Computational fluid dynamics (CFD) simulations

• Validation at lab scale
• Comparison of reactor designs
  – Bubble column, airlift, stirred tank

• Optimization
  – Sensitivity to scale-up
  – Effective mixing – oxygen distribution
  – Geometry and operating conditions

– Coupling to Techno economics and cost prediction
– Systems engineering for overall optimization of conversion process
Mathematical model and numerical methods
Multiphase Euler-Euler equations

- Gas and liquid as continuous interpenetrating phases
  - Bubble sizes are small compared to reactor dimensions
  - Constant bubble size - 6 mm
- Compressible low Mach RANS equations

\[ \alpha_L + \alpha_G = 1 \]

\[ \frac{\partial}{\partial t}(\alpha_i \rho_i) + \vec{\nabla} \cdot (\alpha_i \rho_i \vec{V}_i) = 0 \]

\[ \frac{\partial}{\partial t}(\alpha_i \rho_i \vec{V}_i) + \vec{\nabla} \cdot (\alpha_i \rho_i \vec{V}_i \vec{V}_i) = -\alpha_i \vec{\nabla} P + \alpha_i \rho_i \vec{g} + \vec{\nabla} \cdot (\alpha_i \vec{R}_i) + \vec{F}_i \]

\[ \frac{\partial}{\partial t}(\alpha_i \rho_i Y_{ij}) + \vec{\nabla} \cdot (\alpha_i \rho_i Y_{ij} \vec{V}_i) = \vec{\nabla} \cdot (\alpha_i \rho_i \vec{D}_{ij} \vec{\nabla} Y_{ij}) + \vec{R}_{ij}^{MT} \]
Mass transfer

Oxygen mass transfer (Higbie et al. ¹)

\[
\text{OTR} = k_L a (C_{O_2}^* - C_{O_2})
\]

\[
C_i^* = \frac{X_{i,GP}}{H_i} \frac{\rho_L}{M_L}
\]

\[
k_L = \sqrt{\frac{4D}{\pi}} \frac{|u_{\text{slip}}|}{d_b} \quad a = \frac{6\alpha_G}{d_b}
\]

Microbial oxygen uptake (Monod model)

\[
\text{OUR} = \text{OUR}_{\text{max}} \frac{C_{O_2}}{K_O + C_{O_2}} \alpha_L
\]

Computational model

• Transport properties
  • Fermentation broth properties are similar to water
  • Grace drag model for bubbles
  • Wilke-Chang diffusion of species
  • Multiphase k-ε turbulence model
  • Wall lubrication effects

• Customized solver *TwoPhaseEulerFoam* in OpenFOAM

• Multi-Reference-Frame (MRF) method for rotating cases with impellers

• Simulations performed using
  • 72 Intel Skylake processors
  • 48 hours of run time to simulate 500 seconds

• More details in Rahimi et al., Chem. Engg. Res. Design, 139, 2018
Geometry and meshing

- Bottom inlet with a gas fraction that specifies sparger mass flow rate
- Lateral walls use no-slip condition for liquid and slip for gas
- ~300,000 cells – sufficient for grid convergent solutions
Results
Model validation with small-scale bubble column

- Validation done for a small-scale bubble column (1 m height, 15 cm diameter)
- Average mass transfer coefficient matches *Heijnen and Van’t Riet (1984)*\(^1\)
- Gas holdup matches experiments/simulations by Mcclure et al. (2013)\(^2\)

\[ \nu_g = \frac{V_{\text{mid}}}{A_{\text{reactor}}} \]


Transient fluid dynamics (comparison)

- Superficial gas velocity = 0.1 m/s, impeller speed = 2 rad/s
- Gas hold up is similar for all cases
- Faster time scale to steady state with impellers
- Draft tube and impellers aid better mixing
All reactors show almost the same average concentration without microbial uptake.

Higher mass transfer rate in that case of stir tank reactor.

Stir-tank reactor higher average oxygen concentration with microbial uptake.
Oxygen limited regions are where microbial uptake is sub-optimal < 0.15 mol/m³

- OUR_{max} = 150 mol/m³/h
- Radial transport is limited in bubble column, mitigated in airlift and stir tank
- O₂ limited regions towards the top and the wall boundaries
Streamlines and mixing

- Streamlines obtained from temporal averaging of liquid velocity at steady-state
- Draft tube allows for better top to bottom mixing
- Impellers in the stir tank form Taylor vortices that aid in better mixing
Sensitivity to reactor height

- Cases are at superficial gas velocity of 2 cm/s

- Larger hydrostatic pressure head with greater height
  - Larger oxygen transfer due to higher Henry saturation concentration
Automated meshing of stir-tank reactor

3 impellers, 10 baffles
9 impellers, 5 baffles
5 impellers, 6 baffles

• Automated python script allows for a generic design that can be used for optimization
Stir tank optimization

Sensitivity of stir-tank reactor

- 5 m dia, 17 m height
- $V_{gs} = 2$ cm/s
- Average $O_2$ concentration
  - Rotational speed
  - No: of blades
  - No: of impellers

3 impellers, 4 blades

<table>
<thead>
<tr>
<th>Rotational speed (rad/s)</th>
<th>O$_2$ concentration (mol/m$^3$)</th>
</tr>
</thead>
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<td>0.33</td>
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<tr>
<td>3</td>
<td>0.35</td>
</tr>
</tbody>
</table>

3 impellers, 20 rpm

<table>
<thead>
<tr>
<th>Number of blades</th>
<th>O$_2$ concentration (mol/m$^3$)</th>
</tr>
</thead>
<tbody>
<tr>
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</tr>
<tr>
<td>3</td>
<td>0.30</td>
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<td>0.32</td>
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<td>6</td>
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4 blades, 20 rpm

<table>
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<th>Number of impellers</th>
<th>O$_2$ concentration (mol/m$^3$)</th>
</tr>
</thead>
<tbody>
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Conclusions and future work

• **Conclusions**
  • Computational model
    • OpenFOAM based multiphase solver with oxygen uptake
  • Results
    • Validated small scale bubble column
    • Comparison between bubble column, airlift and stir-tank reactors
      • Better mixing in stir tanks: Taylor vortices aid in mixing
      • Greater pressure heads leads to greater $O_2$ transfer
    • Optimization of stir tank reactor
      • Asymptotic performance for varying
        • Angular velocity, Number of impellers, Rotational speed

• **Future work**
  • Surrogate models for optimizing stir-tank reactors
  • High fidelity LES instead of RANS
  • Bubble size distribution
  • Systems level engineering
    • Coupling with other unit operations
    • Techno-economics
      • Impeller costs may outweigh better mixing
Thank You

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