NATIONAL RENEWABLE ENERGY LABORATORY

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

Image by Dennis Schroeder, NREL

Algae bioreactor

Image by Dennis Schroeder, NREL

Biomethanation reactor (NREL)

[1]Humbird, D., R. Davis, and J. D. McMillan. "Aeration costs in stirred-tank and bubble column bioreactors." *Biochemical engineering journal* 127 (2017): 161-166.

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**

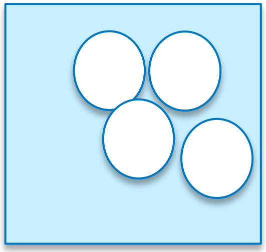
– Coupling to Techno economics and cost prediction

– 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



$$\alpha_{\mathrm{L}} + \alpha_{\mathrm{G}} = 1$$

Volume fraction constraint

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

Mass conservation

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

Momentum conservation

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

Species transport within each phase

Mass transfer

Oxygen mass transfer (Higbie et al. [1])

$$\mathrm{OTR} = k_{\mathrm{L}} a (C^*_{\mathrm{O}_2} - C_{\mathrm{O}_2})$$

Oxygen transfer rate

$$C_i^* = \frac{X_{i,G} P}{H_i} \frac{\rho_L}{M_L}$$

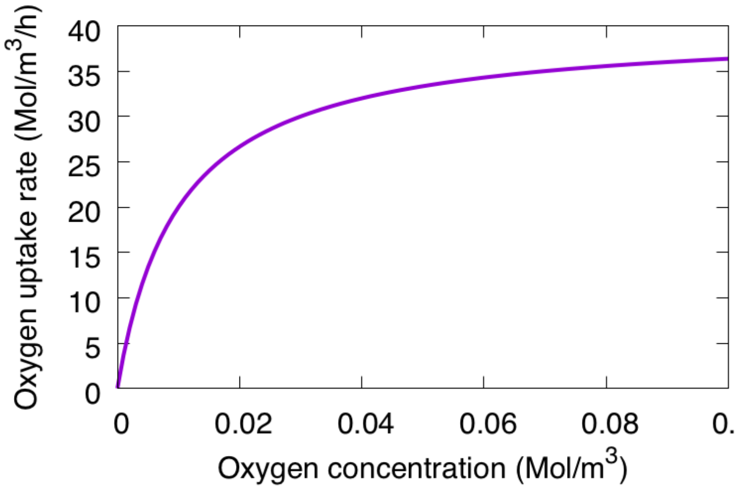
Henry's law

$$k_{\mathrm{L}} = \sqrt{\frac{4D}{\pi} \frac{|\mathbf{u}_{\mathrm{slip}}|}{d_{\mathrm{b}}}} \quad a = \frac{6\alpha_{\mathrm{G}}}{d_{\mathrm{b}}}$$

Mass transfer coefficient

Microbial oxygen uptake (Monod model)

$$\mathrm{OUR} = \mathrm{OUR}_{\max} \frac{C_{\mathrm{O}_2}}{K_O + C_{\mathrm{O}_2}} \alpha_{\mathrm{L}}$$

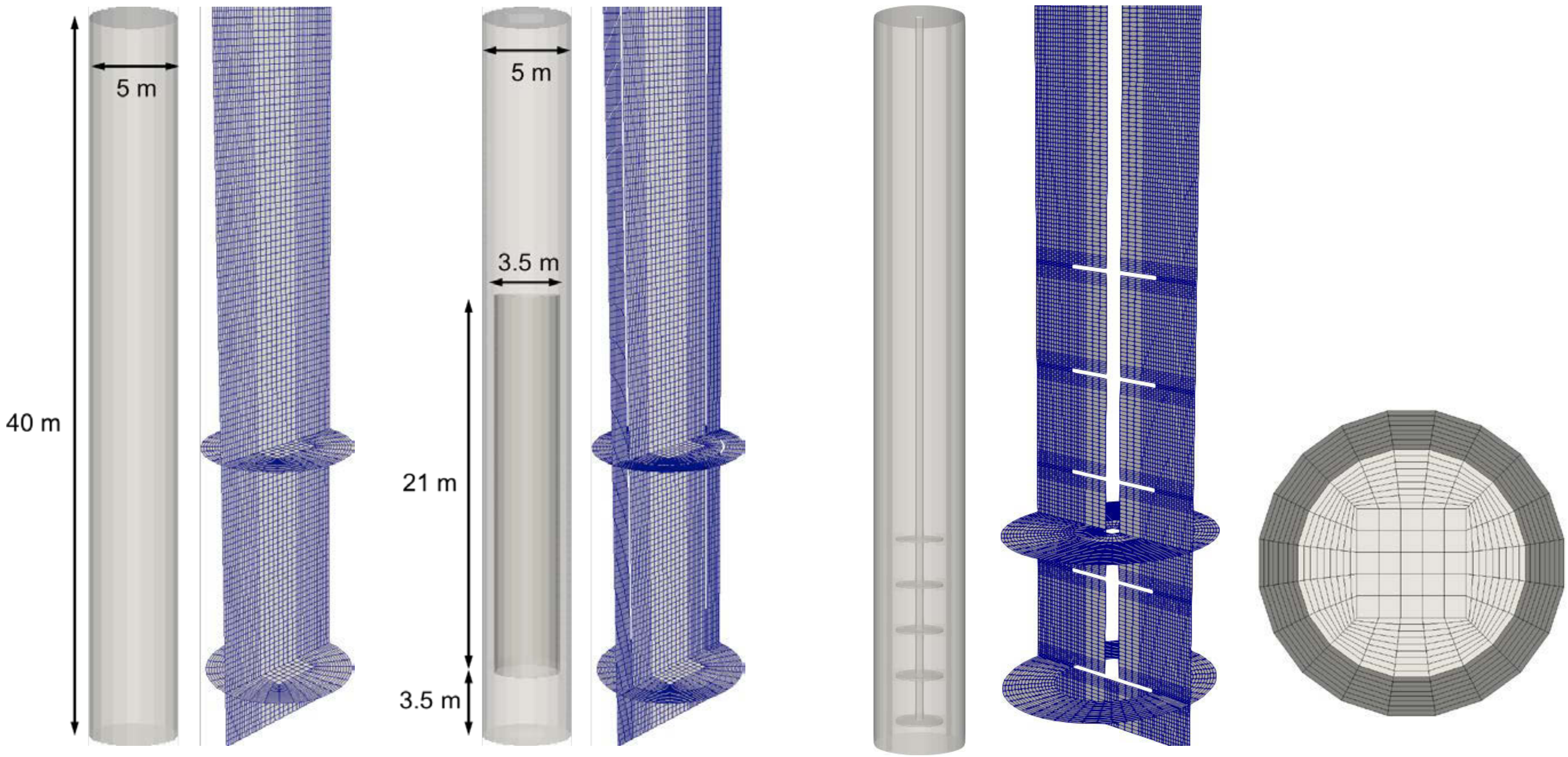


[1] Higbie, R., 1935. The rate of absorption of a pure gas into a still liquid during short periods of exposure. Trans. AIChE 31, 365–389.

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

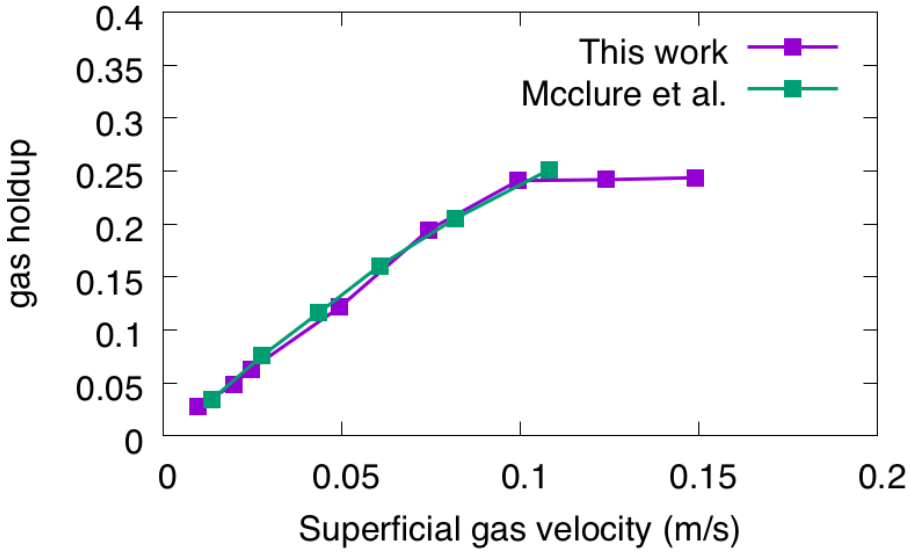


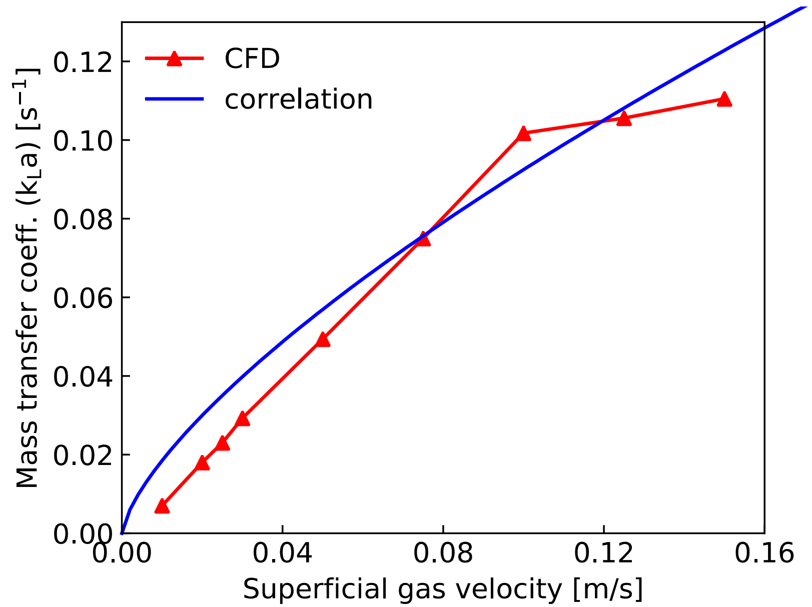
Bubble column airlift Stir tank Sparger

- 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



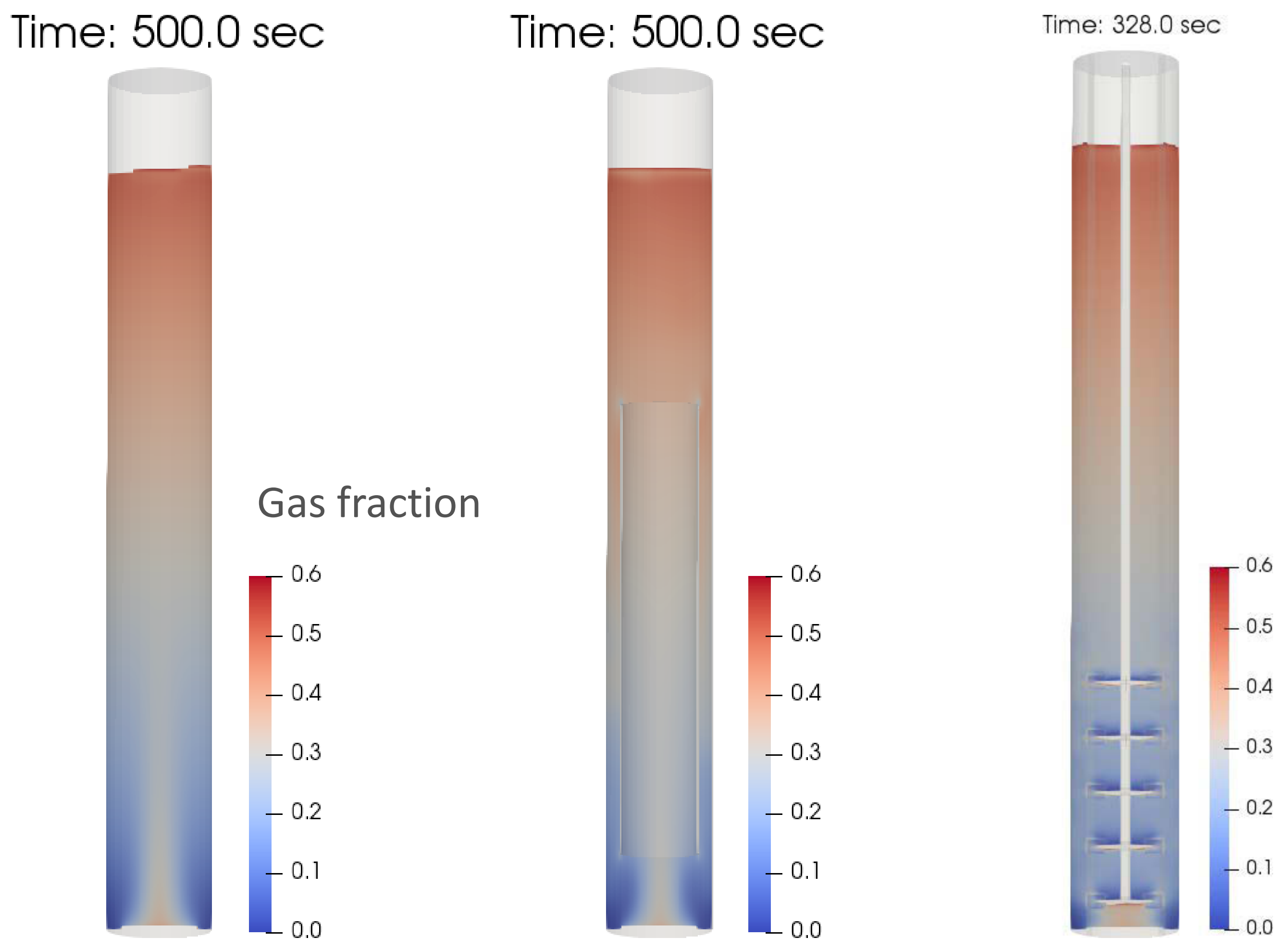


Superficial gas velocity: $vg_s = \frac{\dot{V}_{mid}}{A_{reactor}}$

- 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]

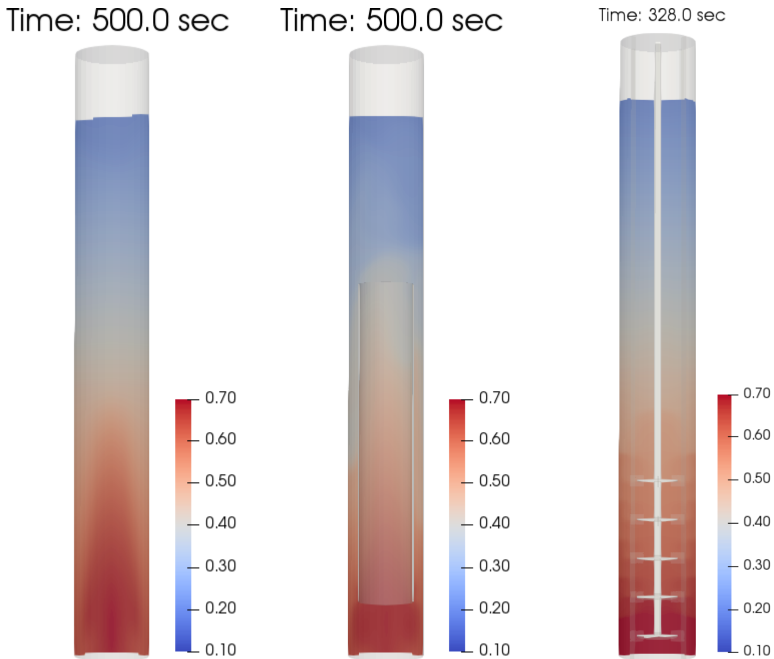
[1] Heijnen, J. J., Van't Riet, K., Apr. 1984. Mass transfer, mixing and heat transfer phenomena in low viscosity bubble column reactors. Chem. Eng. J. 28 (2), B21–B42.
[2] McClure, D. D., Kavanagh, J. M., Fletcher, D. F., Barton, G. W., 2013. Development of a CFD model of bubble column bioreactors: Part one - a detailed experimental study. Chem. Eng. Technol. 36 (12), 2065–2070.

Transient fluid dynamics (comparison)

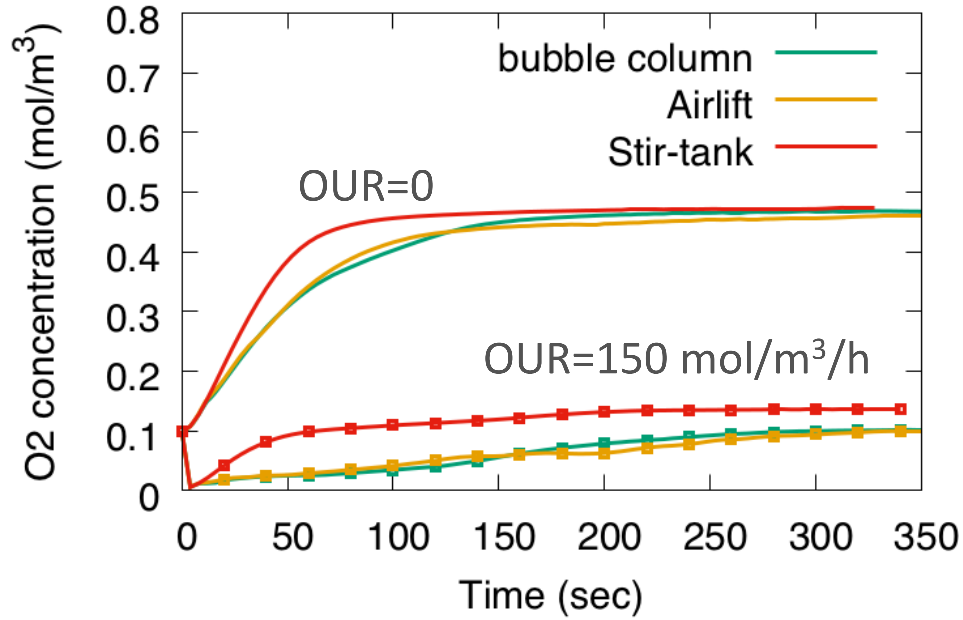


- Superficial gas velocity = 0.1 m/s, impeller speed = 2 rad/s
- Gas hold up is similar for all cases
- Faster time scale to steady state with impellers
- Draft tube and impellers aid better mixing

Oxygen transfer

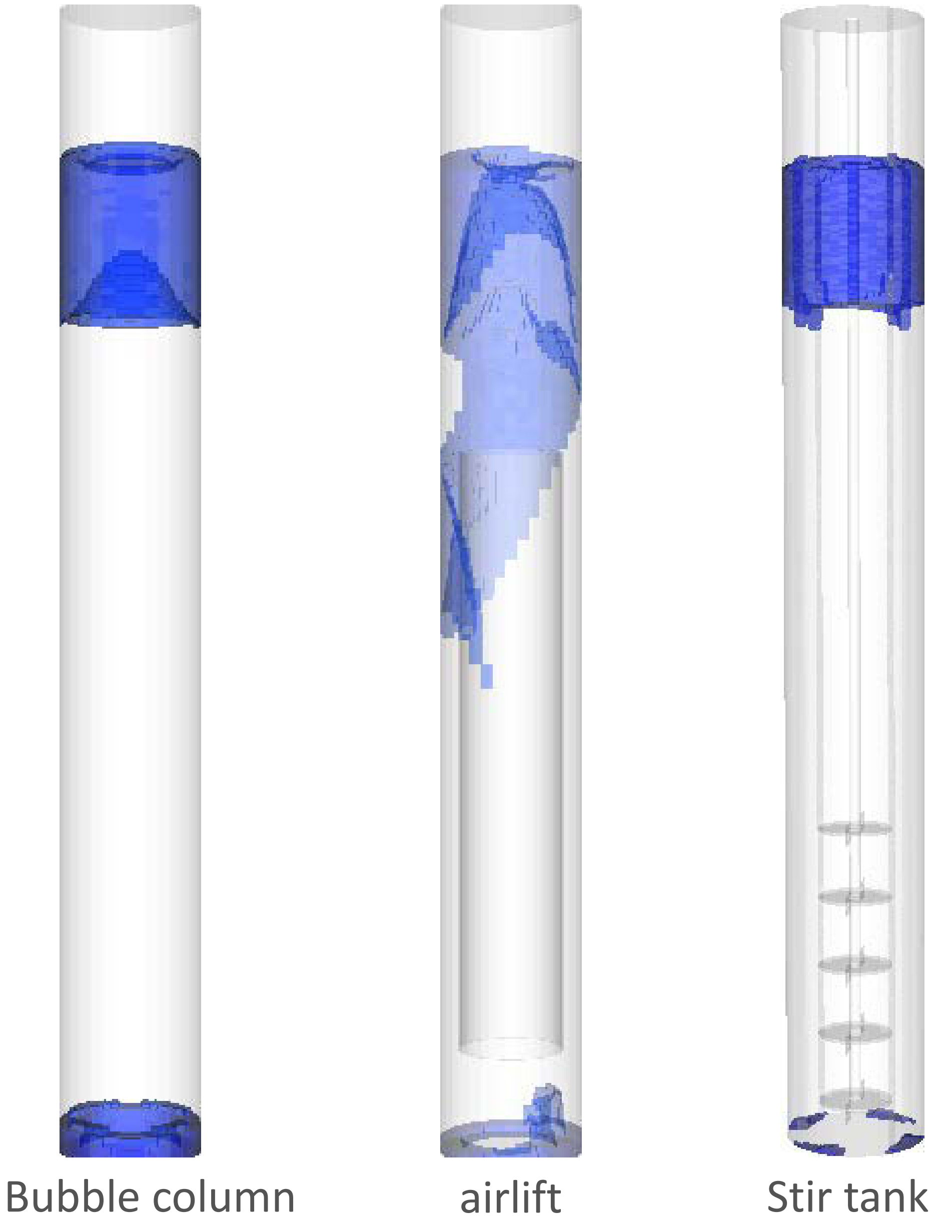


Oxygen concentration in mol/m^3



- 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

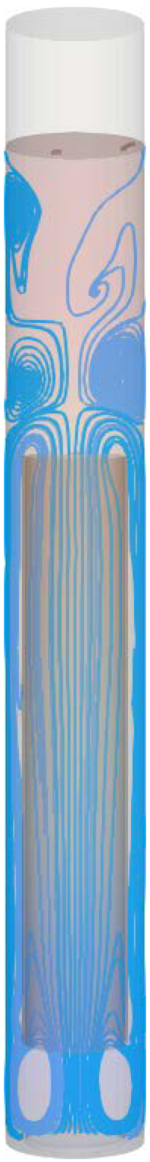
Oxygen limited regions



- Oxygen limited regions are where microbial uptake is sub-optimal < 0.15 mol/m^3
- OUR_{max} = 150 mol/m^3/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

Bubble column

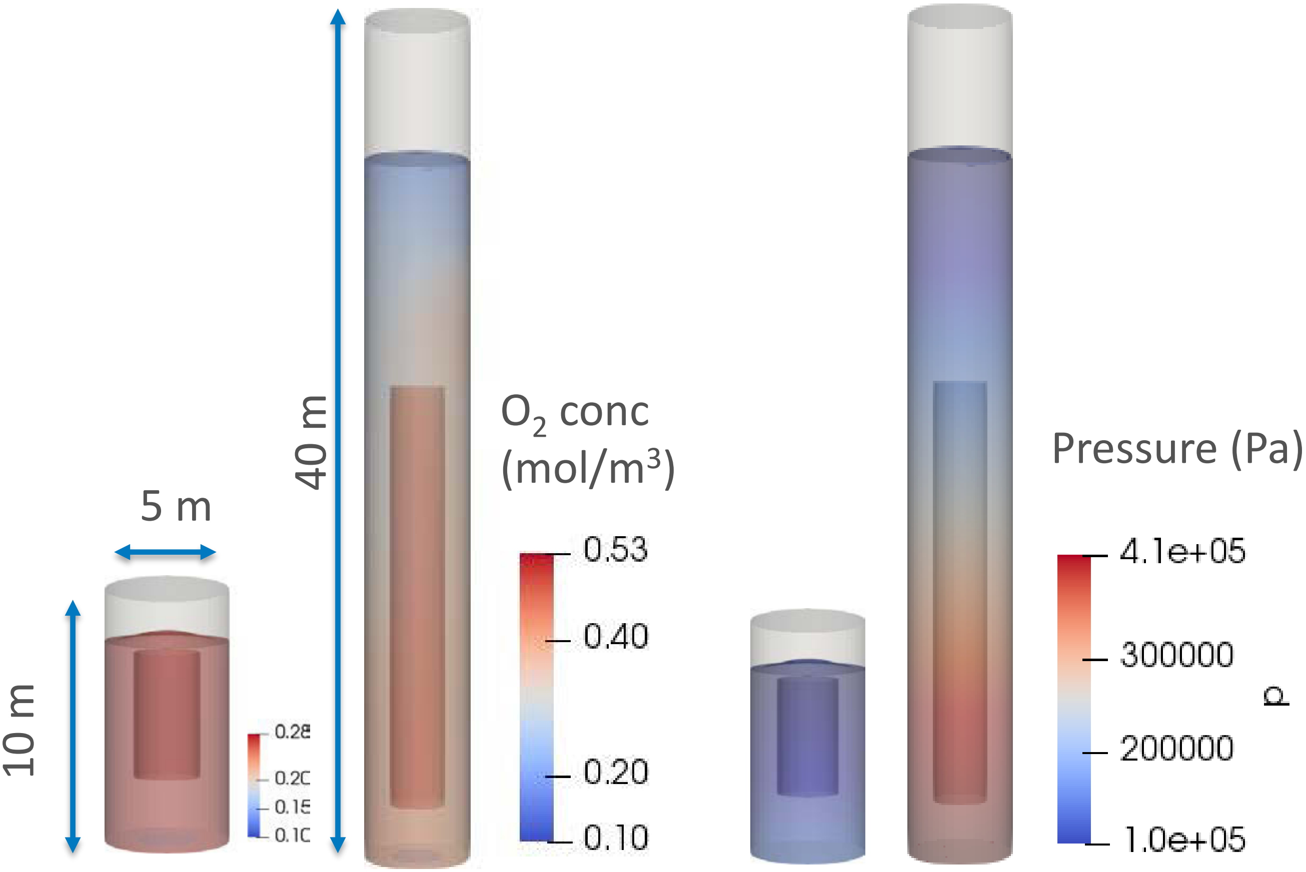


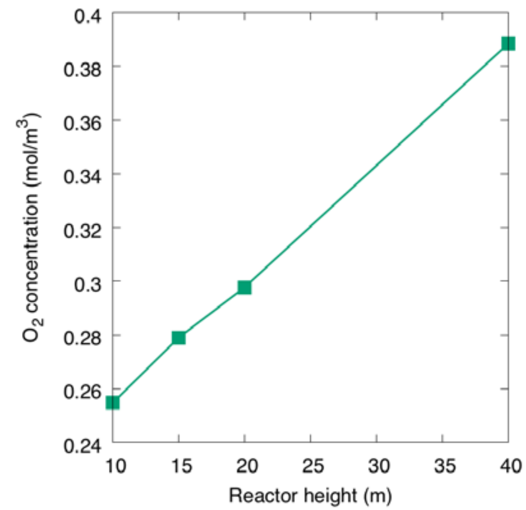
airlift

Stir tank

- 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

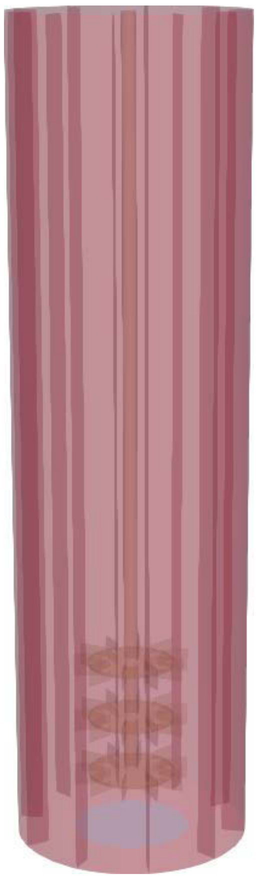
Sensitivity to reactor height



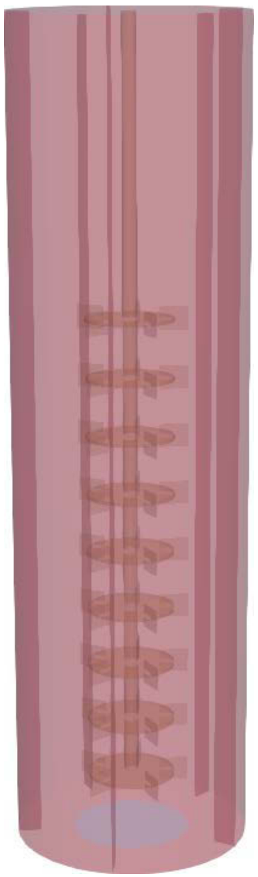


- Cases are at superficial gas velocity of 2 cm/s
- Larger hydrostatic pressure head with greater height
  - Larger oxygen transfer due to higher Henry saturation concentration

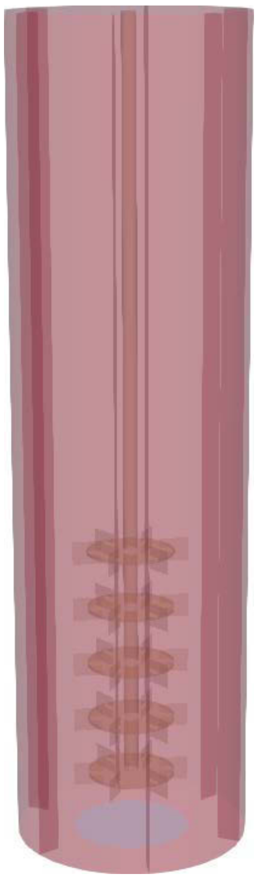
Automated meshing of stir-tank reactor



3 impellers,
10 baffles



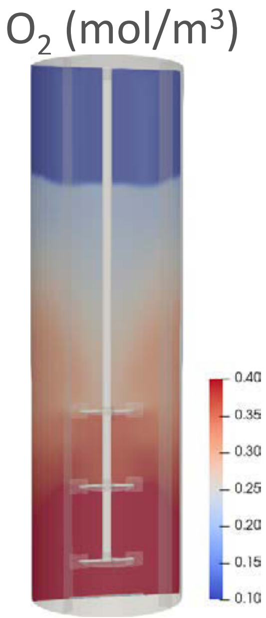
9 impellers,
5 baffles



5 impellers,
6 baffles

- Automated python script allows for a generic design that can be used for optimization

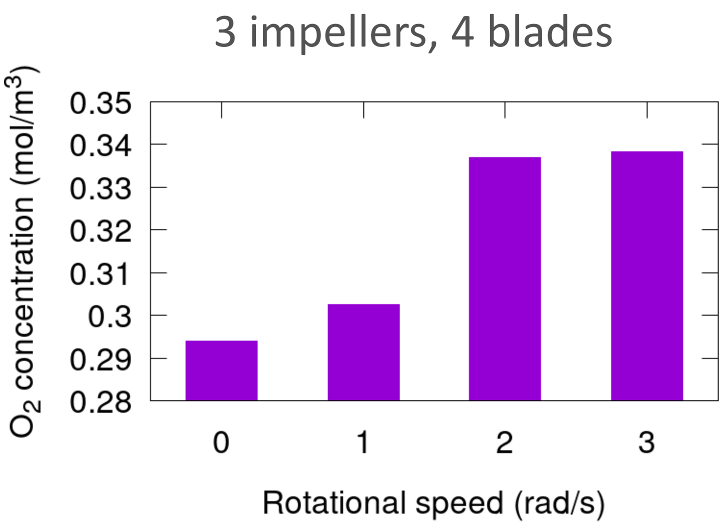
Stir tank optimization

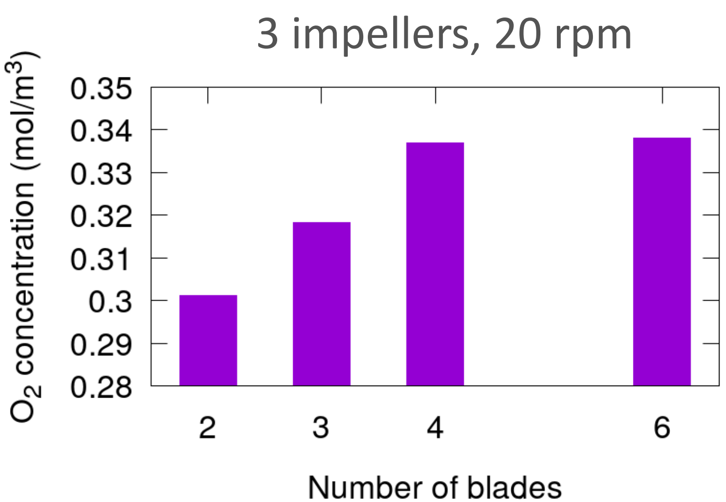


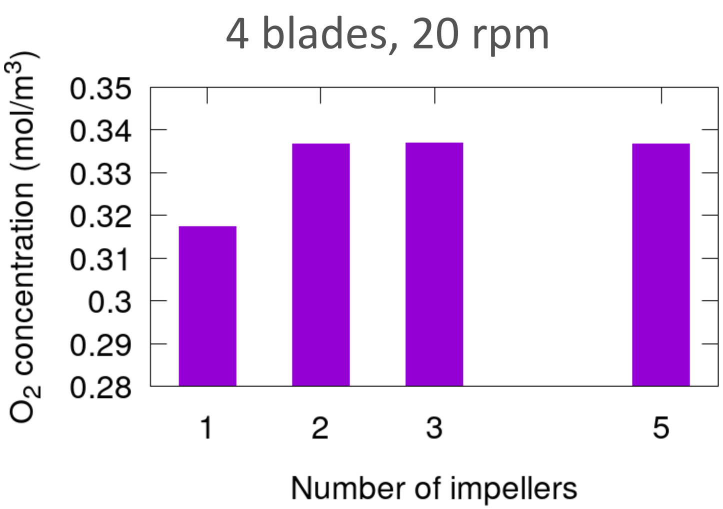
Sensitivity of stir-tank reactor

- 5 m dia, 17 m height
- Vgs=2 cm/s

- average O_2 concentration
  - Rotational speed
  - No: of blades
  - No: of impellers







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

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