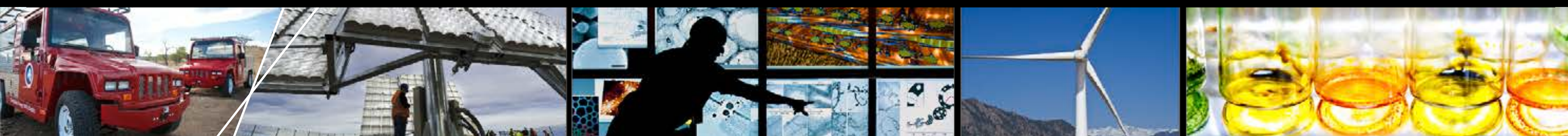
CFD Study of Full-Scale Aerobic Bioreactors

Evaluation of Dynamic O_2 Distribution, Gas-Liquid Mass Transfer and Reaction



David Humbird, Hariswaran Sitaraman, Jonathan Stickel, Michael A. Sprague, Jim McMillan

2016 AIChE Annual Meeting

November 18, 2016

San Francisco, California

NREL/PR-5100-66420
NREL is a national laboratory of the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.

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

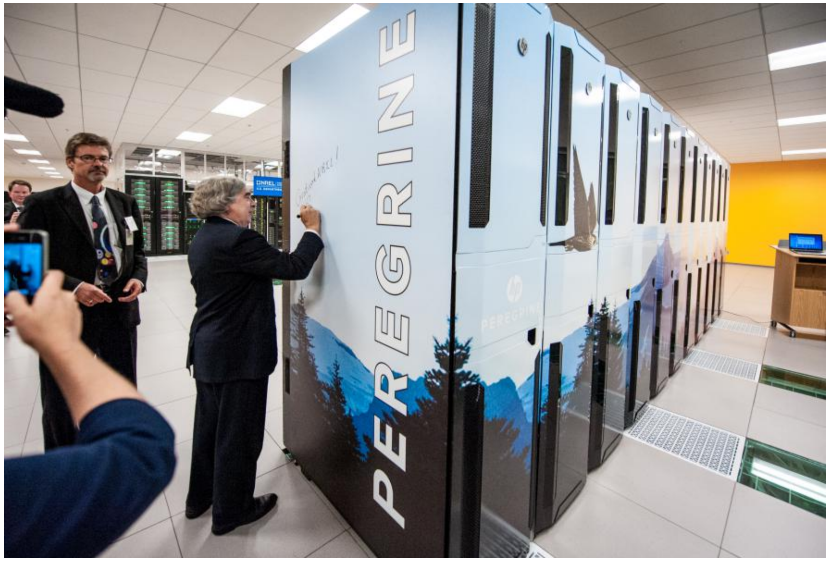


Photo by Dennis Schroeder, NREL 27494

***Peregrine* is NREL's flagship HPC capability:**

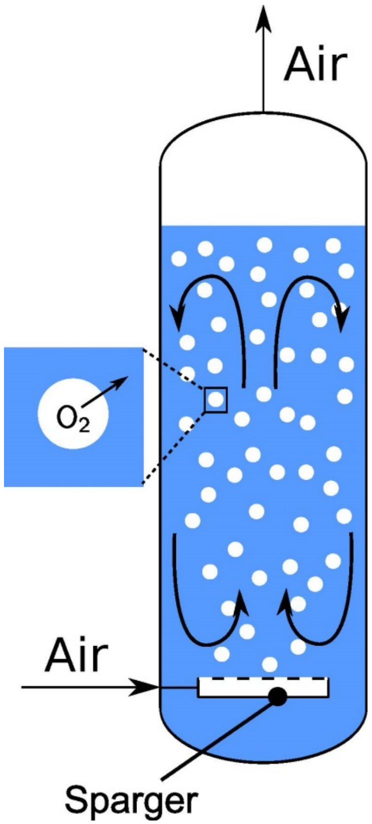
- 1.19 PetaFLOPS
    - 31,104 Intel Xeon processors
    - 576 Intel Phi many-core co-processors
- 3 petabytes of mass storage

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 m^3.
- 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 O_2 mass transfer and consumption to study dissolved O_2 concentration distribution in bubble-column and airlift bioreactors
  - Bubble-columns are expected to have lower CAPEX and OPEX than stirred-tank bioreactors.



CFD Implementation

Numerical Approach

- Euler-Euler multiphase simulation in OpenFOAM
  - `reactingTwoPhaseEulerFoam` (OpenFOAM-3.0)
- Reynolds-averaged Navier-Stokes (RANS)
- *k-ε* turbulence model

Multiphase assumptions

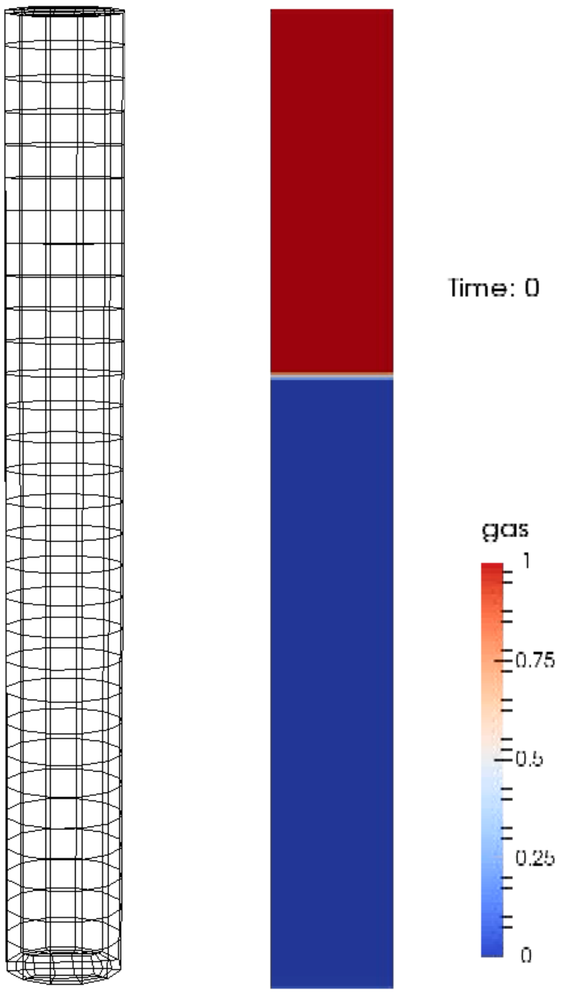
- Bubble diameter << reactor diameter
- Single bubble diameter (5 mm)

Gas-liquid mass transfer

- Oxygen transfer rate: $\mathrm{OTR} = k_\mathrm{L} a \left(C^*_{\mathrm{O_2}} - C_{\mathrm{O_2}} \right)$
- Mass transfer coefficient (Higbie): $k_\mathrm{L} = \sqrt{\frac{4D}{\pi} \frac{u_\mathrm{slip}}{d_\mathrm{b}}}$
- Specific interfacial area: $a = \frac{6}{d_\mathrm{b}} \frac{\alpha_\mathrm{G}}{1-\alpha_\mathrm{G}}$

CFD model validation (small scale)

- Simulate lab-scale bubble column
  - 0.15 m diameter x 1.2 m height
  - Initial liquid height 0.75 m
  - 1,350 cells (45 x 30)
  - Air/water at 20 °C
  - Zero initial dissolved O_2 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]

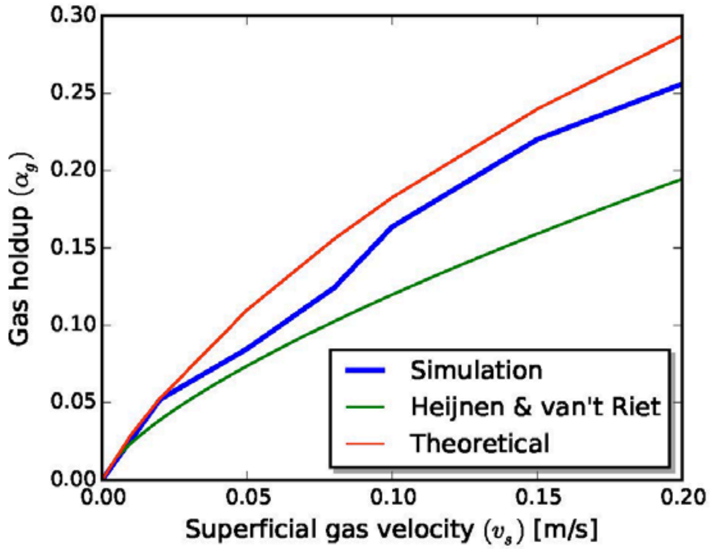
$$\alpha_{\mathrm{G}} = 0.6 v_{\mathrm{Gs}}^{0.7}$$

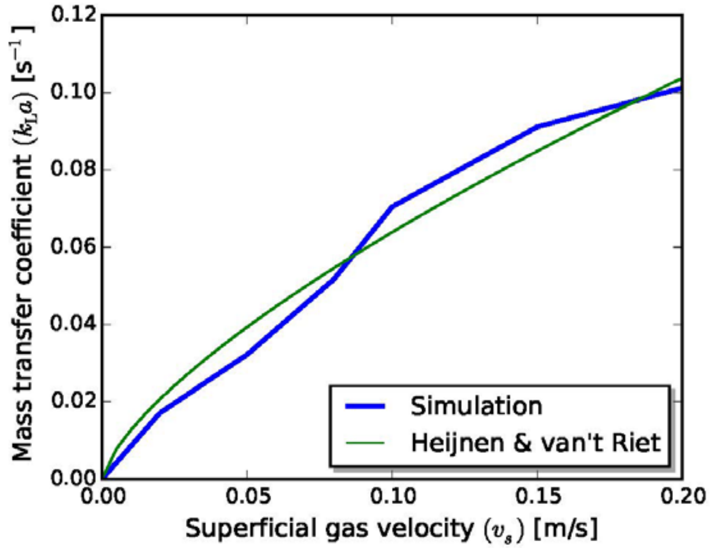
- Rise in O_2 concentration to saturation over time is fit to exponential

$$C_{\mathrm{O_2}} = C_{\mathrm{O_2}}^{*}\left(1 - \exp(-k_{\mathrm{L}} a t)\right)$$

- Mass transfer coeff compares favorably to design equation of Heijnen and van't Riet[2]

$$k_{\mathrm{L}} a = 0.32 v_{\mathrm{Gs}}^{0.7}$$





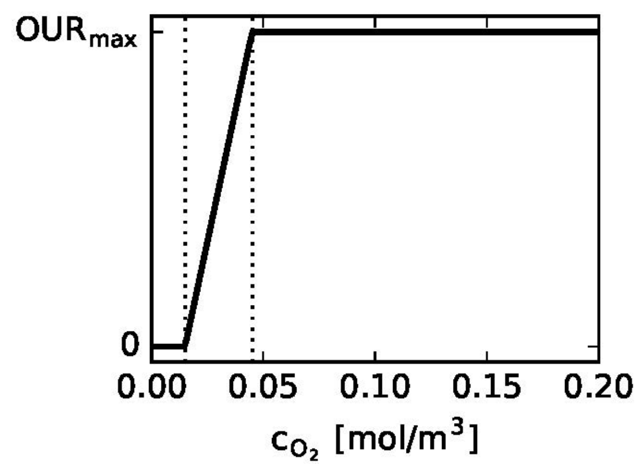
1. Iordache and Muntean, 1981
2. Heijnen and van't Riet, 1984

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 → micro-aerobic → fully aerobic

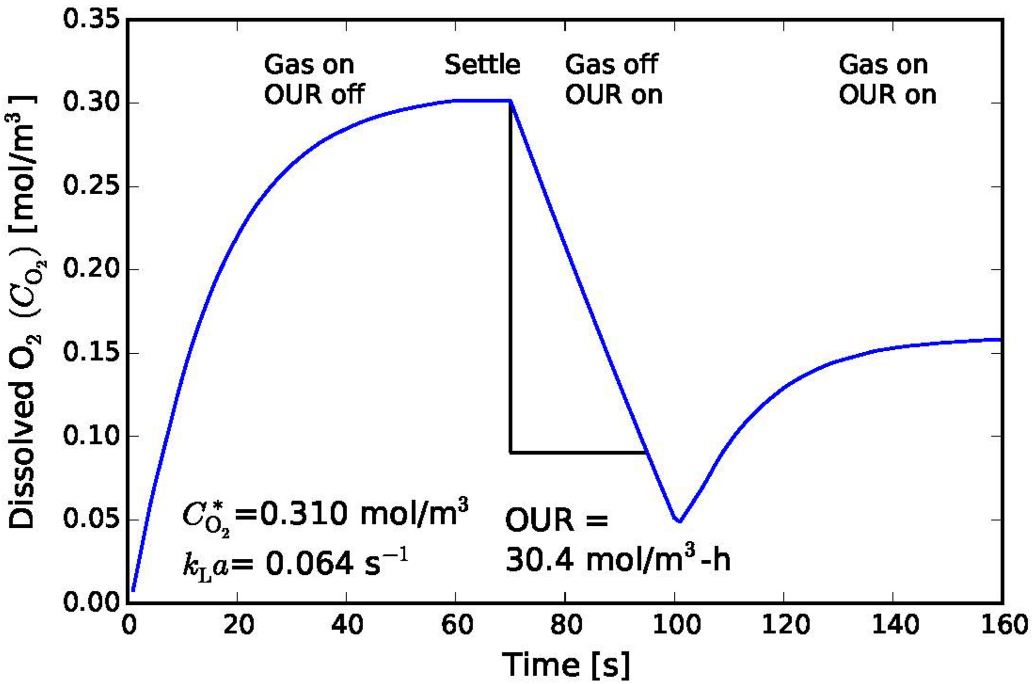
$$\mathrm{OUR} = \begin{cases} 0, & \text{if } C_{\mathrm{O_2}} < C_{\mathrm{O_2}}^{\min} \\ \mathrm{OUR}_{\max}\left[\dfrac{C_{\mathrm{O_2}} - C_{\mathrm{O_2}}^{\min}}{C_{\mathrm{O_2}}^{\max} - C_{\mathrm{O_2}}^{\min}}\right], & \text{if } C_{\mathrm{O_2}}^{\min} \leq C_{\mathrm{O_2}} < C_{\mathrm{O_2}}^{\max} \\ \mathrm{OUR}_{\max}, & \text{if } C_{\mathrm{O_2}} \geq C_{\mathrm{O_2}}^{\max} \end{cases}$$



Gas-on/gas-off simulation

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

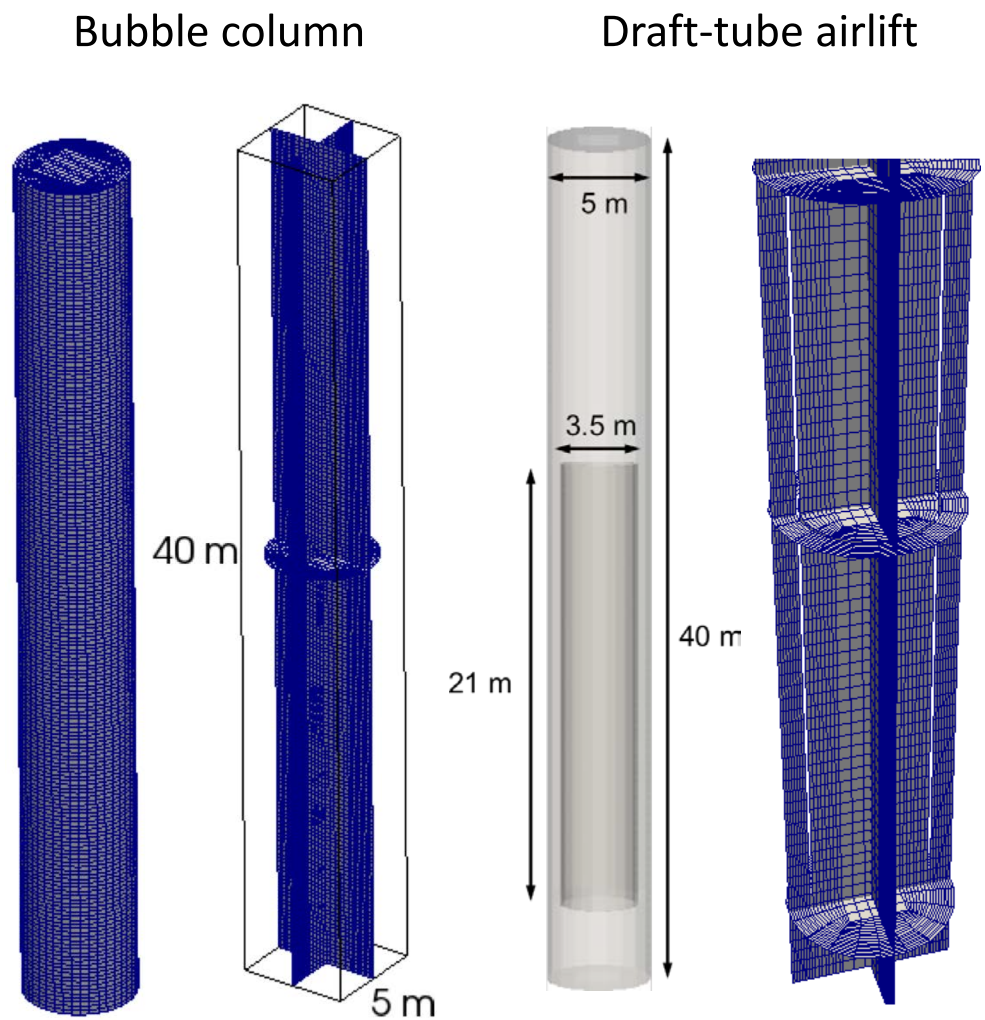
1. t=0 s: Air introduced with v_{Gs}=0.10 m/s
2. t=60 s: Air turned off
3. t=70 s: O_2 sink function activated
4. t=85 s: Air reintroduced with v_{Gs}=0.10 m/s, sink function still active



Simulation of commercial-scale reactor

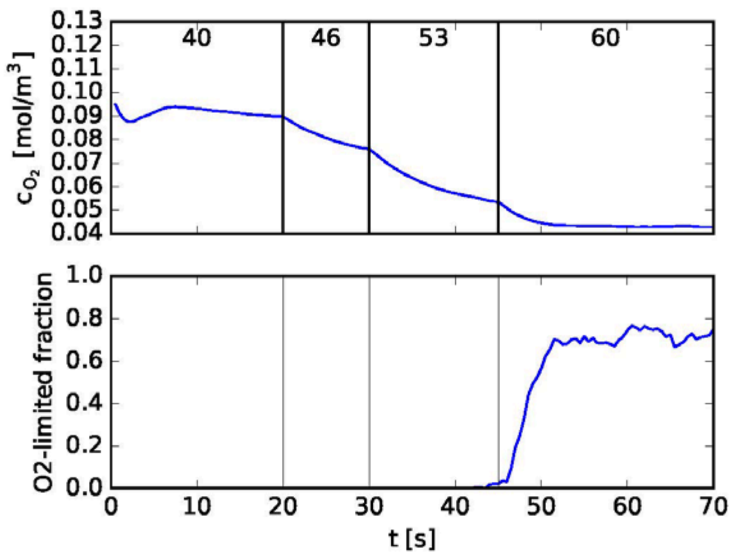
- Fully-coupled simulations
  - Two-phase flow
  - Interphase O_2 mass transfer
  - O_2 uptake model
- Probe for oxygen-depleted areas in full-size reactors

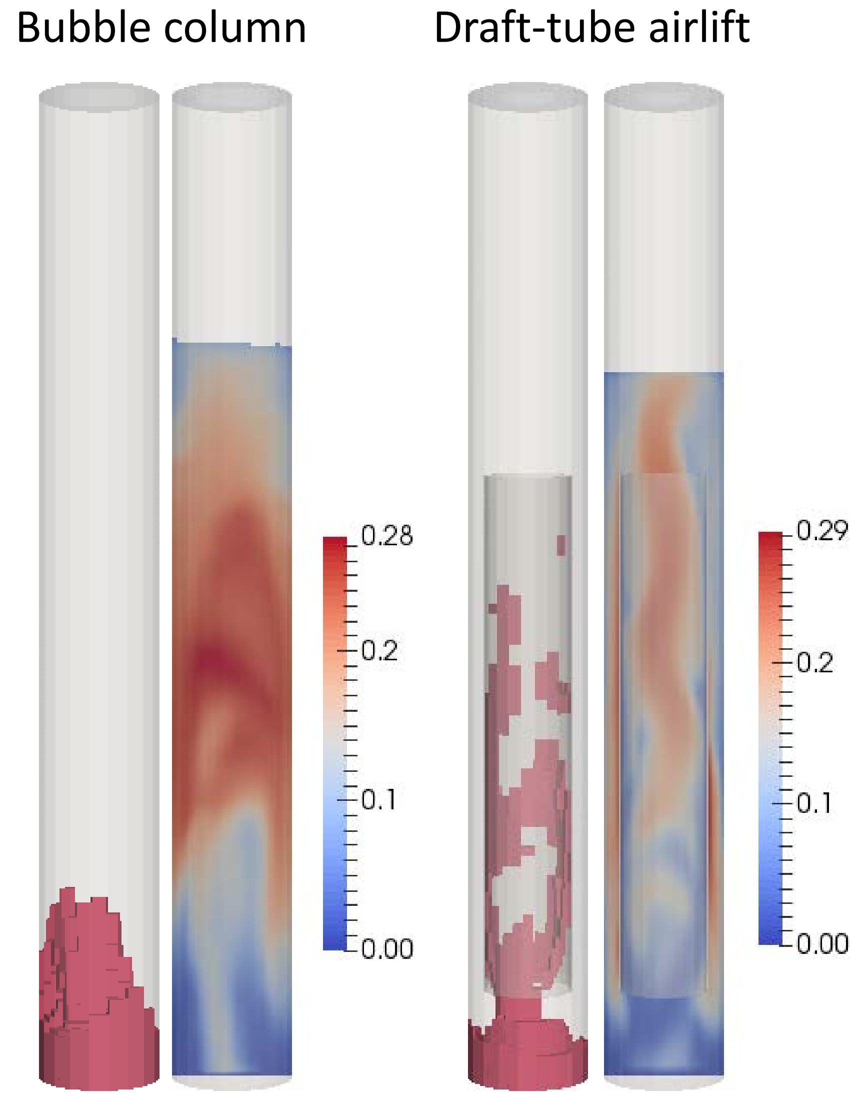
- Bubble column:
  - 5m diameter x 40m height
  - 25m initial liquid height
  - 25,000 cells (125x200)
- Draft-tube airlift
  - 3.5m draft tube in 5m column x 40m height
  - 25m initial liquid height
  - 38,000 cells (190x200)



Oxygen-limited regions

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



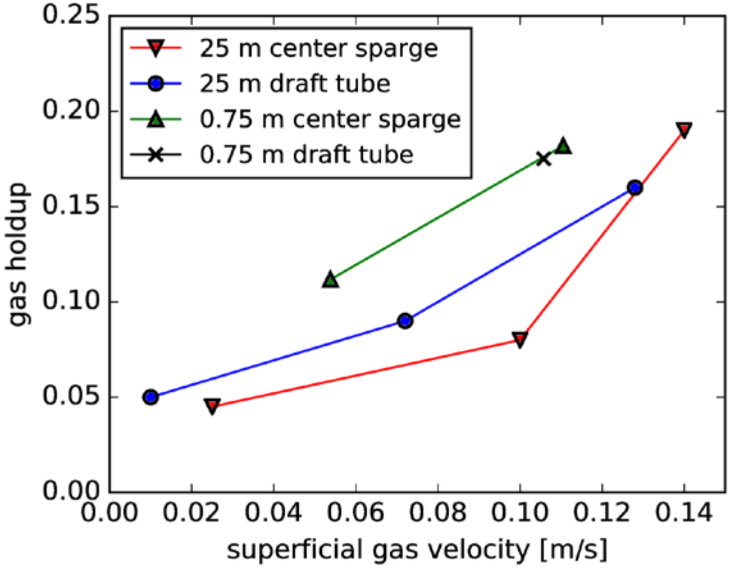


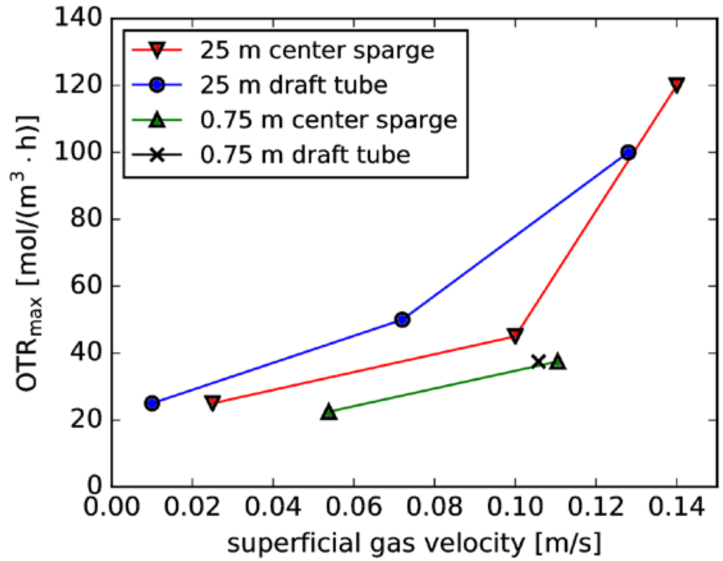
15% oxygen-limited volume in each

Maximum OTR simulation

- OTR_{max} significantly larger in commercial-scale reactor
  - More oxygen transferred near reactor inlet where pressure is high
- Observed OTR_{max} is in line with bubble column design heuristics

  ~100 mol/m^3-h at 0.14 m/s
- Additional data currently in production

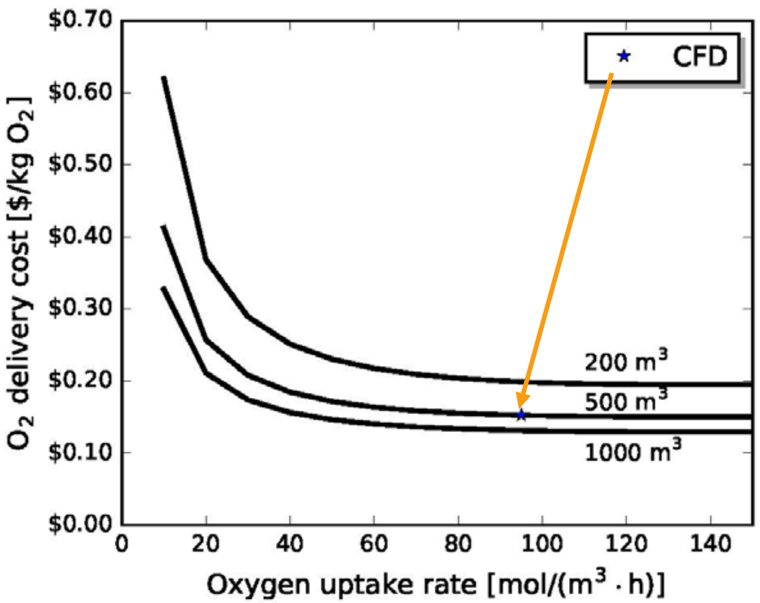




Economic considerations

- Previously demonstrated that CFD validates the reactor design equations used in techno-economic analysis
- $OTR_{max} = f(v_{Gs})$ data from commercial-scale simulations gives O_2 delivery cost equivalent to design equations
- Additional $OTR_{max} = f(v_{Gs})$ results will supplement or replace the design equations
- CFD simulations will inform minimum superficial velocity and maximum reactor size

Aggregate (CAPEX+OPEX) 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

Acknowledgements

Co-Authors

NREL National Bioenergy Center

Jonathan J. Stickel
James D. McMillan

NREL Computational Science Center

Hariswaran Sitaraman
Michael A. Sprague

Funding

US DOE Contract# DE-AC36-08-GO2308
EERE Bioenergy Technology Office (BETO) http://www.eere.energy.gov/biomass

NREL's High Performance Computing resources were used to perform the CFD simulations http://hpc.nrel.gov/

OpenFOAM Project http://openfoam.org

Speaker information:
Dave Humbird, DWH Process Consulting LLC
dave@dwhpc.com