CO_2 Reduction and Upgrading for e-Fuels Consortium

U.S. DEPARTMENT OF ENERGY

Analysis and Modeling

Multiphysics Computational-Fluid-Dynamics (CFD) for Design and Scale-Up of Gas Bioreactors that Utilize CO_2

Date: April 7, 2023

Technology Area Session: CO_2 utilization Technology

Principal Investigator: Hari Sitaraman

Team members: Malik Hassanaly, Milo Parra-Alvarez, Mohammad Rahimi

Organization: NREL

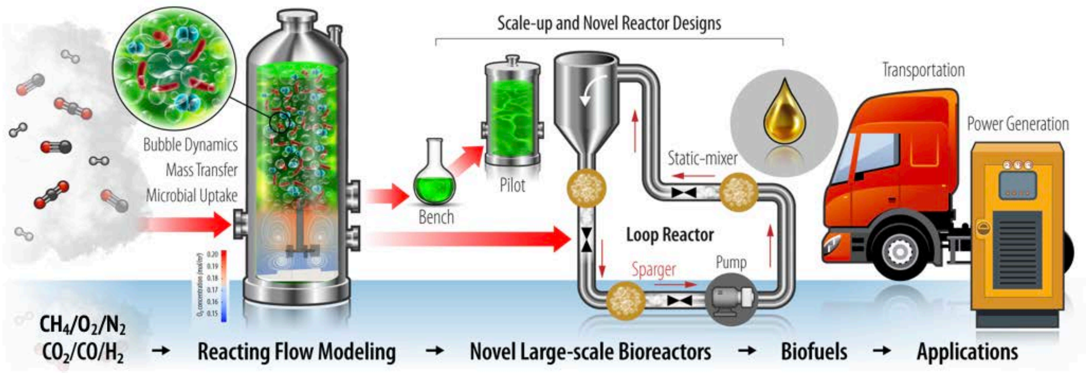
Project Overview: introduction

- **Funding:** through 2021 BETO CO_2 lab call, $250k per year from Jan 1, 2022 – Sep 30, 2024.
- **What are we trying to do?:** Develop validated high fidelity computational models for gas fermentation-based CO_2 conversion.
- **How is it done today?:** microbiological advances are made at the lab scale in well mixed reactors. We are trying to answer what happens when we scale-up to millions of liters.
- **Why is it important?:** lab-to-production scale transition is required to achieve CO_2 conversion at Mton-Gton scale and computational models can derisk/accelerate this transition.
- **What are the risks?:** Need significant industry engagement to assess feasibility/economics of optimal reactors developed in this work.

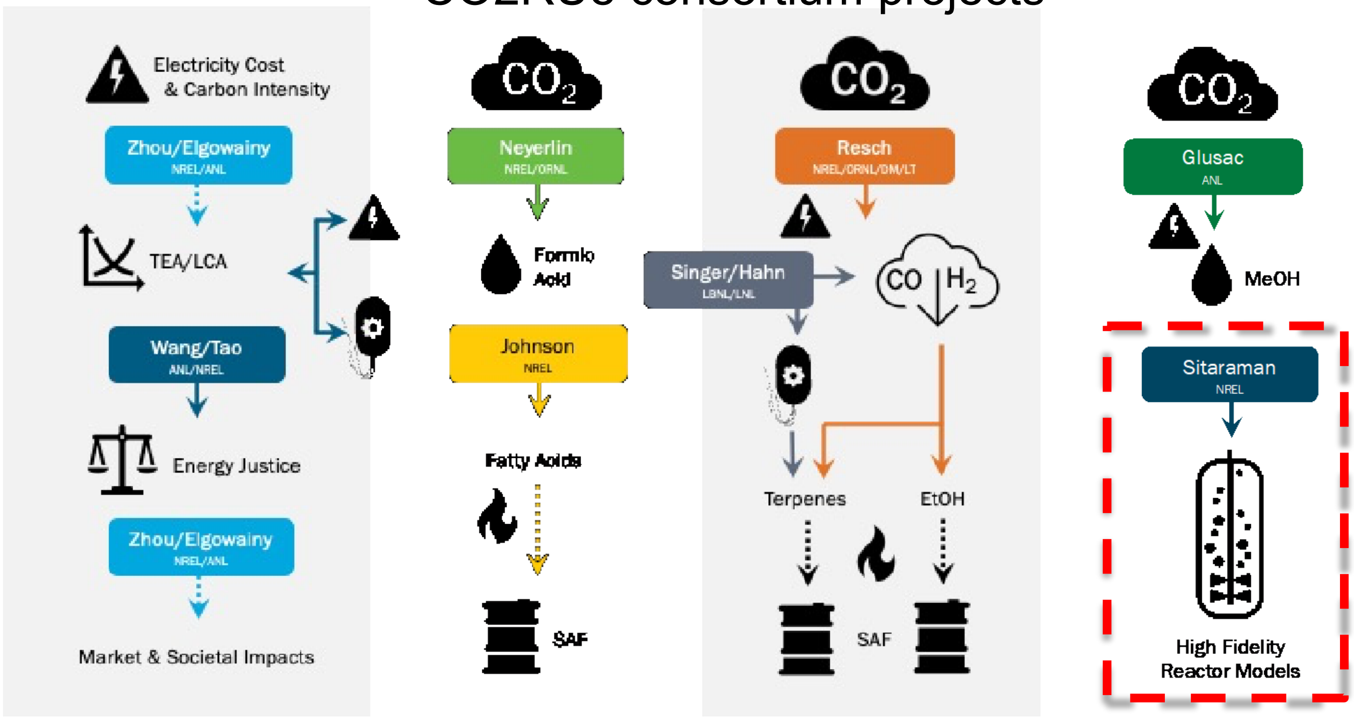
Project Overview: over-arching goals

- **Goal**
  - Enable scaled-up bioreactor design and optimization for CO_2 conversion through validated high fidelity multiphysics simulations

- **Supports CO2 consortium goals**
  - Develop technologies to upgrade CO2 to fuels and chemicals
  - reduction of greenhouse gas emissions
  - Derisk technologies toward commercialization/deployment

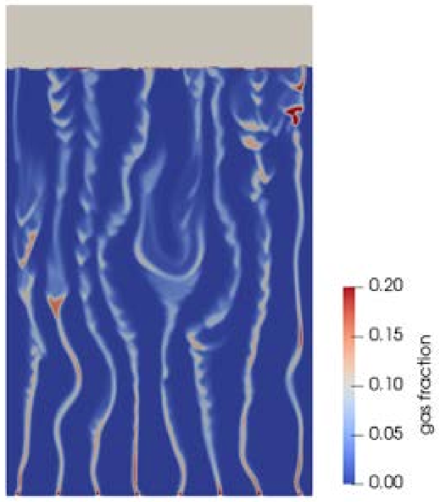


CO2RUe consortium projects



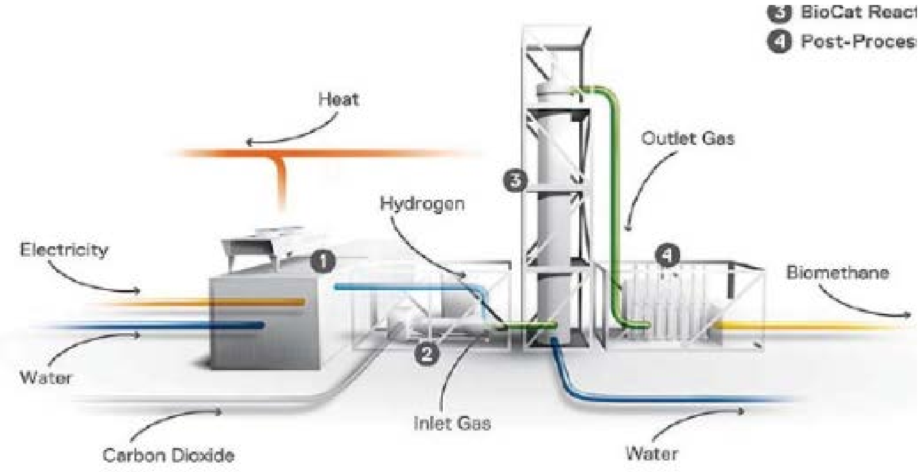
Project overview: previous work

- Previously worked with industry partners
  - NovoNutrients – CO_2/H_2 to food
  - SoCAL gas/Electrochaea (biomethanation)
  - Lumen biosciences – flat panel bioreactors
  - Exxon/Viridos – algae ponds
- BETO funded work– sugars to alcohols



Flat panel bioreactor modeling

novonutrients
food and feed from co2™



Biomethanation (Electrochaea)

Impeller mixing in biomethanation reactor

Technical approach

Technical approach: challenging questions

Task 1: Bubble dynamics

How do gas mixtures Impact ($CO/CO_2/H_2$) bubble size distributions and mass transfer?

Task 2: Microbial kinetics

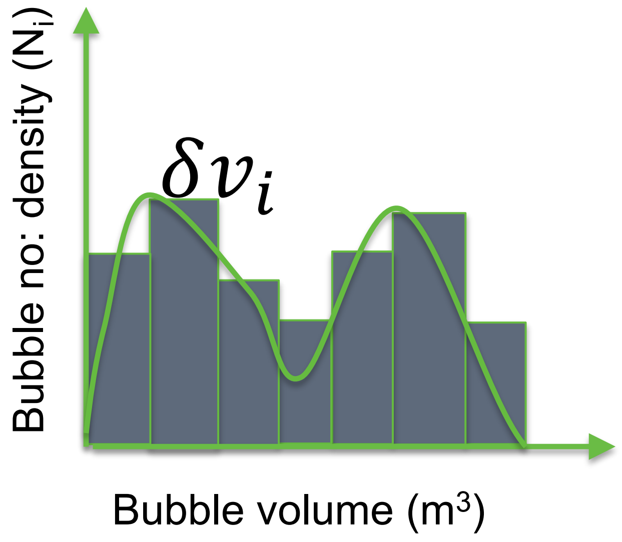
How does component-wise microbial uptake influence species distribution and hydrodynamics?

Task 3: Novel reactor design

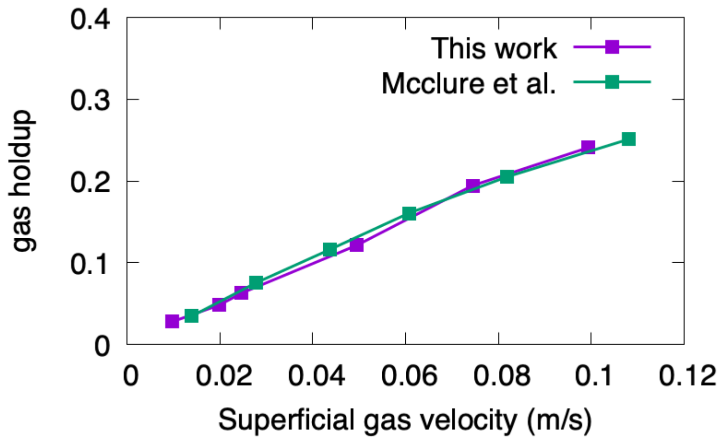
How do we design large-scale reactors (~ 500 m^3) with improved mixing and energy requirements?

Technical approach: computational model

- Gas/liquid as continuous interpenetrating phases
- Population balance model for bubble size
- Computational fluid dynamics solvers in this work:
    - Uses high performance computing resources
    - Open-source code development with specific models for $CO_2/CO/H_2$ mixtures: mass transfer, microbial uptake, bubble size distribution, turbulence
- Bubble column validation with literature – air or pure CO_2

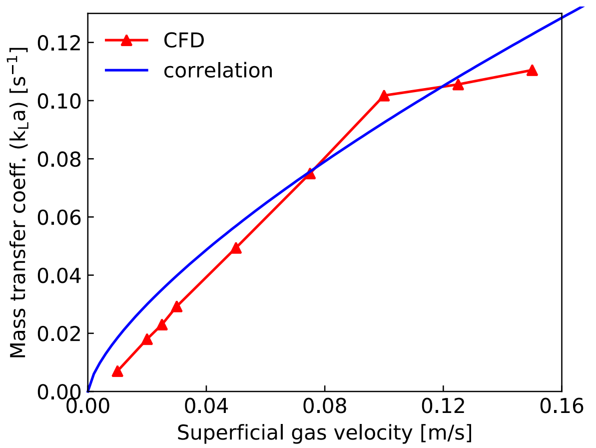


Comparison with Mcclure et al., Chem. Engg. Tech., 36,12,



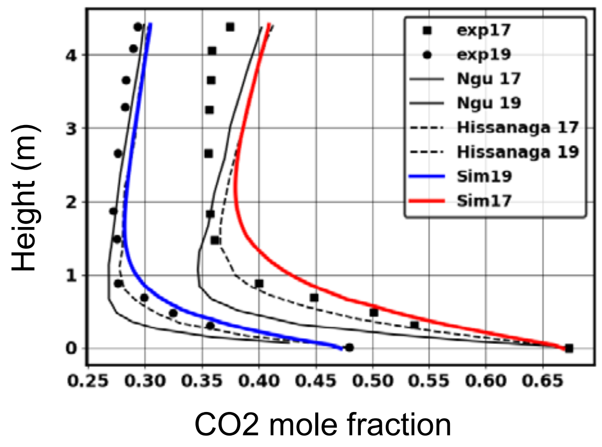
Air validation

Comparison with Van't Riet and Tramper, 1991



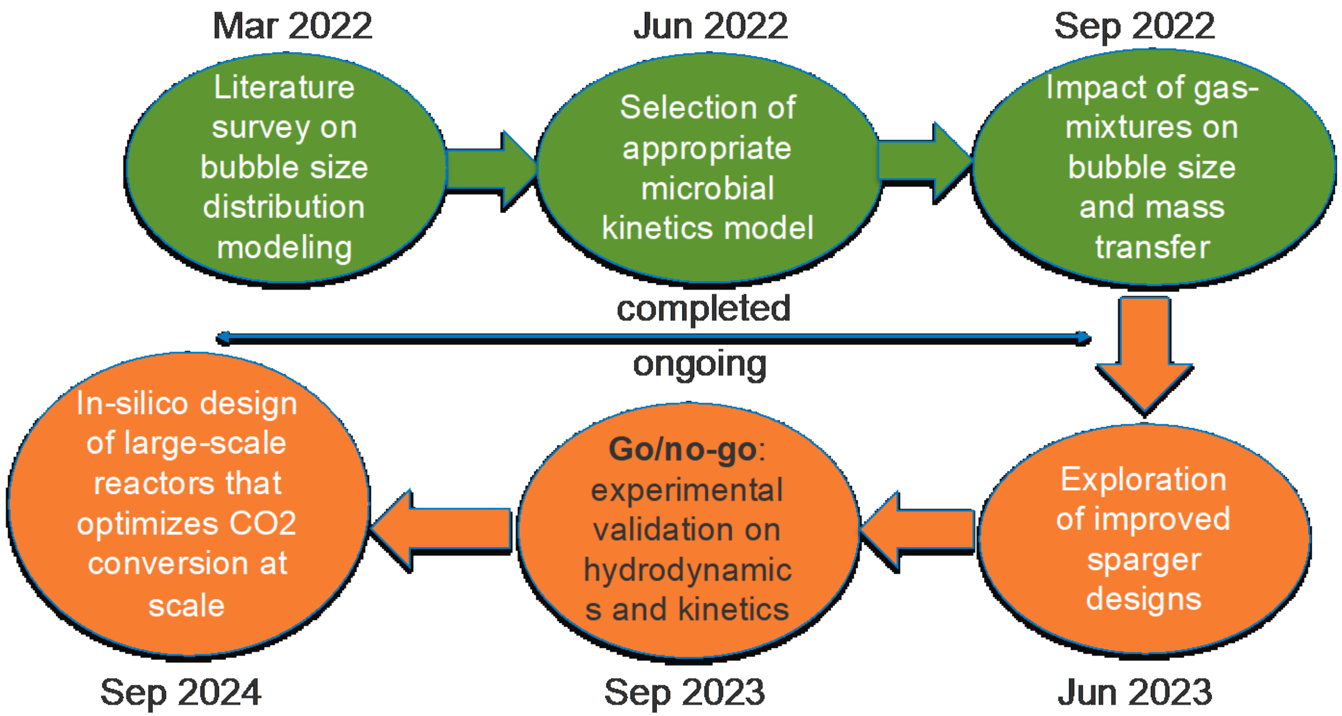
Air validation

Comparison with Hissanaga et al., Chem. Engg. Sci, 2020 and Ngu et al., Chem. Engg. Sci., 2022



Pure CO_2 validation

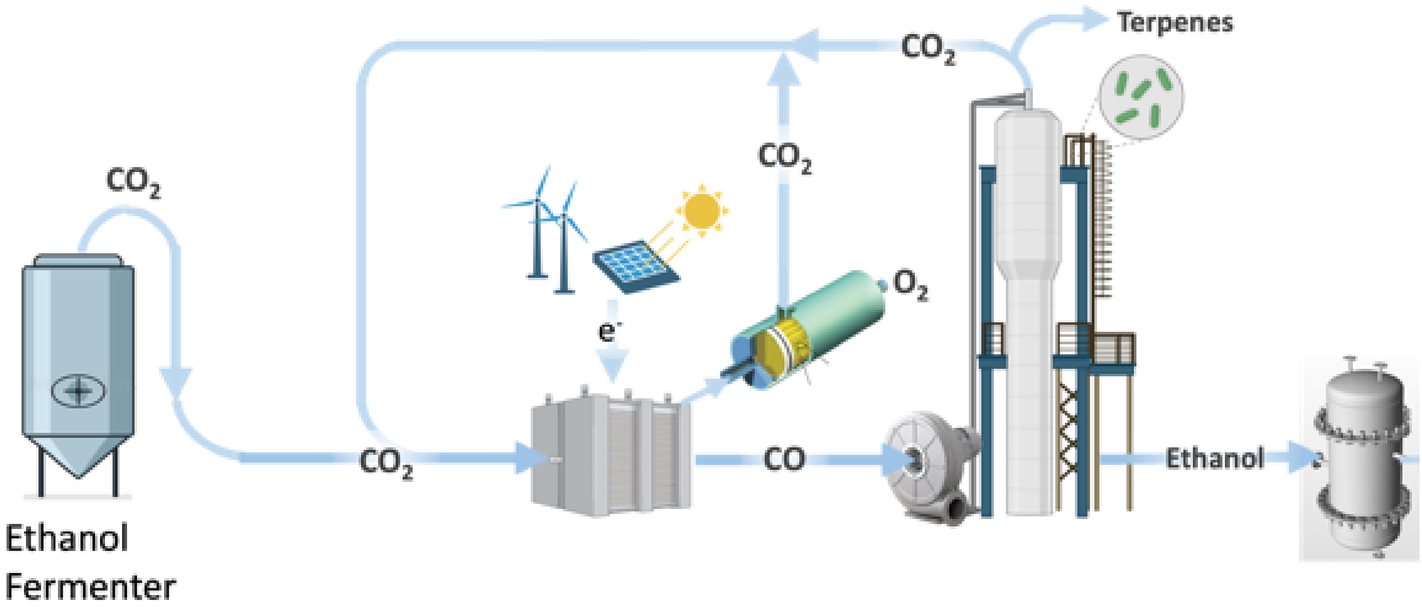
Technical approach: milestones/risk management

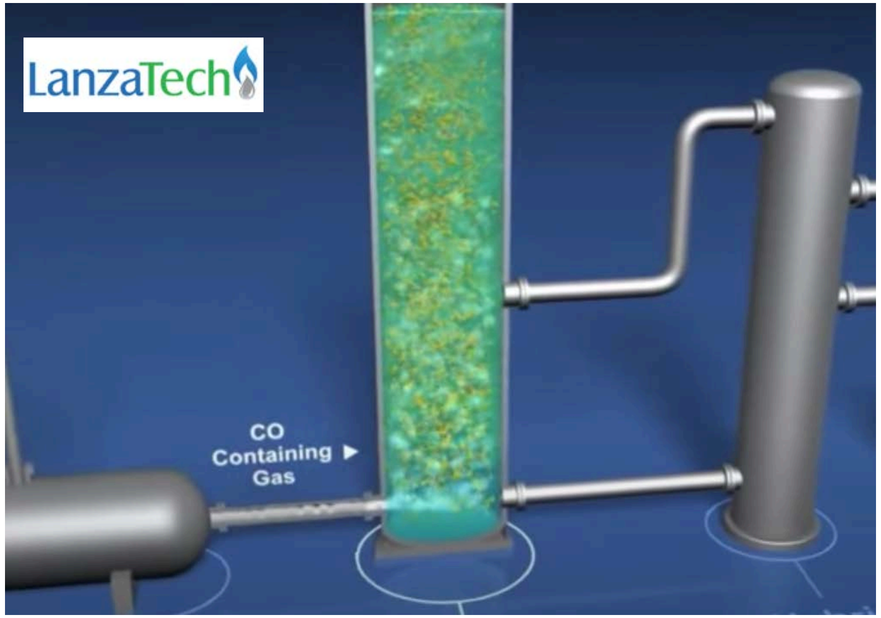


Date	Annual milestones
Sep 30, 2022	Impact of gas mixtures on bubble size/mass transfer
Sep 30, 2023	Experimental validation of hydrodynamics/kinetics
Sep 30, 2024	Large scale reactor design and optimization

- Risk/Mitigation 1: Experimental data for go/no-go: we are now collaborating and working closely with NREL biomethanation group and LanzaTech.
- Risk/Mitigation 2: Translating optimal reactor designs to industry: now working with CO2RUe advisory board on engaging reactor manufacturers.

Technical approach: collaborations

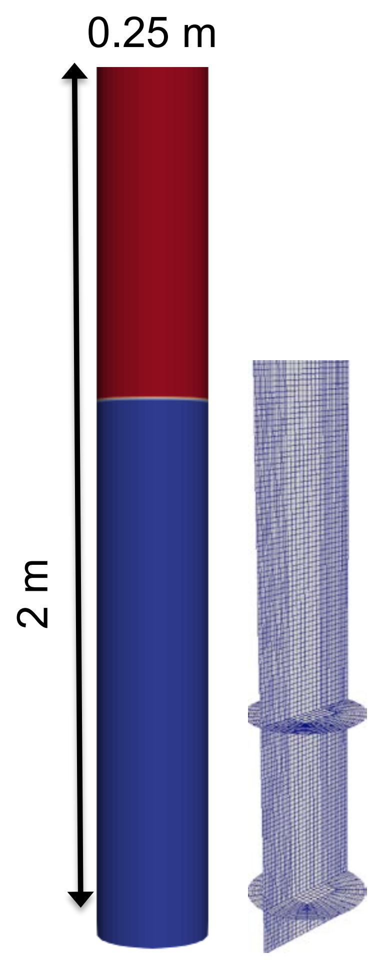


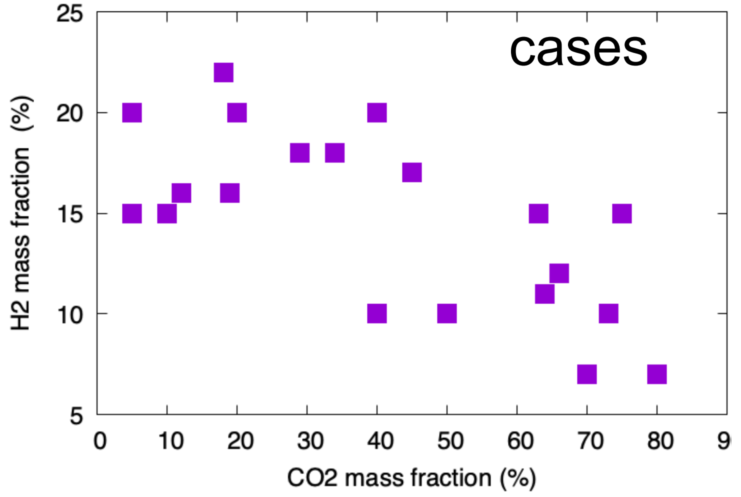


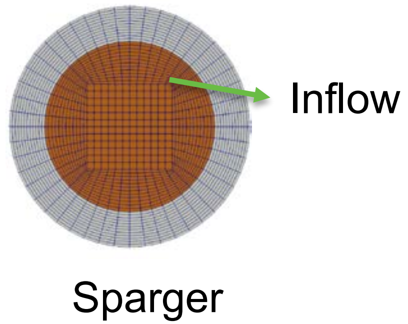
- Syngas upgrading project in CO2RUe consortium (Resch, NREL)
- LanzaTech is providing experimental data on bubble dynamics and mass-transfer
- NREL Biomethanation project: high speed visualization of bubble dynamics
- Electrochaea: advisory role on reactor scale-up for biomethanation

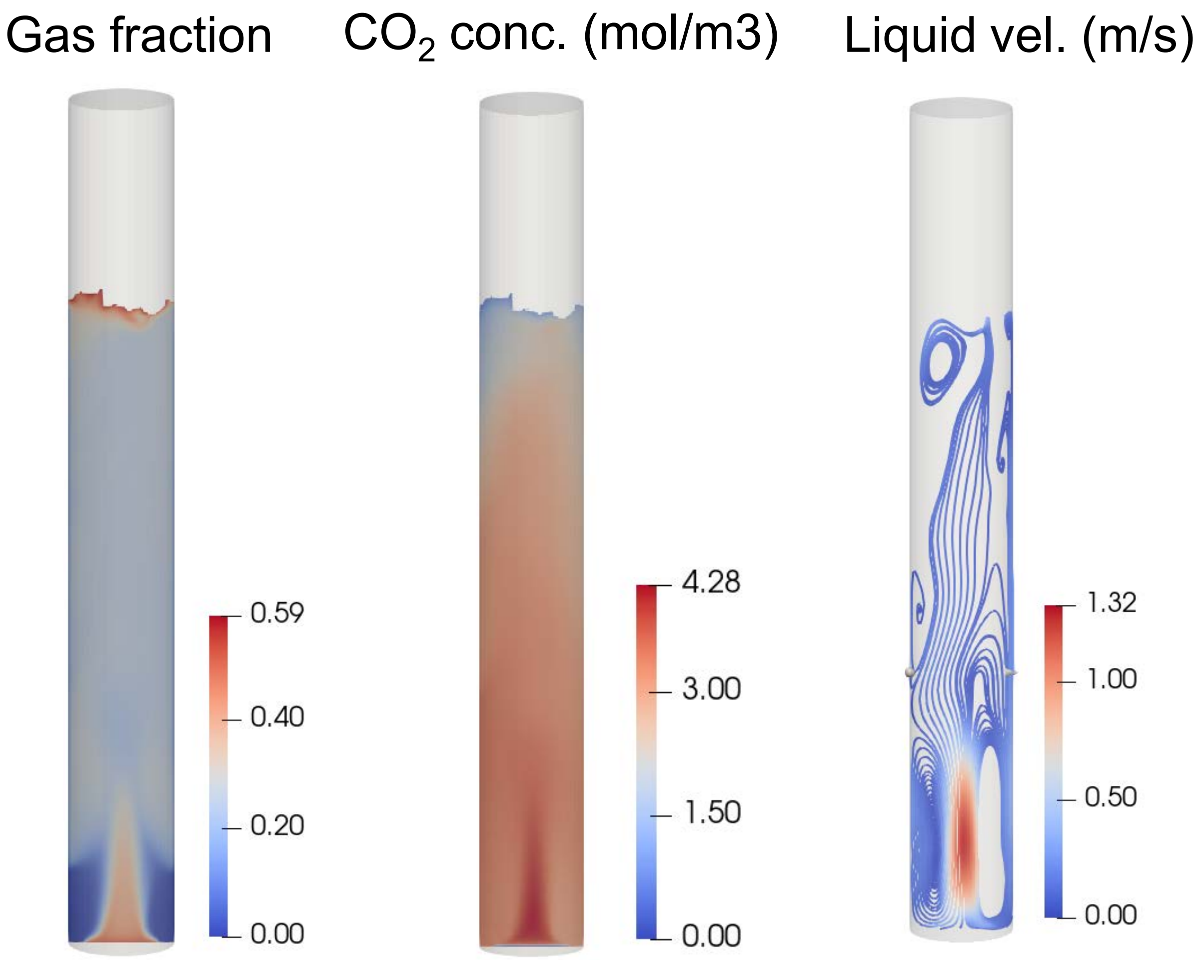
Progress

Progress: influence of gas mixtures (milestone 1)



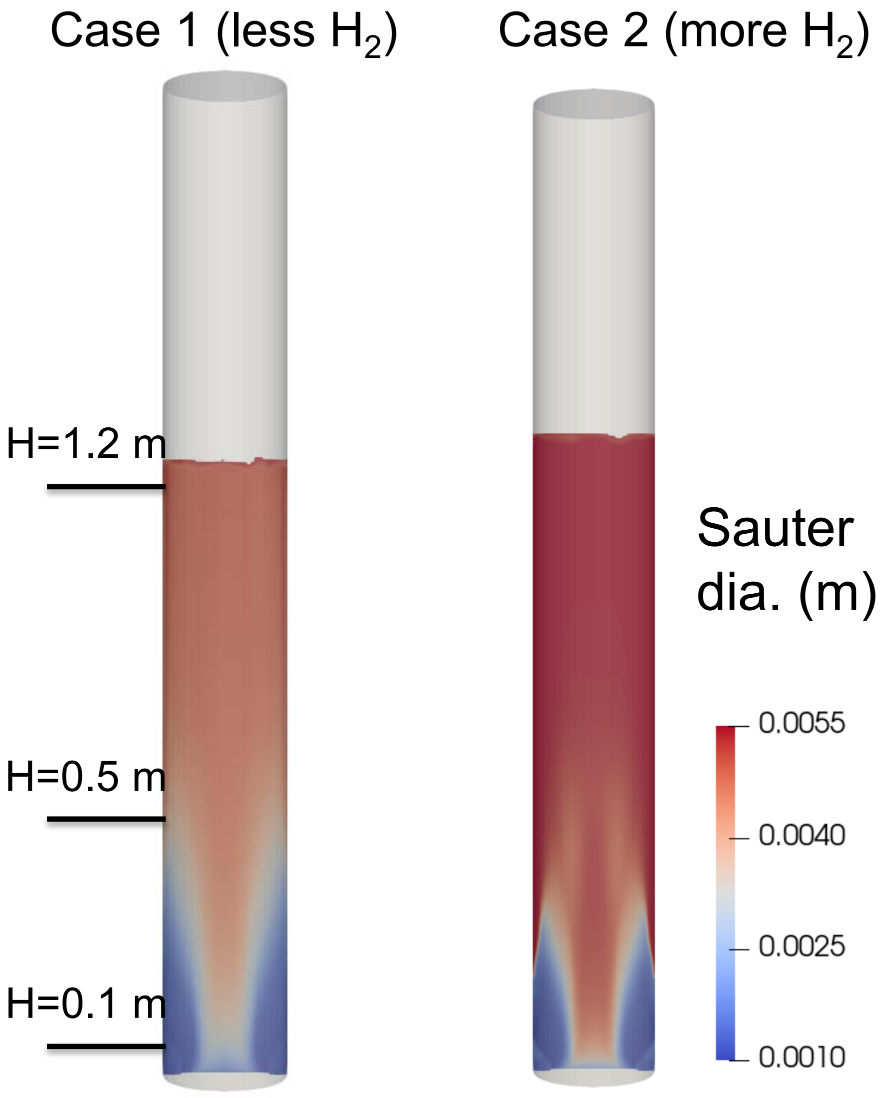


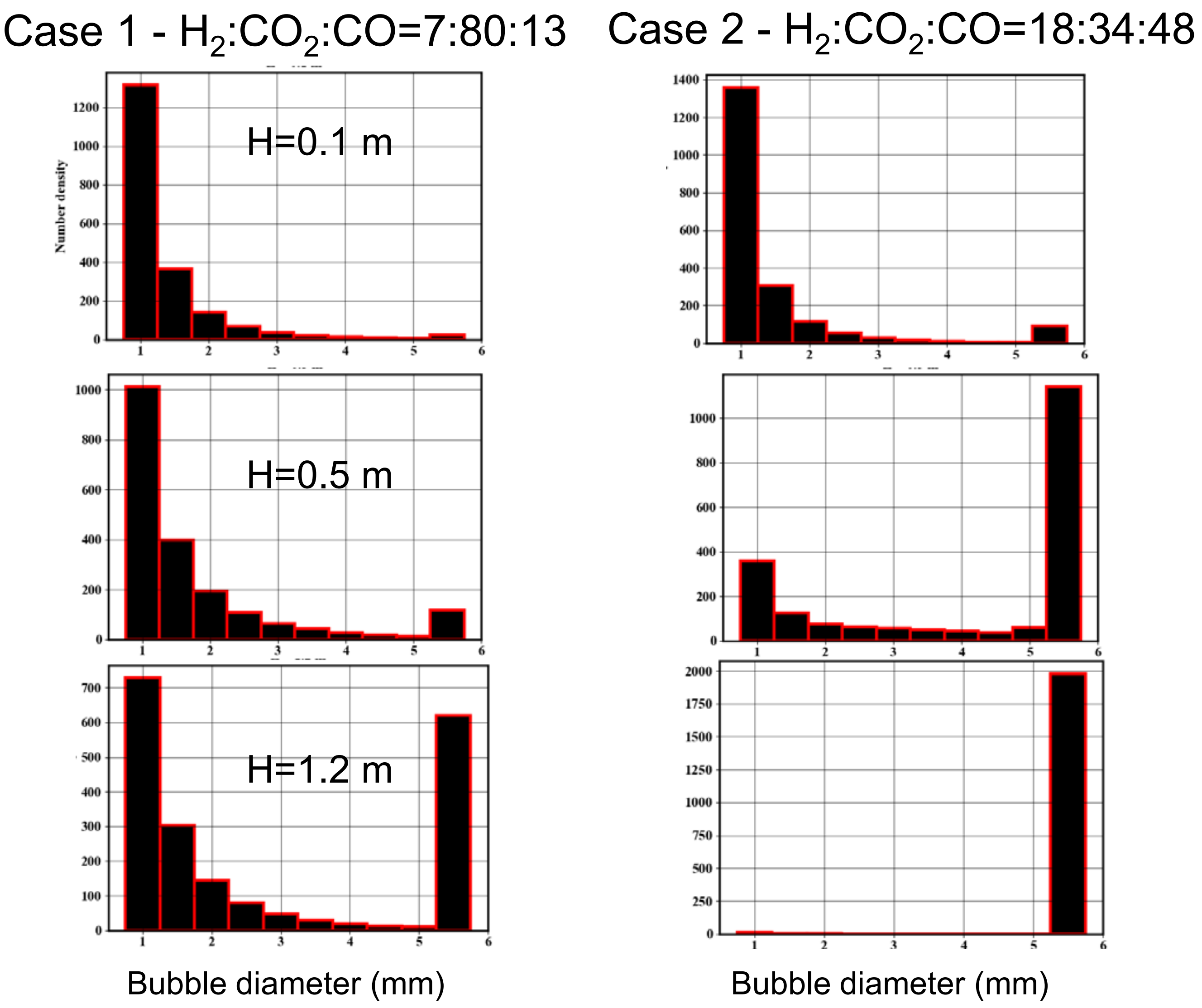




- Bottom inlet with a gas fraction that specifies sparger mass flow rate
- Vary gas mixture (H_2:CO_2:CO) while keeping constant mass flow rate of 0.45 g/s

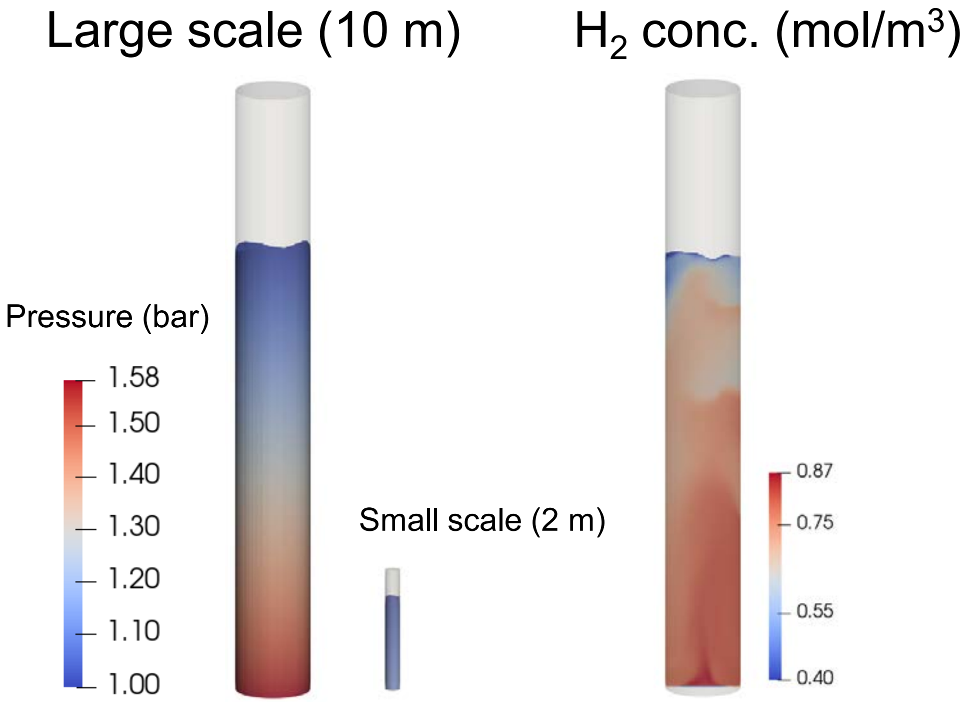
Progress: influence of H_2 (milestone 1)

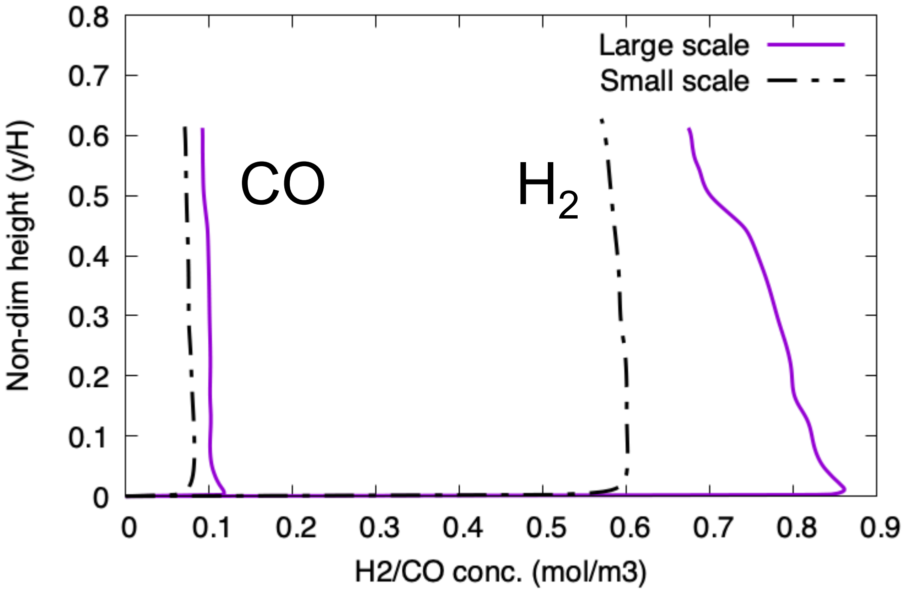




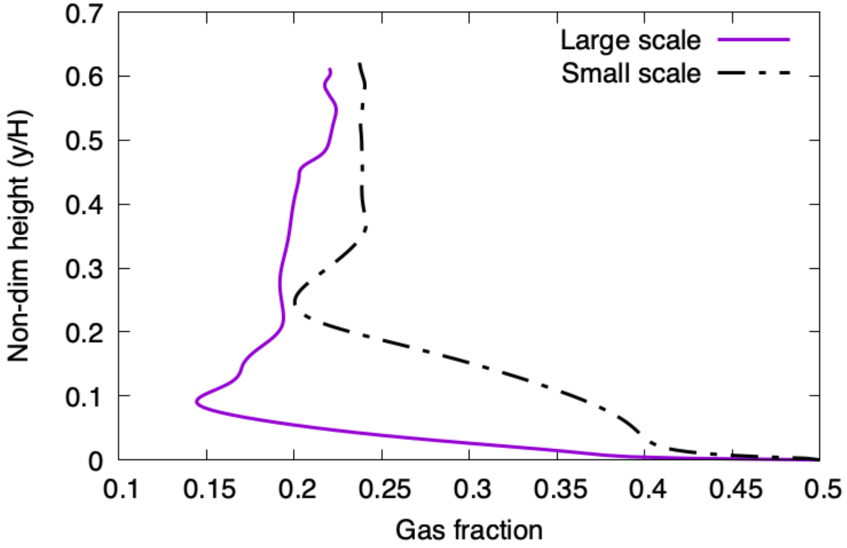
- Higher H_2 fraction results in faster bubble coalescence and higher average Sauter diameter

Progress: effect of scale-up (milestone 3)





- Higher hydrostatic pressure head enables greater mass transfer
- Superficial velocity of 5 cm/s is kept the same between cases
- Spatial inhomogenities in species concentration and gas fraction

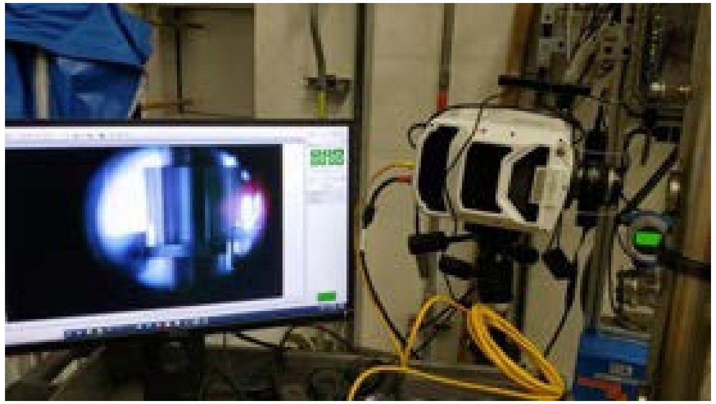


Progress: ongoing work

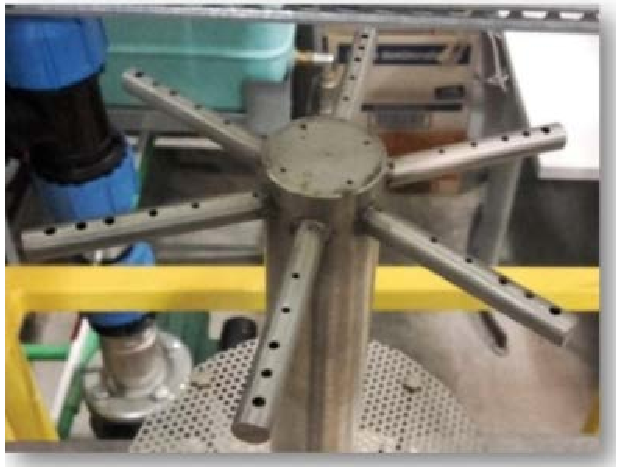
- Validation (FY23 annual go/no-go)
  - Bubble size distribution validation
    - LanzaTech experiments
    - NREL in-house bubble imaging
  - Kinetics/hydro validation
    - Biomethanation reactor (NREL)

- Sparger design (FY23 Q3)
  - Study impact of sparger designs
    - Ring/porous plates/Spider

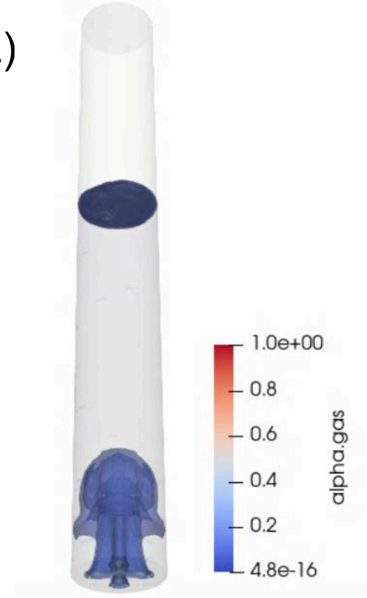
- Novel reactor designs (FY24)
  - Full scale simulations at scale (~ 500 m^3)
    - Include all physics from previous FYs
    - Show improvements in productivity



High speed imaging (Harrison, NREL)



Sparger designs (Besagni, Chem. Engg. Sci., 2018)



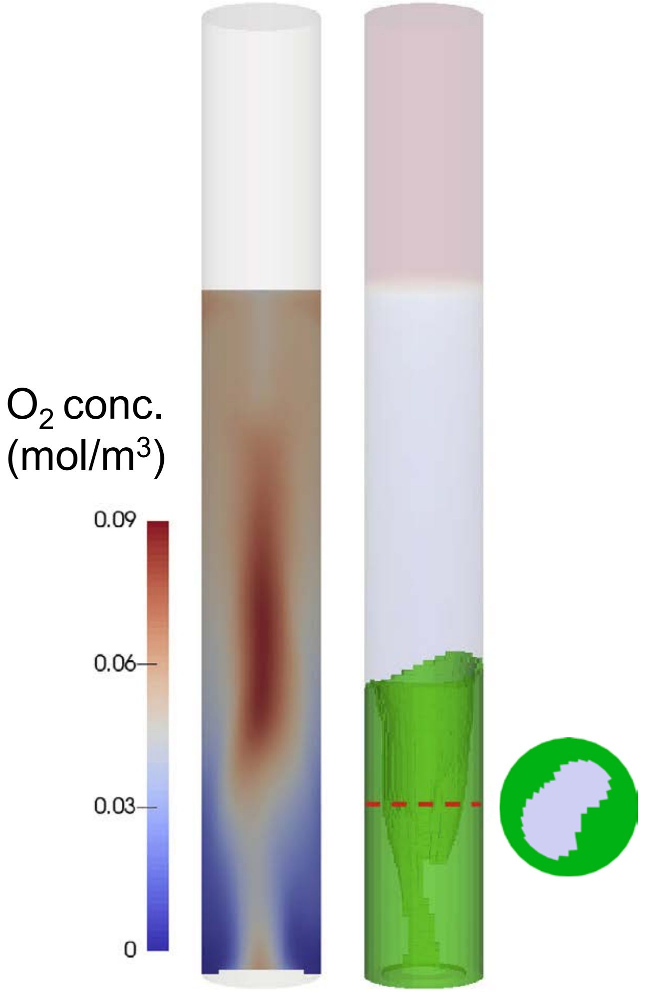
Gas fraction transient with a spider style sparger

Impact

- This work will enable design of large-scale fermenters for fuel production through:
  - CO_2/syngas conversion to fuels
  - Sugar conversion to sustainable aviation fuels
  - Fills the gap for CO_2 conversion specific physics models lacking in widely available software:
    - mass transfer, microbial uptake
    - bubble size distribution, turbulence models

- Industry engagement
  - Ongoing work with LanzaTech and Electrochaea
  - Future efforts to engage reactor manufacturers

- Accelerate lab scale microbiology research to industrial scale by reducing testing and design cycles and derisking scale-up

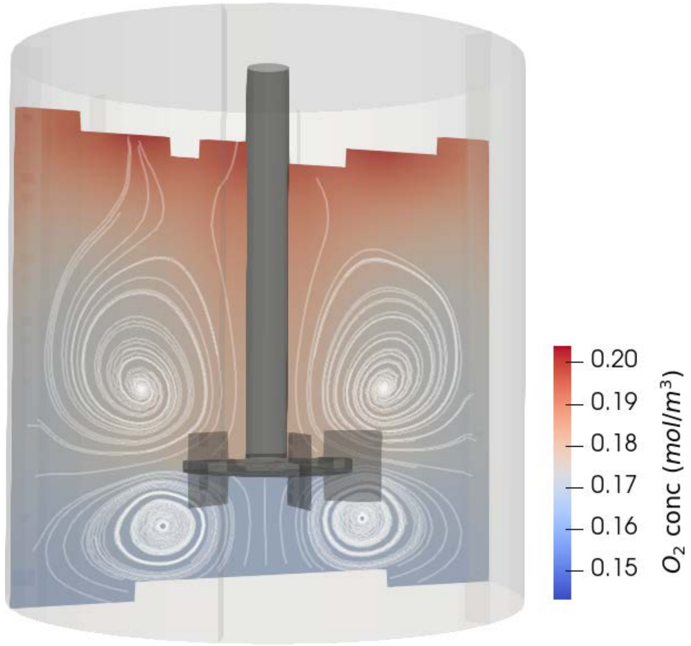


Oxygen depleted regions in a 40 m bubble column

Summary

- This project will use high-fidelity simulations to
  - quantify mass transfer in large-scale gas fermenters
  - Propose novel reactor designs and accelerate scale-up

- Achieve BETO goals
  - greenhouse gas reduction
  - Derisk technologies and support techno-economics
  - Sustainable aviation fuel production



- Publications/Presentations
  - Sitaraman et al., Impact of Variable Gas Mixtures on Bubble Size Distribution and Mass Transfer in Gas Fermentation Reactors, AIChE Annual meeting 2022

  - Rahimi et al., Computational fluid dynamics study of full-scale aerobic bioreactors: Evaluation of gas-liquid mass transfer, oxygen uptake and dynamic oxygen distribution, Chem. Engg. Res. Design, 189, 2018

Quad Chart Overview

Timeline

- Project start date: Jan 1st, 2022
- Project end date: Sep 30th , 2024

	FY22 Costed	Total Award
DOE Funding	$ 250,000	$ 750,000

TRL at Project Start:1
TRL at Project End:2

Project Partners*

- LanzaTech (no-cost partner)
- NREL Biomethanation project (no-cost partner)

Project Goal

Develop accurate computational models to quantify gas-liquid mass-transfer and mixing dynamics in scaled-up CO_2/syngas fermentation systems (~ 500 m^3 capacity), thus accelerating the path from lab-to-industry via optimal reactor designs.

End of Project Milestone

In-silco design of novel industrial-scale bioreactors that show 50% improvement for productivity compared to simulations of at-scale stirred-tank reactors.

Funding Mechanism

CO2 utilization lab call, 2021

Thank You

NREL/PR-2C00-85603

NREL Transforming ENERGY

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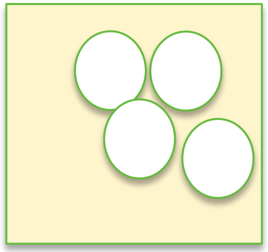
Multiphase Euler-Euler equations

- Gas and liquid as continuous interpenetrating phases
- 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

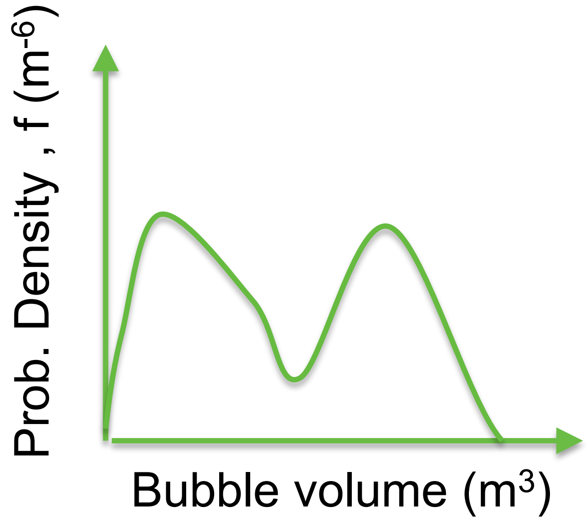
$$\frac{\partial}{\partial t}(\alpha_i \rho_i \mathbf{V}_i) + \vec{\nabla} \cdot (\alpha_i \rho_i \mathbf{V}_i \mathbf{V}_i)$$
$$= -\alpha_i \vec{\nabla} P + \alpha_i \rho_i \mathbf{g} + \vec{\nabla} \cdot (\alpha_i \bar{\mathbf{R}}_i) + \mathbf{F}_i$$

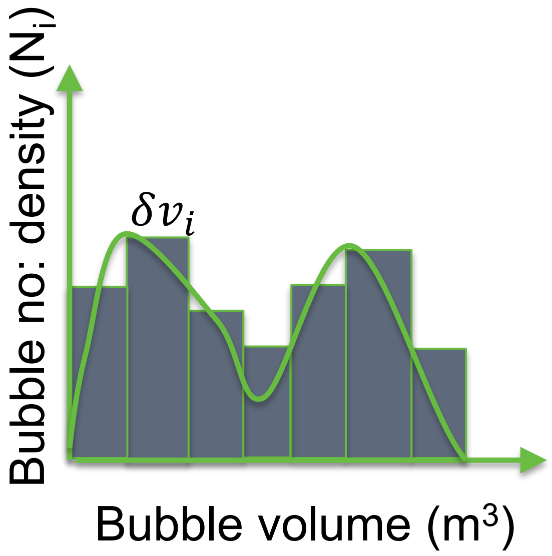
Momentum conservation

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

Species transport within each phase

Bubble size distribution* modeling





$$\textit{number of bubbles per unit volume } N_i = f\ \delta v_i$$

$$\textit{phase fraction of each group } f_i = \frac{N_i v_i}{\sum_j N_j v_j}$$

$$\frac{\partial n_v}{\partial t} + \nabla \cdot (v_{ph} n_v) = h_v$$

$$h_v = \underbrace{\frac{1}{2}\int_0^v n_{v'} n_{v-v'} C_{v',v-v'} dv'}_{\text{coalescence}(+)} - \underbrace{n_v \int_0^\infty n_{v'} C_{v,v'} dv'}_{\text{coalescence}(-)} +$$

$$\underbrace{\int_v^\infty n'_v B_{v'} \beta_{v,v'} dv'}_{\text{breakup}(+)} - \underbrace{n_v B_v}_{\text{breakup}(-)} - \underbrace{\frac{\partial(\dot{v} n_v)}{\partial v}}_{\text{drift}} + \underbrace{\dot{n_v}}_{\text{nucleation}}$$

PDF transport equation

Bubble dynamics source terms

*Lehnigk et al., AIChE Journal, 68,3, 2022

Drag and mass transfer model

$$F_D = \frac{3}{4}(C_D/d)\alpha\rho_l U_r^2 * sign(U_r)$$

Drag force

$$C_D = f(Re, Eo, \alpha_g)$$

Ishii Zuber drag model

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

$$\mathrm{MTR} = k_\mathrm{L} a(C_j^* - C_j)$$

Oxygen transfer rate

$$C_j^* = \frac{X_{j,G}P}{H_i}\frac{\rho_L}{M_L}$$

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

[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.

Numerical methods and solver

- Transport properties
  - Fermentation broth properties are similar to water
  - Multiphase k-ω SST turbulence model
  - Population balance over 1-5 mm bubbles with 10 classes
- Customized *multiphaseEulerFoam* in OpenFOAM
  - Higbie mass transfer model
  - Microbial uptake
- Simulations performed using
  - 128 Intel Skylake processors
  - 48 hours of run time to simulate 30 seconds for 0.5 million cells
- More details in Rahimi et al., Chem. Engg. Res. Design, 139, 2018