Subtask 4.1.5 Pipeline MVA

CFD Modeling Hypothetical CO_2 Releases At High Island 10L Using ANSYS Fluent

Napoli Rosario and Daniel Chen, Dan F. Smith Dept. Chem. & Bio. Eng.,
Lamar University, Beaumont, TX

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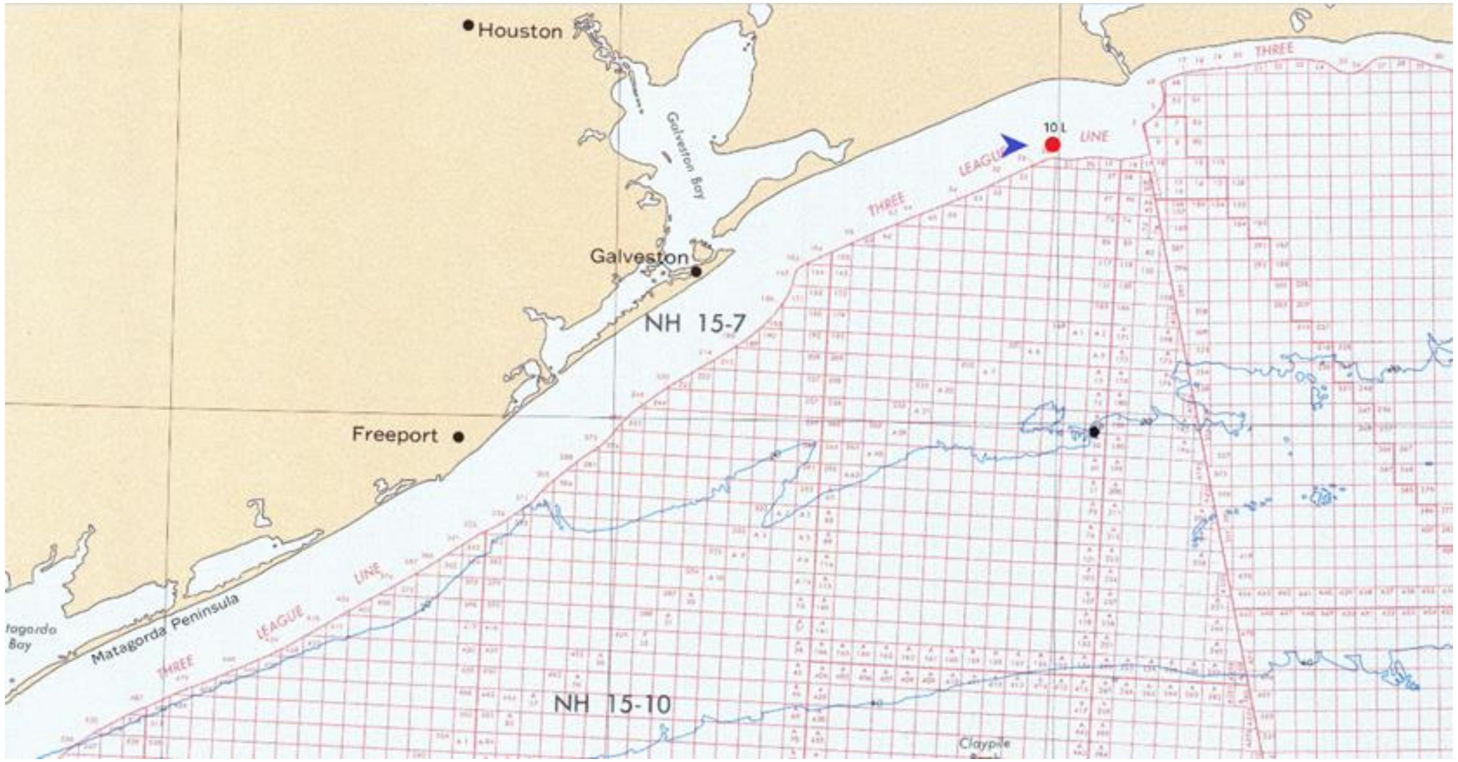
Problem Statement

- A potential CO_2 leak from an offshore High Island 10 L reservoir can affect the marine environment and the safety of the marine traffic.
  - The absorbed CO_2 can react with carbonate in seawater and reduce the pH
  - The CO_2 emitted at the seawater surface can lower the oxygen levels and impact surface traffic.
- The objective is to employ the ANSYS Fluent CFD tool for a 3-D modeling with chemistry & mass transfer for CO2 leaks into the water column from a High Island 10L well to determine CO_2 absorption in seawater, the pH change, and CO_2 emission at the seawater surface.

High Island 10L Field Location

- In the state of Texas, a geologic formation suitable for storage of CO_2 has been identified (Ramirez 2019). The geologic formation is the High Island 10-L, a depleted oil and gas reservoir, located off Jefferson County coast on the Gulf of Mexico.
- The cumulative production of the High Island 10-L from 1950 to 1984 is 830,416 barrels of oil and 30,940,973 cubic feet of dry gas (Fowler and Caughey 1987). According to the barometric map shown, High Island 10L is close to the Texas coast at a water depth between approximately 10 and 20 meters.



ANSYS Fluent Simulation

- For this work, the Eulerian, Turbulence (k-ε), Mass Transfer, Drag and Lift Force, Chemical Reaction and Population Balance models (PBM) were selected.
- This a stiff, 2-Phase, transient, and reactive system
  - involving the mass transfer of CO_2 gas to water, then the reaction of absorbed aqueous CO_2 with carbonate in alkaline seawater, and release of unabsorbed CO_2 to atmosphere
  - impact on water and air will be evaluated.

EULERIAN MODEL

- The Eulerian Model simulates the interaction between a gas and liquid.

- **Continuity:**

Volume fraction for the q^{th} phase

$$\frac{\partial(\alpha_q \rho_q)}{\partial t} + \nabla \cdot (\alpha_q \rho_q \mathbf{u}_q) = \sum_{p=1}^{n} \dot{m}_{pq}$$

- **Momentum for q^{th} phase:**

$$\frac{\partial(\alpha_q \rho_q \mathbf{u}_q)}{\partial t} + \nabla \cdot (\alpha_q \rho_q \mathbf{u}_q \mathbf{u}_q) = -\alpha_q \nabla p + \alpha_q \rho_q \mathbf{g} + \nabla \cdot \boldsymbol{\tau}_q + \sum_{p=1}^{n} (\mathbf{R}_{pq} + \dot{m}_{pq} \mathbf{u}_q) + \alpha_q \rho_q (\mathbf{F}_q + \mathbf{F}_{\text{lift},q} + \mathbf{F}_{\text{vm},q})$$

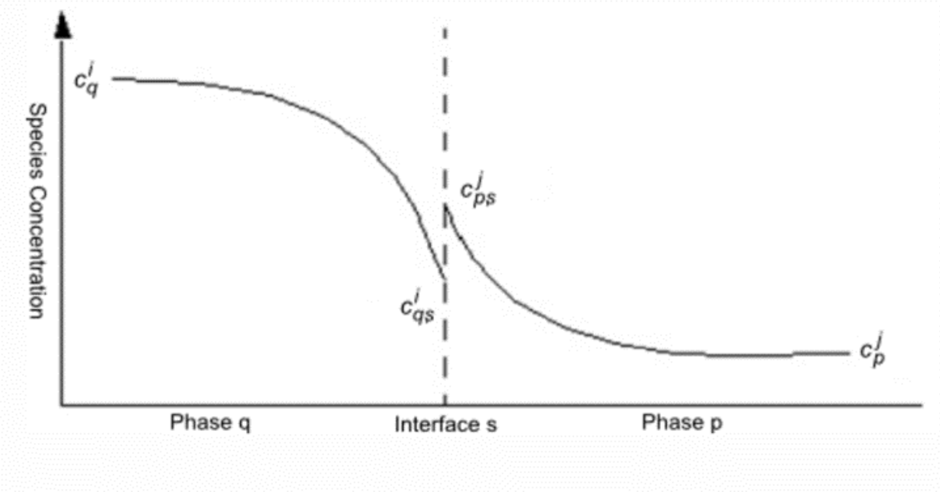
transient | convection | pressure | body | shear | interphase forces exchange | interphase mass exchange | external, lift, and virtual mass forces

Solids pressure term is included for granular model.

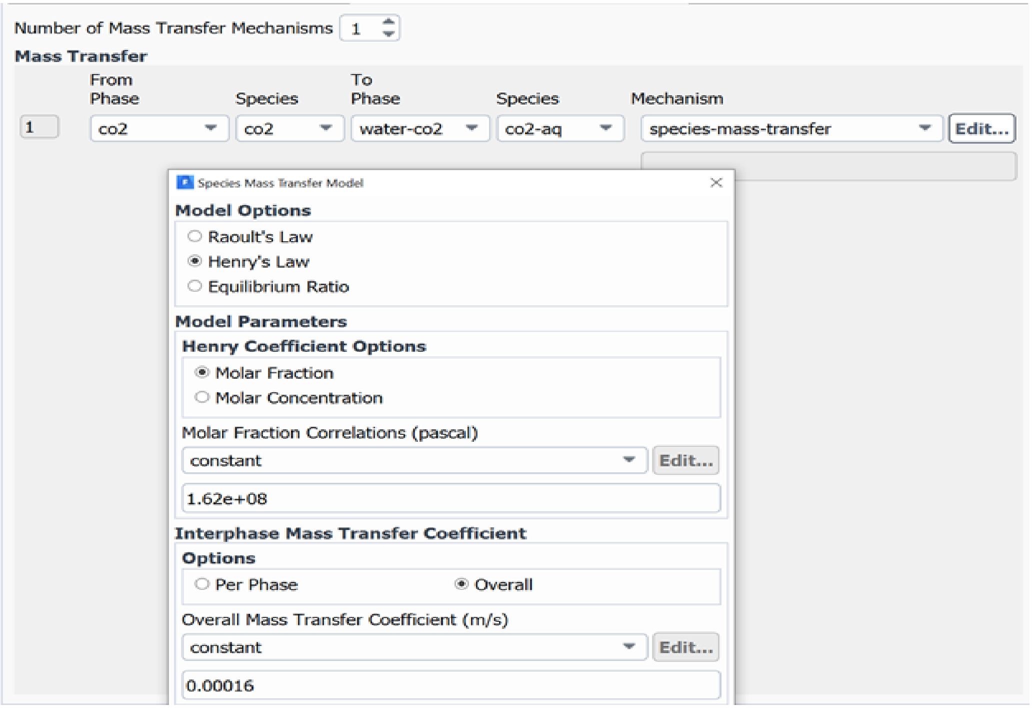
$$\alpha = \frac{Volume\ of\ Phase\ in\ Cell}{Volume\ of\ Cell}$$

- The Eulerian model was selected with two phases, water-CO2 (aqueous phase) and CO2 (gas phase). The water-CO2 phase consists of $H_2O_{(l)}$, $H_2CO_{3(l)}$, $HCO_3^-{}_{(l)}$, $CO_3^{-2}{}_{(l)}$, $CO_{2(l)}$ and $H^+_{(l)}$. While the CO2 phase consists of $CO_{2\ (gas)}$ and $N_{2(gas)}$.

MASS TRANSFER: Two Film Theory



- For gases that are not very soluble in water like CO2, the mass transfer is controlled by the liquid phase resistance.
- The overall mass transfer can be expressed as $1/K_L = 1/k_L$
- $\dot{m}_q = K_L A (C_{(p,s)} - C_{p,\infty})$, mass transfer rate in kg/s.
- $(dm/dt)/V = K_L\, a\, (C_s - C_b)$ where $(dm/dt)/V$ is mass transfer rate in $kg/(m^3 *s)$, a is specific surface area in m^2/m^3, C_s is CO_2 conc. at bubble interface, C_b is bulk CO_2 conc. In the aqueous phase.
- The mass transfer coefficient was set constant at 0.00016 m/s.



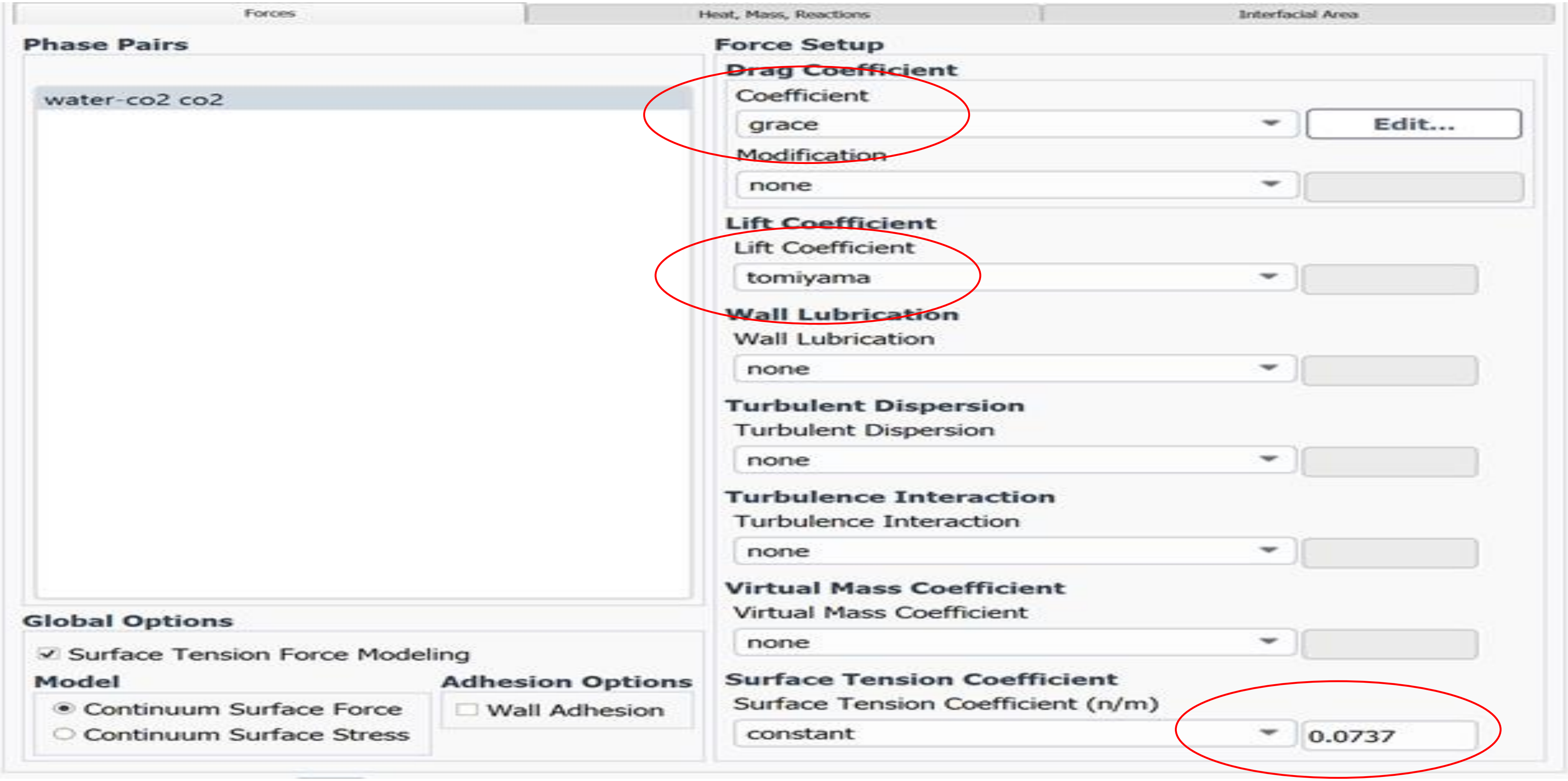
The Hughmark correlation:

$$k_p = \frac{ShD}{L} \qquad Sc = \frac{\mu}{\rho D} \qquad Re = \frac{\rho |V_q - V_p| d}{\mu} \qquad Sh = 2 + 0.95 Re^{\frac{1}{2}} Sc^{\frac{1}{3}}$$

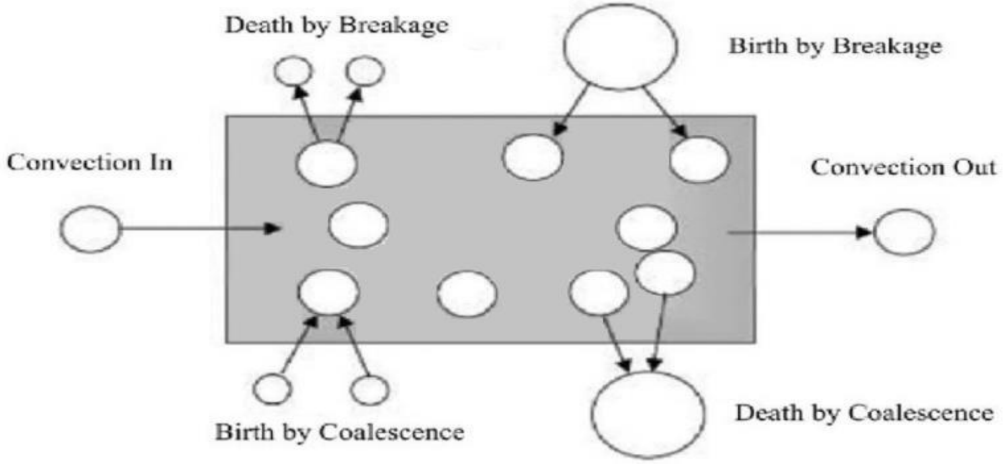
Where kd is the mass transfer coefficient, Sh the Sherwood number, Sc the Schmidt number, Re the Reynolds number, L and d the CO_2 bubble diameter, μ_{water} dynamic viscosity, ρ_{water} the density and $|V_{water} - V_{CO2}|$ the magnitude relative velocities of the phases. The correlation is a function of the CO_2 diameter and the velocities of seawater and CO_2

DRAG AND LIFT MODELS

- The surface tension was set constant at 0.0737 n/m.
- The drag and lift coefficients were estimated with the Grace and Tomiyama models (Fluent Image below).



POPULATION BALANCE MODEL: BUBBLE INTERACTIONS



$$\frac{\partial}{\partial t}[n(V,t)] + \nabla.[\vec{u}n(V,t)] + \underbrace{\nabla_V.[G_V n(V,t)]}_{\text{Growth term}}$$
$$= \frac{1}{2}\int_0^V \underbrace{a(V-V',V')n(V-V',t)n(V',t)\,dV'}_{\text{Birth due to aggregation}}$$
$$- \int_0^\infty \underbrace{a(V,V')n(V,t)n(V',t)dV'}_{\text{Death due to aggregation}}$$
$$+ \int_{\Omega_V} \underbrace{pg(V')\beta(V|V')n(V',t)dV'}_{\text{Birth due to breakage}} - \underbrace{g(V)n(V,t)}_{\text{Death due to breakage}}$$

REACTION RATE and EQUILIBRIUM CONSTANTS

Reaction Rates (Mitchell. 2010)

Reaction	$k_{forward}$	$k_{reverse}$	$K_{equilibrium}$
$H_2O + CO_{2(aq)} \leftrightarrow H_2CO_3$	$6*10^{-2}\ s^{-1}$	$2*10\ s^{-1}$	0.003
$H_2CO_3 \leftrightarrow H^+ + HCO_3^-$	$1*10^{7}\ s^{-1}$	$5*10^{10}\ M^{-1}\ s^{-1}$	$2*10^{-4}$ M
$HCO_3^- \leftrightarrow H^+ + CO_3^{-2}$	$3\ s^{-1}$	$5*10^{10}\ M^{-1}\ s^{-1}$	$6*10^{-11}$ M

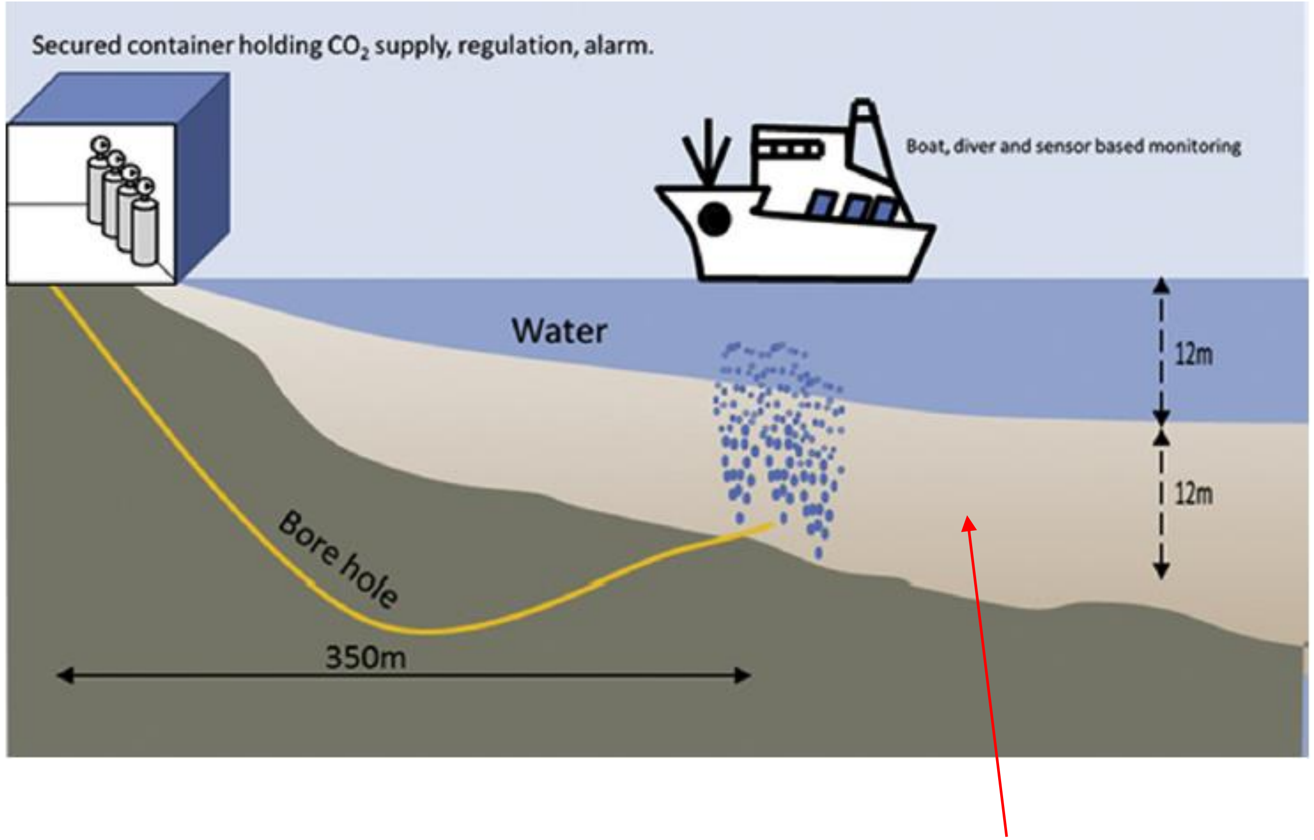
Overall Reaction: $H_2O + CO_{2(aq)} + CO_3^{-2} \leftrightarrow 2HCO_3^-$

Properties of Seawater and CO_2 :

Seawater is a buffer solution with weak acids and their conjugate bases as in human blood

Properties	Values
Seawater pH	8.2
Seawater Velocity	0.15 m/s
Seawater Temperature	298 K
Seawater Carbonate Ion Concentration (CO_3^{-2})	0.245mol/m3
CO_{2g} Temperature	205 F

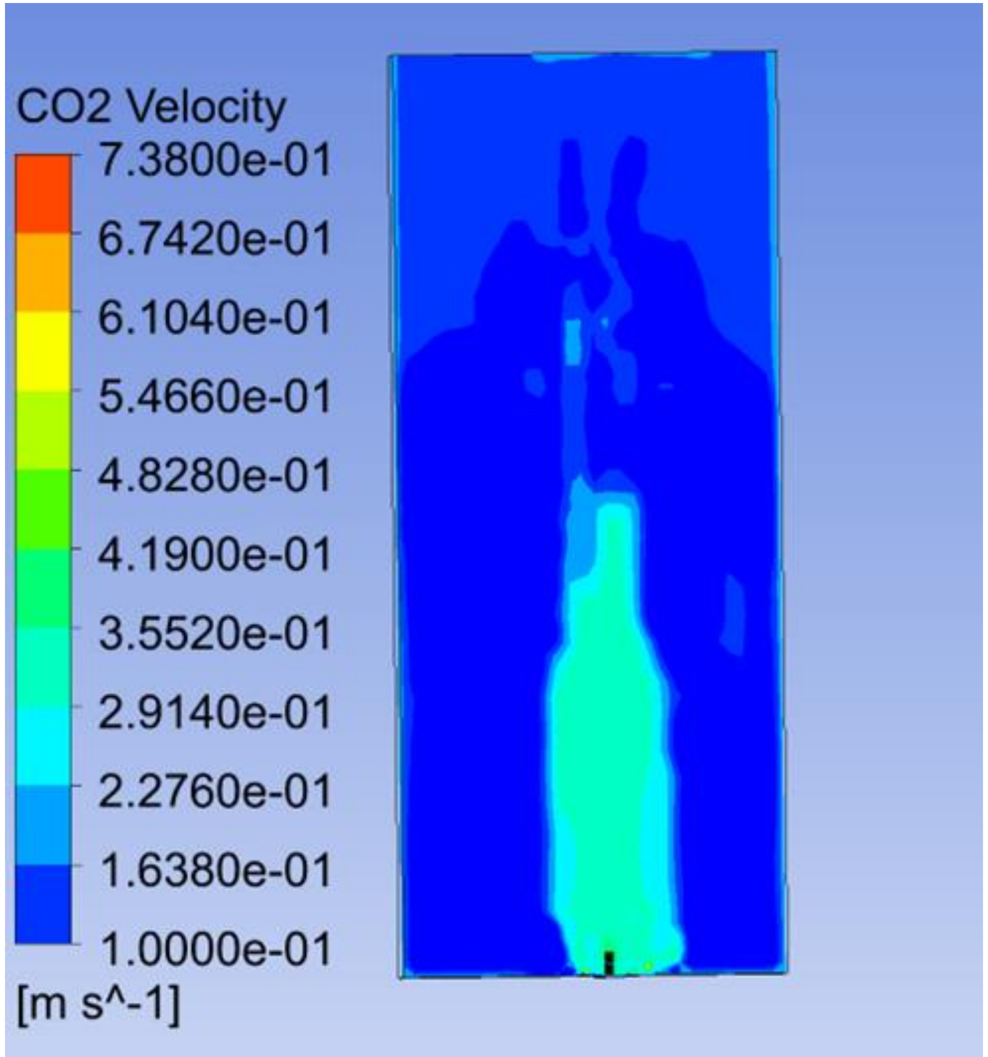
Validation with QICS experiments

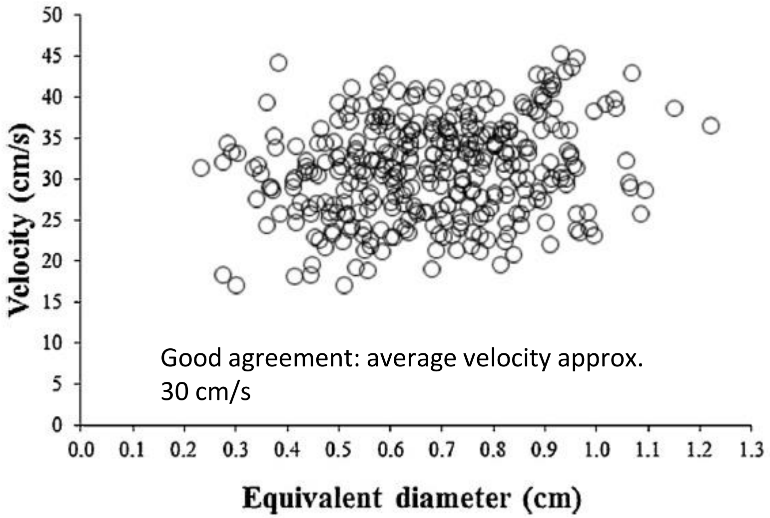


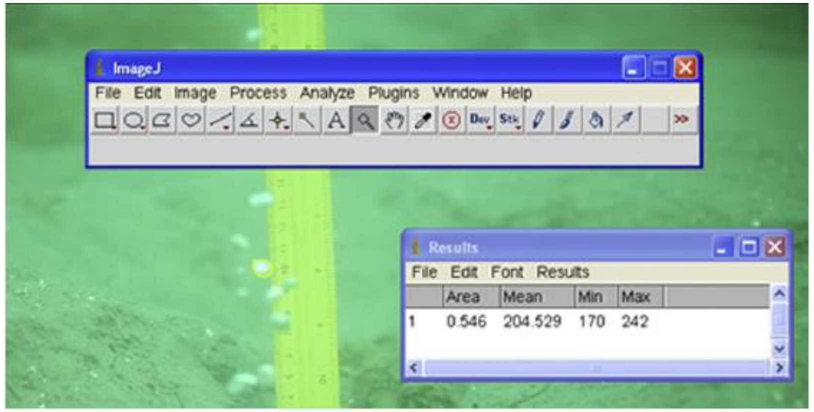
Sediments

- The CFD simulation was validated with the Quantifying and Monitoring Potential Ecosystem Impacts of Geological Carbon Storage (QICS) experiment conducted by Sellami et al. in Ardmucknish Bay, Scotland (2015).
- CO_2 (0.002896 kg/s or 91.3 ton/yr) was injected at the seafloor and the velocity of the bubbles was measured.

Results: CFD (L) vs QICS Experiments (R)



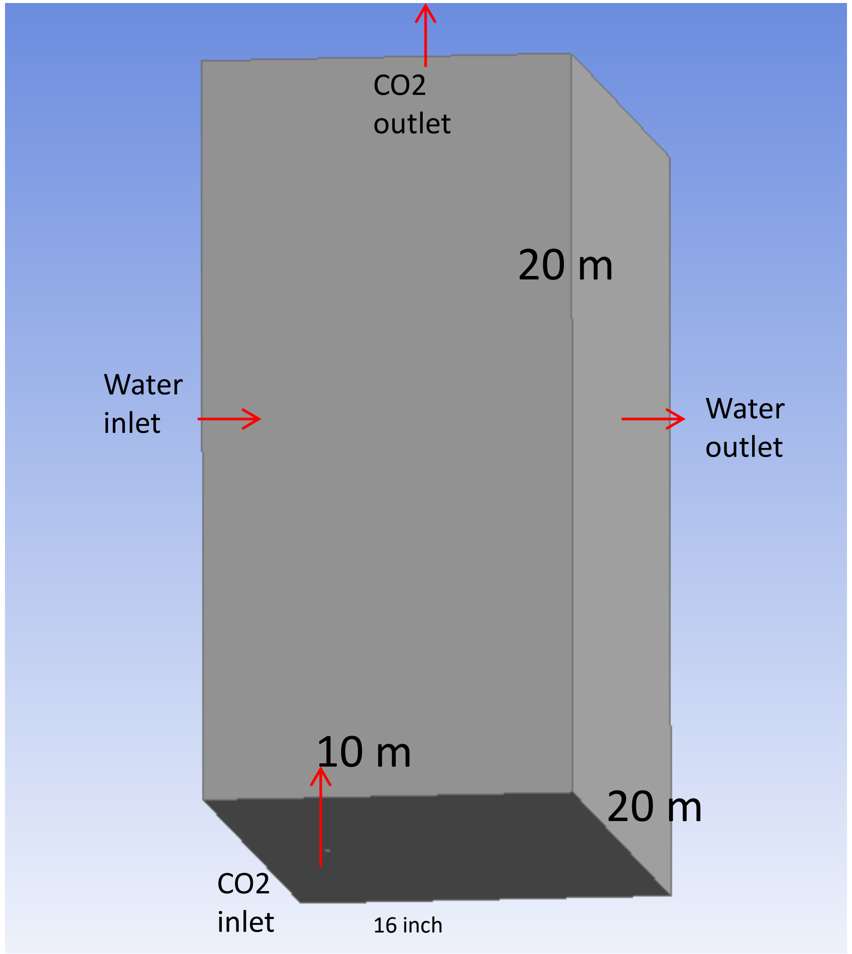




Bubble velocity ranges 23-48 cm/s in good agreement with 12m depth and 5m width, 3-D

QICS data measured at 20-30 cm above sea floor (Sellami et al, 2015); Bubble rise velocity: 20-45 cm/s,

Validated Model Used In High Island 10L Simulation



- This is transient simulation with initial time step 0.0001s.
- The simulation time to steady state was 163s.
- Leakage of 0.1 kg/s & 35 kg/s (3154 ton/yr & 1.104 E6 ton/yr) at 20m depth
- Hole size 16 in
- Seawater Current at 0.15 m/s

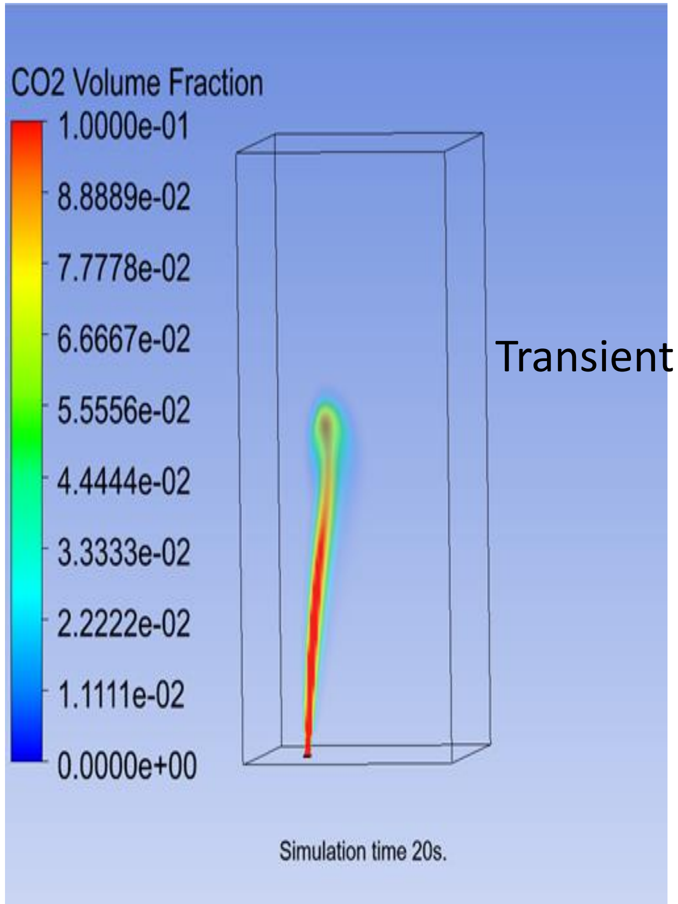
Boundary Conditions

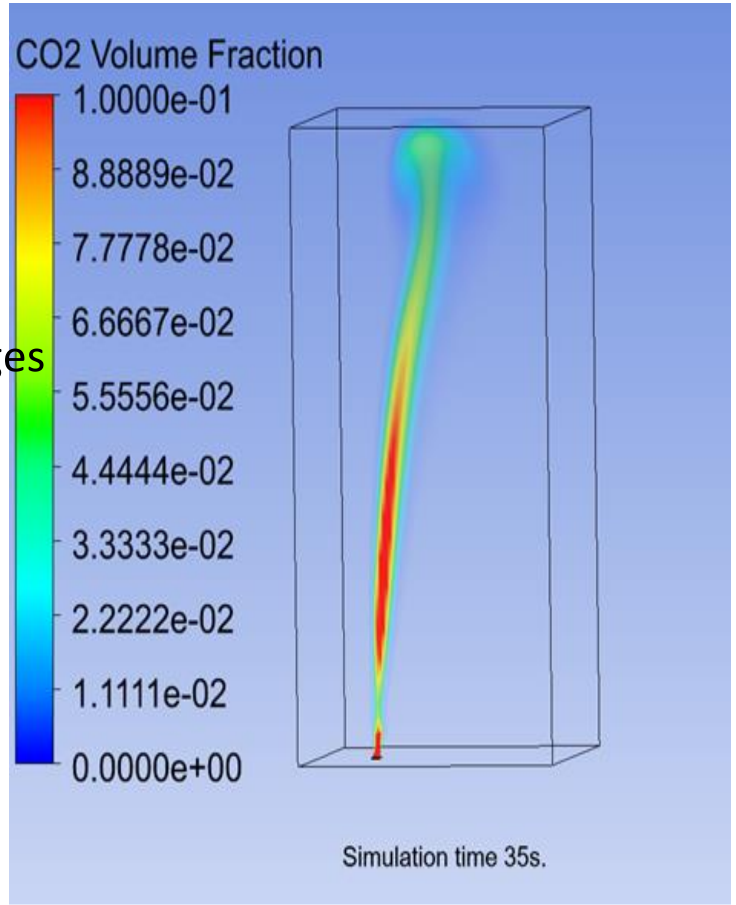
- The boundary conditions: CO2inlet, interior-fluid, wall, waterinlet, wateroutlet and wateroutlettop.
  - The CO2inlet boundary type was set as mass flow inlet. The flow rate, pressure, temp. (28.4 psig & 205 F) and composition (pure CO2) are specified .
  - The waterinlet boundary type was set as velocity inlet. The velocity of the fluid and composition are specified (temp. 298 K, p= 10084.2 [Pa/m]*y)
  - The wateroutlet boundary type was set as pressure outlet. This boundary condition allows the exit of liquid and gases.
  - The wateroutlettop boundary type was set as degassing. It allows to the exit of gases.

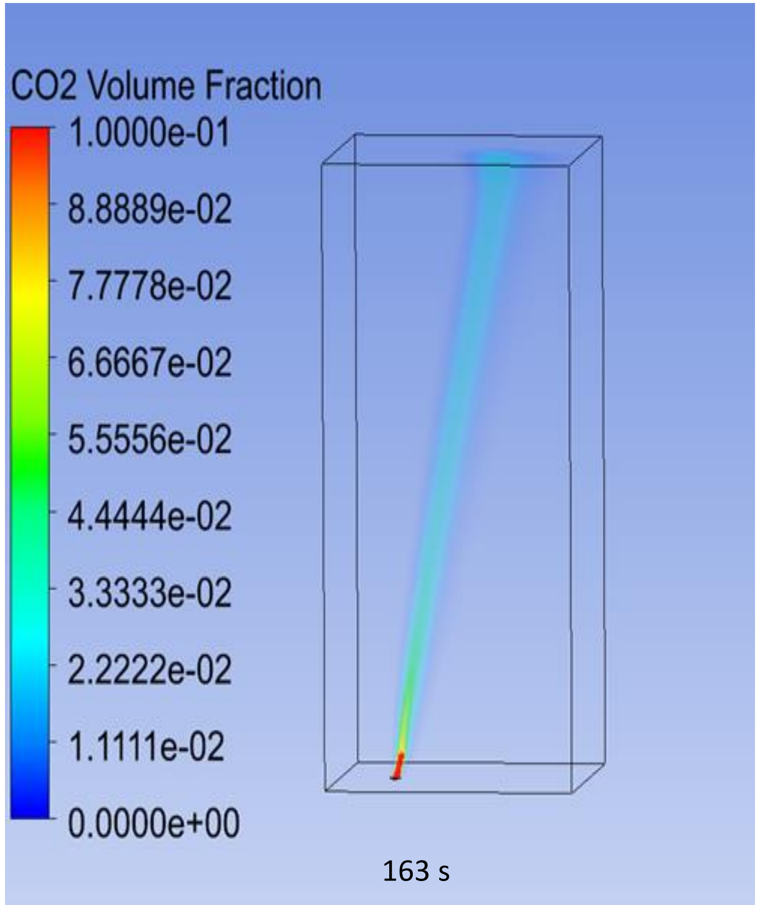
Simulation for water column depth 20 m for 0.1 kg/s; Seawater Current at 0.15 m/s

Transient Images

Transient Images

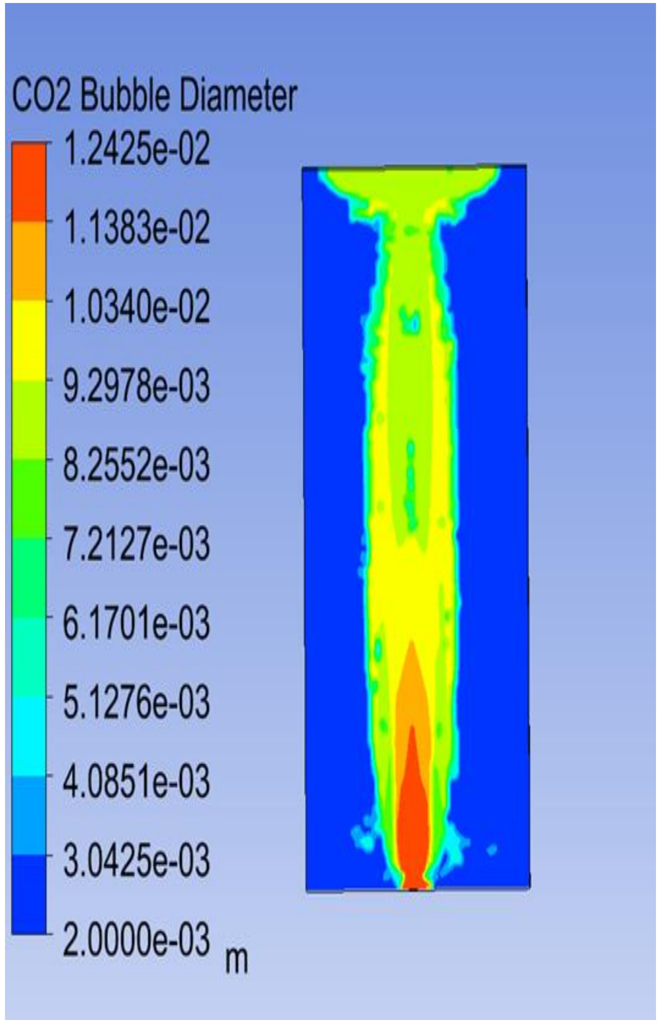


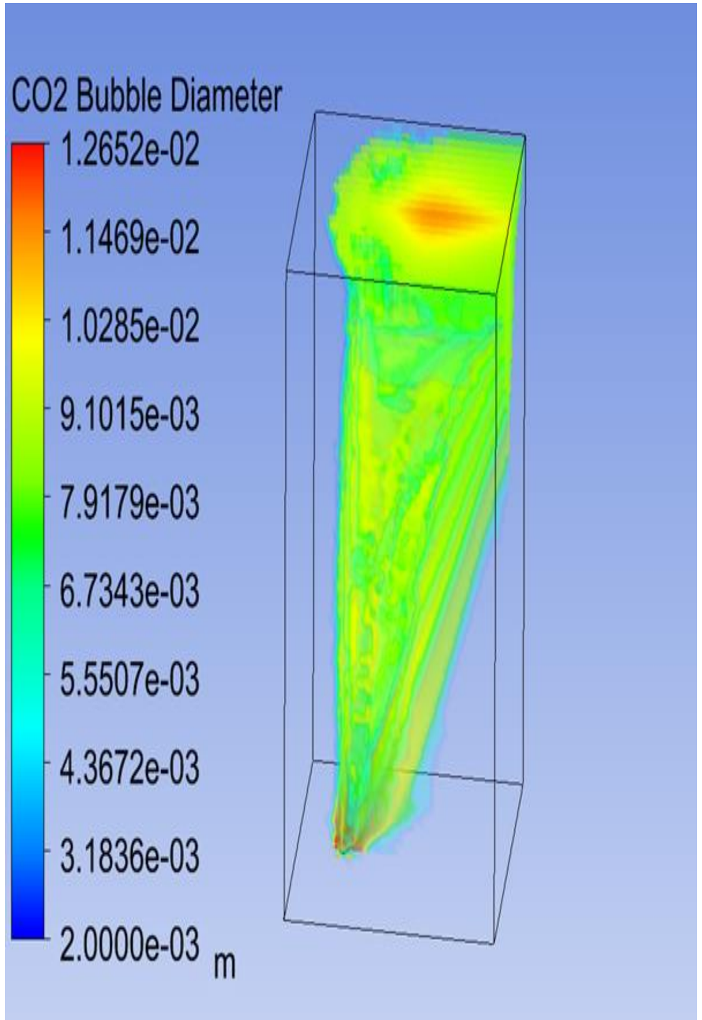


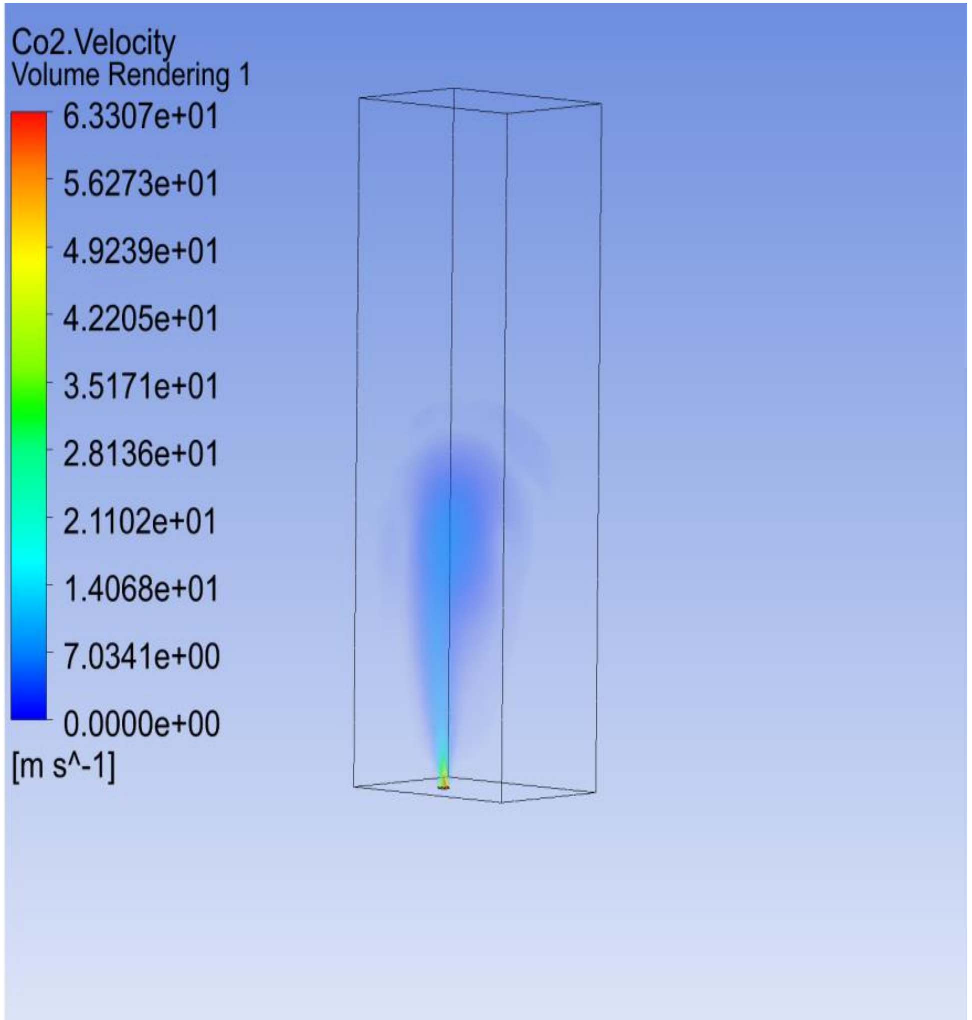


CO_2 Bubble Diameter (2-13 mm, 0.1 kg/s)

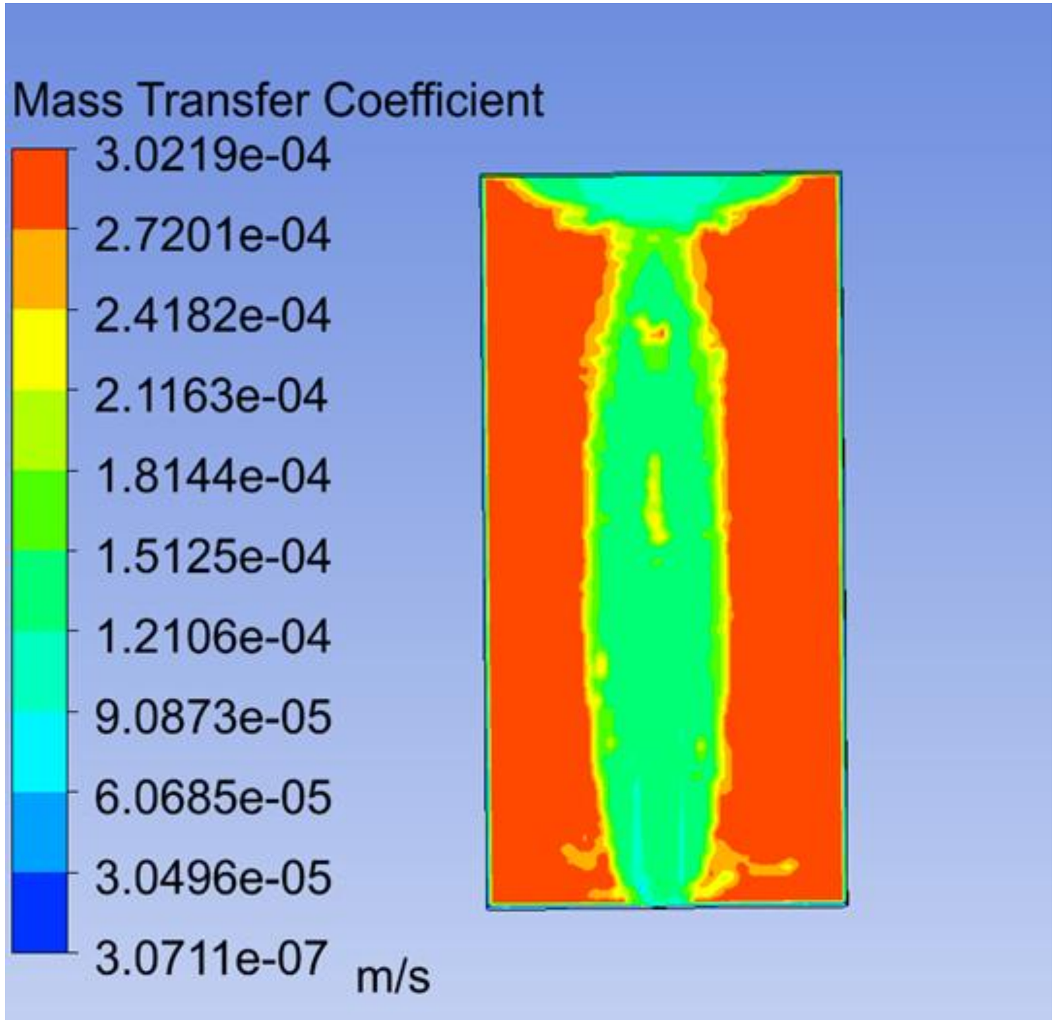
CO_2 Bubble velocity (7-63 m/s at simulation time 4 s, transient, 0.1 kg/s).

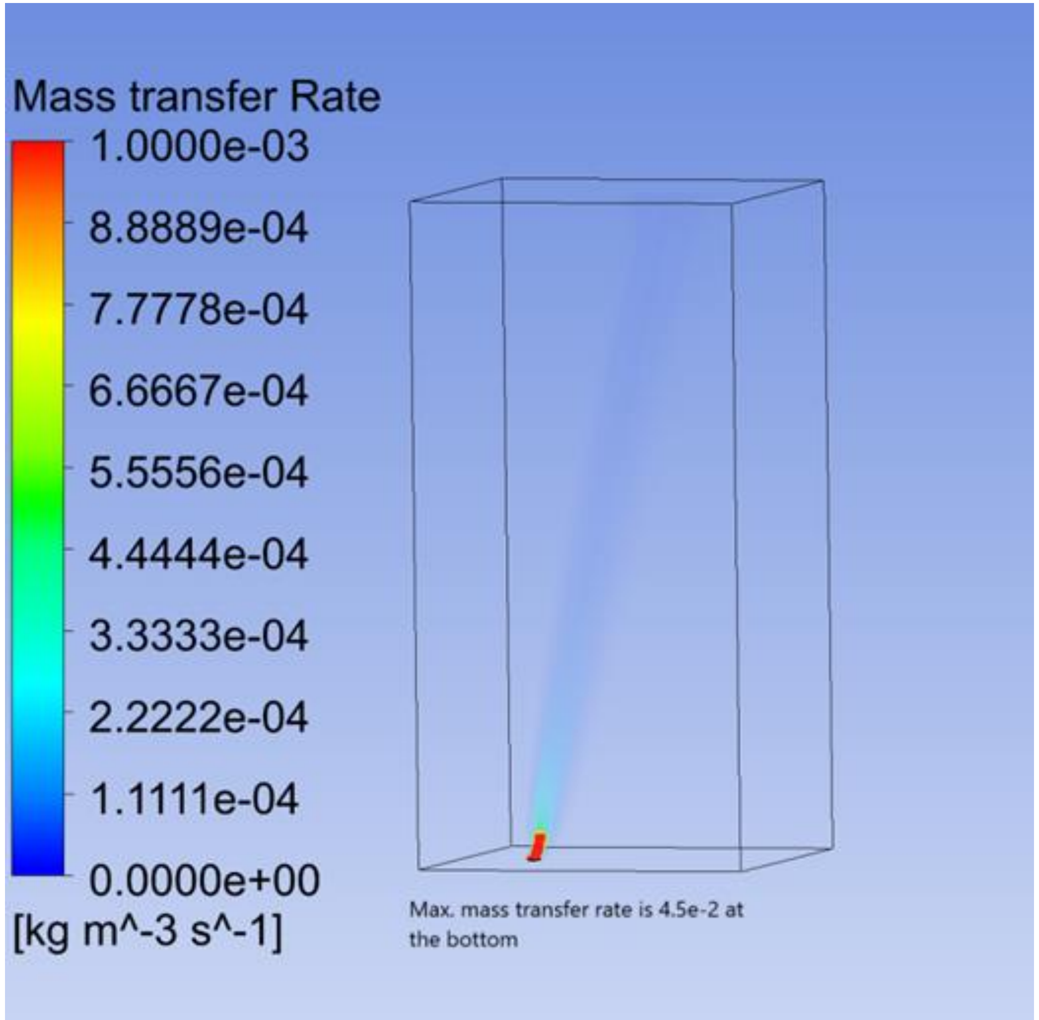




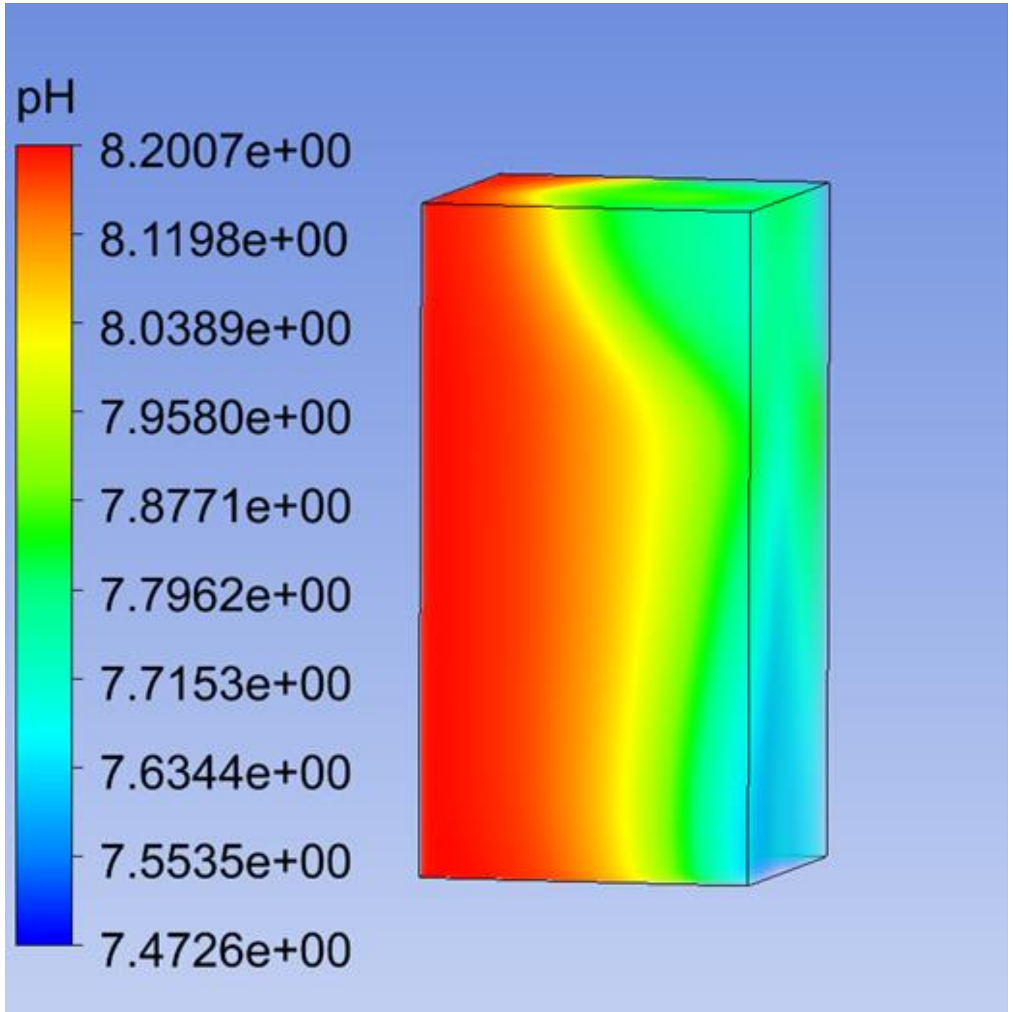


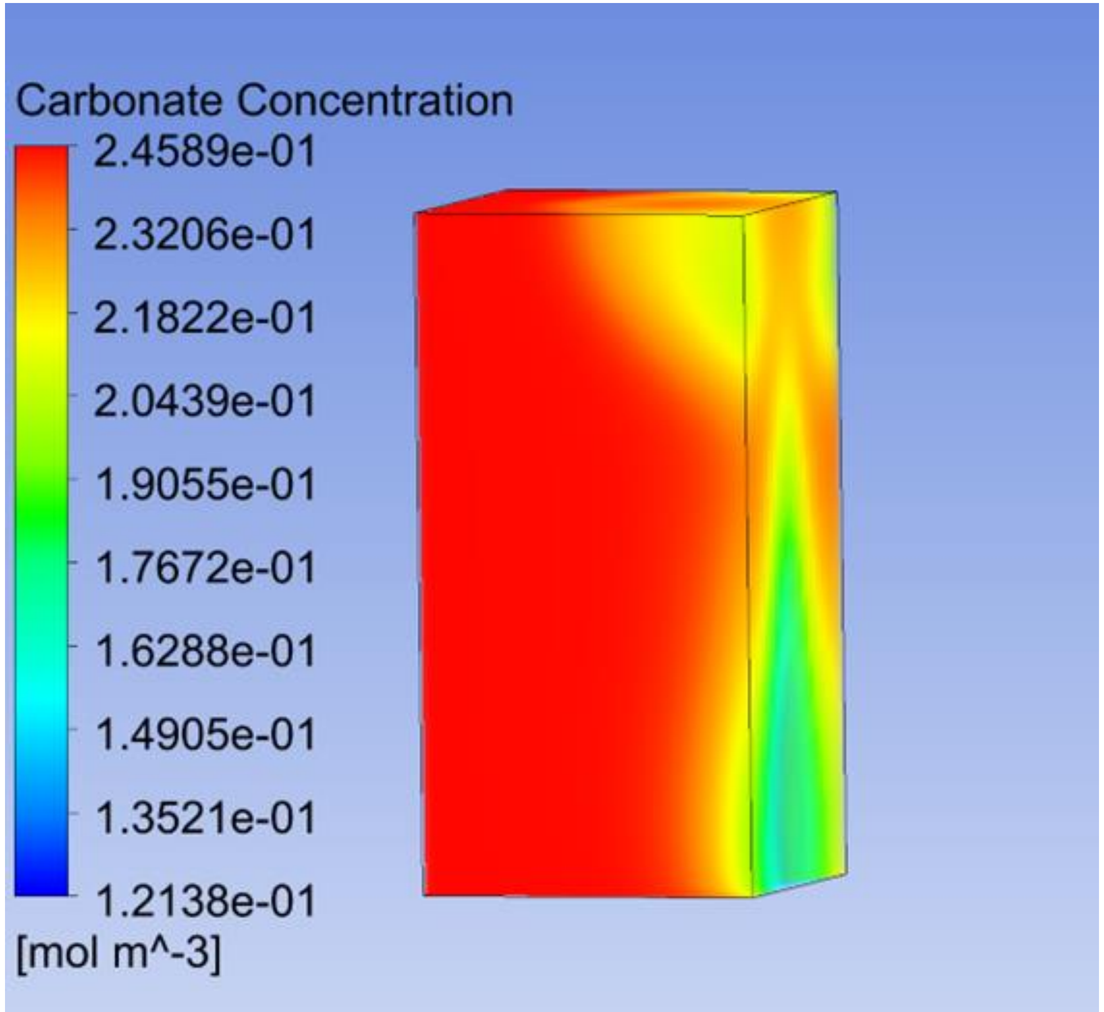
Mass Transfer Coefficient & Mass Transfer Rate (0.1 kg/s)



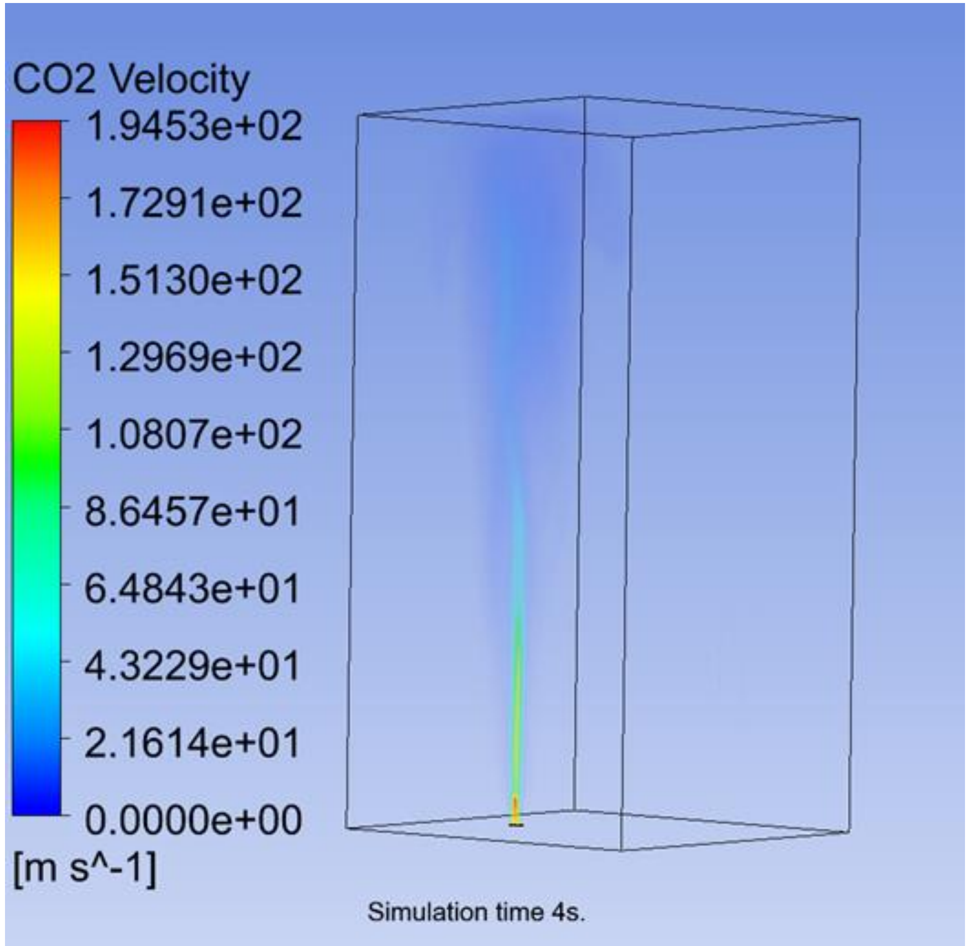


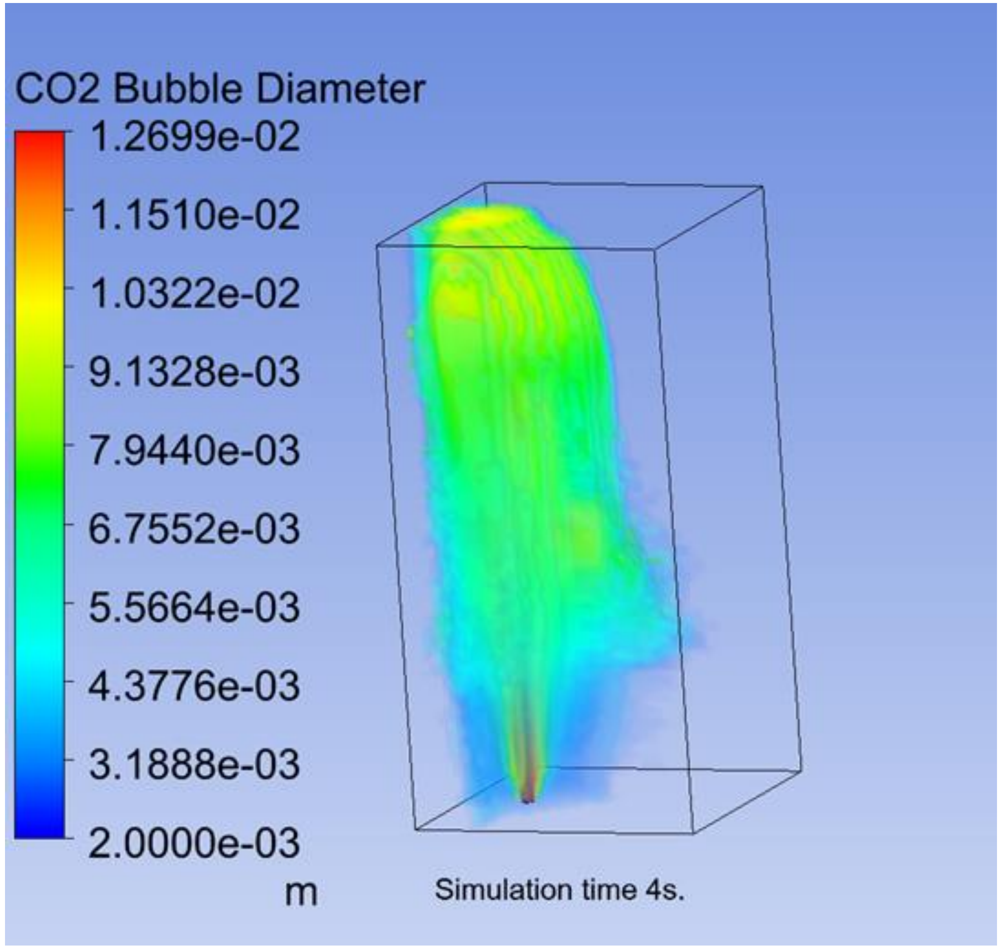
pH and Carbonate Concentration (0.1 kg/s)





Source @ 20 m depth at 35 kg/s





Speed 194 - < 22 m/s

Bubble size 3-13 mm

Results between Oldenburg and Pan (2020) and this Study at 20m water depth & 35 kg/s release rate

Factors to Compare	Oldenburg and Pan (2020) Study	CFD Simulation
Release	35 Kg/s	35Kg/s
CO_2 absorbed	26%	3%
Time of Plume to Reach Surface	0.5s	0.45s
Bubble Diameter Average (Log mean)	0.0005 m	0.005 m
Average Mass Transfer Coefficient	0.0001 m/s	.00016 m/s
Hole Diameter	2 in	16 in
Orifice Pressure	4 MPa	0.3 MPa

- Mass transfer rate per plume volume $(1/V)*(dm/dt)=k_L*a*(C_s-C_b)$
    - Where k_L is the mass transfer coeff. in m/s, *a* is specific surface in m^2/m^3, and C_s and C_b represent CO_2 conc. at the CO_2 bubble surface and the bulk seawater
- **POSSIBLE CAUSES OF DISCREPANCY**
- Bubble sizes are 10 times smaller in Oldenburg & Pan's work (**Hole size, Orifice pressure, jet speed, and others?)**
- No chemical reactions are used in Oldenburg and Pan; rather, TAMOC's simple mass conservation approach to decrease local CO_2 gradient as bubbles dissolve is used in Oldenburg & Pan

Conclusion

- Transient, multi-phase 3-D CFD simulations with mass transfer and CO2 neutralization reactions considered were performed on hypothetical CO2 releases (0.1 kg/s and 35 kg/s) from a High Island 10L injection well (It's challenging with convergence issues!).
- Model has been validated with QICS CO_2 bubble rise velocity data.
- CFD models predict : CO_2 bubble velocity, bubble diameter, mass transfer rate, and pH in the CO2 water column (plume).
- The main hazard appears to be CO_2 release to the atmosphere.
- pH change is rather limited (pH drops from 8.2 to 7.5 and $CO_3^{=}$ conc. drops from 0.25 – 0.12 mol/m^3).
- Absorption of CO_2 was much lower compared to Odenburg and Pan (2020)'s work (These are only preliminary results!)
  - ➢ The possible causes: hole diameter, orifice pressure, bubble size, and bulk CO_2 concentration.

Future Work

- Extend CO_2 bubble bin size range in Population Balance Model
- Calc. pCO_2 from pH
- Sensitivity Analysis
  - Orifice P (0.3 MPa - 4 MPa)
  - Hole size (2 -16 in)
  - Water Depth (10m – 100 m)
  - Current Speed (0.03 - 1.4m/s)

Acknowledgement

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Questions?