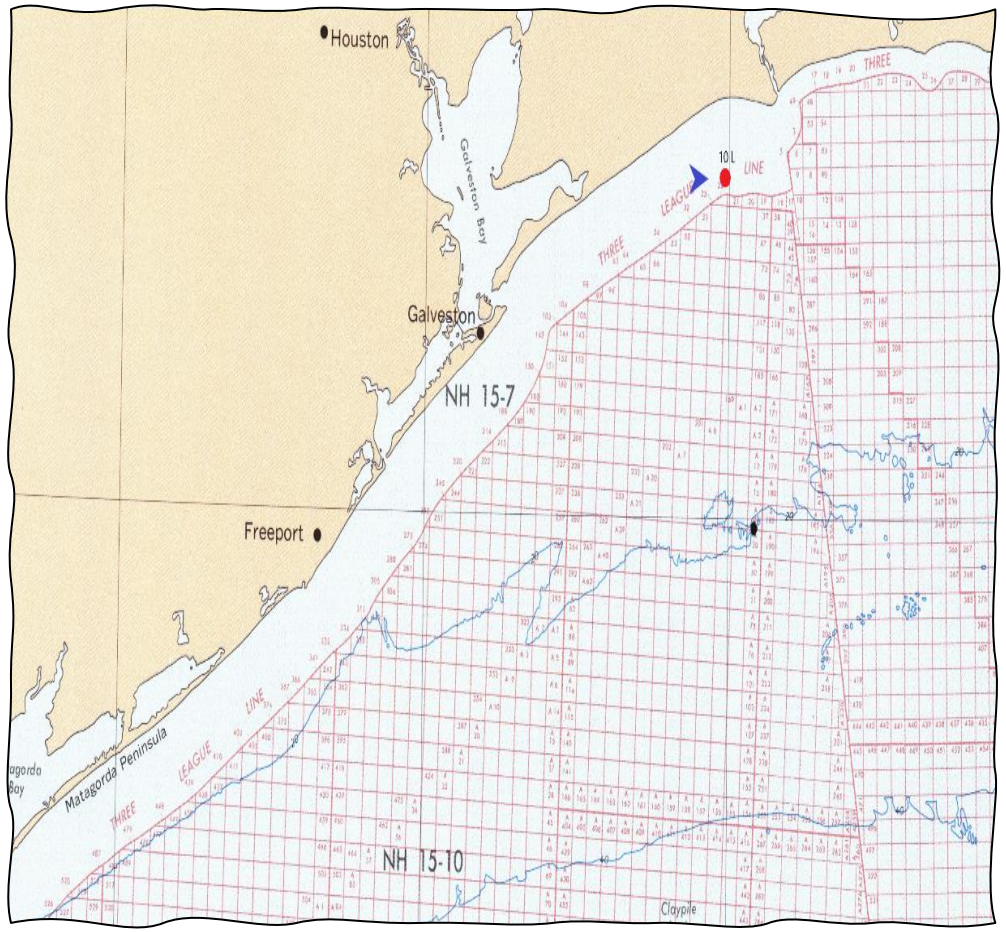
Subtask 4.1.5 Pipeline MVA
3-D CFD Modeling of Subsea CO_2 Pipeline Leaks

Vinayak Babu Rajan and Daniel Chen, Dan F. Smith Dept. Chem. & Bio. Eng., Lamar University, Beaumont, TX

GoMCarb Annual Meeting, April 7th, 2023

Problem Statement



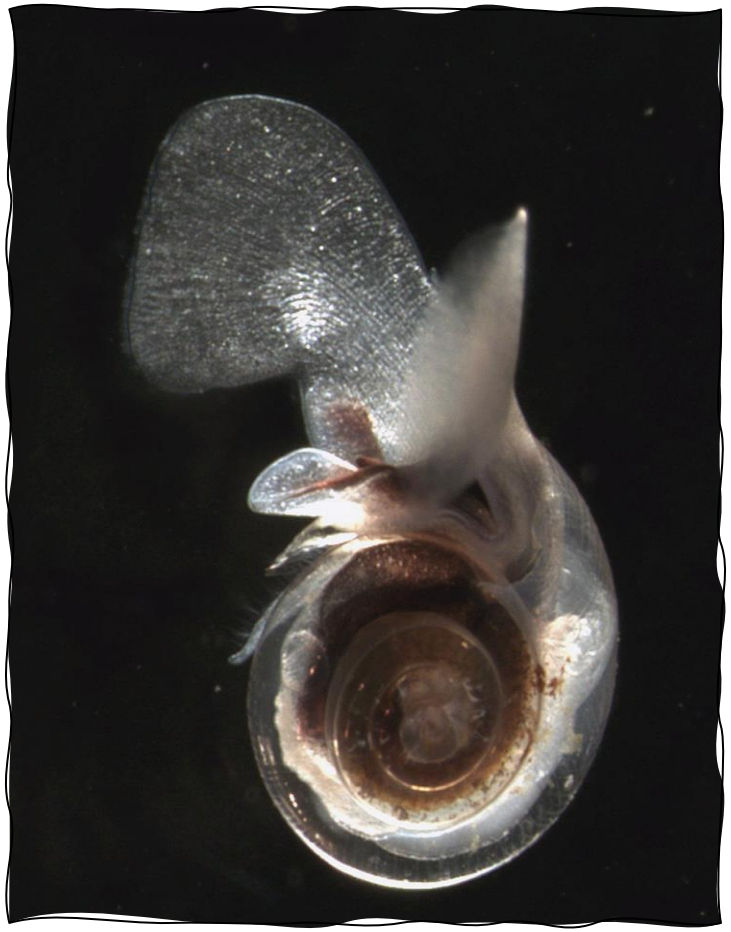
- A CO_2 leak from the offshore reservoir (High Island 10L) might threaten the survival of many marine animals, notably calcifying ones like oysters and corals.
- A geological formation suitable for CO_2 storage has been reported in the state of Texas (Ramirez, 2019). The High Island 10-L is a depleted oil and gas reservoir found off the coast of Jefferson County in the Gulf of Mexico.
- High Island 10L is located along the Texas coast at a sea depth of 10 to 20 meters, according to the barometric map.
- The goal is to use ANSYS Fluent to simulate the hydrodynamics and kinetics of CO_2 leaks into the water column from a High Island 10L well.

CO_2 Chemistry in Seawater

Acidic Mechanism: $CO_2 + H_2O \rightleftharpoons H_2CO_3 \rightleftharpoons H^+ + HCO_3^- \rightleftharpoons 2H^+ + CO_3^{2-}$

- Reactions shift to the right as the seawater absorbs more carbon dioxide, leading to an increase in bicarbonate and hydrogen ions, and decreasing pH.
- The reactions shift back to the left in the presence of seawater carbonate; this buffering prevents from rapid decrease in pH.

- Ocean is a CO_2 Sink !!! But Acidification poses a threat to the ocean's complex chemical equilibrium and marine life.



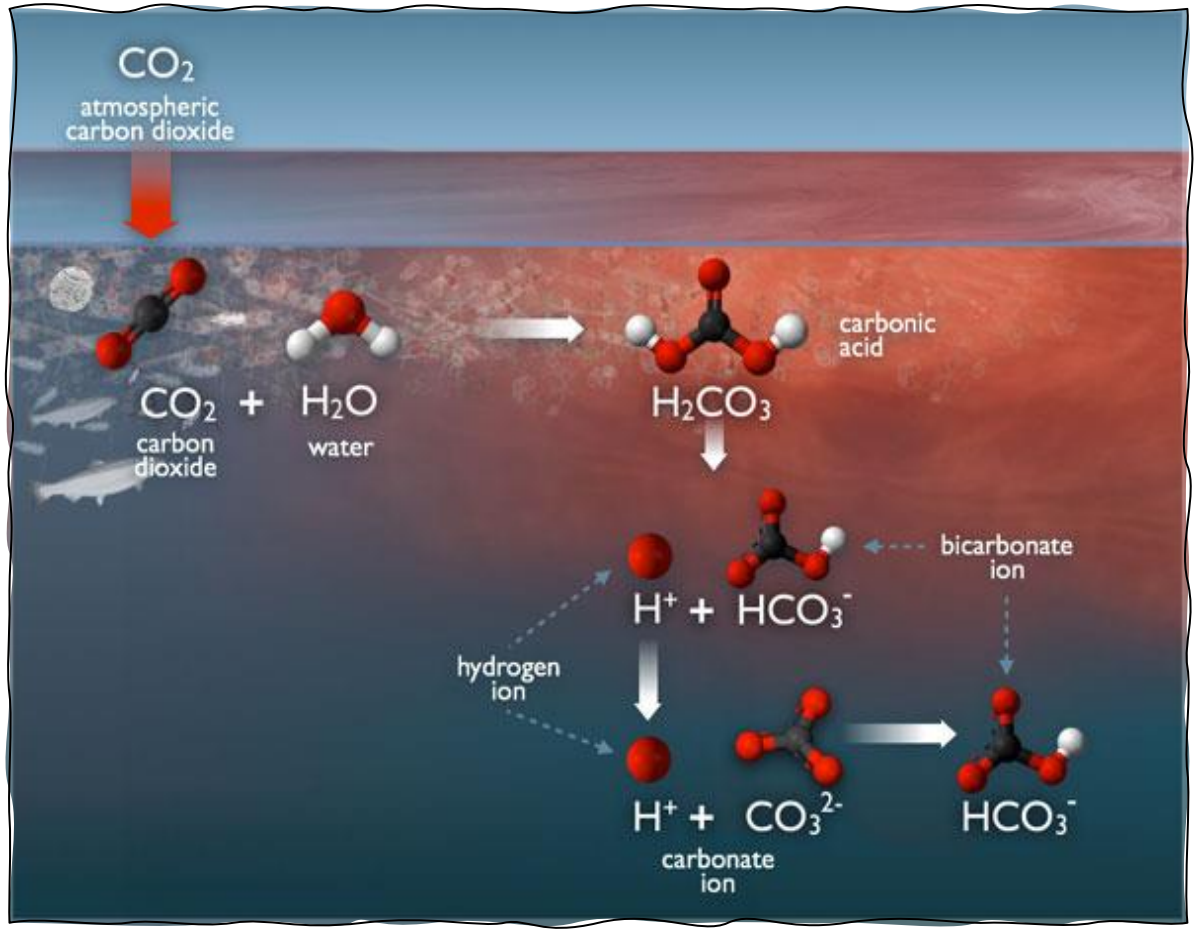
Seawater Composition Estimation

Initial Composition of seawater is estimated using pH, Salinity, $pCO_{2(initial)}$ and temperature data.

Seawater Species of Interest: CO_3^{2-}, HCO_3^-, $CO_{2(aq)}$, H^+, OH^-

Seawater chemical properties at High Island 10L

- pH = 8.2
- Salinity = 34.5 ppt
- $pCO_{2(initial)}$ = 360 µatm
- Temperature = 22.8 C
- Density = 1025 kg/m^3



Correlations used for coupling seawater properties to the simulation

Using Seawater chemical properties at High Island 10L : pH, Salinity, $pCO_{2(initial)}$ & Temperature

Compute:
Dissociation Constants &
Henry's Law Constant

Estimate:
$[CO_3^{2-}]$, $[HCO_3^-]$,
$[CO_{2(aq)}]$, $[H^+]$, $[OH^-]$

- Dissociation constant of carbonic acid in seawater on the basis mol/kg solution (K_1^{SW}) as a function of T

$H_2CO_3 \leftrightarrow H^+ + HCO_3^-$

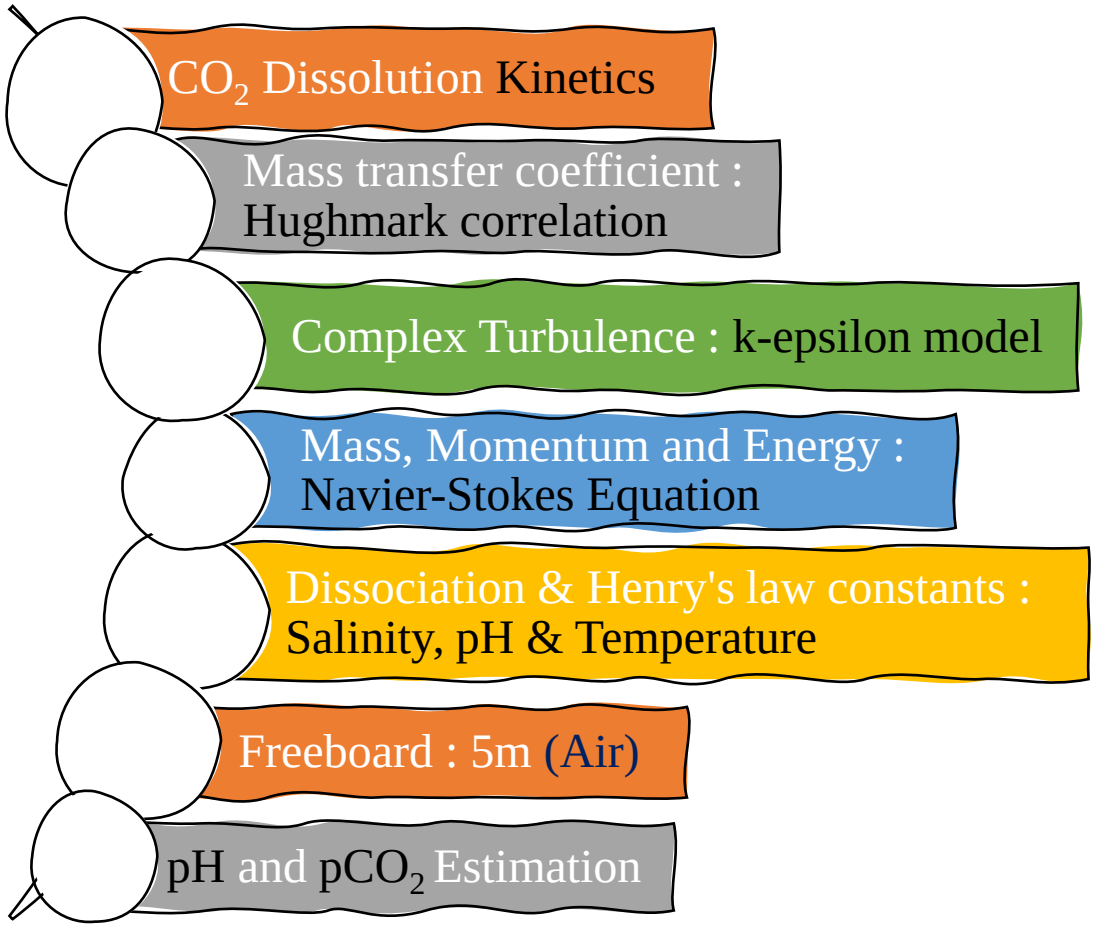
$$\ln K_1^{SW} = 2.18867 - \frac{2275.036}{T} - 1.468591 \ln T + \left(-0.138681 - \frac{9.33291}{T}\right) S^{0.5} + 0.0726483S - 0.00574938S^{1.5}$$

- Henry's Law Constant of CO_2 in pure water (mol/kg. atm)

$$\log H_{CO_2,W} = 108.3865 + 0.01985076 \cdot T - \frac{6919.53}{T} - 40.45154 \cdot \log T + \frac{669365}{T^2}$$

- Henry's law coefficient of CO_2 in the seawater (mol/kg. atm) can be determined by
- $\log\left(\frac{H_{G,W}}{H_{G,Sw}}\right) = hI$

Eulerian Model coupled with CO_2 Dissolution Kinetics using Ansys Fluent



Kinetics:

$H_2O + CO_{2(aq)} \leftrightarrow H_2CO_3$

$k_f = 6*10^{-2}\ s^{-1}$

$k_r = 2*10\ s^{-1}$

$H_2CO_3 \leftrightarrow H^+ + HCO_3^-$

$k_f = 1*10^{7}\ s^{-1}$

$k_r = 5*10^{10}\ M^{-1}\ s^{-1}$

$HCO_3^- \leftrightarrow H^+ + CO_3^{-2}$

$k_f = 3\ s^{-1}$

$k_r = 5*10^{10}\ M^{-1}\ s^{-1}$

Validation Study - QICS

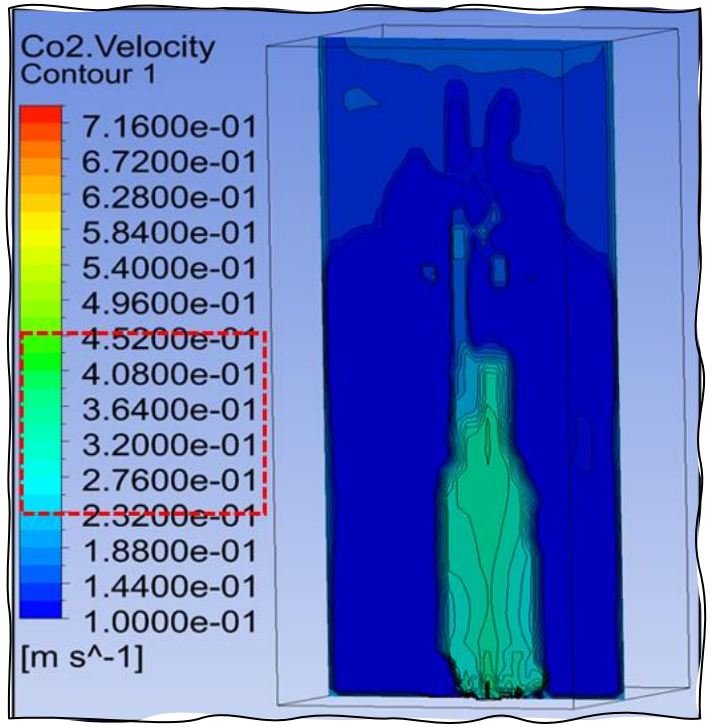


Fig : QICS Simulation

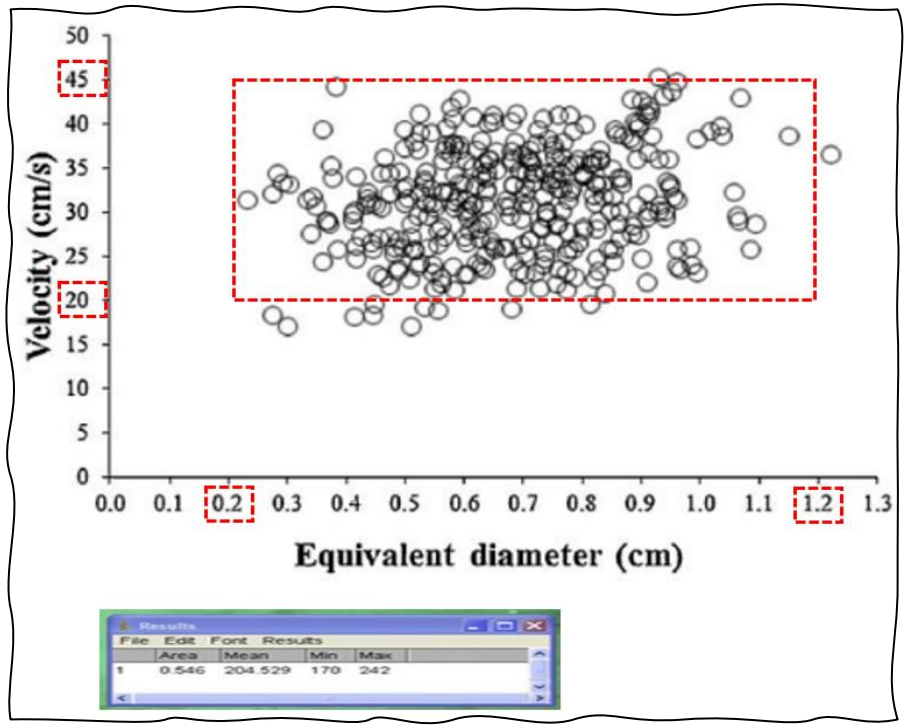


Fig : QICS Experiment (Sellami et al, 2015)

The velocity of bubbles in our simulation (3-D) agrees well with QICS experiment velocity measurements.

- Simulation Bubble Velocity : **24-36 cm/s**
- QICS Experiment Bubble Velocity : **20 – 45 cm/s**

Validated results used for High Island 10L

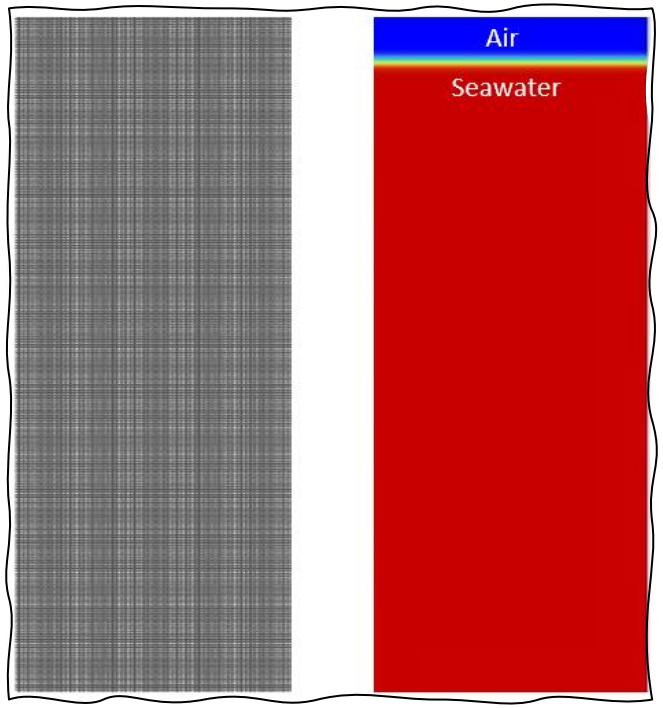


Fig : Meshing & Air-Water Patching

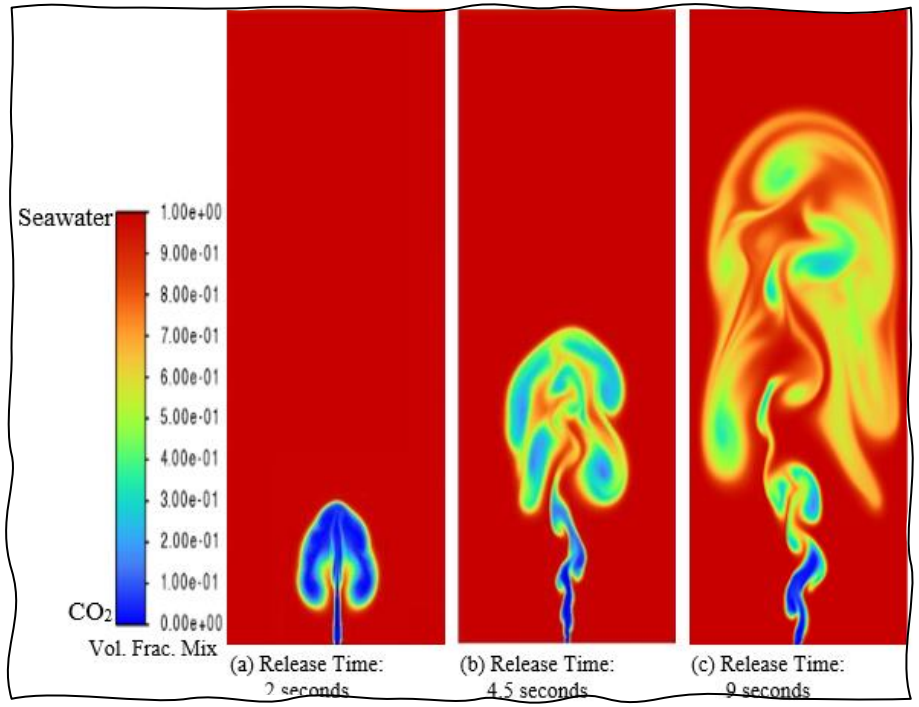
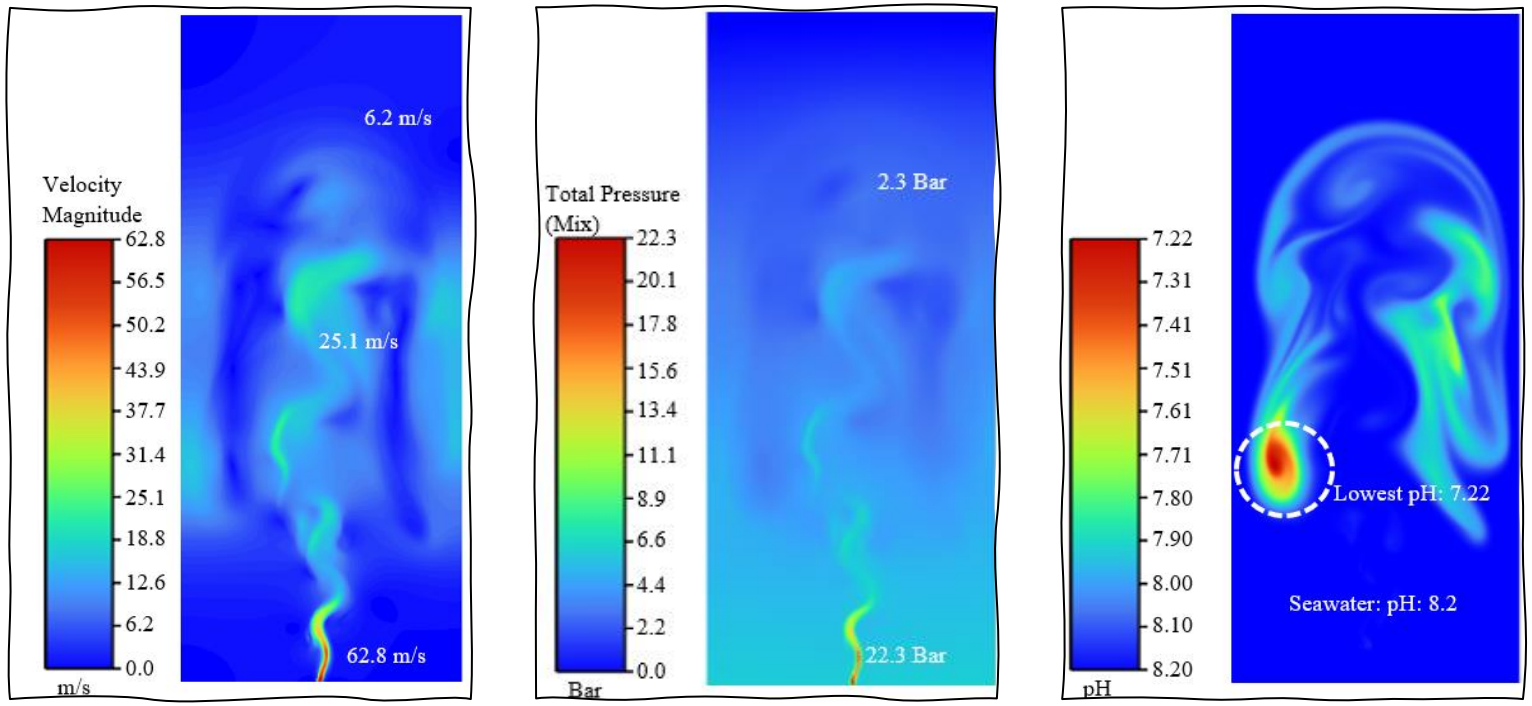


Fig : Volume Fraction of Mix at Release Time = 2, 4.5 & 9 sec's

- Transient, multi-phase, CFD simulation including mass transfer and CO_2 reactions were performed.
- Time step of 0.001s.
- Leakage hole size of 2 in.
- Leakage flowrate of 35 kg/s.
- Water column depth 50 m and Air freeboard of 5m.

CFD Contours



- At 9 seconds; Plume Height = 48m, Plume Width =16m.
- The lowest pH obtained in simulation is of 7.22 after 9 seconds of leak.
- Length scale for transitioning from jet to buoyant plume is around 3-4 m, in 50m water column case

Fig : CFD Contours for Velocity, Pressure and pH change(35 kg/s, High Island 10L)

Conclusions

- CO_2 dissolution kinetics is considered.
- Mass transfer coefficient is estimated by the Hughmark correlation (not constant).
- The dependence of Henry's law constant on seawater salinity is considered.
- Meshes in the CO_2 plume are refined (using structured mesh)
- Model has been verified using CO_2 rise velocity data from the QICS experiment.
- CFD Model predicts: Hydrodynamics(Plume velocity, rise time, height and width) & Kinetics (pH & pCO_2)

Acknowledgement

- Special thanks are due to Curtis Oldenburg at the Lawrence Berkeley National Laboratory (LBL) for useful discussions and Margaret A Murakami, Susan D. Horvoka, and Ramon H. Trevino at the University of Texas, Austin (UT) for providing marine environmental data near 10L and 24L lease blocks in Texas State Waters and other communications are acknowledged.
- Financial support from “Offshore Gulf of Mexico Partnership for Carbon Storage--Resources and Technology Development GoMCarb," Department of Energy Offshore Gulf of Mexico; UT Prime Award # DE-FE0031558, LU Subaward UTA18-000644, $153,123, 4/1/2018-3/31/2023” is greatly acknowledged.