CAAP Quarterly Report

June 26, 2023

Project Name: Determination of Potential Impact Radius for CO_2 Pipelines using Machine Learning Approach

Contract Number: 693JK32250011CAAP

Prime University: Texas A&M University

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Reporting Period: 3/27/2023 – 6/26/2023

Project Activities for Reporting Period:

The following relevant tasks in the proposal have been completed:

- Collected more publications related to CO_2 dispersion experiments and CO_2 CFD simulations for the review paper.
- Conducted literature review to identify the widely applied numeric simulation setup for improvement of CO_2 dispersion modeling in Ansys Fluent:
    - Model
        - Energy model
        - Viscous model: SST k-ω turbulence model
        - Species model: Species transport (CO_2 and air)
    - Boundary conditions:
        - Wind inlet: Velocity inlet (wind profile power law)
        - CO_2 source: Mass flow rate (CO_2 evaporates at 1 atm and 194 K)
        - Outlet: Pressure outlet
        - Ground: Wall
        - Top and sides: Symmetry
- With the setup mentioned above to perform CFD simulations of CO_2 dispersion and validated the results against full-scale CO_2 release experiments, CO2PIPETRANS JIP project. More details are provided in the Appendix.
- Conducted a systematic literature review to summarize common CO_2 pipeline operating conditions, locations, and corresponding geometries in the US. More details are provided in the Appendix.

Project Financial Activities Incurred during the Reporting Period:

Based on the proposed budget, the cost is broken down into two parts:

- Efforts from the PI Dr. Wang for about 0.25 month.
- Efforts and work by graduate students, Chi-Yang Li and Jazmine Aiya D. Marquez, totally for about 3 months for each of them.

Project Activities with Cost Share Partners:

Dr. Wang's time and efforts (0.25 month) in this quarterly period are used as cost share. He devoted his time to supervise the graduate students, review all paperwork, travel to Orlando to give a presentation in the PRCI CO_2 Workshop, and prepare the progress report.

Project Activities with External Partners:

Dr. Wang was invited by Tom Marlow from PRCI to present this project idea in the PRCI CO_2 Workshop in Orlando, June 7-9, 2023. The presentation was well-received in the workshop. One main comment from the workshop group is how to validate the developed tool. When we submitted the proposal in 2022, we encountered challenges in conducting extensive large-scale testing and gathering experimental data. Consequently, we made the decision to exclude this task from the proposal.

Following in-depth discussions with esteemed colleagues and industry experts during the workshop, including Bob Smith from DOE, Rick Noecker from Exxon Mobil, Kevin Dahncke and Steve Bevers from Denbury, and Tom Marlow from PRCI, a unanimous consensus emerged that validating the machine learning tool is imperative. In this regard, Denbury graciously offered to contribute valuable data and extend necessary support for this ongoing study beyond current scope of work.

I will engage in further discussions with Denbury regarding the project. Bob Smith has informed me that the initial award for this project was granted for a duration of two years. However, considering that typical CAAP projects span three years, I am currently exploring the feasibility of extending the project for an additional year for the validation study.

Potential Project Risks:

For the future parametric study using Ansys Fluent, incorporating terrain information has increased the computation time. We anticipate that performing hundreds of CFD simulations in the future will require a significant amount of time. I have assigned two PhD students to work on this project to accelerate the project.

Future Project Work:

- Continue to write the review paper, titled "***CO_2 pipelines release and dispersion: a review***".
- Perform parametric studies at HPRC for all dispersion scenarios by using Ansys Fluent with the numeric simulation setup mentioned above. For other parameters of concern, besides the 5 categories of terrains, the variables for pipeline characteristics and weather conditions are as Table 1.

Table 1. The variables for pipeline characteristics and weather conditions.

	Variable	High	Medium	Low
Pipeline characteristics	pressure (MPa)	20	10	1
	diameter (inch)	30	16	4
	flow rate (MMcfd)	1300	590	30
Weather conditions	wind speed (mph)	50	25	1
	temperature (°F)	100	60	20

- Construct the database for the PIR for CO_2 pipelines dispersion based on the simulation results with the setup above.

Potential Impacts to Pipeline Safety:

- The variables for pipeline characteristics and weather conditions cover the upper limits and lower limits of the current industrial practices; therefore, the machine learning model is believed to have accurate predictions for other pipelines in the range.

Appendix

1. CFD Modeling Discussion

Because we assume CO_2 evaporates immediately after release in the simulation, there is no liquid CO_2 near the source; therefore, near-field is believed to have a little higher error. Meanwhile, the far-field is believed to have good performance, because the liquid CO_2 have little influence for the far-field CO_2 concentration. The comparison of experimental results and current simulation results is shown in Table 22. Additionally, the mesh is shown in Figure 1 and the CO_2 concentration contours as a point at 5 m is shown in Figure 2.

Table 2. The comparison of CO_2 concentrations between experiments and simulations.

Downstream distance from source (m)	Highest molar fraction (%) Experiment	Simulation	Error (%)
5	≒21	16.65	-20
15	≒4.2	4.09	-3
40	≒0.9	0.82	-9

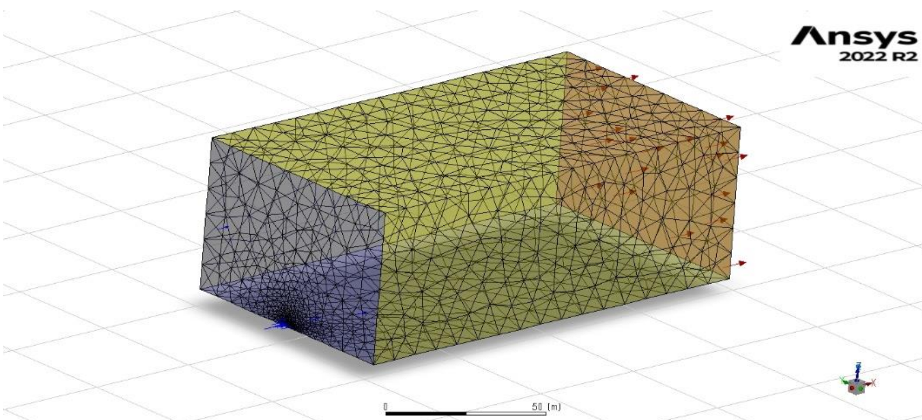

Figure 1. Mesh for the geometry.

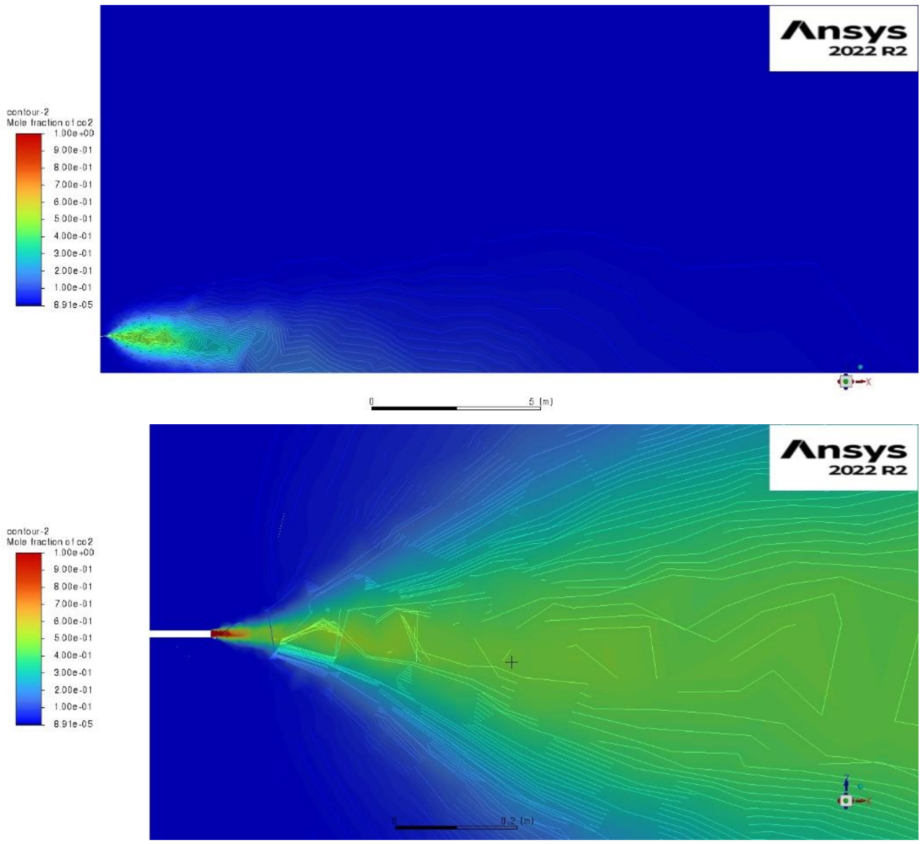

Figure 2. CO_2 concentration contours at distance of 5 m.

2. Terrain Information

The terrains where CO_2 pipelines might locate could be roughly classified into 5 categories, including plain, moderate slope, steep slope, valley with moderate slope, and valley with steep slope. To simulate the CO_2 dispersion with real terrains, the geometries in Monticello Mississippi (Figure 3), Raton New Mexico (Figure 4), Walsenburg Colorado (Figure 5), Vernal Utah (Figure 6), and Calistoga California (Figure 7) were chosen to represent these 5 categories.

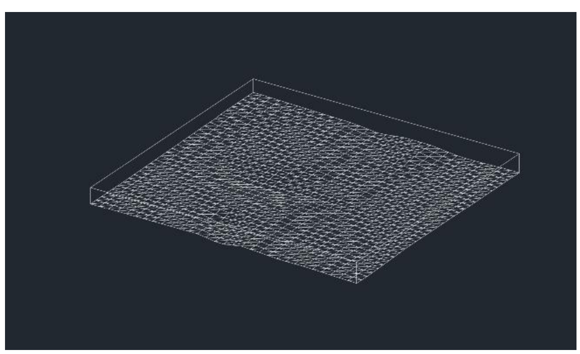

Figure 3. Monticello Mississippi

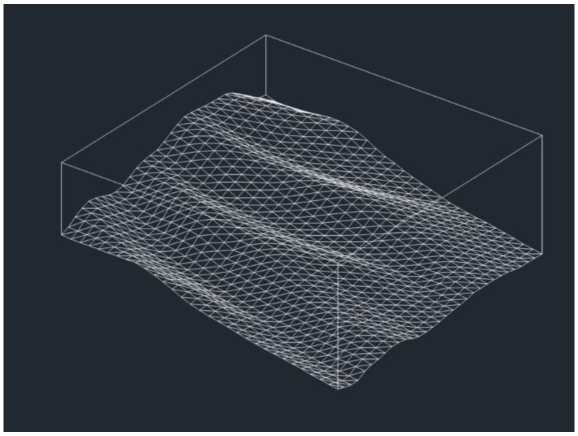

Figure 4. Raton New Mexico

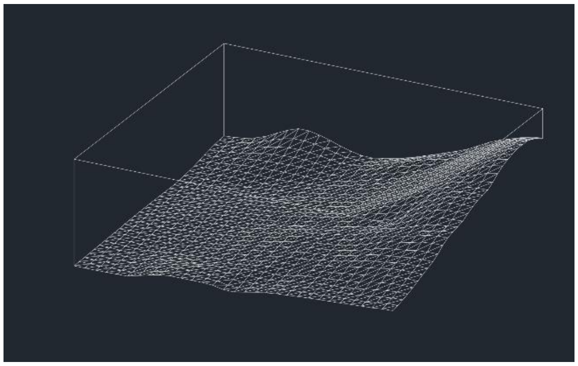

Figure 5. Walsenburg Colorado

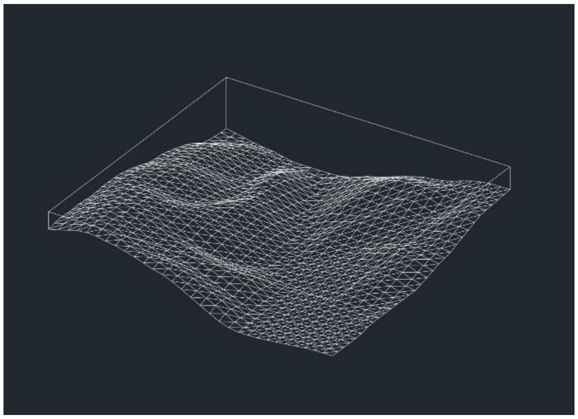

Figure 6. Vernal Utah

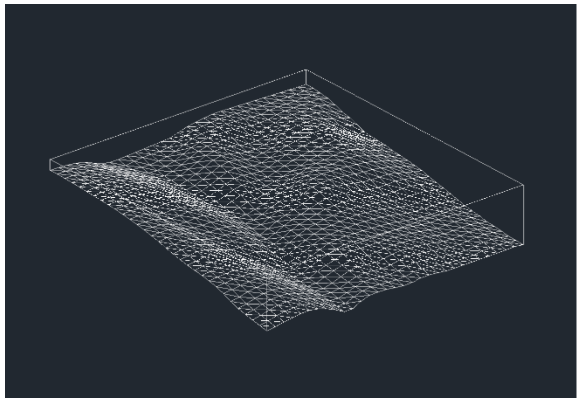

Figure 7. Calistoga California