CAAP Quarterly Report

December 22, 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: 9/27/2023 – 12/26/2023

Project Activities for Reporting Period:

The following relevant tasks in the proposal have been completed:

- Adjusted the procedure for calculating the CO_2 behavior in the near field based on assumption of isentropic flow relationships. More details are provided in the Appendix.
- Used Ansys Fluent to conduct CFD simulation for the 28 cases based on the results of the calculation for the near field. More details are provided in the Appendix.
- Held the second TAP meeting with PHMSA representatives.
- Present in the 2023 PHMSA R&D Forum.
- The review paper of CO2 pipeline release and dispersion was officially published in the *Journal of Loss Prevention in the Process Industries*.

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, organize the second TAP meeting, travel to Washington DC to attend PHMSA R&D Forum, and prepare the progress report.

Project Activities with External Partners:

During the 2023 PHMSA R&D Forum, Dr. Wang discussed the intention to participate in the ongoing planning of the **Skylark Joint Industry Project (JIP)** with Simon Gant (Project Leader, UK HSE) and Mary McDaniel. Simon Gant expressed agreement with TAMU/PHMSA involvement, particularly in the Computational Fluid Dynamics (CFD) modeling component. Mary McDaniel also conveyed strong interest and support for this initiative. Subsequently, a meeting took place on Teams with PHMSA staff (Nusnin Akter, Ashley Kroon, Basim Bacenty) and Dr. Wang to explore the potential extension of the CAAP project, including additional tasks within the Skylark JIP framework. On December 6, 2023, Dr. Wang officially submitted a statement of work, along with a budget and budget justification, to PHMSA for their consideration in joining the Skylark JIP.

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:

- Continuously perform parametric studies at TAMU HPRC for all dispersion scenarios by using Ansys Fluent with the numeric simulation setup with the calculation results. For other parameters of concern, besides the 5 categories of terrains, the variables for pipeline characteristics and weather conditions are as Table 1 (updated after recommendations from technical panel).

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)	25	14	3
	temperature (°F)	100	60	0

- Continuously expand the database for the PIR for CO_2 pipelines dispersion based on the simulation results with the setup above.
- Perform parametric studies to search for the suitable machine learning techniques and corresponding hyper-parameters for the machine-learning model.

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 CO_2 pipelines in the range.

Appendix

1. Calculating the CO_2 behavior in the near field

As mentioned in the previous report, the 10 times of the distance of Mach disc (x_m) from the pipe could be considered as the distance of near field.

$$x_m = 0.6455 \times d_e \times \sqrt{\frac{P_0}{P_a}}$$

Where d_e is the diameter of the nozzle exit, P_0 is the stagnation pressure, and P_a is the ambient pressure.

Then, we could calculate the velocity at the end of the near field based on the assumptions of no entrainment of ambient fluid, isentropic flow relationships, and constant pressure at the release point of rupture pipeline.

$$V_{CO_2} = V_0 \left\{ C_D + \frac{\left[1 - \frac{P_a}{P_0} \times \left(\frac{2}{\gamma + 1}\right)^{\frac{-\gamma}{\gamma-1}}\right]}{\gamma C_D} \right\}$$

Where V_{CO_2} is the velocity of CO_2 in the atmosphere, V_0 is the velocity in the pipeline, C_D (1 for the well-rounded nozzle) is the volume discharge coefficient, γ (1.30 for CO_2) is the ratio of the heat capacities.

In our previous simulations on the near field, huge amount of air entrained and occupied nearly 70% weight at the end of the near field, due to the significant pressure drops for the CO_2 pipelines from pipeline to atmosphere. We assumed the fluid composition at the end of near field are 30% CO_2 and 70% air. Therefore, we could obtain the velocity of fluid as below.

$$V_a = V_{wind} \times 0.7 + V_{CO_2} \times 0.3$$

Where V_a is the velocity of fluid in the atmosphere, and V_{wind} is the velocity of wind.

Because the pressure in the atmosphere is relatively low (1 atm), we could derive the cross-sectional area of the fluid based on the ideal gas law and the conservation of mass equation.

Additionally, because the scenario of concern is that CO_2 release from both ends of the ruptured pipeline, we apply twice the mass flow rate for the simulations. Due to the velocity of the fluid is a critical factor for the dispersion, we apply twice the release cross-sectional area of the fluid with the velocity obtained above to run the simulations.

Consequently, we could use the composition, velocity, and area to represent the behavior of near field and use Ansys Fluent to simulate the dispersion in the far field.

According to Table 1, take the situation of 1 MPa gauge pressure, 30 inch pipeline diameter, 1300 mmcfd mass flow rate, 3 mph wind speed, and 100 °F ambient temperature as an example. We could calculate the velocity of fluid, the distance of near field, and the radius of cross-sectional area of fluid, as 2.25 meter per second, 49.11 meter, and 24.32 meter, respectively.

2. Simulation results for 28 cases

With the information of the calculations on the near field, we could create suitable geometry and use the necessary factors for the subsequent CFD simulation on Ansys Fluent. Then, we ran simulations for 28 cases and the results are shown in Table 2.

For the situation of 1 MPa gauge pressure, 30 inch pipeline diameter, 1300 MMcfd mass flow rate, 3 mph wind speed, and 100 °F ambient temperature, we simulated the CO_2 dispersion over the plain geometry (Figure 1). The contour for CO_2 mole fraction on the top view and side view are shown in Figure 2 and Figure 3. Moreover, the CO_2 mole fraction dispersion profile is as Figure 4.

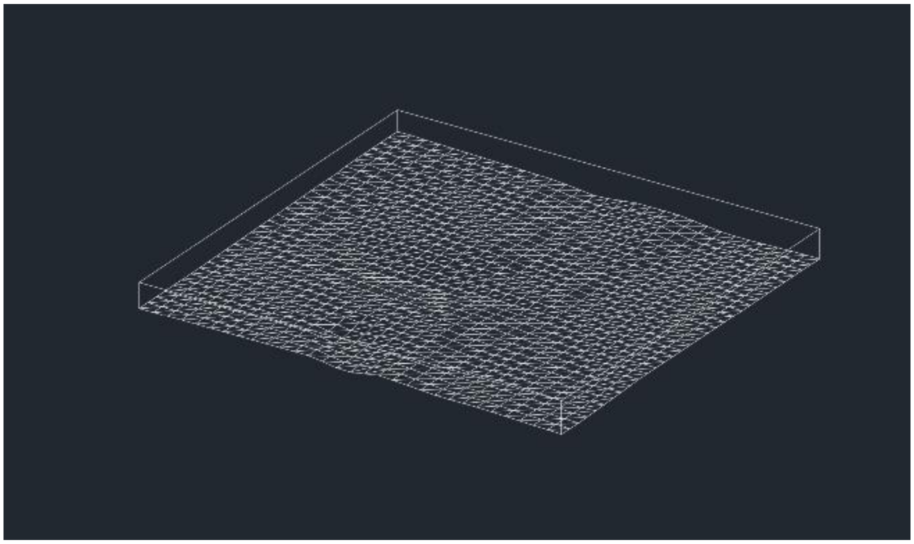

Figure 1. Plain (Monticello, Mississippi).

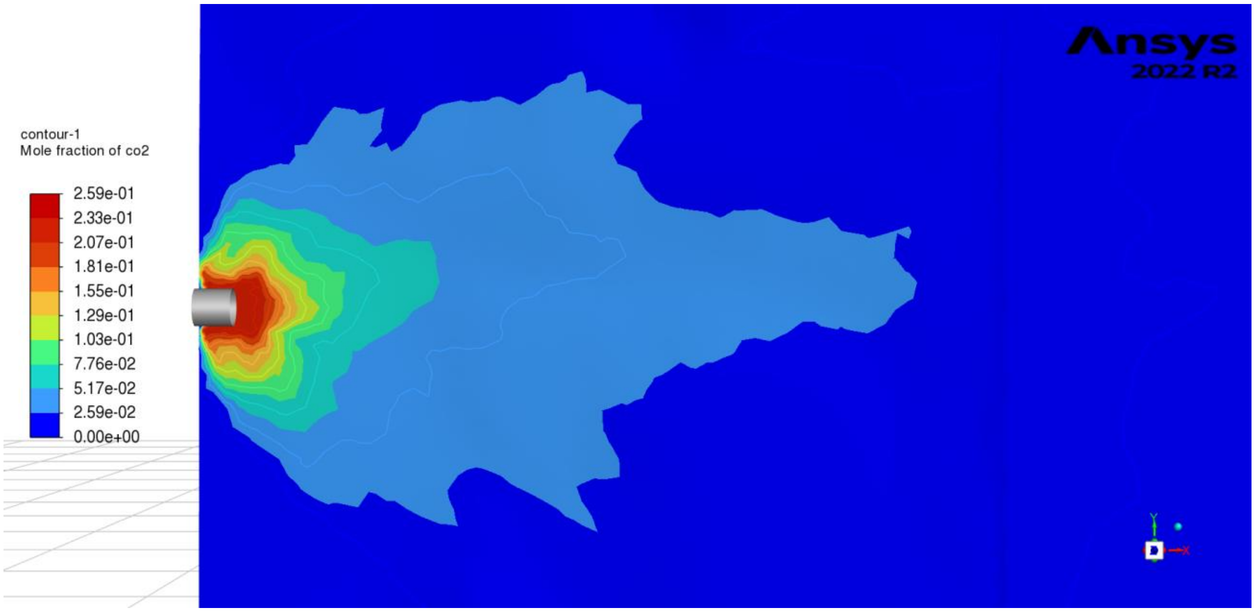

Figure 2. The contour for CO_2 mole fraction on the top view.

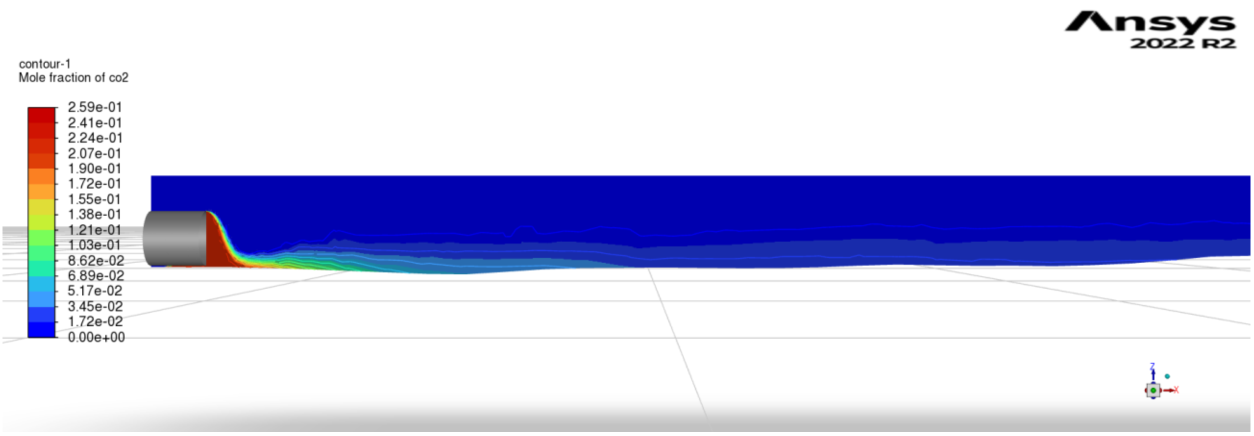

Figure 3. The contour for CO_2 mole fraction on the side view.

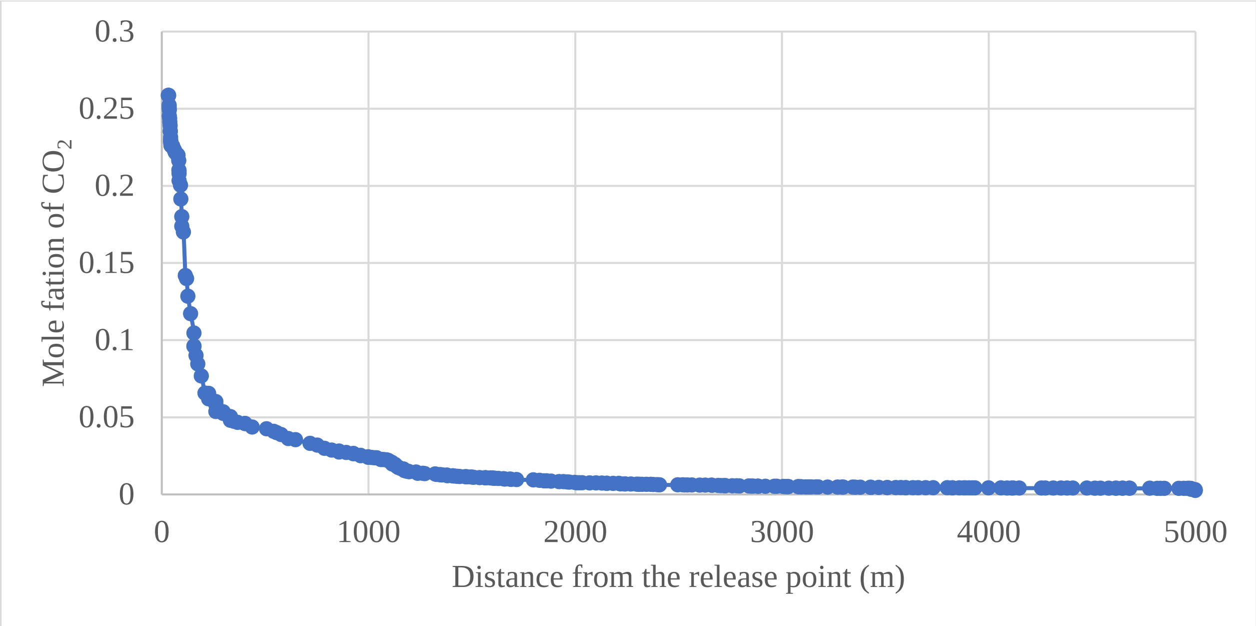

Figure 4. CO_2 mole fraction versus distance from the release point.

Table 2. Simulation results for 28 cases.

Geometry	gauge pressure (MPa)	diameter (inch)	flow rate (mmcfd)	wind speed (mph)	ambient temperature (°F)	Distance for 9% (m)	Distance for 4% (m)	Distance for 1% (m)
Plain (Monticello Mississippi)	10	30	1300	3	100	166.17	556.07	1657.27
	1	4	30	25	0	14.50	28.59	62.64
	1	4	30	14	0	14.78	31.19	81.18
	1	4	30	3	0	15.04	34.18	100.89
	1	4	30	25	60	14.50	28.59	62.67
	1	4	30	14	60	14.78	31.20	80.92
	1	4	30	25	100	14.49	28.84	55.57
	1	4	30	3	60	15.09	34.68	102.67
	1	4	30	14	100	14.77	31.37	79.99
	1	4	30	3	100	15.04	34.17	100.65
Hill with steep slope (Raton, New Mexico)	1	4	30	25	0	9.42	20.56	49.61
	1	4	30	14	0	9.55	22.56	60.38
	1	4	30	3	0	9.72	29.99	93.56
	1	4	30	25	60	9.42	20.51	49.74
	1	4	30	14	60	9.55	22.42	60.13
	1	4	30	25	100	9.42	20.50	49.80
	1	4	30	3	60	9.72	30.37	93.42
	1	4	30	14	100	9.55	22.56	60.36
	1	4	30	3	100	9.72	30.38	93.41
Valley with moderate slope (Vernal, Utah)	1	4	30	25	0	8.45	18.22	82.37
	1	4	30	14	0	8.57	18.78	85.53
	1	4	30	3	0	8.79	28.46	111.57
	1	4	30	25	60	8.44	18.18	82.60
	1	4	30	14	60	8.57	18.78	85.30
	1	4	30	25	100	8.45	18.22	82.49
	1	4	30	3	60	8.79	28.55	111.67
	1	4	30	14	100	8.57	18.78	85.39
	1	4	30	3	100	8.79	28.46	111.68