CAAP Quarterly Report

October 4, 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: 6/27/2023 – 9/26/2023

Project Activities for Reporting Period:

The following relevant tasks in the proposal have been completed:

- Published a review paper for CO_2 pipelines dispersion:
  C. Li, J.A.D. Marquez, P. Hu, Q. Wang, CO_2 pipelines release and dispersion: A review. *Journal of Loss Prevention in the Process Industries* **2023**, *85*, 105177.
- Adjusted the procedure for the simulation and validated the results against full-scale CO_2 release experiments, CO2PIPETRANS JIP project. More details are provided in the Appendix.
- Conducted simulations on two cases in practices. More details are provided in the Appendix.
- Held a meeting with technical panel and collected the recommendations for further study. 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 work, and prepare the progress report.

Project Activities with External Partners:

I continue the discussions with Denbury regarding the extension of project on 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*, much higher than we expected. One PhD student graduated and a *new PhD* joined the project. These factors cause some delays and we will require more time to finish this project. Although I have assigned two PhD students to work on this project to accelerate the project, a *no-cost extension* of this project is needed.

Future Project Work:

Perform parametric studies at TAMU 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 (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	12	1
	temperature (˚F)	100	60	0

- Create 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

According to the process of collecting for the review, separating the simulation scope to near-field stage and far-field stage is the widely used method on simulating the dispersion behavior from high pressure CO_2 pipelines (Figure 1). In near-field stage, we analyze the depressurization behavior from the pipe, while in far-field, we obtain the dispersion result in far-field stage.

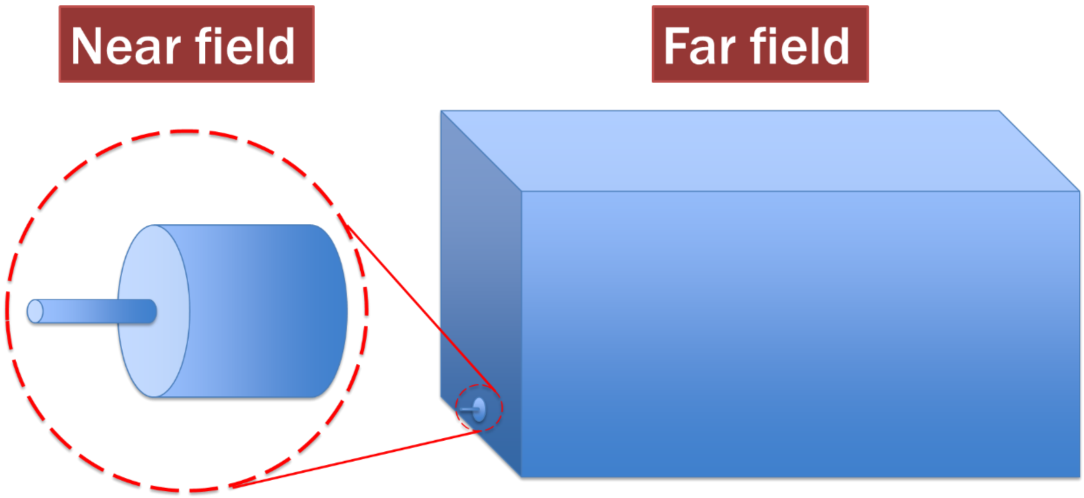

Figure 1. Near-field and far-field.

In the near-field stage, the pressure drops rapidly, while temperature reduces accordingly, and velocity increases promptly. Thus, the behavior in the near-field stage is complicated. In Ansys Fluent, as the Mach number exceed 0.3, the density-based solver (rather than pressure-based solver) is recommended to use. Therefore, we used the density-based solver for the near-field stage, and pressure-based solver for far-field stage. Furthermore, we applied very fine mesh to make sure the simulation could work and utilized 2-D axisymmetric model to simplify the calculation. Therefore, the geometry and mesh of the BP test 8 (15.74 MPa and 420.3 K) from CO2PIPETRANS JIP project is as Figure 2, and simulation results is as Figure 3.

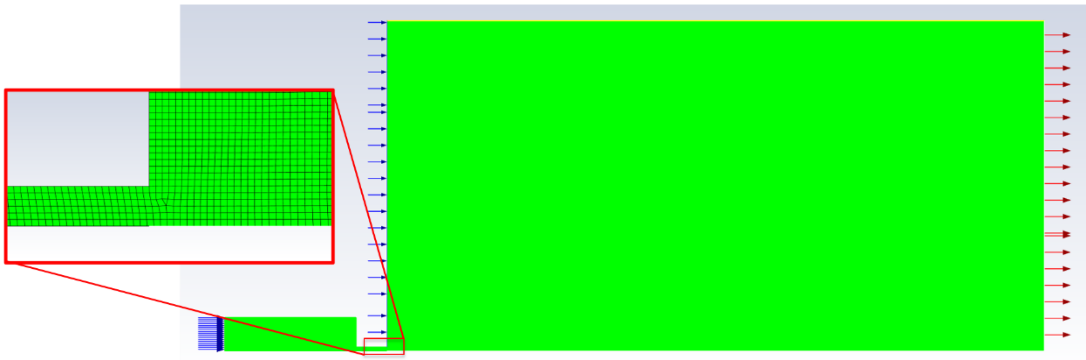

Figure 2. Geometry and mesh of BP test.

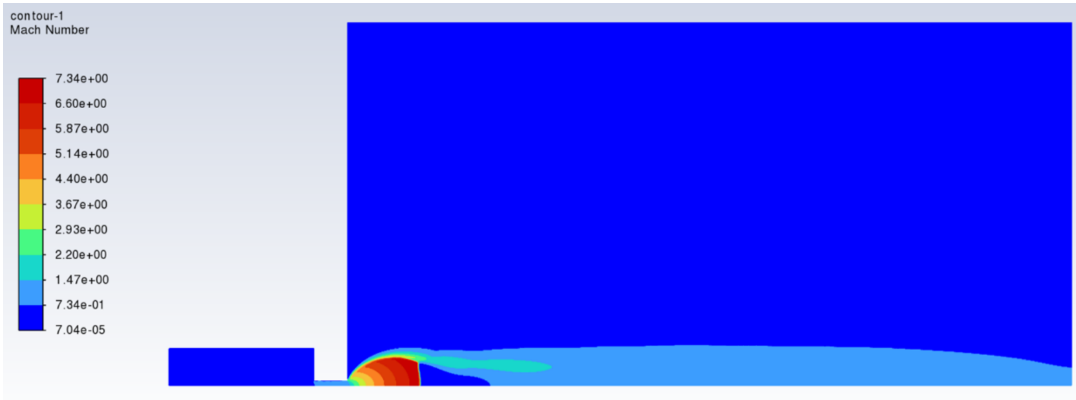

Figure 3. Simulation results.

From Figure 3, we could observe the Mach disc, which manifests as a notable characteristic within specific shock wave occurrences, especially within the realm of swift supersonic or hypersonic flows (Figure 4). Moreover, we also could get the accurate mass flow rate from this simulation, whose observed value was 4.07 kg/s (Figure 5).

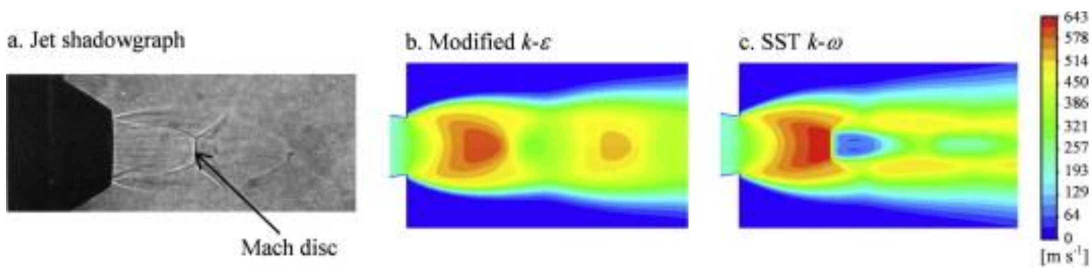

Figure 4. Mach disc (adopted from Liu et al., 2014).

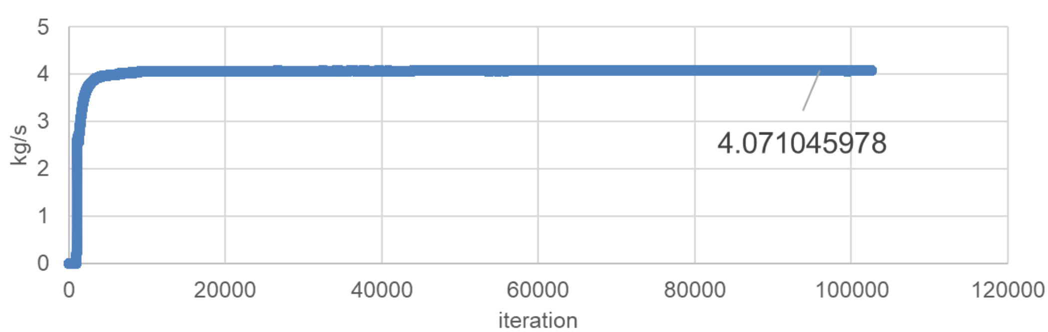

Figure 5. Mass flow rate from the near-field simulation.

However, the near-field stage for this relatively simple BP test 8 case took TAMU HPRC a day to run the simulation, not to mention the CO_2 pipelines with higher pressure and temperature. Therefore, it would take too much time to create the database for our further machine learning step, so we need to adjust the procedure on predicting the near-field stage.

Thus, we used the conservation equation of energy to do the calculation for near-field stage:

$$\Delta H + \Delta KE + \Delta PE = Q + W_s$$

Where, H is enthalpy, KE is kinetic energy, PE is potential energy, Q is heat, and W_s is shaft work.

In the near-field stage, there is some fraction of CO_2 would disperse to atmosphere, while some air entrains and mixes with CO_2. According to the simulation from Ansys Fluent, 3.8 kg/s (out of total 4.07 kg/s CO_2 from the pipe) CO_2 blended with air and accounted for 28.22 %. The initial state (420.3 K and 15.74MPa) is the CO_2 in the pipe and the final state (281 K and 96020 Pa) is the mixture of CO_2 and air at the 10 times of the distance of Mach disc (x_m) from the pipe, which is believed the pressure and temperature from the pipe is reduced to ambient temperature and ambient pressure. In this case, the corresponding distance is 1 meter.

$$\left(m_a H_{a,i} + m_c H_{c,i} - m_a H_{a,f} - m_c H_{c,f}\right) + \left(\frac{1}{2} m_a {v_{a,i}}^2 + \frac{1}{2} m_c {v_{c,i}}^2 - \frac{1}{2} m_a {v_f}^2 - \frac{1}{2} m_c {v_f}^2\right) + 0 = Q + W_s$$

$$\rho_{mix} = \frac{PM_{mix}}{RT}$$

$$A_f = \frac{m_a + m_c}{\rho_{mix} v_f}$$

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

Where m_a is the mass flow of air, m_c is the mass flow of CO_2, $H_{a,i}$ is the enthalpy of air in initial state, $H_{c,i}$ is the enthalpy of CO_2 in initial state, $H_{a,f}$ is the enthalpy of air in final state, $H_{c,f}$ is the enthalpy of CO_2 in final state, $v_{a,i}$ is the velocity of air in initial state, $v_{c,i}$ is the velocity of CO_2 in initial state, v_f is the velocity of the mixture in final state, ρ_{mix} is the density of mixture, P is the pressure, M_{mix} is the molecular weight of mixture, R is the gas constant, T is the temperature, A_f is the input area for far-field statge, x_m is the distance of the Mach disc, d_e is the diameter of the nozzle exit, P_0 is the stagnation pressure, and P_∞ is the ambient pressure.

For the W_s, Joule-Tompson coefficient (μ_{JT}) and Peng-Robinson equation of state applied to escaped CO_2 to calculate the shaft work on the surrounding based on isothermal expansion.

$$P = \frac{RT}{V_m - b} - \frac{a\alpha}{{V_m}^2 + 2bV_m - b^2}$$

$$a = \frac{0.45724R^2{T_c}^2}{P_c}$$

$$b = \frac{0.07789RT_c}{P_c}$$

$$\alpha = \left(1 + (0.37464 + 1.54226\omega - 0.26992\omega^2)\left(1 - {T_r}^{0.5}\right)\right)$$

$$T_r = \frac{T}{T_c}$$

$$\mu_{JT} = \left(\frac{\partial T}{\partial P}\right)_H$$

$$W_s = \Delta\left(P \times m_{c,e} \times V_m\right)$$

Where $m_{c,e}$ is the mass flow of escaped CO_2, and V_m is the specific volume of the CO_2 at corresponding conditions with considering Joule-Tompson coefficient (μ_{JT}) and Peng-Robinson equation of state.

Therefore, we could calculate the temperature, specific volume of CO_2, and through the depressurization process. Consequently, we could calculate the shaft work on surrounding.

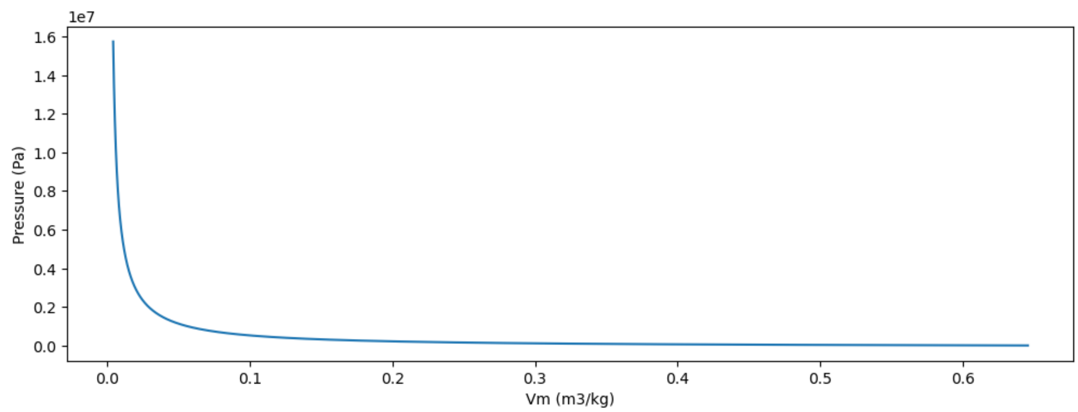

Figure 6. Shaft work of escaped CO_2.

Additionally, there is some heat loss from the dispersion. For this case, CO_2 will be passing through three sections before it can be released into the atmosphere. From the storage tank, it will traverse a flexible hose, a metering spool, and an orifice plate (Table 2).

Table 2. The properties of the material.

Transport path	Material	Length (m)	Inner radius (in)	Outer radius (in)	Thermal conductivity (W/m·K)
Flexible hose	Hydrogenated Nitrile Butadiene Rubber (HNBR)	3	2	1.25	0.23
Metering spool (pipe)	Steel	2	0.5	0.42	45
Orifice plate	Stainless Steel	0.5	0.5	2.2	15

These transport paths were based on common materials used for CO_2 transportation. To account for the heat lost from transport between the storage tank and the orifice, the heat generated by the fluid through each of the materials was calculated using the following equation:

$$Q = \frac{2\pi k L (T_i - T_o)}{\ln\left(\frac{r_o}{r_i}\right)}$$

Where, k is the thermal conductivity; L is the length of the pipe; T_i is the temperature inside the pipe; T_o is the temperature outside the pipe; r_o is the outer radius of the pipe; and r_i is the inner radius of the pipe. Hence, the heat loss from CO_2 transport can be summed as:

$$Q = Q_{FlexibleHose} + Q_{MeteringSpool} + Q_{OrificePlate}$$

With the equations mentioned above, we could get the velocity, composition of CO_2, and area from the near-field stage (Table 3). Thus, we could use them in the far field to simulate the dispersion behavior.

Table 3. Parameters obtained from near-field stage.

Parameter	Value
Mass fraction (%)	28.22
Velocity (m/s)	21.33
Area (m^2)	0.46

For the far-field stage, the geometry and mesh, composed of 192,627 nodes and 1,059,276 elements, for the scope is as Figure 7. The CO_2 concentration contours is shown in Figure 8. The CO_2 concentration along the downstream is as Figure 9. The comparison of experimental results and current simulation results is shown in Table 4.

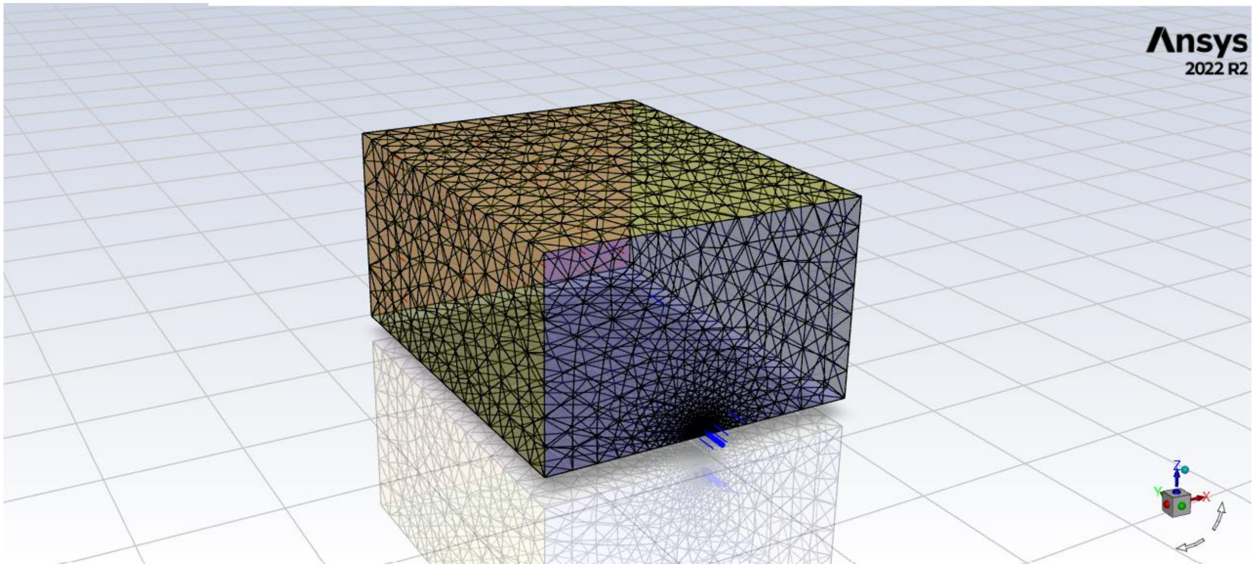

Figure 7. Geometry and mesh for the scope of simulation.

Figure 8. CO_2 concentration contours.

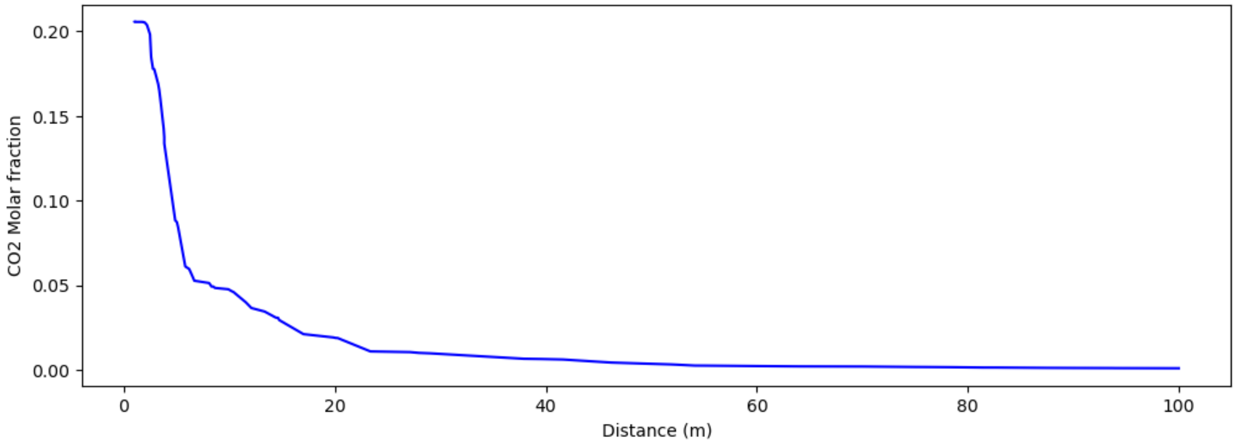

Figure 9. The CO_2 concentration along the downstream for BP test 8.

Table 4. The comparison of CO_2 concentrations between experiments and simulations.

Downstream distance from source (m)	Highest molar fraction (%) Experiment	Simulation
5	8.22%	8.69%
10	3.36%	3.52%
20	1.85%	1.61%
40	1.49%	0.70%

2. Case studies on real cases

Two case studies (Table 5) have been conducted based on the above-mentioned method, which is the combination of calculation on near-field and CFD simulation on far-field.

Table 5. Parameters for two case studies.

	Variable	Case 1	Case 2
Pipeline characteristics	pressure (MPa)	20	20
	diameter (inch)	4	30
	flow rate (MMcfd)	30	1300
Weather conditions	wind speed (mph)	1	1
	temperature (°F)	60	60

The CO_2 concentration along the downstream and the distance for CO_2 concentration at 1%, 4%, and 9% are as Figure 10, Figure 11, and

Table 1.

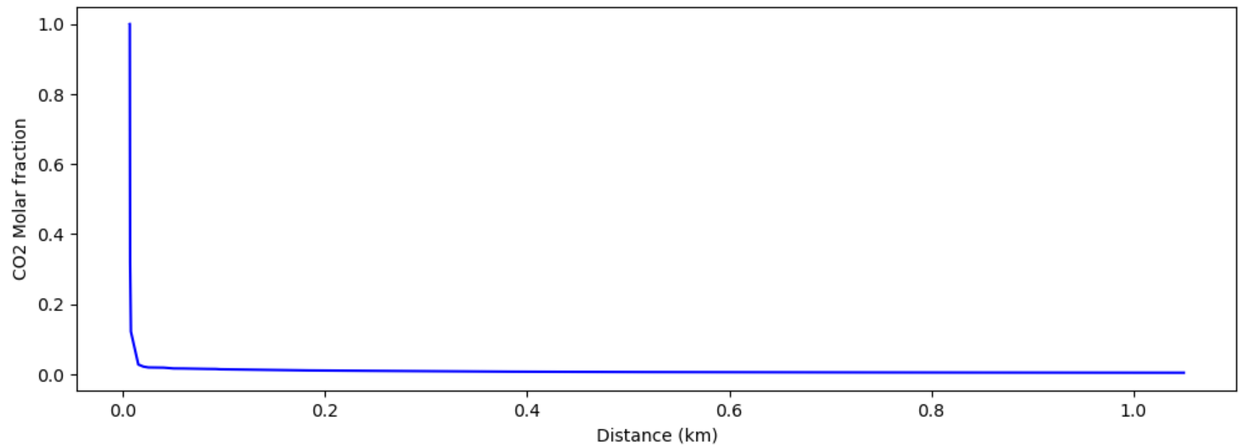

Figure 10. The CO_2 concentration along the downstream for Case 1.

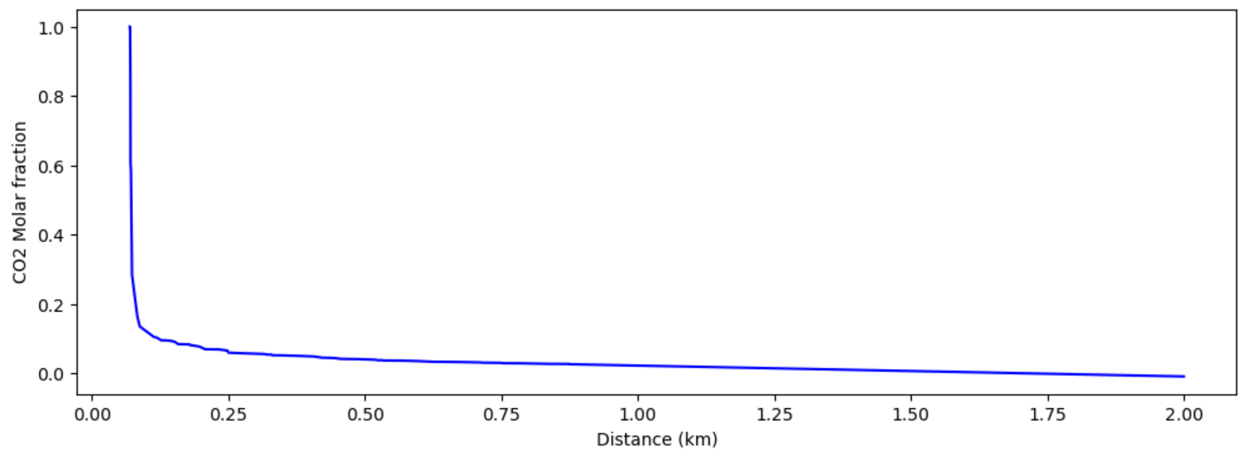

Figure 11. The CO_2 concentration along the downstream for Case 2.

Table 6. The distance for CO_2 concentration at 1%, 4%, and 9%.

Concentration	1%	4%	9%
Case 1	210	10	6
Case 2	1810	450	155

3. To-do list after technical panel meeting (Sep 27, 2023)

A. Check the influence of the roughness of ground.

B. Check the influence of the temperature in pipelines.