CAAP Quarterly Report

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

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Business and Activity Section

(a) Contract Activity

Contract was officially signed between PHMSA and Texas A&M Engineering Experiment Station.

(b) Status Update of Past Quarter Activities

- Formed a Technical Advisory Panel (TAP) and held a kickoff meeting with PHMSA and TAP.
- Conducted a literature review on existing field tests related to CO_2 release and dispersion.
- Conducted a literature review about how PIR was addressed for natural gas pipelines.
- Established an initial CFD model using ANSYS Fluent based on the BP DF1 CO_2 dispersion experiments conducted by DNV.

(c) Cost Share Activity

Dr. Wang's time and efforts (0.5 month) in this quarterly period are used as cost share. He devoted his time to supervise the research with the graduate students, review all paperwork, prepare and host the kickoff meeting.

(d) Task 1: Establish the CFD models of CO_2 release and dispersion from a high-pressure pipeline

In this quarter, we went through the regulations related to PIR and conducted literature review on CO_2 release and dispersion experiments. Then, we chose a suitable setup to establish the initial CFD model and compared the simulation results with the experimental data for the purpose of validation. The model will be refined further at both steady state and transient state in the second quarter.

The following is a detailed discussion of current progress and completed work in the first Quarter.

1. Background and Objectives

1.1 Background

With the increasing attention on global climate change, carbon capture and storage (CCS) projects are receiving greater importance in the current worldwide discussion. For these operations, the safe transportation of carbon dioxide (CO_2) is a critical element to continue growth in the field. Although CO_2 is neither toxic nor flammable, in the event of a catastrophic release from a pipeline rupture, its asphyxiant nature could pose a significant threat to the people and other living animals in the vicinity. Therefore, the determination of the potential impact radius (PIR) for CO_2 pipelines is important to ensure the safety of the nearby communities.

1.1.1 Potential impact radius in the DOT regulation

The calculation of the PIR of the potential impact circle within which the failure of a pipeline could have a significant impact on people or property is the key step of 49 CFR 192 Subpart O - Gas Transmission Pipeline Integrity Management (Gas Transmission Pipeline Integrity Management, 2003). The specific formula for the PIR of natural gas is calculated as:

$$r = 0.69\sqrt{p \cdot d^2}$$

where: r is the PIR in feet, p is the maximum allowable operating pressure (MAOP) in the pipeline segment in pounds per square inch, and d is the nominal diameter of the pipeline in inches.

For the transportation of gases other than natural gas, the operator should apply different factors to calculate the corresponding PIR, as shown below (Gas Transmission Pipeline Integrity Management, 2003; The American Society of Mechanical Engineers, 2004; Michael Baker Jr., Inc., 2005):

$$r = \sqrt{\frac{14490 \cdot \mu \cdot \chi_g \cdot \lambda \cdot C_d \cdot H_C \cdot Q \cdot p \cdot d^2}{a_0 \cdot I_{th}}}$$

where: r is the PIR in feet, μ is combustion efficiency factor, χ_g is emissivity factor, λ is release rate decay factor, C_d is discharge coefficient, H_C is heat of combustion in BTU per pound, Q is flow factor, p is the maximum allowable operating pressure (MAOP) in the pipeline segment in pounds per square inch, d is the nominal diameter of the pipeline in inches, a_0 is sonic velocity of gas in feet per second, and I_{th} is threshold heat flux in BTU per hour square feet.

However, the premise to applying these formulas is that thermal radiation from a sustained jet or trench fire is the dominant hazard from the pipe rupture, because these formulas are derived from a fire model which considers the threat to human life from the thermal radiation (Stephens et al., 2002; Michael Baker Jr., Inc., 2005). For natural gas or other flammable gases whose specific gravity are significantly lower than air, gases barely accumulate around the ground to form the vapor cloud, which could turn into vapor cloud explosion with the ignition source, so the application of these equations are valid. However, for gases with a specific gravity close to or higher than 1, the dispersion along the ground and concentration of the gases are the dominant hazards to the people and property, thus the above equations could not be applied to calculate the PIR.

The hazardous characteristic for CO_2 is asphyxia and the specific gravity of CO_2 is higher than 1, so we could not apply the above formulas to determine the PIR for CO_2 pipelines. In this project, we plan to combine computational fluid dynamics (CFD) models and machine learning techniques to develop a tool to determine the PIR for CO_2 pipelines.

1.1.2 CO_2 release experiments

Because this project will utilize simulation methods, the comparison of simulation and experimental results to validate the model applicability is an important task. Therefore, we have conducted a literature review to search for suitable experiments to conduct the validation. Currently, there have been many applications for simulating dispersion of CO_2 using CFD with reasonably good results (Godbole et al., 2018; Rian, 2014). We have also performed CFD simulations of CO_2 dispersion and validated the results against full-scale CO_2 release experiments to demonstrate the applicability of CFD simulation in the dispersion of CO_2 (Joshi et al., 2016; Shen et al., 2020).

There have been many CO_2 release experiments conducted, such as CO2PIPETRANS joint industry project, CO2Safe-Arrest joint industry project, COSHER joint industry project, CO_2QUEST project, and COOLTRANS research program. We then decide on an applicable experiment and use the setup information from that specific experiment to establish the CFD simulation and compare the simulation results with the experimental results.

For the CO2PIPETRANS joint industry project, there are two CO_2 release experiment projects funded by BP and Shell; the experiments included high-pressure steady state and time-varying liquid storage releases, and high-pressure time-varying supercritical vapor storage releases (Witlox et al., 2014). In this project, there are many publicly available parameters and data; thus, it is convenient for the public to apply them to conduct the simulation and compare the simulation with the experimental results (Rian et al., 2014; Witlox et al., 2014).

For the CO2Safe-Arrest joint industry project, the project is composed of two objectives, respectively investigating the fracture propagation and arrest characteristics of steel pipelines carrying anthropogenic CO_2, and investigating the dispersion of CO_2 following its release into the atmosphere. An explosive charge was applied to generate an explosive release of CO_2 from the pipe in less than 12 seconds (Godbole et al., 2018).

For the CO_2QUEST project, the project mainly focusses on addressing fundamental issues regarding the typical impurities in a CO_2 stream from the fossil fuel sources (Porter et al., 2016). For the COSHER joint industry project, the experiment, whose CO_2 release was also initiated by an explosive charge, was similar to that of CO2Safe-Arrest joint industry project (Ahmad et al., 2015). Lastly, for the COOLTRANS research program, the project consisted of a venting experiment and scaled rupture experiments, however, the experiment data are not publicly available (Allason et al., 2014). The comparison of CO_2 experiments is provided below in **Table 1**.

Table 1. Comparison of CO_2 release and dispersion experiments

Project	Objective	Setup	Results
CO2PIPETRANS JIP	Demonstrating large scale CO_2 pipeline release, to validate the computer models for assessing the consequence of an accidental release from CO_2 pipeline	High-pressure steady-state liquid storage releases (9 experiments) Time-varying liquid storage releases (3 experiments) Time-varying supercritical vapor storage releases (5 experiments)	• Many experimental data are available to validate the results from models • The raw data is not publicly accessible currently
CO2Safe-Arrest JIP Part 3: Dispersion model	Investigating the dispersion of CO_2 following its release into the atmosphere	Time-varying storage releases (an explosive release of 91% CO_2 and 9% N_2 pressurized to 15 MPa)	• The results from CFD are in reasonably good agree with the experiments • The raw data is not publicly accessible
COSHER JIP	Demonstrating large scale CO_2 pipeline release to provide release and dispersion data	Time-varying liquid storage releases (an explosive release of 99.99% CO_2 pressurized to 15 MPa)	• The data are useful for model development and validation • The raw data is not publicly accessible
CO_2QUEST WP2: CO_2 transport	Addressing fundamentally issues regarding to the typical impurities in CO_2 stream from the fossil fuel sources	Time-varying liquid storage releases (29 experiments performed; 2 experiments discussed in the article)	• CFD models were developed to simulate impure CO_2 releases following puncture or rupture of a CO_2 pipeline • The raw data is not publicly accessible
COOLTRANS puncture and scaled rupture experiments	Investigating the behavior of releases of CO_2 mixtures in the gaseous and liquid phase	Time-varying liquid storage releases (8 experiments)	• The information could be applied to support risk assessment • The raw data is not publicly available

Although the raw data of CO2PIPETRANS joint industry project is not publicly accessible currently, we could use data published in an article. Furthermore, because the wind direction of BP DF1 field test 11 is very close to the release direction, there are many comparisons in the article (Witlox et al., 2014). Thus, this experiment is selected to validate our CFD models.

1.2 Objectives

In the first quarter, the objective is to setup the initial CFD model using ANSYS Fluent. Another objective is to validate the initial CFD model using the experimental results from the BP DF1 field test 11.

2. Modeling Program

2.1 Implementation

SolidWorks was used for the development of the CFD model. ANSYS Fluent 2022 R1 was used to simulate the CO_2 dispersion from the pipeline. The numerical simulation was performed on the Texas A&M University High Performance Research Computing (HPRC) Grace cluster. Grace is an Intel x86-64 Linux cluster with 925 compute nodes (44,656 total cores) and 5 login nodes. There are 800 compute nodes with 384 GB of memory, and 117 GPU nodes with 384 GB of memory. The computation time for each trial takes around 2 hrs.

2.2 Model setup

The layout and dimensions of the CFD model are presented in **Figure 1**. The CFD model is developed for a region of $100 \times 50 \times 80\ m^3$ around the release, using ANSYS Fluent. For validation of the CFD model, its simulation results are compared with the experimental results from the BP DF1 field test (Witlox et al., 2014). The mesh topology was determined by refining the mesh until grid independence of the flow field solutions was achieved. The final mesh of the computational domain for the case contains 599,394 nodes and 3,485,414 elements in total. The mesh details and mesh report are shown in **Figure 2**.

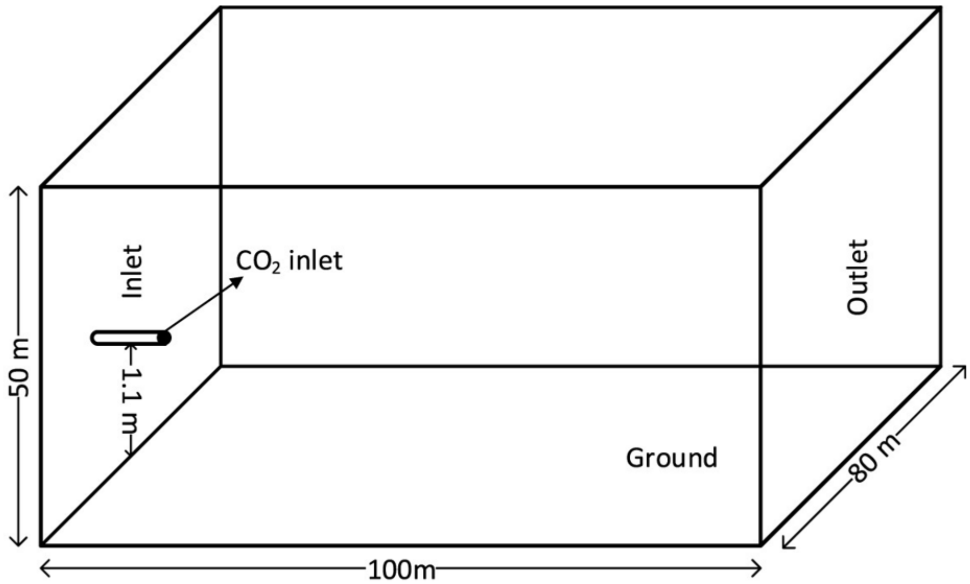

Figure 1. The CFD model setup for the CO_2 release (dimensions not to be scaled).

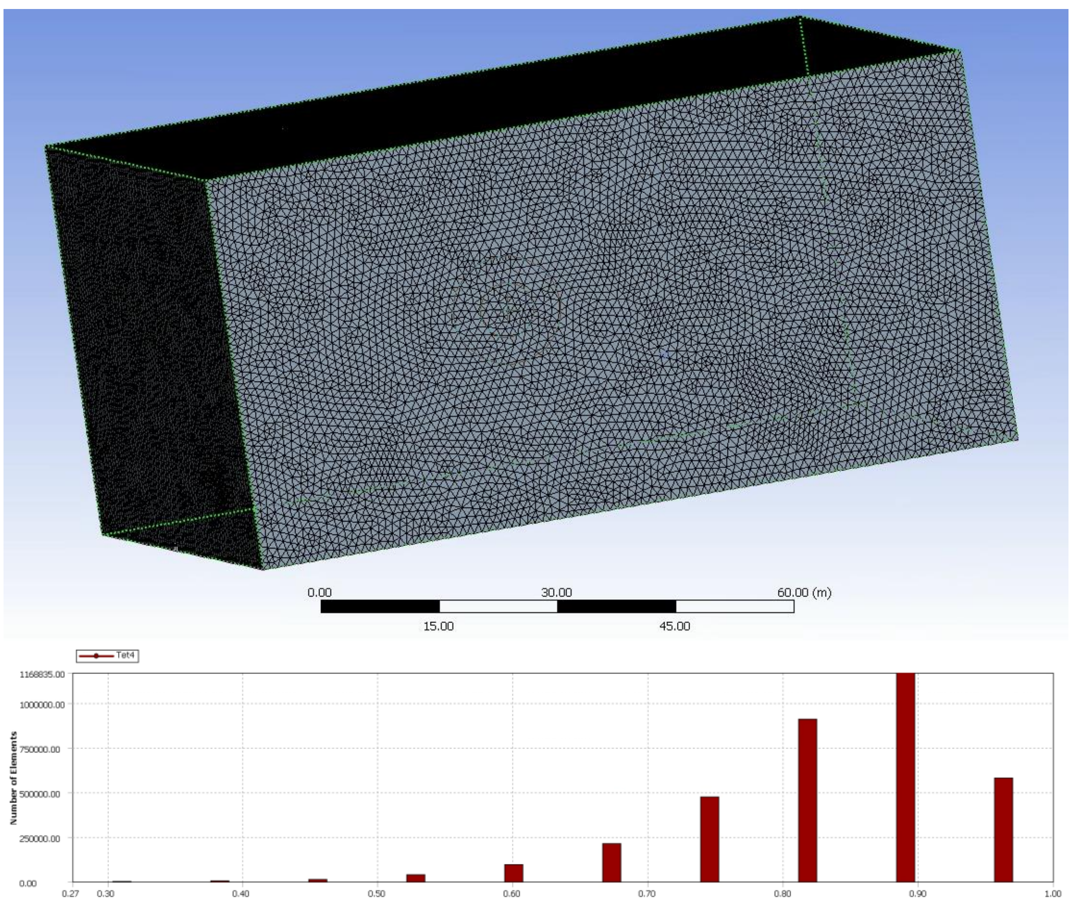

Figure 2. Mesh details and mesh report.

An energy model and a viscous model are applied to the system. The energy model equation is given in tensor form as *Energy Model:*

$$\frac{d(\rho E)}{dt} + \nabla\cdot\left[\vec{V}(\rho E + p)\right] = \nabla\cdot\left[k_{eff}\nabla T - \sum_j h_j J_j + \left(\bar{\bar{\tau}}_{eff}.\vec{V}\right)\right] + S_h \qquad \text{Equation 1}$$

The first three terms on the right-hand side of Equation 1 represent energy transfer due to conduction, species diffusion, and viscous dissipation, respectively. S_h includes the heat of chemical reaction, and any other volumetric heat sources that are defined.

The energy E per unit mass used in Equation 1 is defined as *Viscous Model:*

$$E = h - \frac{p}{\rho} + \frac{V^2}{2} \qquad \text{Equation 2}$$

The RNG-based k-epsilon turbulence model is derived from the instantaneous Navier-Stokes equation, using a mathematical technique called “renormalization group” (RNG) methods. Full Buoyancy effects were applied to enable the inclusion of buoyancy effects on epsilon.

3. Results and Discussion

The CFD simulation results were inspected carefully in terms of convergence, CO_2 concentration distribution etc., to make sure that the model setting is appropriate. It is to be noted that the fluctuations observed in the field test concentration profile are due to sensor noise. As the distance from the source of release increases, the fluctuations in the concentration profiles also increase because sensor noise is relatively large in comparison to small concentration values. The simulation results matched the experimental results from the BP DF1 field test 11 (**Table 2**), especially within the close region (5 m). The experimental results validated the model settings, and the simulation can therefore be applied as the base model.

Table 2. Comparison between raw data and simulation results

	Test 11 experimental data	Simulation result
Sensor 01 (5 m)	20 mol%	23 mol%
Sensor 03 (15 m)	4 mol%	9 mol%
Sensor 16 (40 m)	0.5 mol%	0.8 mol%

4. Future Work

Pipeline incident reports are available from the U.S. National Transportation Safety Board and Canada's Transportation Safety Board. These reports could be reviewed to compare the CFD simulation, incident results, and the harm of different CO_2 concentrations to human health.

For future model development, a more accurate steady-state model can be created. A transient model can also be used to validate the results.

Additionally, the identification of the scenario is a critical step in hazard assessment. To determine the PIR for the dispersion, the release time is a very basic parameter to apply. Therefore, an agreement should be established on the release time for our prediction on the PIR. For example, to assess the worst-case release scenario for toxic gases, the owner or operator shall assume the quantity is released over 10 minutes (Hazard Assessment, 1999).

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