CAAP Quarterly Report

March 22, 2024

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

Contract Number: 693JK32250011CAAP

Prime University: Texas A&M University

Prepared By: Sam Wang, qwang@tamu.edu, 979-845-9803

Reporting Period: 12/27/2023 – 3/26/2024

Project Activities for Reporting Period:

The following relevant tasks in the proposal have been completed:

- Created the procedure for conducting simulations on Ansys Fluent. More details are provided in the Appendix.
- Created *PyFluent* package file and applied Python to run the parameter combinations. More details are provided in the Appendix.
- Used Ansys Fluent to conduct CFD simulation for 131 cases based on the results of the calculation for the near field. 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 0.75 month.
- Efforts and work by three graduate students, Chi-Yang Li (3 months), Jazmine Aiya D. Marquez (2 months), and Haoyu Yang (1 month).

Project Activities with Cost Share Partners:

Dr. Wang's time and efforts (0.75 month) in this quarterly period are used as cost share. He devoted his time to supervise the graduate students, review all paperwork, coordinate university staff and PhD students to setup *PyFluent* package, 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. 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. The extension of the CAAP project is currently pending on the status of the Skylark JIP. Simon Gant is working with UK Department for Energy Security and Net Zero to explain why DNV Spadeadam and Arkansas have been selected for the experimental parts. This is progressing well.

Potential Project Risks:

For the parametric study using Ansys Fluent, incorporating terrain information has increased the computation time. Performing hundreds of CFD simulations requires a significant amount of time. With three PhD students to work on this project and the development of Python code, we already collected good amount of data. CFD simulations are expected to be finished by this summer.

Future Project Work:

- With the tool created in this quarter, we could run the simulations in more efficient ways. The future work is to conduct ongoing parametric studies at TAMU HPRC for various dispersion scenarios using Ansys Fluent, incorporating the numerical simulation setup and calculating the results. In addition to the five terrain categories, consider pipeline characteristics and weather conditions as outlined in 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)	25	14	3
	temperature (°F)	100	60	0

- Continuously enhance the PIR database for CO_2 pipeline dispersion using the simulation results obtained with the aforementioned setup.
- Conduct parametric studies to identify appropriate machine learning techniques and their corresponding hyperparameters 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.

<u>**Appendix**</u>

1. Manual for conducting simulations on Ansys Fluent with HPRC at TAMU

Basic Setup (Ansys Workbench is already open): Simulation on HPRC

- Create a directory in /scratch/user/*Your_NetID* for a new case; Open Ansys Fluent Workbench; Create an Ansys Fluent task: Analysis Systems > Fluid Flow (Fluent); Import the case: Right click "*Setup*", click "*Import Fluent Case*" and "*Browse*" the corresponding cas.h5 file.
- Lauch Ansys Fluent: double clicks "*Setup*", check "*Double Precision*", fill the number of "*Solver Processes*".
- As you run a new mesh. Replace the mesh: (Top tabs) File > Import > Mesh. In the "*Read Mesh Options*" tab, check "*Replace Mesh*" and "*Show Scale Mesh Panel after Replacing Mesh*". Then, click "*Continue*" and choose the corresponding msh file (Select the "Files of Type" as "All Mesh Files (*.msh* *.MSH*)".). Once the "*Scale Mesh*" window pops up, click "*close*". Then, an <u>*information*</u> window will open, just click "*OK*".
- Match the mesh: File > Recorded Mesh Operations > Match Zone Names. Click the one in "*Missing Zones*" and the one in "*New Zones*". Then, click "*Apply*". (Each geometry with several simulations). A window will ask if you want to reload the set-up, just click "*Yes*". Once the set-up has been reloaded, click "*close*".

Simulation: Atmosphere Stability

- Change wind speed: (Top tabs) User-Defined > Named Expressions > Manage. Choose "*wind_velocity_reference*" and "Edit" it to the corresponding value (the unit is meters per second).
- Change temperature and check species composition: (Outline View on the side) Setup > Boundary Conditions (double click) > Operating Conditions. Change "*Operating Temperature*" to the corresponding value (the unit is degree F). and click "*OK*". Setup > Boundary Conditions (click on the + sign to show different boundary conditions) > inlet (click on the + sign)> inlet_wind (double click) > Thermal. Fill the blank with the corresponding value (the unit is degree F) and click "*Apply*". After checking Thermal, go to Species. Make sure that the mole fraction box is checked, and the mole fraction is 0.000421 and click "*Apply*". Note: The window will not automatically close so make sure to click apply before closing the window manually. Setup > Boundary Conditions > Outlet (click on the + sign) > outlet (double click) > Thermal. Fill the blank with the corresponding value (the unit is degree F). and click "*Apply*". After checking Thermal, go to Species. Make sure that the mole fraction box is NOT checked, and the mass fraction is 0.0006395131737702 and click "*Apply*".
- Meanwhile, "*Type*" of "*inlet_co2*" should be under <u>**Wall**</u>. If it is not under WALL, right click "*inlet_co2*" and change its "*Type*" to "wall" and click apply then close the window.
- Initialization: (Outline View on the side) Solution > Initialization (double click). Check

"*Standard Initialization*". Fill the "*Temperature*" blank with the corresponding value (the unit is degree F) and check "*co2*" is 0.0006395131737702. Then, "*Initialize*".

- Run Atmosphere Stability case: (Outline View on the side) Solution > Run Calculation. Change "Number of Iterations" and click "*Calculate*".
- Save the file: (Top tabs) File > Save Project.

Simulation: Introduce CO_2

- Introduce CO_2: (Outline View on the side) Setup > Boundary Conditions (double click this)> Wall (click on the + sign). Right click on "*inlet_co2*" and change its "*Type*" to "*velocity-inlet*". Change "*Velocity Magnitude*" (in Momentum tab) to the corresponding value (the unit is meters per second). Change "*Temperature*" (in Thermal tab) to the corresponding value (the unit is degree F). Change "*Species Mass Fraction*" to **0.3**. Then, click "*Apply*".
- Run CO_2 Dispersion case: (Outline View on the side) Solution > Run Calculation. Change "Number of Iterations" and click "*Calculate*". A window will appear because some settings have changed, just click on "*ok*"
- Save the XY plot: (Outline View on the side) Results > Plots > XY plot (double click). Change to right plot direction. Change "*Y Axis Function*" as "*Species*" and "*Mole fraction of co2*". Select "*wall_ground*" and the appropriate surface from "*Surfaces*". Check the "*Write to File*" in "*Options*". Then, click "*Write*" and name the file.
- Save the profile: (Top tabs) File > Export > Profile. Choose "*wall_ground*" in "*Surface*" and choose "*Mole fraction of co2*" in "*Values*". Then, click "*Write*" and name the file.
- Save the file: (Top tabs) File > Save Project.

Results Collection

- Download and save .dat.h5 files.
- Download and save XY plot file.
- Download and save profile file.

2. *PyFluent* file for conducting simulations on Ansys Fluent.

In Ansys Fluent simulations, meshes need to be created. The following simulation process involves much repetitive work, which are replacing the parameter, waiting simulations, and saving the results. Therefore, we applied Python with *PyFluent* package to repeatedly execute the steps to conduct the simulations. The code in the file is as follows:

```
import ansys.fluent.core as pyfluent

import pandas as pd

from tqdm import tqdm

#from ansys.fluent.core.filereader.case_file import CaseFile
```

```python
#import inspect
import shutil
import os
import glob
#Access the combination of parameters
parameter_path = ……
df = pd.read_excel(parameter_path)

# Define how to access the corresponding meshse
def Mesh_Switch(vd): ……

# Open Fluent
solver = pyfluent.launch_fluent(precision='double', mode='solver', show_gui=True,
processor_count=10)
solver.execute_tui('/display/set/rendering-options/driver msw') # This is essential to write data
solver.tui.define.units("temperature", "F")

starting_point = 0

for i in tqdm(range(0, len(df)), desc="Processing"):
    if i < starting_point:
        continue
    # Read case, depending on the size parameter
    if i == starting_point or df.iloc[i]['Size'] != df.iloc[i-1]['Size']:
        if df.iloc[i]['Size'] == '1x1':
            case_name = "FLAT_1x1.cas.h5"
            solver.file.read(file_type="case", file_name=case_name)
        else:
            case_name = "FLAT_3x5.cas.h5"
```

```
        solver.file.read(file_type="case", file_name=case_name)
    # Read mesh, depending on the Virtual diameter parameter
    if i == starting_point:
        mesh_name = Mesh_Switch(df.iloc[i]['Virtual diameter'])
        solver.execute_tui(f'/file/replace-mesh \n {mesh_name}')

    elif df.iloc[i]['Virtual diameter'] != df.iloc[i-1]['Virtual diameter']:
        mesh_name = Mesh_Switch(df.iloc[i]['Virtual diameter'])
        solver.execute_tui(f'/file/replace-mesh \n {mesh_name}')

    # Edit wind_velocity_reference to corresponding value
    solver.tui.define.named_expressions.edit('wind_velocity_reference', 'definition',
df.iloc[i]['wind speed (m/s)'])
    # Edit the operating temperature
    solver.tui.define.operating_conditions.operating_temperature(df.iloc[i]['ambient
temperature (F)'])
    # Edit inlet wind temperature
     inlet_dict = solver.setup.boundary_conditions.velocity_inlet["inlet_wind"].get_state()
    inlet_dict["t"]["constant"] = (df.iloc[i]['ambient temperature (F)'] - 32) * 5/9 + 273.15
    inlet_dict["mf"]["co2"]["constant"] = 0.0006395131737702
    solver.setup.boundary_conditions.velocity_inlet["inlet_wind"].set_state(inlet_dict)

    # Edit outlet temperature
    outlet_dict = solver.setup.boundary_conditions.pressure_outlet["outlet"].get_state()
    outlet_dict["t0"]["constant"] = (df.iloc[i]['ambient temperature (F)'] - 32) * 5/9 + 273.15
    outlet_dict["mf"]["co2"]["constant"] = 0.0006395131737702
    solver.setup.boundary_conditions.pressure_outlet["outlet"].set_state(outlet_dict)

 # Change boundary condition of inlet co2 to wall
```

```
solver.setup.boundary_conditions.velocity_inlet.change_type(zone_list=["inlet_co2"],
new_type="wall")

# Initialization from inlet wind
solver.tui.solve.initialize.compute_defaults.velocity_inlet('inlet_wind')
solver.tui.solve.initialize.initialize_flow()

# Run atm stability, here the number may be edited based on the task
solver.tui.solve.iterate(200)

# Start introducing CO2
# Change type to velocity inlet
solver.setup.boundary_conditions.wall.change_type(zone_list=["inlet_co2"],
new_type="velocity-inlet")
# Change inlet BCs
inlet_dict = solver.setup.boundary_conditions.velocity_inlet["inlet_co2"].get_state()
inlet_dict["vmag"]["constant"] = df.iloc[i]["in-let CO2 velocity (m/s)"]
inlet_dict["t"]["constant"] = (df.iloc[i]['ambient temperature (F)'] - 32) * 5/9 + 273.15
inlet_dict["mf"]["co2"]["constant"] = 0.3
solver.setup.boundary_conditions.velocity_inlet["inlet_co2"].set_state(inlet_dict)

# Run calc, the number may be edited based on the task
solver.tui.solve.iterate(200)
```

 # Save XY plot

xyname = ……

solver.execute_tui(f'/plot/plot \n yes \n {xyname}\n no \n no \n no \n molef-co2 \n yes \n 1 \n 0 \n 0 \n xzplane \n wall_ground \n \n')

 # Save the data

dataname = ……

solver.execute_tui(f'/file/write-data \n {dataname} \n')

3. *The results of Ansys Fluent simulations.*

After the Ansys Fluent simulations, we save the XYplot and data. Then, we conduct the data processing on the XYplot to obtain the distances as the CO_2 mole fraction reach 9%, 4%, and 1%. Besides the 28 cases we got in the previous report, we obtained an additional 131 cases in this quarter. With the help of tools created in this quarter, we could run the simulations in more efficient ways. The results are shown in Table 2.

Table 2. Current simulation results for various 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	556	1657
	1	4	30	3	0	15	34	100
	1	4	30	3	60	15	34	101
	1	4	30	3	100	15	34	100
	1	4	30	14	0	15	31	79
	1	4	30	14	60	15	31	79
	1	4	30	14	100	15	31	79
	1	4	30	25	0	14	28	56
	1	4	30	25	60	14	28	56
	1	4	30	25	100	14	28	56
	1	16	30	3	0	63	107	402
	1	16	30	3	60	53	102	297
	1	16	30	3	100	58	108	311
	1	16	30	14	0	61	126	700
	1	16	30	14	60	61	131	712
	1	16	30	14	100	61	131	674
	1	16	30	25	0	63	149	1032
	1	16	30	25	60	63	149	1008
	1	16	590	25	60	59	121	959
	1	16	30	25	100	46	61	137
	1	16	590	25	100	59	121	959
	10	4	30	3	0	39	60	198
	10	4	590	3	0	96	229	1164
	10	4	30	3	60	39	60	196
	10	4	590	3	60	96	227	1164
	10	4	30	3	100	39	60	199
	10	4	590	3	100	96	227	1164
	10	4	30	14	0	56	89	196
	10	4	590	14	0	85	122	1040

	10	4	30	14	60	56	89	196
	10	4	590	14	60	85	122	1040
	10	4	30	14	100	56	89	196
	10	4	590	14	100	85	122	1040
	10	4	30	25	0	48	84	138
	10	4	590	25	0	80	122	1054
	10	4	30	25	60	48	84	138
	10	4	590	25	60	80	122	1051
	10	4	30	25	100	48	84	138
	10	4	590	25	100	81	122	1054
	10	4	1300	3	0	99	309	1609
	10	4	1300	3	60	100	306	1598
	10	4	1300	3	100	99	305	1597
	10	4	1300	14	0	90	219	1724
	10	4	1300	14	60	90	217	1708
	10	4	1300	14	100	90	214	1699
	10	4	1300	25	0	84	159	1585
	10	4	1300	25	60	84	159	1542
	10	4	1300	25	100	84	159	1539
	20	4	30	3	0	40	61	196
	20	4	590	3	0	101	251	1176
	20	4	30	3	60	35	61	201
	20	4	590	3	60	101	251	1178
	20	4	30	3	100	35	61	194
	20	4	590	3	100	101	251	1178
	20	4	30	14	0	61	92	217
	20	4	590	14	0	87	172	1054
	20	4	30	14	60	61	92	217
	20	4	590	14	60	87	172	1054
	20	4	30	14	100	61	92	217
	20	4	590	14	100	87	172	1053
	20	4	30	25	0	60	86	157

	20	4	590	25	0	62	146	1070
	20	4	30	25	60	60	86	163
	20	4	590	25	60	62	146	1069
	20	4	30	25	100	60	86	163
	20	4	590	25	100	62	146	1068
	20	4	1300	3	0	103	332	1600
	20	4	1300	3	60	103	329	1598
	20	4	1300	3	100	101	329	1592
	20	4	1300	14	0	93	269	1744
	20	4	1300	14	60	93	269	1733
	20	4	1300	14	100	93	268	1729
	20	4	1300	25	0	62	156	1649
	20	4	1300	25	60	62	156	1649
	20	4	1300	25	100	62	156	1665
	10	16	30	3	0	46	63	140
	10	16	30	14	0	82	92	192
	10	16	30	14	60	82	92	231
	10	16	30	14	100	82	92	231
	10	16	30	25	0	87	111	224
	10	16	30	25	60	87	111	224
	10	16	30	25	100	87	111	224
	20	16	30	3	0	55	73	151
	20	16	30	3	60	57	74	160
	20	16	30	3	100	58	75	163
	20	16	30	14	0	90	111	268
	20	16	30	14	60	90	111	268
	20	16	30	14	100	90	111	269
	20	16	30	25	0	86	121	251
	20	16	30	25	60	86	121	251
	20	16	30	25	100	86	121	251
	1	30	30	3	0	43	68	219
	1	30	590	3	0	122	245	1172

	1	30	1300	3	0	128	378	1581
	1	30	30	3	60	45	68	213
	1	30	590	3	60	122	245	1172
	1	30	1300	3	60	128	376	1576
	1	30	30	3	100	46	68	215
	1	30	590	3	100	122	245	1172
	1	30	1300	3	100	128	374	1587
	1	30	30	14	0	79	115	295
	1	30	30	14	60	79	115	295
	1	30	590	14	60	114	175	1046
	1	30	1300	14	60	118	314	1737
	1	30	30	14	100	79	115	295
	1	30	590	14	100	114	175	1046
	1	30	1300	14	100	118	314	1732
	1	30	30	25	0	61	94	191
	1	30	590	25	0	102	149	1092
	1	30	1300	25	0	109	157	1811
	1	30	30	25	60	61	94	191
	1	30	590	25	60	102	149	1089
	1	30	1300	25	60	109	157	1786
	1	30	30	25	100	61	94	191
	1	30	590	25	100	102	149	1093
	1	30	1300	25	100	109	157	1758
	20	30	30	3	0	32	51	125
	20	30	30	3	60	32	52	123
	20	30	30	3	100	32	51	128
	20	30	30	14	0	73	96	185
	20	30	30	14	60	73	96	185
	20	30	30	14	100	73	96	185
	20	30	30	25	0	61	92	181
	20	30	30	25	60	61	92	181
	20	30	30	25	100	61	92	181

	10	16	30	3	60	31	53	137
	10	16	30	3	100	156	274	1214
	10	16	590	14	0	448	972	3014
	10	16	590	14	60	429	973	3012
	10	16	590	14	100	461	980	3012
	10	16	590	25	0	578	1043	4145
	10	16	590	25	60	578	1043	4191
	10	16	590	25	100	578	1043	4140
	20	30	590	14	0	186	367	1091
	20	30	1300	14	0	192	368	1308
	20	30	590	14	60	186	367	1091
	20	30	590	14	100	186	366	1104
	20	30	590	25	0	237	423	1808
	20	30	1300	25	0	247	452	1888
	20	30	590	25	60	228	426	1799
	20	30	1300	25	60	247	452	1864
Hill with steep slope (Raton, New Mexico)	1	4	30	25	0	9	21	50
	1	4	30	14	0	10	23	60
	1	4	30	3	0	10	30	94
	1	4	30	25	60	9	21	50
	1	4	30	14	60	10	22	60
	1	4	30	25	100	9	21	50
	1	4	30	3	60	10	30	93
	1	4	30	14	100	10	23	60
	1	4	30	3	100	10	30	93
Valley with moderate slope (Vernal, Utah)	1	4	30	25	0	8	18	82
	1	4	30	14	0	9	19	86
	1	4	30	3	0	9	28	112
	1	4	30	25	60	8	18	83
	1	4	30	14	60	9	19	85
	1	4	30	25	100	8	18	82
	1	4	30	3	60	9	29	112

	1	4	30	14	100	9	19	85
	1	4	30	3	100	9	28	112