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Dispersion Study of Pressurised CO_2 Release with Obstacles

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Abstract: Carbon Capture and Storage (CCS) is an alternative for decreasing greenhouse gas (GHG) emissions by removing carbon dioxide (CO_2) from power plants. Accidental discharges from CCS plant will result in a release of dense CO_2 gas cloud to the ambience at high concentration which becomes a dominated threat to human health. However, there is a knowledge gap in assessing the release of CO_2 via pipeline leakage. Thus, it is necessary to develop an accurate consequence model for CO_2 release in order to demonstrate a safe layout and other safeguards. In this study, pure CO_2 discharge and dispersion have been detailed out using a three-dimension model with presence of obstacles in a Computational Fluid Dynamics (CFD) software. The realizable κ-ε turbulence model was chosen for simulating the dispersion of pure CO_2-air. A case study based on Kit Fox gas experiments of pure CO_2 instantaneous release is developed to evaluate the discharge scenario. The results obtained from the model are compared with experimental data available in literatures and validation is achieved.

Key words: Fluent, ambient boundary layer, dense gas dispersion, CO_2

INTRODUCTION

Carbon dioxide (CO_2) is a product of burning solid waste and wood. It is also discharged when fossil fuels (e.g., oil, natural gas, coal) are combusted. For instance, CO_2 emissions from fossil fuel power generation (23 Gton-CO_2/year) represent approximately 26% the total emissions (Holloway *et al*., 2007; IPCC, 2005, 2007). CO_2 concentration in the atmosphere was observed up to 391 ppm_v in 2011 (VijayaVenkataRaman *et al*., 2012). The high CO_2 concentration is the main cause of global warming due to its heat-trapping behaviour. Barker *et al*. (2007) have reported the increase of the average global temperature near the earth's surface about 0.78±0.18°C between 1906 and 2005. The consequence from the global warming can be noticed in several phenomena such as a rising of sea levels, melting snow and changing weather patterns (VijayaVenkataRaman *et al*., 2012). The global warming was determined as the greatest environmental challenge in the 21st century (Akorede *et al*., 2012).

Carbon Capture and Storage (CCS) is a new technology in decreasing the CO_2 emissions. The CCS will assist in achieving 19% of CO_2 reduction in 2050 where 9% reduction from industry and transportation and 10% from power generation (IEA, 2009). Over 3000 CCS projects are being planned by 2050. In the CCS system, CO_2 is separated by different capture technologies (e.g., post-combustion, pre-combustion and oxy-fuel) from big sources such as fossil fuel power generation. Captured CO_2 will be then transported by pipelines across all countries and population areas to storage areas (McCoy and Rubin, 2008; Haugen *et al*., 2009). Accidental discharges from the CCS are highly likely to happen due to a rupture or puncture of CO_2 pipelines (Koornneef *et al*., 2010). Possible impacts of the accidental CO_2 discharges are potential asphyxiant hazards CO_2 on human and also the environment due to released CO_2 displacing oxygen in the air (Wilday *et al*., 2011; Koornneef *et al*., 2012). Exposure to elevated concentration of CO_2 can increase the acidity of the blood triggering adverse effects on the respiratory, cardiovascular and central nervous systems of human. It was reported by HSE UK (Wilday *et al*., 2011) that the allowable exposure limit of CO_2 is 0.5% (5000 ppm_v) for an 8 h time-weighted average and with a Short Term Exposure Limit (STEL) of 1.5% (15000 ppm_v) for 15 min. There are several tragic disasters occurred due to CO_2 exposure such as the Noyos Lake on 21st August, 1986 which caused deaths of at least 1700 people and many livestock near the lake and up to 14 km distance from the area in the northwest area of Cameroon, West Africa (Kling *et al*., 1987). The CCS technology is still under development. A number of knowledge gaps in terms of safety have been identified which require further development (Shuter *et al*., 2011). One of the knowledge gaps which give rise to research priorities is the modelling of the dispersion of supercritical CO_2 releases from pipelines where fracture propagation is a possibility

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(Koornneef *et al*., 2012; Shuter *et al*., 2011; Bilio *et al*., 2009). This is one of the most important issues in the environmental assessment of CO_2 transport pipelines (Bilio *et al*., 2009).

In the case of accidental release, CO_2 will disperse from accidental sources to the atmosphere. An important impact on the CO_2 dispersion is the presence of the obstacles such as buildings and trees surrounding the point of release (DNV, 2010). The dense CO_2 release may sink in low-lying areas, for example valleys, streams and ditches. Thus, the mechanism of the CO_2 dispersion will depend on the mechanical turbulence (Mo *et al*., 2012). Therefore, numerical dispersion simulation tools for predicting the pure CO_2 dispersion should include assessing the impacts of the obstacles.

Numerical codes and models are increasingly used to investigate the behaviour of a released substance and to predict the consequences of a hypothetical hazardous scenario. A large number of consequence tools include two dimension analysis (2D) such as PHAST, SAFETI and EFFECT and three dimension analysis (3D) such as FLUENT, PANACHE and CFX. Computational Fluid Dynamics (CFD) is able to take into account the effects of obstacles and complexity of the geometry for the realistic accidental loss of contaminants consequence (Tauseef *et al*., 2011a). FLUENT is widely used for a wide range of industrial applications and has an extensive use all over Europe due to its capability of simulating boundary layer (Di Sabatino *et al*., 2007). A recent comparison between FLUENT and Atmospheric Dispersion Modelling System (ADMS) stressed that the CFD models were more appropriate for situations in complex environments than ADMS (Riddle *et al*., 2004). The current approach for the dispersion of dense gas is based on the calculation using the realizable κ-ε model with the presence of the obstacles in FLUENT (Tauseef *et al*., 2011b). Validation of numerical codes and models is a necessary step before the application of the models to safety and risk assessment analysis. This study will use the realizable κ-ε turbulent model in FLUENT 14.0 to simulate dispersion of pure CO_2 instantaneous release. A case of the Kit Fox field experiments will be chosen to set up parameters in a 3D-CFD model (WRI, 1998; Hanna and Chang, 2001). Impacts of obstacles and wind on the CO_2 dispersion will be evaluated. Highest peak concentration of CO_2 at a sensor closest to the point of release will be predicted and compared with experimental data.

MATERIALS AND METHODS

Kit Fox CO_2 dense gas field experiment: The Kit Fox CO_2 dense gas experiment was conducted to test the dispersion of pure CO_2 gas to the atmosphere with presence of obstacles. This experiment was part of the Petroleum Environmental Research Forum (PERF) 93-16 project carried out in late summer 1995 at the US Department of Energy (DOE) Nevada Test Site (WRI, 1998; Hanna and Chang, 2001). The geometry in the experiment has been used for several modelling of the CO_2 dispersion (Hanna and Chang, 2001; Mazzoldi *et al*., 2008a; Papanikolaou *et al*., 2011).

Pure CO_2 gas was released from the ground level area source of 1.5×1.5 m. An entire experiment in term of size was built to represent 1/10 of actual chemical plant or oil refinery (WRI, 1998; Hanna and Steinberg, 2001). In order to do that, thousands of plywood were installed in 120×314 m whole field size to increase the surface roughness of the experiment area. The plywood obstacles were installed in two different arrays of Equivalent Roughness Pattern (ERP) and Uniform Roughness Array (URA). Details of ERP and URA arrays are explained in the Table 1.

The trial 3-7 of the Kit Fox experiment was chosen to simulate the pure CO_2 instantaneous release. Details of the trial obtained from WRI (1998) and Hanna and Chang (2001) are described in the Table 2. Thus, the maximum observed concentration of CO_2 at detector closest to release section was a value of 8500 ppm_v.

Description of CFD-setup: A three dimension domain was created by a box with 315 m length×120 m width×30 m height. Figure 1 describes computational geometry for simulated process. A pure CO_2 release area was set at original coordinator (0, 0, 0). The height of release is at ground level (z = 0 m). For reducing the computational costs and simulation time, a total of 75 ERP obstacles were used without the presence of URA obstacles in the domain. The 3D model, as shown in Fig. 1, is designed using the Design Modeller in ANSYS FLUENT 14.0. The mesh of the domain was created at 385,349 cells. Fine mesh has been created near the ground and the obstacles. The mesh becomes coarser near other domain boundaries.

Table 1: Details of obstacles in the Kit Fox experiment

Obstacle	Size (m)	Spacing (m)
URA	0.2 (high)×0.8 (wide)	2.4 (lateral) and 2.4 (longitudinal)
ERP	2.4 (high)×2.4 (wide)	6.1 (lateral) and 8.1 (along-wind)

Table 2: Kit Fox experimental used in FLUENT simulation

Release category	Plume
Mass rate	3.65 (kg sec^{-1})
Duration of release	20 sec
Temperature of CO_2 release	298.15 K
Temperature of ground	302 K
Temperature of wind	304 K at 2 m
Velocity of wind	1.10 at 2 m
Pasquil-Gifford stability class	F (stable)
Friction velocity (u_*)	0.21 (m sec^{-1})
Roughness length for EPA only configuration	0.03 (m)
Monin-Obukhov length	17 (m)
Wind direction	Horizontal

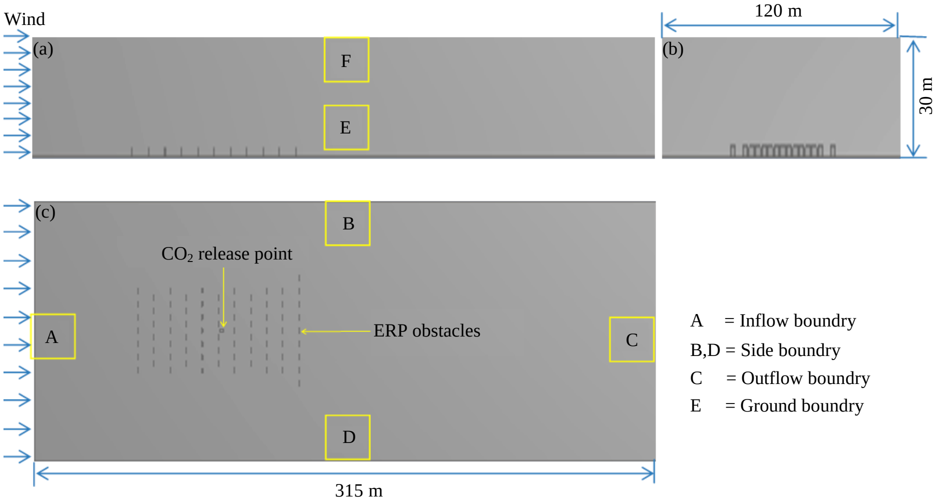

Fig. 1(a-c): Computational domain with ERP obstacles and CO_2 release point, (a) Side view, (b) Front view and (c) Top view

Boundary conditions

Inflow boundary condition: A wind profile includes wind velocity, temperature, turbulent kinetic energy (κ) and its dissipation (ε) was defined at the inflow boundary condition. Horizontal wind direction was shown as in Fig. 1. The calculation for the wind profile of the Ambient Boundary Layer (ABL) was successfully obtained in Papanikolaou *et al.* (2011). It showed that the stable conditions of the atmosphere were accurately simulated for the wind profile of Kit Fox experiment. Thus, user defined functions were created on C^{++} to link into Fluent 14.0 based on Papanikolaou *et al.* (2011) to model parameters of the wind in the domain.

The wind profile was modelled using the approach of the Monin-Obukhov similarity (Kaimal and Finnigan, 1994; Pontiggia *et al.*, 2009):

$$u(z)=\frac{u_*}{\kappa}\left[\ln\left(\frac{z}{z_0}\right)+\varphi_m\left(\frac{z}{L}\right)-1\right] \tag{1}$$

$$T(z)=T_w+\frac{T_*}{\kappa}\left[\ln\left(\frac{z}{z_0}\right)+\varphi_m\left(\frac{z}{L}\right)-1\right]-\frac{g}{C_p}(z-z_0) \tag{2}$$

$$k(z)=\frac{u_*^2}{\sqrt{C_\mu}}\sqrt{\frac{\varphi_h\left(\frac{z}{L}\right)}{\varphi_m\left(\frac{z}{L}\right)}} \tag{3}$$

$$\varepsilon(z)=\frac{u_*^3}{z\kappa}\varphi_h\left(\frac{z}{L}\right) \tag{4}$$

$$T_*=\frac{u_*^2 T_w}{gL\kappa} \tag{5}$$

where, $C\mu$ is equal to 0.09, κ is von Karman constant (0.4), friction velocity, u_*, is taken from the experimental data. C_p is specific heat capacity of dry air (1020 J kg^{-1} K), g is acceleration of gravity (9.81 m sec^{-2}), k is turbulence kinetic energy (m^2 sec^{-2}), ε is the turbulence dissipation rate (m^2 sec^{-3}), L is Monin-Obukhov length scale (m), T is temperature (K), T_w is ground temperature (K), T_* is dynamical temperature (K), u is velocity (m sec^{-1}), z is height of domain (m), z_0 is roughness length (m). The wind conditions of the simulated case are stable (F). For the stable condition, the function ϕ_h, ϕ_m were given by Eq. 6, 7:

$$\varphi_h\left(\frac{z}{L}\right)=1+5\frac{z}{L}\qquad \text{for } \frac{z}{L}\geq 0 \tag{6}$$

$$\varphi_m\left(\frac{z}{L}\right)=1+4\frac{z}{L}\qquad \text{for } \frac{z}{L}\geq 0 \tag{7}$$

Outflow boundary condition: The outflow boundary condition was set at this boundary because the flow pressure and velocity are not previously indicated.

Top and two sides boundary conditions: Zero gradients of flow through these boundary conditions was made. The symmetry boundary condition was chosen to calculate for this assumption.

Ground boundary condition: A standard wall function was applied at the bottom to specify a no-slip condition. A zero value of velocity will gain at this boundary. This approach is useful for decreasing the numbers of cells near to the bottom to avoid resolving the ground surface roughness in the simulation. Fluent version 14.0 (Fluent Inc., 2012) allowed to simulate wall function of sand-grain in ABL. Thus, the roughness of the wall is modelled by following Eq. 8:

$$K_s = \frac{9.793z_0}{C_s} \quad (8)$$

where, K_s is corresponding height, C_s is a model constant required for the wall function (using the default value of C_s is equal to 0.5 in Fluent), z_0 is roughness length. In the present simulation, the roughness constant, C_s, is defined through user defined function.

CFD-setup

Step 1: Simulation of the wind flow: To obtain a steady flow of wind field into the domain before CO_2 release, a realizable κ-ε turbulence model was implemented. The wind flow is able to get a full development over the computational domain before gas release at the convergence of 160-240 iterations.

Step 2: CO_2 releases: From above initial condition, the CO_2 release was simulated by using a realizable κ-ε turbulence model and transient condition state simulation. "Wall" boundary was changed to "mass flow rate" at CO_2 release area. The release duration of trial experiment is 20 sec. The mass flow inlet boundary condition is a constant value of 3.65 kg sec^{-1}.

Step 3: Dispersion of pure CO_2 into the ambience: In this step, the discharge of CO_2 was stopped and the released CO_2 was entered into the atmosphere. The "mass flow rate" was changed back to the "wall". The dispersion was simulated up to 135 sec. The time step in running simulations was set at 0.1 sec.

RESULTS AND DISCUSSIONS

Simulation of a horizontally Ambient Boundary Layer (ABL): A horizontally ambient boundary layer flow was accurately simulated using the CFD code to predict the dispersion occurs without presence of the obstacles (Blocken *et al*., 2007). Thus, a test of the same speed profile has been conducted from the inlet to outlet boundary. Three different locations in the present computational domain have been set as was shown in Fig. 2. Mean wind speed plot (Fig. 3) illustrates the result of the wind velocity profile at different locations. It shows that the wind flow is horizontally non-homogeneous at the set-up locations. Particularly, the wind speed increases after the wind moves through the obstacle region. The wind velocity at z = 2 m of the inlet in Kit Fox experiment is a value of 2.7 m sec^{-1}. The predicted wind speed at this location is a value of 3.0 m sec^{-1}.

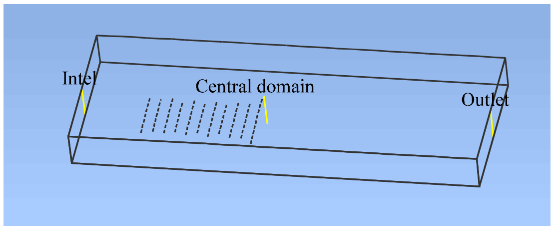

Fig. 2: Locations of predicted wind velocity in computational domain

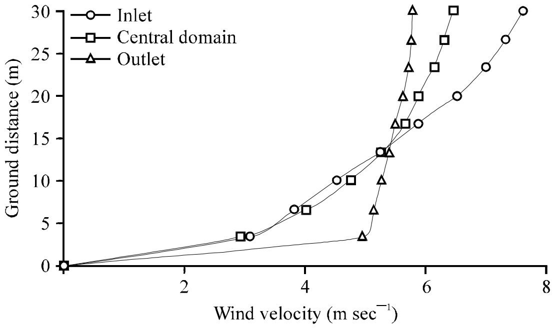

Fig. 3: Mean wind speed before CO_2 releases

From contour of wind velocity in Fig. 4, it is shown that the velocity rises up to the height of domain and reduces to a value of zero near the obstacles. The CO_2 will not disperse well in the obstacle region. Thus, CO_2 may be trapped and promote accumulation of high concentration in this region.

Analysis of CO_2 cloud concentration simulation: Pure CO_2 of 3.65 kg sec^{-1} has been released from the release point at ground level (z = 0 m). The CFD set-up for solving this problem has been shown above. After the wind flow has fully developed over the computational domain, CO_2 has started to release at initial condition (t = 0 sec). Figure 5 shows the mole fraction of CO_2 in created cloud. It is observed that toxic cloud gets wider as distance increases from the release point, as shown in. Fraction of CO_2 is high at the region close to the release point, indicating very high toxic concentration in that area. The nature of CO_2, which is denser and less viscous than air,

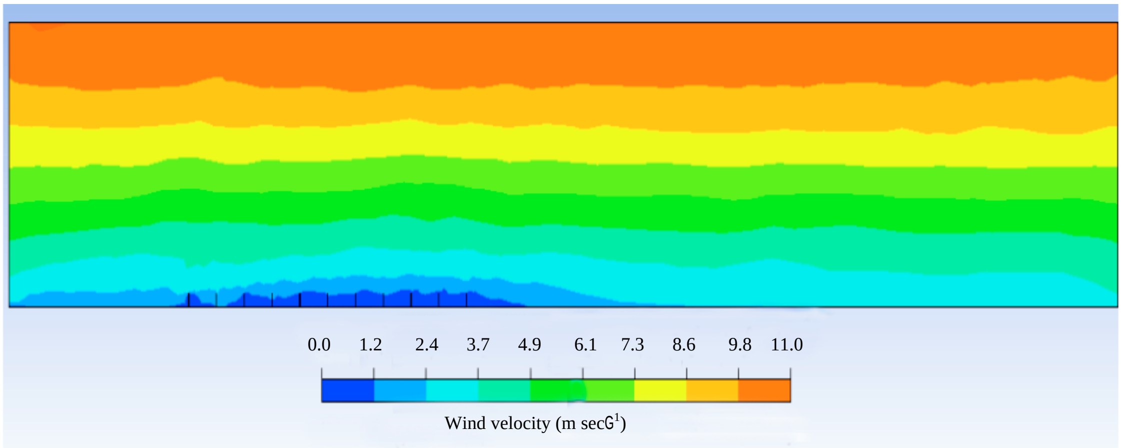

Fig. 4: Contour of wind velocity at central plane before CO_2 releases

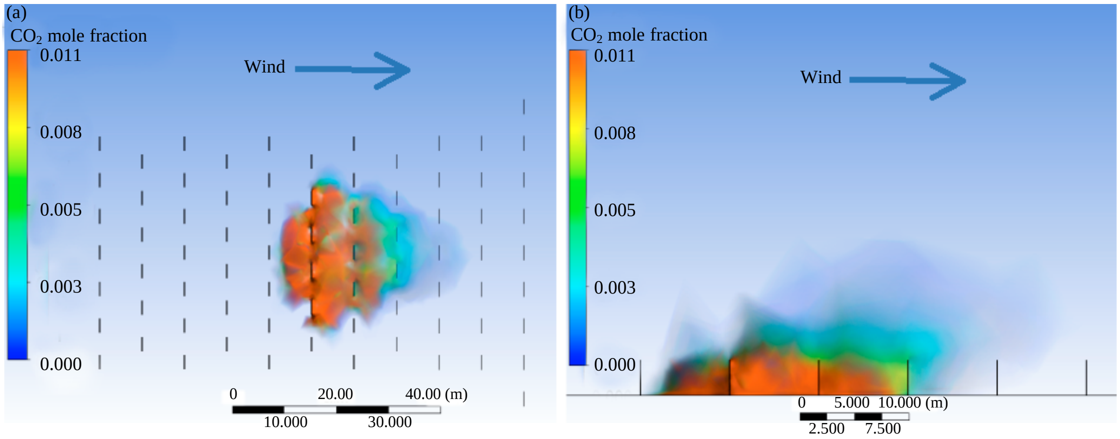

Fig. 5(a-b): The mole fraction of CO_2 in created cloud, (a) Top view and (b) Side view

therefore, CO_2 tends to come down to the ground, imposing major risks to humans especially in the condition of complex geometry and low wind speed.

CO_2 predicted concentration at location of sensor (x = 25 m, y = 0 m, z = 0.3 m) closest to the release point is illustrated in Fig. 6. These simulation results were compared with CO_2 experimental data. The CO_2 concentration plot (Fig. 6) shows that the CO_2 predicted concentration peaks at a higher value and at an earlier time than was determined during the experiment. The CO_2 predicted concentration then becomes lower than the experimental data and remains lower for the remainder of the simulation. The maximum volumetric predicted concentration of CO_2 is 9,411 ppm$_v$. It indicates that the maximum CO_2 concentration was over predicted compared to the concentration from the experiment.

In the present study, the realizable κ-ε turbulence model in FLUENT 14.0 predicted a value of maximum CO_2 concentration of 9,411 ppm$_v$ at a distance of 25 m while the experimental data is 8,500 ppm$_v$ at the same location. The UK occupational reported exposure limit of CO_2 is 0.5% (5,000 ppm$_v$) for an 8 h time-weighted average (Wilday *et al*., 2011). Thus, the FLUENT 14.0 model is able to predict approximately the harmful threshold concentration to determine the safety distance.

It should be noted that the developed model in this study is to simulate the mixing of CO_2 with air and subsequent dispersion of the toxic cloud within the obstacles. Therefore, the impacts of impurities in CO_2 stream (such as hydrogen sulfide) on phase, temperature and pressure during release process were not strictly addressed. Dispersion may differ between pure CO_2-air and CO_2-H_2S-air due to the above impacts (Koornneef *et al*., 2012). In addition, the conditions of CO_2 release such as pressure and temperature drop, phase change and sublimation were not calculated. A source

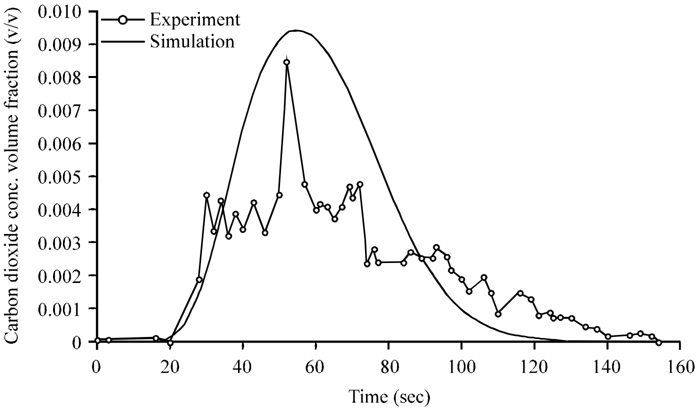

Fig. 6: Comparison of CO_2 volume fraction between experimental data and simulation results at a point of x = 25 m, y = 0 m, z = 0.3 m

term model was developed based on choked conditions to calculate the condition of the CO_2 outflow in the near field (Mazzoldi *et al*., 2008b). Hence, CO_2 discharged from a 10 mm hole of a pipeline at 10 Mpa pressure and 3.7 kg sec^{-1} leakage flow rate. The leakage flow rate is similar with the present study (3.65 kg sec^{-1}). However, the flow conditions during release process are various. For supercritical/liquid CO_2 releases, a dry ice bank may be formed in the outflow.

CONCLUSIONS

A 3D model has been developed to simulate the dispersion of pure CO_2 from accidental releases using FLUENT 14.0. The realizable κ-ε turbulence model was used to predict the dispersion of pure CO_2 instantaneous release from the ground. A wind profile and description of surface roughness were defined at the inlet and the ground boundary respectively through user defined functions. The simulation results have a good agreement with the experiment. FLUENT-CFD can be used as a tool for CO_2 concentration prediction in atmospheric release with certain over prediction as a case study of CO_2 in the far field.

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