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CO2 Dispersion Consequences Study using 3D CFD method in a CCUS facility

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Abstrak.

Carbon Capture Utilization and Storage (CCUS) adalah metode dan teknologi injeksi gas CO_2 yang memungkinkan penangkapan dan penyimpanan CO_2 di bawah tanah. Tujuannya adalah pengurangan emisi CO_2 ke atmosfer serta meningkatkan pemulihan minyak/gas/panas. Tidak seperti rekan-rekan mereka di Amerika Serikat dan Eropa, bagaimanapun, teknologi CCUS di Cina belum matang atau masih dalam skala percontohan. Mengingat jumlah besar dan laju aliran yang akan digunakan untuk CCUS, akibatnya, pelepasan besar dapat menghasilkan rentang bahaya yang signifikan pada konsentrasi yang cukup tinggi untuk memiliki efek toksik. Makalah ini berfokus pada konsekuensi pelepasan CO_2 ke lingkungan atau lingkungan yang bervariasi ketinggiannya untuk mempelajari pengaruhnya terhadap variasi permukaan tanah dari titik pelepasan hingga tingkat dispersi CO_2. Pengaruh peralatan besar terhadap luasan konsentrasi CO_2 juga dibahas.

Kata kunci: *Penangkapan Karbon, Dispersi CO2, Pengurangan Emisi*

Abstract.

Carbon Capture Utilization and Storage (CCUS) is a method and technology for CO_2 gas injection that enables the capture and storage of CO_2 underground. The aim is the CO_2 emission reduction into the atmosphere as well as enhancing oil/gas/heat recovery. Unlike their counterparts in USA and Europe, however, the CCUS technology in China is not yet mature or still at a pilot scale. Given the large quantities and flow rates which will be used for CCUS, consequently, major releases could produce significant hazard ranges at concentration high enough to have toxic effects. This paper focuses on the consequence of CO_2 releases to the neighbourhood or environment which varies in elevations to study the effect to the varied ground levels from the release points to the extent of CO_2 dispersion. The effect of large equipment to the CO_2 concentration extents is also discussed.

Keywords: *Carbon Capture, CO2 Dispersion, Emission Reduction*

Introduction

CO_2 is most commonly handled near its critical pressure (73.82 bar) where its properties tends to be close to that of a liquid in a CCUS operations [9]. This large pressure is prone to leak at the pipe flanges, storage nozzles, valves etc and can cause loss of containment. Although it is not classified as "toxic", CO_2 is more than just an asphyxiant and causes physiological effects including increased breathing rate and acidosis. In addition to the hazard of asphyxiation due to released CO_2 displacing oxygen in the air, the inhalation of elevated concentration of CO_2 can increase the acidity of the blood triggering adverse effects on the respiratory, cardiovascular and central nervous systems. CO_2, like nitrogen, will displace oxygen but unlike nitrogen, which does not have a neurological impact on humans, people would be at severe threat from increasing CO_2 concentration well before they were from the reducing oxygen concentrations [18]. Low temperatures release or blowdown causing potential damage to elastomer seals on decompression could be another potential hazard. [15].

Any release of liquid or supercritical CO_2 will, upon expansion, change phase to either a vapour or a vapour/solid depend upon inventory pressure and temperature. The heavier than air release cloud will tend to follow slopes and dents in the ground downwards and collect at low points. Modelling liquid and supercritical CO_2 releases in level open space has been validated with acceptable results for PHAST v.6.6, but for releases where ground topography or into confined spaces it is generally recommended to use Computational Fluid Dynamics (CFD) type modelling tools, enabling obstruction and confinement to be accounted for [1].

This paper briefly explains the use of 3D CFD tools FLACS for CO_2 consequence modelling considering varied ground topography and complex environment in a CCUS pilot test facility. The result might be useful for the assessment of potential hazard presented by a CCUS infrastructure.

Review of Previous Studies

There have been many studies in the recent years which investigated the release and dispersion of CO_2. Witlox et.al discussed the validation of discharge and subsequent atmospheric dispersion for carbon dioxide releases in open space using consequence modelling package Phast. The experimental work on CO_2 releases was also carried out at the Spadeadam site (UK) by Advantica for BP [19]. Subsequent study with sensitivity analysis for a wide range of scenarios (base cases) including high-pressure cold releases (liquid storage) and high-pressure supercritical releases (vapour storage) from vessels, short pipes or long pipes was also carried out [20]. Witlox et.al. had also previously described an extension to the existing model in Phast version 6.53.1 to account for the effects of solid CO_2 [21]. However, no experimental validation was presented due to data confidentiality.

Comparison to a wider range of experimental data currently available regarding near-field liquid CO_2 dispersion was carried out by Wareing et.al. [17]. For all these studies, the effect of turbulence generated by confinement at the locations of releases were not considered. Vianello, et.al. compared the maximum dispersion distance from CO_2 dense gas models of US-EPA Degasis+ and Phast 6.6. This study showed that even when release rates are similar consequences calculated with different software may be very different. Here, the maximum distance calculated with PHAST was half of that calculated with Degasis+ due to different heavy gas dispersion models. However, the critical assessment of various models in this study is hampered by the absence of reliable experimental data.

The CO_2 dispersion simulations were conducted by Dixon and Hasson using Ansys-CFX CFD code without considering solid CO_2 particles but instead using a scalar representing the particle concentration to avoid significant computation time [6]. However, it was assumed that the particles diameters were constant in calculating the heat and mass exchange between particles and gas phase resulting in poor prediction of CO_2 gas distribution from particle sublimation. Dixon et.al. also carried out CO_2 dispersion simulations using Lagrangian particle tracking approach to model CO_2 solid phase [7]. Both studies calculated release rate using Homogenous Equilibrium Model (HEM) rather than Bernoulli Equation. In this study, particles were assumed to remain at a constant temperature of -78oC which in reality the particles temperature are expected to fall as low as -100°C. Dixon et.al also carried out validation of CO_2 dispersion models in CFX, Open Foam and FRED for high pressure CO_2 releases against experimental works [5]. This study showed that all the 3(three) tools had good agreement with the experimental data. However, these studies were also performed in open space and flat ground.

The CO_2 dispersion simulations using KFX as well as its validation within a realistic environment for the purpose of improving CCS facility had been performed by Kjell et.al. [14]. However, the simulations and experimental works were only involving medium size storage tank as obstruction.

Release and Dispersion Modelling

Release models are used to quantitively define the release scenario by estimating discharge rates, total quantity release (or total release duration). Discharge rate models require a careful consideration of the released material. In the consequence calculation, release rates must be calculated very accurately because of the consequences analysis is very sensitive to its results. Even when release rates are similar consequences calculated with different software may be very different due to different gas dispersion models. The critical assessment of various model is hampered by the absence of reliable experimental data.

Release depends on the conditions of CO_2 transport which can be in three states: liquid, gas or supercritical. In cases where CO_2 is transported in the liquid phase, the release following a full-bore rupture is usually calculated using a model for non-stationary two-phase outflow from a large pipeline. In cases where the CO_2 is transported in the gas phase, a model for a non-stationary outflow from a gas pipeline is generally used or coupled with a spray-release model.

At atmospheric pressure carbon dioxide may only exist as a gas or in solid form; the sublimation temperature is at -78.5C. However, CO_2 intended for injection (storage tanks, pipelines) will for technical and economic reasons mostly be compressed into liquid or even supercritical form before transportation. In consequence, it is expected that a high-pressure CO2 release will first experience a significant pressure drop, followed by a substantial temperature drop due to the Joule-Thomson effect. As a result, the CO_2 will undergo a phase change from liquid to solid/gas and potentially result in the formation of dry ice and/or of a sonic jet flow during the process of pressure decompression. Currently, many of the physical processes associated with the rapid release of CO_2 have not been explicitly modelled in dense gas dispersion model. Nevertheless, Mazzoldi et.al. (2010) argued that most rapid releases of a liquid/vapor mixture of CO_2 would transform rapidly into the gas phase due to the frictional heating and mixing provided by the ambient air (following rapid entrainment of air into the initial dense gas cloud). Accordingly, we will simply assume that the CO_2 liquid/gas mixture has been converted entirely into the gas phase immediately after its release from the source.

A large number of parameters affect the dispersion of gases. These include atmospheric stability, wind speed, local terrain effects and buoyancy of the material released to mention some. CO_2 can be categorized as a dense (heavier than air) gas. A dense gas is defined as any gas whose density is greater than the density of the ambient air through which it is being dispersed. This result can be due to a gas with a molecular weight greater than that of air, or a gas with a low temperature due to auto-refrigeration during release or other processes.

The Shell FRED (Fire Release Explosion Dispersion) software is composed of a suite of hazard modelling codes with a common interface. For the calculation presented here the Pressurized Release (PR) model is employed, which makes calls to a number of underlying codes. Following the flashing calculation, the dispersion of CO_2 is calculated using a jet dispersion model, AEROPLUME, the results of which may then be passed on the dense gas dispersion model HEGADAS. An important aspect of the code to note in the present context is that it is assumed that a homogenous equilibrium exists between the particles and the air, i.e. the velocity, temperature and pressure of the two phases are assumed to be equal.

In the present work, the thermodynamics library employed by FRED did not account for solid CO_2 but instead the liquid vapour saturation line was extrapolated to atmospheric pressure. Hence, following the flash process, FRED gave a gas/liquid mixture with liquid drops rather than solid particles. The subsequent gas plume consisted of a mixture of vapour and liquid CO_2, together with liquid and vapour water, and air.

FLACS Modelling

FLACS at present only simulates gaseous flow while two-phase flow of aerosol is not directly modelled. The solid CO_2 phase is also not accounted in FLACS dispersion model. Consequently, in the present study, the CO_2 with initial phase of liquid is considered instantaneously turned into gas that the released gas temperature is in normal boiling pont after flashing while the mass and momentum of flow through the orifice are basically the same. This modelling approach seems reasonable in the case of CO_2 release considering the liquid CO_2 never exists in the normal atmospheric pressure. The drawback of this assumption will be discussed in this paper.

FLACS uses single planar shock model to compute expanded-jet properties and air entrainment modelling techniques for modelling releases. The 1-D model of release of ideal gas through a nozzele from pressurized reservoir is the basis of single planar shock model. The model assumes single-phase compressible (gas) flow at all stages and neglects the possible entrainment of air in the region up to expanded jet area. After the expanded jet area, the general fluid dynamics equation is employed which allows the entrainment model to be included. The equation of mass and momentum balance equations, together with formulations of entrainment rate are utilized and are supplemented with the conservation of mixture fractions as well as ideal gas equation for the jet entrainment model.

Dispersion Model Validation

For the purpose of model validation, the dispersion predictions from the FLACS and FRED can be compared to experimental results. The experimental study turned into executed by way of Dixon et.al. [5]. Figure 1 shows the comparison of FLACS, FRED and experimental results for centreline distance of various concentrations. The simulations as well as experimental results consider wind speed of 2.7 m/s downwind of the release and hole size of 1/2 in. Centreline predictions of the CO_2 concentration are compared to the measured values at a height of 1m above ground level (at the release height).

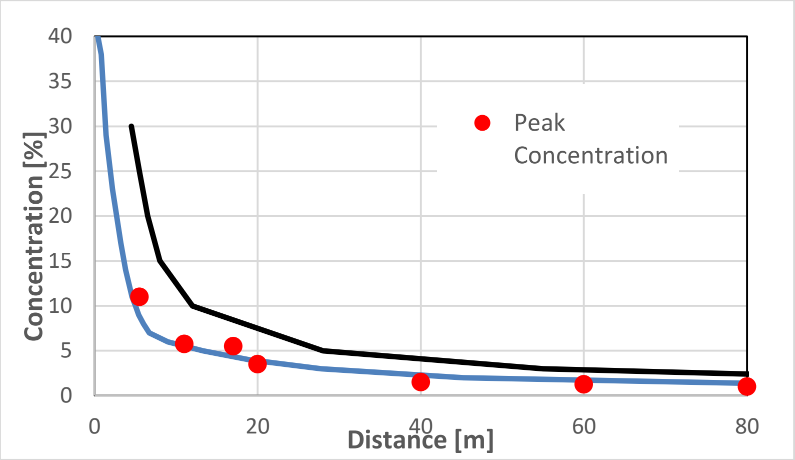

Figure 1 Validation Results of FLACS and FRED CO_2 concentration extents with Experiment

From the graph, there is generally good agreement between the experiments and the model predictions for both FLACS and FRED models. FLACS results have better agreement to the experimental results compared to FRED.

Simulated Scenarios

The CCUS facility in the study is divided into 3 areas. Area 1 comprises heating, process as well as gathering area. Basically, CO_2 in this area is mostly in gas phase. The leak rate from hole size of 1" is considered in this area which results in 3kg/s release rate. Area 1 is located at relatively higher ground level compared to other areas and is also located in the near vicinity of a neighbouring facility. The prevailing wind speed of 3.1m/s is used in the simulations with the direction to the other area of the facility as well as to the direction of neighbouring facility. The leak is chosen with the elevation of 1.5m from the ground.

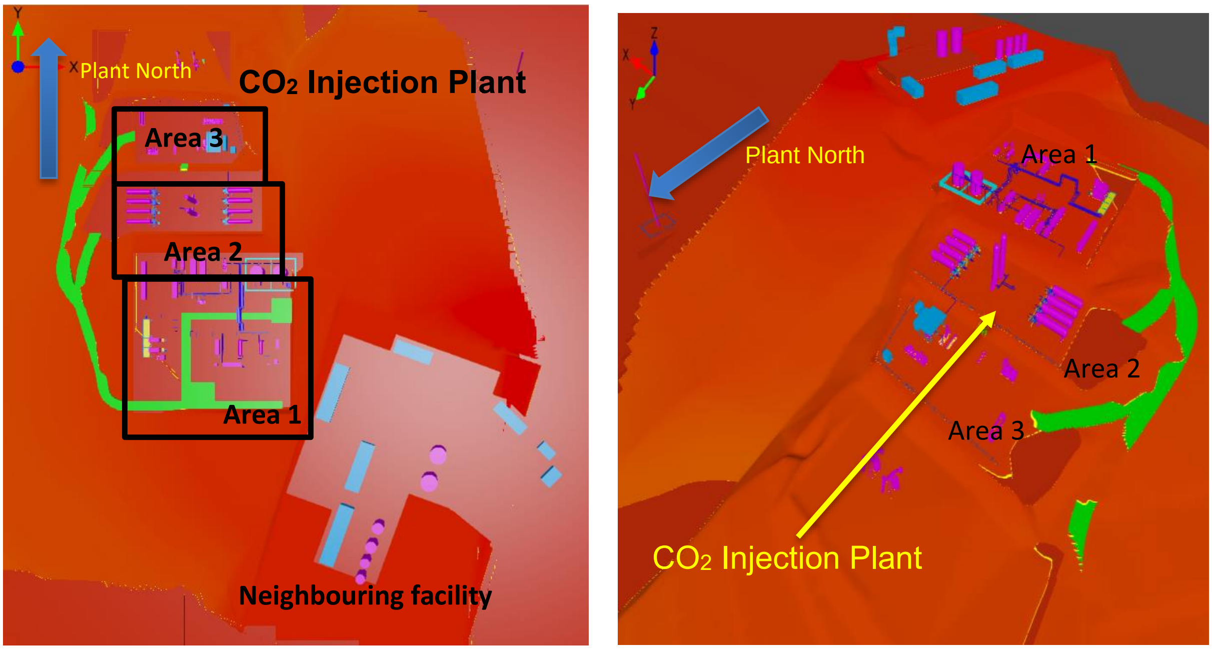

Figure 2 FLACS geometry model showing 3 areas in the facility (left: top view, right: isometric view)

Figure 2 shows the aerial view of planned CCUS pilot test facility at Changqing. Top view showing area divisions and neighbouring facility (left). Illustration of ground contour variation between different areas in the facility is illustrated on the right figure showing that Area 1 is the highest elevation in the facility and Area 3 is the lowest. The neighbouring facility is slightly higher than Area 1. It is noteworthy to say that the facility is slightly inclined clockwise relative to the true north.

The leak location in Area 1 is chosen to study the effect of large equipment parallel to the leak and wind direction as well as the variation of ground elevation to the CO_2 dispersion extent as shown in Figure 3.

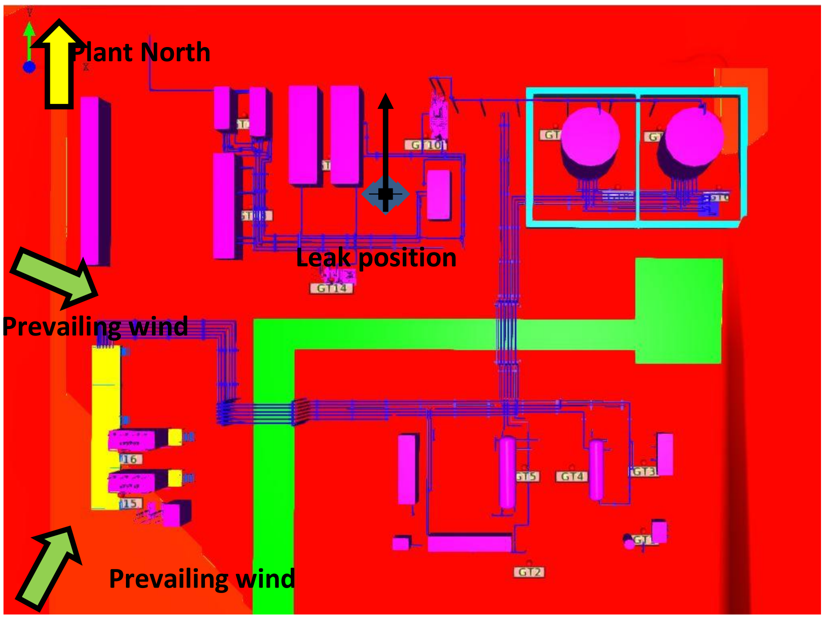

Figure 3 Leak position and direction for CO_2 dispersion simulation in Area 1

Figure 4 shows leak position and leak direction in Area 2 for CO_2 dispersion simulation to study the effect of different elevation and the present of large equipment perpendicular to leak and wind direction. Moreover, the long equipment on the left in the figure were added as part of the project expansion.

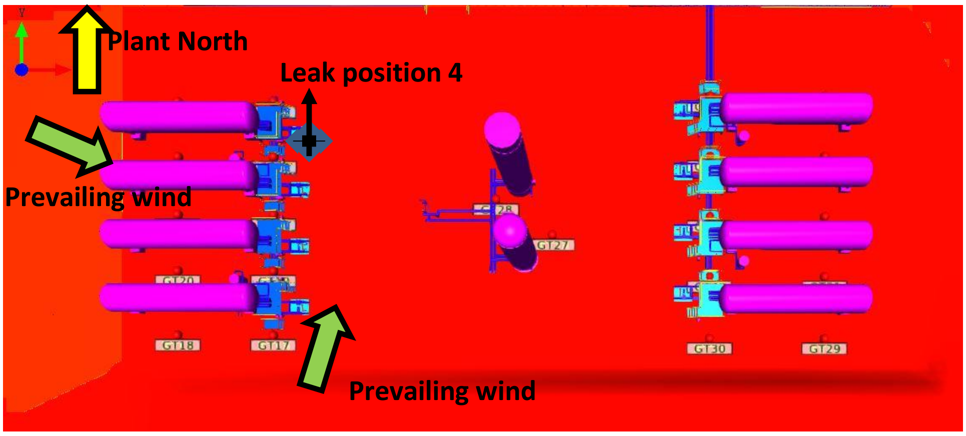

Figure 4 Leak position and direction simulated in Area 2

Figure 5 illustrates the leak position and leak direction in Area 2 for CO_2 dispersion simulation to study the effect of different elevation and the present of small equipment to the CO_2 dispersion extent.

Figure 5 Leak position and leak direction in Area 3 for CO_2 dispersion simulation

Area 2 is at slightly lower elevation compared to Area 1. This area comprises compression equipment which contains CO_2 in the form of liquid in its stream and the leak rate of 52 kg/s from small piping full bore rupture (34mm) is used in the simulations considering higher pressure and lower temperature of CO_2. The wind speed and wind directions are similar with Area 1.

Area 3 is also located at the elevation below the elevation of Area 2. This area includes injection pump and is also containing CO_2 in the liquid form. The leak rate, wind speed and wind directions are similar with the other areas.

The simulated scenarios performed are summarized in Table 1.

Table 1 List of simulated scenarios in each area at CCUS facility

Area	Storage Pressure and Temperature	Hole Size (mm)	Leak Rate	Initial Phase	Ambient Temp (oC)	Wind Direction (from)
1	2.7MPa, 40°C	76	3	Gas	37.7°C (maximum), 8.8°C(average)	S (prevailing), W(prevailing)
2	2.5MPa, -26°C	38	52	Liquid	37.7°C (maximum), 8.8°C(average)	S (prevailing), W(prevailing)
3	2.5MPa, -26°C	38	52	Liquid	37.7°C (maximum), 8.8°C(average)	S (prevailing), W(prevailing)

Simulations Result

An example of CO_2 dispersion contours from FLACS dispersion simulation for several concentration ranges in the case of southerly wind is illustrated in Figure 6.

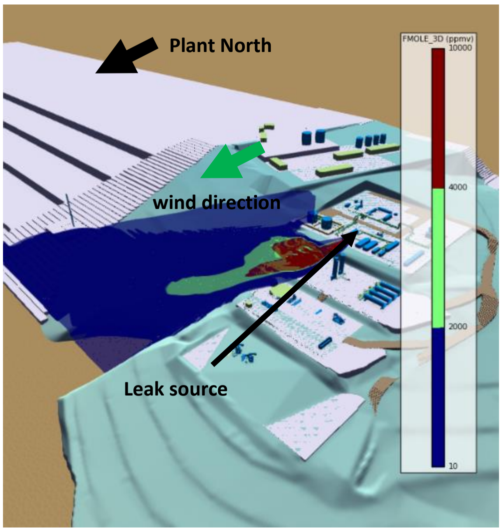

Figure 6 Example of CO_2 dispersion contours from FLACS simulation results

The CO_2 dispersion extent result from FLACS simulation was compared to FRED simulation for several concentration levels and is shown in Figure 7.

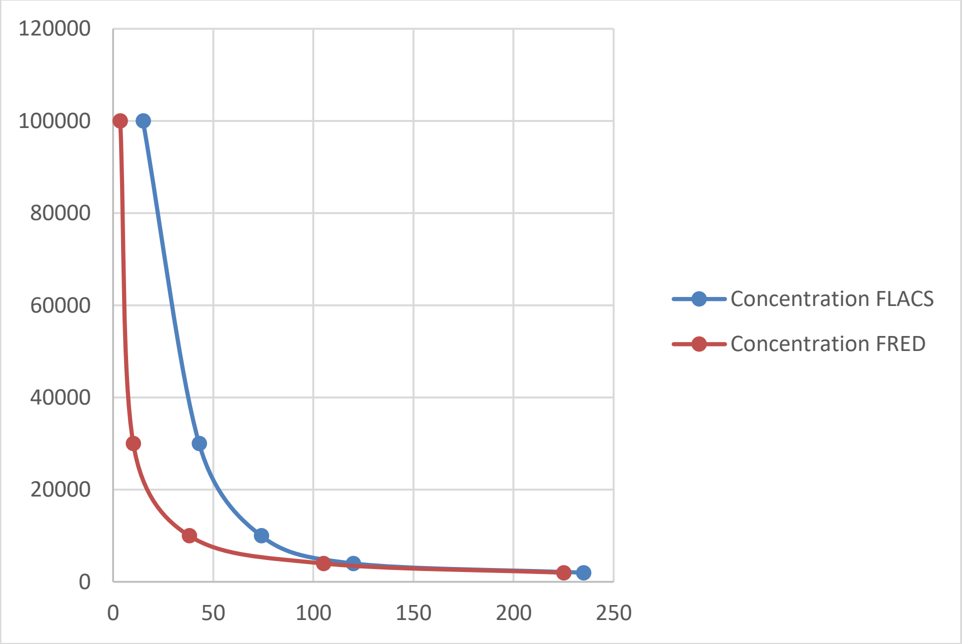

Figure 7 CO_2 dispersion concentrations distances from FLACS and FRED simulations (Area 1, 37.7°C ambient temperature)

From the graph, the dispersion extents from FLACS simulation are much longer compared to FRED results for some high concentrations ranges. The effect of turbulence caused by the long and large equipment parallel to the wind and leak direction made the CO_2 dispersion extents longer than the open space for concentrations up to 10,000ppm. The dense gas behaviour of CO_2 is also affecting the dispersion extent which tends to follow the ground contour below the leak source location. For Area 2, the CO_2 dispersion extents from FLACS and FRED for the case of southerly wind are also compared in Figure 8. From the simulations, the CO_2 dispersion extents are slightly longer compared to simulations without obstructions with FRED. However, the differences are not as long as the dispersion extent in Area 2 due to the absence of long equipment parallel to the wind and leak direction.

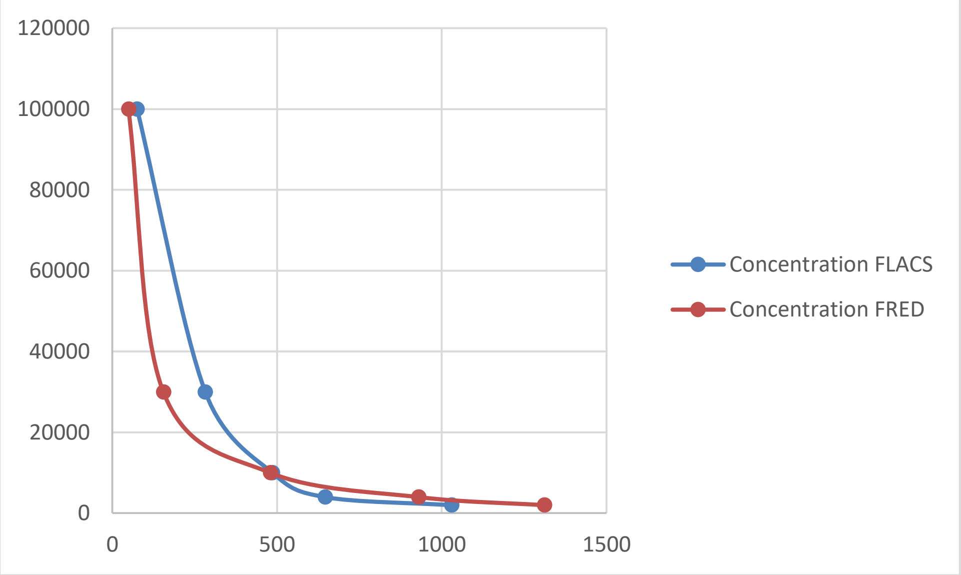

Figure 8 CO_2 dispersion concentrations distances from FLACS and FRED simulations (Area 2, 37.7°C ambient temperature)

In Area 3, similar comparison is provided in Figure 9.

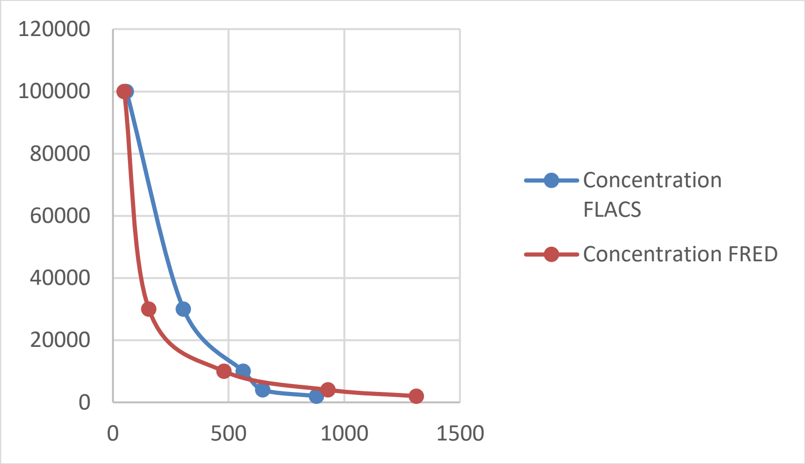

Figure 9 CO_2 dispersion concentrations distances from FLACS and FRED simulations (Area 3, 37.7°C ambient temperature)

The dispersion simulations were also conducted with the wind direction toward the neighbouring facility. One of the worst simulation results is illustrated in Figure 10 which shows the CO_2 dispersion concentration extents mapped onto surface from leak at Area 1. From the simulation, it is shown that the CO_2 concentration up to 2000ppm almost completely engulfs the neighbouring facility. The higher ground elevation of the neighbouring facility made the higher concentration of CO_2 dispersion could not reach its location.

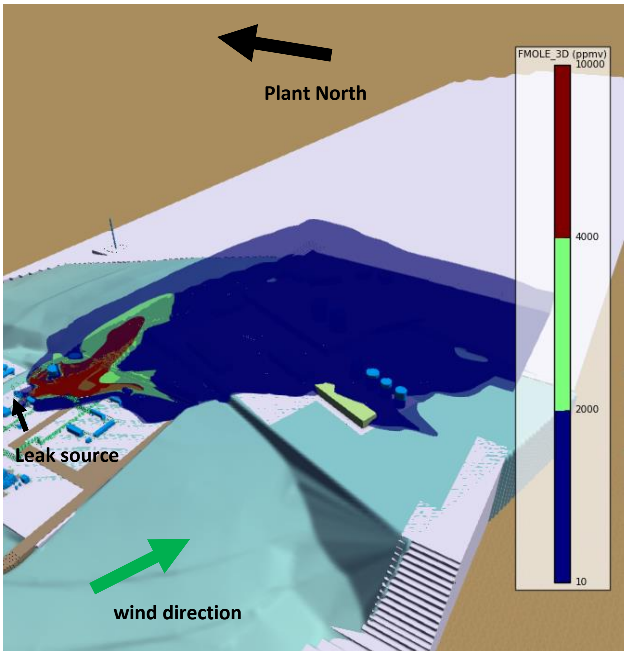

Figure 10 Illustration of the worst scenario with wind direction from West in Area 2

The CO_2 dispersion simulations were also conducted using colder ambient temperature (average in the facility location). For this cold ambient temperature, the simulations results for each area are provided in Figure **11**, Figure **12** and Figure 13, respectively.

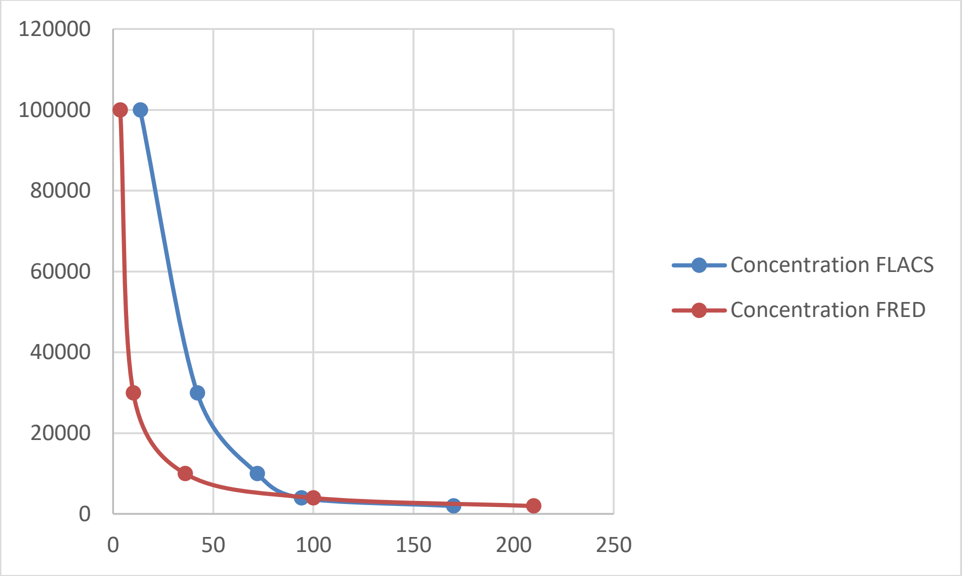

Figure 11 CO_2 dispersion concentrations distances from FLACS and FRED simulations (Area 1, 8.8°C ambient temperature)

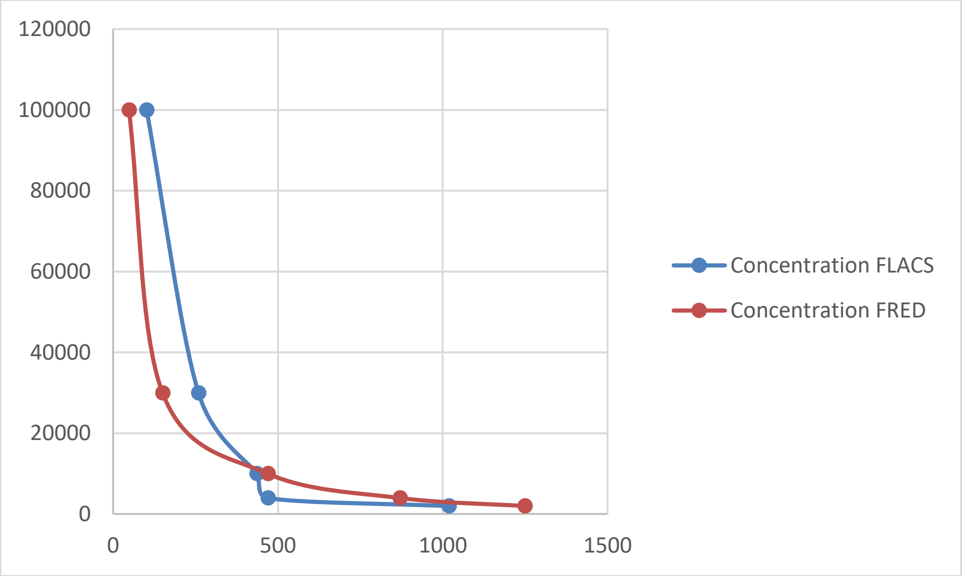

Figure 12 CO_2 dispersion concentrations distances from FLACS and FRED simulations (Area 2, 8.8°C ambient temperature)

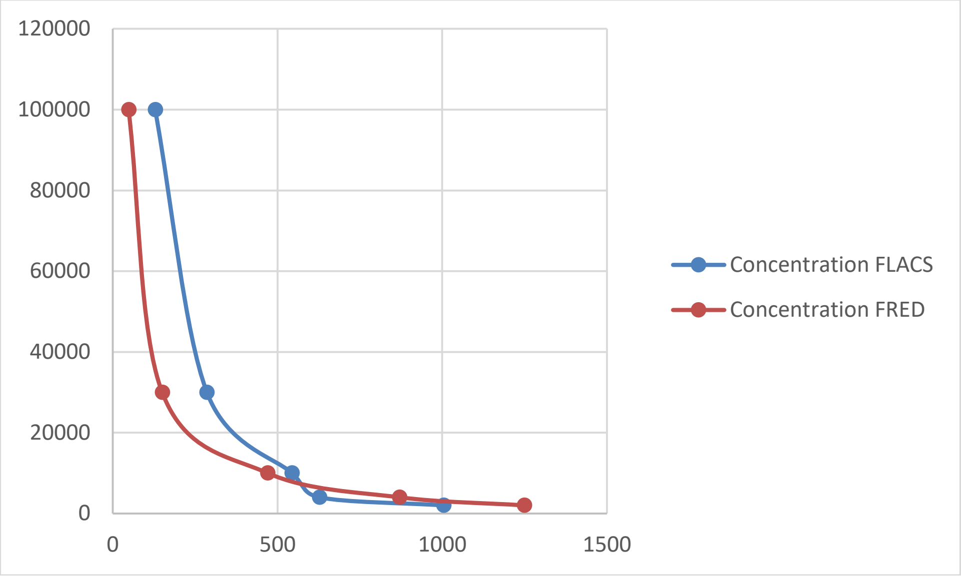

Figure 13 CO_2 dispersion concentrations distances from FLACS and FRED simulations (Area 3, 37.7°C ambient temperature)

The simulations results show that colder temperature made the CO_2 dispersion extents slightly shorter compared to high temperature due to density changes. The colder temperature tends to cause the CO_2 denser/heavier resulting in the shorter dispersion extents.

Conclusions and Recommendations

The CO_2 dispersions simulations in the CCUS facility have been performed to simulate the effect of varied ground elevations as well as the presence of large equipment around the release points. Both FRED and FLACS used release rates that were calculated using the Bernoulli equation which was found to provide reasonable predictions of the flow rate for the releases conditions considered here.

For the simulated scenarios performed, the terrain contours as well as large equipment surrounding the leak locations had some effects on the CO_2 dispersion distance particularly for high concentrations up to 10,000 ppm. For lower concentrations, the ground contours seem to give minimum effect to the dispersion extent.

For simulation having wind direction toward the neighbouring facility, the CO_2 concentration reached up to 2000ppm engulfing the facility. The CO_2 dispersion concentration in the neighbouring facility resulting from accidental release at the CCUS facility was not reaching the concentration of concern (10,000 by standard).

From the simulations, the cold ambient temperature made the CO_2 dispersion extent slightly lower for all areas compared to the simulations using relatively hotter ambient temperature.

The effect of varied ground contours and the presence of large equipment/piping should be validated against experiment to study the suitable turbulence models in 3D CFD tools.

In cases where CO_2 is stored or transported in its liquid phase, the two-phase outflow model should be used instead to model the expansion and flashing as well as rain out.

CO_2 in reality exists in solid phase experiencing sublimation and heat exchange to the surrounding which will affect the dispersion concentration extent. The solid phase model might have to be included in the dispersion modelling to have a more agreement results with the experiment.

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