Investigation of terrain effects on the consequence distance of CO2 released from high-pressure pipelines

Xiong Liu
University of Wollongong, xiong@uow.edu.au

Ajit R. Godbole
University of Wollongong, agodbole@uow.edu.au

Cheng Lu
University of Wollongong, chenglu@uow.edu.au

Guillaume Michal
University of Wollongong, gmichal@uow.edu.au

Follow this and additional works at: https://ro.uow.edu.au/eispapers1

Part of the Engineering Commons, and the Science and Technology Studies Commons

Recommended Citation
Liu, Xiong; Godbole, Ajit R.; Lu, Cheng; and Michal, Guillaume, "Investigation of terrain effects on the consequence distance of CO2 released from high-pressure pipelines" (2017). Faculty of Engineering and Information Sciences - Papers: Part B. 995.
https://ro.uow.edu.au/eispapers1/995

Research Online is the open access institutional repository for the University of Wollongong. For further information contact the UOW Library: research-pubs@uow.edu.au
Investigation of terrain effects on the consequence distance of CO2 released from high-pressure pipelines

Abstract
As part of Carbon Capture and Storage (CCS) projects, Carbon Dioxide (CO₂) is usually transported via pipelines from source to sequestration location. Ensuring the safety of the operation is of great importance, as CO₂ is a hazardous substance and an accidental release may have catastrophic consequences. Therefore, a comprehensive understanding of the effects of a CO₂ release from CCS facilities is essential to allow the appropriate safety precautions to be taken. The majority of prior studies that address this topic do so by simulating CO₂ dispersion over a flat horizontal terrain. However, CO₂ pipelines may be deployed near topographically complex locations such as congested industrial or urban areas. The extent to which the complexity of the terrain may affect the area affected by an accidental release has not been explored in detail. In this paper, we present Computational Fluid Dynamics (CFD) models for the prediction of atmospheric dispersion of CO₂ over complex terrains, in order to evaluate the ‘consequence distance’ relating to accidental CO₂ releases from high-pressure pipelines. The CFD model is validated against the results of a heavy gas dispersion experiment carried out at Thorney Island. Simulations of CO₂ dispersion over seven types of complex terrain are carried out, considering ‘full-bore’ rupture of a pipeline carrying a pre-combustion CO₂ mixture. The influence of different terrain features on the consequence distance is studied. In addition, the dispersion of a (CO₂ + H₂S) mixture is simulated to investigate the threshold value of the fraction of Hydrogen Sulphide (H₂S) for which the hazardous effects of H₂S become significant for a release over complex terrains.

Disciplines
Engineering | Science and Technology Studies

Publication Details

This journal article is available at Research Online: https://ro.uow.edu.au/eispapers1/995
Investigation of terrain effects on the consequence distance of CO$_2$

released from high-pressure pipelines

Xiong Liu, Ajit Godbole, Cheng Lu*, Guillaume Michal

School of Mechanical, Materials and Mechatronic Engineering, University of Wollongong, NSW 2522, Australia

Abstract

As part of Carbon Capture and Storage (CCS) projects, Carbon Dioxide (CO$_2$) is usually transported via pipelines from source to sequestration location. Ensuring the safety of the operation is of great importance, as CO$_2$ is a hazardous substance and an accidental release may have catastrophic consequences. Therefore, a comprehensive understanding of the effects of a CO$_2$ release from CCS facilities is essential to allow the appropriate safety precautions to be taken. The majority of prior studies that address this topic do so by simulating CO$_2$ dispersion over a flat horizontal terrain. However, CO$_2$ pipelines may be deployed near topographically complex locations such as congested industrial or urban areas. The extent to which the complexity of the terrain may affect the area affected by an accidental release has not been explored in detail. In this paper, we present Computational Fluid Dynamics (CFD) models for the prediction of atmospheric dispersion of CO$_2$ over complex terrains, in order to evaluate the ‘consequence distance’ relating to accidental CO$_2$ releases from high-pressure pipelines. The CFD model is validated against the results of a heavy gas dispersion experiment carried out at Thorney Island. Simulations of CO$_2$ dispersion over seven types of complex terrain are carried out, considering ‘full-bore’ rupture of a pipeline carrying a pre-combustion CO$_2$ mixture. The influence of different terrain features on the consequence distance is studied. In addition, the dispersion of a (CO$_2$ + H$_2$S) mixture is simulated to investigate the threshold value of the fraction of Hydrogen Sulphide (H$_2$S) for which the hazardous effects of H$_2$S become significant for a release over complex terrains.

Keywords: Carbon Capture and Storage; CO$_2$ pipeline; CO$_2$ dispersion; CFD modelling; Complex terrain

* Corresponding author. Tel.: +61-2-4221-4639; Fax: +61-2-4221-5474.
1. Introduction

It is widely acknowledged that global warming is mainly due to excessive concentrations of Carbon Dioxide (CO$_2$) in the atmosphere. Such excessive concentrations result in part from CO$_2$ emissions from fossil fuel-powered electricity generation, vehicular exhausts, depleting forest covers, etc. Currently, power stations contribute about 40% of the total anthropogenic generation of CO$_2$. If the current trends continue, it is expected that the emissions will triple by 2050 (Seevam et al., 2008). The Carbon Capture and Storage (CCS) technique is considered to be the most effective and economical way to reduce the excessive CO$_2$ concentrations. The technique is expected to potentially reduce 19% of CO$_2$ emissions into the atmosphere by 2050 (Global CCS Institute, 2009; Mazzoldi et al., 2012). In the CCS chain, it is preferred that CO$_2$ is transported from source to storage location using high-pressure pipelines, especially when transporting large quantities of CO$_2$ over long distances (Liu et al., 2014b; Metz et al., 2005). In the near future, extensive networks of CO$_2$ pipelines may be constructed to facilitate the increasing application of CCS (Liu et al., 2014b; Mazzoldi et al., 2012).

In the deployment of CO$_2$ pipelines, safety is of great importance because CO$_2$ is a toxic gas as well as an asphyxiant that can lead to coma or even death. For humans, the short term exposure limit of 15,000 ppm is used as a guide for maximum allowable exposure (HSE, 2005). Exposure levels above 10% (100,000 ppm) will lead to rapid loss of consciousness. Further exposure at higher concentrations leads to asphyxiation (Standards Australia, 2012). If an accident occurs leading to release of CO$_2$ from the pipeline, the consequences may be catastrophic for human and animal populations. Therefore, in order to provide sufficient separation between CO$_2$ pipelines and residential areas, it is necessary to obtain a better understanding of the consequences of a CO$_2$ release when an accident occurs. This requires a reliable and accurate atmospheric dispersion model that takes into account various meteorological and terrain conditions.

Atmospheric dispersion models generally fall into three categories (Koopman et al., 1989; Liu et al., 2015a): (1) Gaussian models; (2) ‘Similarity-profile’ models and (3) Computational Fluid Dynamics (CFD) models.
Both Gaussian and similarity-profile models can provide quick estimates and are widely used in the industry. However, these models have a limited range of validity since they cannot capture the effects of obstacles and complex terrains. On the contrary, CFD models use more detailed mathematical descriptions of the laws of nature (conservation principles) that govern the process of dispersion. CFD models can be set up to solve the equations of fluid mechanics in three spatial dimensions and time, thus enabling an accurate and detailed representation of the flow fields in complicated geometries (Ahmed et al., 2016; Efthimiou et al., 2017; Liu et al., 2015a).

Due to an increasing interest in the application of CCS-related technologies, CFD techniques have been used in CO\textsubscript{2} dispersion simulations. Mazzoldi et al. (2008) simulated the ‘Kit Fox’ CO\textsubscript{2} dispersion experiment (Western Research Institute, 1998) using both CFD and ‘Gaussian plume’ models. They found that CFD models were able to produce better concentration estimations than Gaussian plume models. Gaussian plume models have very limited capabilities of simulating dense gas dispersion, as they are very simple and take no account of the density of the released gases. Liu et al. (2015a) compared the performance of CFD models with a similarity-profile model, SLAB, in the simulation of Kit Fox experiments. It was found that SLAB fared reasonably well. However, CFD models performed much better as indicated by all performance measures. As part of the COOLTRANS research programme (Cooper, 2012), Wareing et al. (2014, 2015, 2016) investigated the near-field CO\textsubscript{2} dispersion using CFD models employing the Reynolds-Averaged Navier-Stokes (RANS) hydrodynamic method with adaptive mesh refinement. Comparison of the simulation results against experimental data showed broad agreement. Investigation of far-field CO\textsubscript{2} dispersion in the COOLTRANS programme was undertaken by Wen et al. (2013, 2016). They simulated the dispersion of CO\textsubscript{2} released from a vertical vent as well as from a horizontal ‘shock tube’ test rig using the open source CFD code OpenFOAM (Wen et al., 2013). The results of the CFD simulations were found to agree well with measurements. In addition, they developed a dedicated CFD solver, CO\textsubscript{2}FOAM, within the framework of OpenFOAM, specifically for the dispersion of CO\textsubscript{2} from pipeline releases. Simulation using CO\textsubscript{2}FOAM was validated against experimental measurements in Case Study 3 in the COOLTRANS programme, in which CO\textsubscript{2} was released through a puncture in a buried pipe (Wareing et al., 2016). Xing et al. (2013) performed CFD simulations of vertical CO\textsubscript{2} releases from a circular source. Various turbulence models were
tested and it was found that the results predicted using the $k-\varepsilon$ and shear stress transport (SST) $k-\omega$ models were in better agreement with measurements. Liu et al. (2014b) simulated the dispersion of CO$_2$ released from high-pressure pipelines using the commercial CFD code ANSYS Fluent. The models for the prediction of source strength as well as the far-field dispersion were validated by simulating CO$_2$ dispersion experiments conducted by DNV BP (Witlox, 2012). In this work, Liu et al. carried out a comparison between CFD models and a similarity-profile model, Phast UDM. It was found that CFD models performed well in predicting the time-varying CO$_2$ concentration pattern, but Phast UDM tended to considerably under-predict the concentration. The above studies focused on validation of the model rather than application of the model in a realistic release scenario. The source strength (mass flow rate specified at the inlet to the dispersion domain) used in the simulation was hypothetical or suggested by small-scale release experiments, which may not reflect a realistic release adequately. To evaluate the possible consequences of a realistic CO$_2$ release, Mazzoldi et al. (2012) modelled full-bore ruptures of pipelines of various sizes carrying CO$_2$ mixtures. The CFD dispersion code ‘fluidyn-PANACHE’ was used to perform the simulations and ‘consequence distances’ corresponding to specific CO$_2$ concentration levels were obtained. Liu et al. (2015b) studied the consequence distances of full-bore ruptures of CO$_2$ pipelines carrying pre-combustion and post-combustion CO$_2$ mixtures, with the pipe Internal Diameter (ID) ranging from 400 to 800 mm, and stagnation pressure ranging from 10 to 20 MPa. To achieve a conservative prediction of the consequence distance, the release direction was considered horizontal and the dispersion source was assumed as a gaseous CO$_2$ mixture. These studies give a clear picture of the area which may be affected when an accident occurs. However, in their studies, only a flat horizontal terrain was considered in the dispersion modelling, so that how and to what extent a complex terrain may affect the consequence distance remained unexplored.

In recent years, due to the enhanced availability of computing resources, CFD techniques have also been used in the studies of hazardous gas dispersion over complex terrains. Typically, dispersion patterns over a flat horizontal terrain with an isolated building (Blocken et al., 2008; Gousseau et al., 2011; Tominaga and Stathopoulos, 2009) or a fence (Tomas et al., 2015) have been studied. These studies were usually intended to validate the performance of CFD techniques in modelling pollutant dispersion around obstacles. Further studies include dispersion over a group of buildings representing urban areas (Bijad et al., 2016; Kumar et
al., 2015; Liu et al., 2016; Nazridoust and Ahmadi, 2006; Stabile et al., 2015; Wingstedt et al., 2017). In such terrains, pollutants can be trapped in the street ‘canyons’ formed by the buildings, and also in the ‘wakes’ of the buildings. Research has been carried out on the influence of pollutant transport modelling and the influence of inflow conditions, canyon configurations, and building dimensions. As the goal of gas dispersion modelling is to predict dispersion in an actual environment, studies of dispersion around actual building complexes or over real terrains are critical. In several studies, CFD techniques have been applied to gas dispersion around actual groups of building in an industrial environment (Efthimiou et al., 2017; Michioka et al., 2013; Pontiggia et al., 2011; Tseng et al., 2006), and reasonable qualitative outcomes have been obtained. Some studies take more complex features of the terrain into account, using hypothetical topographical elements (Meroney, 2012) or using topographical data of real sites to generate computational meshes that conform to the terrain (Scargiali et al., 2005; Woolley et al., 2014). It seems that the current techniques are capable of modelling CO$_2$ dispersion over complex terrains. Although studies have already been carried out to evaluate the impact area on a flat terrain due to releases from CO$_2$ pipelines, studies about the influence of particular terrain features on the consequence distance are still very limited. However, such information is likely to be very helpful for estimating the required separation between CO$_2$ pipelines and residential areas.

In this paper, CFD models designed to simulate CO$_2$ dispersion over complex terrains are presented, with the objective of evaluating the effects of particular terrain features on the consequence distances. The basic numerical methods employed are validated through simulations of trials in the Thorney Island experiment involving large-scale dispersion of a heavy gas (Davies and Singh, 1985). CO$_2$ dispersion over seven types of terrain is investigated, five of these simulating basic terrain features, one representing an urban landscape, and one modelling an undulating real terrain. The influence of the complex terrain on the consequence distance is then discussed. In addition, as Hydrogen Sulphide (H$_2$S) is a common component in CO$_2$ mixtures in CCS operations and is harmful even at very low concentration levels, the effects of terrain features on the dispersion of H$_2$S in a CO$_2$ mixture are also studied.

2. Numerical method

In this study, the CFD code ANSYS Fluent was used to carry out the simulations, which utilises the Finite
Volume Method (FVM) to discretise the governing differential equations of fluid flow. The method involves solving the conservation equations of mass, momentum, and energy based on the RANS approach (ANSYS, 2011; Versteeg and Malalasekera, 2007):

**Mass:**
\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \bar{v}) = 0
\]  
(1)

**Momentum:**
\[
\frac{\partial (\rho \bar{v})}{\partial t} + \nabla \cdot (\rho \bar{v} \bar{v}) = -\nabla p + \nabla \cdot (\tau) + \rho g
\]  
(2)

**Energy:**
\[
\frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\rho E + p) = \nabla \cdot \left[ k_{\text{eff}} \nabla T - \sum_i h_i \frac{\rho}{\rho + \tau} + \rho \nabla \cdot \bar{J}_i \right]
\]  
(3)

with the auxiliary equations:
\[
\tau = \mu \left[ (\nabla \bar{v} + (\nabla \bar{v})^T) - \frac{2}{3} \nabla \cdot \bar{v} I \right]
\]
\[
E = h - \frac{p}{\rho} + \frac{v^2}{2}
\]

where \( \rho \) is the density, \( t \) the time, \( \bar{v} \) the velocity vector, \( p \) the pressure, \( \tau \) the stress tensor, \( \rho g \) the gravitational body force per unit volume, \( \mu \) the dynamic viscosity, \( I \) the unit tensor, \( E \) the total energy, \( k_{\text{eff}} \) the effective thermal conductivity, \( T \) the temperature, \( h_i \) the specific enthalpy of species \( i \), and \( J_i \) the diffusion flux of species \( i \).

The local mass fraction of each species is predicted by solving a convection-diffusion equation for each species. This conservation equation is given by (ANSYS, 2011):
\[
\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho \bar{J}_i) = -\nabla \cdot \bar{J}_i + R_i
\]  
(4)

where \( Y_i \) is the mass fraction of species \( i \), \( \bar{J}_i \) the mass diffusion vector, and \( R_i \) the net rate of production of species \( i \). The mass diffusion vector is given by:
\[
\bar{J}_i = -\left( \rho D_{i,m} + \frac{\mu_i}{S_{ci}} \right) \nabla Y_i - D_{T,i} \frac{\nabla T}{T}
\]  
(5)

where \( D_{i,m} \) the mass diffusion coefficient for species \( i \), \( S_{ci} \) the turbulent Schmidt number and \( D_{T,i} \) the thermal diffusion coefficient for species \( i \).
Turbulence was modelled using the extensively validated $k$-$\varepsilon$ model. This model introduces two transport equations for turbulent kinetic energy $k$ and eddy dissipation rate $\varepsilon$ respectively (ANSYS, 2011; Versteeg and Malalasekera, 2007):

\[
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_j} (\rho k u_j) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon \quad (6)
\]
\[
\frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_j} (\rho \varepsilon u_j) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{1\varepsilon} \frac{\varepsilon}{k} G_k - C_2 \varepsilon \frac{\varepsilon^2}{k} \quad (7)
\]

where $u_i$ is the velocity component along the $x_i$ direction, $t$ the time, $\mu$ the dynamic viscosity, $\mu_t$ the turbulent dynamic viscosity ($\mu_t = c_{f}k^{2}/\varepsilon$), and $G_k$ the generation of turbulent kinetic energy per unit volume due to the mean velocity gradients.

The prevailing wind at the site being considered affects the dispersion patterns of a pollutant released near ground level. Friction and other features of the ground surface lead to the formation of an ‘atmospheric boundary layer’ (ABL) that affects the wind velocity profile at the inlet to the dispersion domain. Here, the wind velocity profile is described using a power law correlation (Peterson and Hennessey, 1978):

\[
u = u_r \left( \frac{z}{z_r} \right)^{\alpha} \quad (8)
\]

where $u$ is the wind velocity at height $z$, $u_r$ a reference wind velocity measured at the reference height $z_r$, and $\alpha$ is the ‘wind shear exponent’. This description of the wind velocity profile allows the construction of a shorter computational domain upstream of the release location.

It is also necessary to define appropriate turbulence levels at the wind inlet to maintain appropriate levels of turbulent kinetic energy and the eddy dissipation rate within the computational domain. In this study, $k$ and $\varepsilon$ profiles recommended by Han et al. (2000) were employed:

\[
k = 6u^2 \quad (9)
\]
\[
\varepsilon = \frac{u^3}{Kz} \left( 1.24 + 4.3 \frac{z}{L} \right) \quad (10)
\]

where $u_r$ is the ‘friction velocity’, $L$ the ‘Monin-Obukhov’ length, and $K$ the von Karman constant ($\approx 0.4$).
Trial 29 of the Thorney Island field experiment Phase II was simulated to validate the numerical methods adopted. Three phases of the Thorney Island tests (Davies and Singh, 1985) were designed to study the dispersion of dense gas clouds which might result from catastrophic releases. The objective of Phase II was to study the dispersion of heavy gases over a complex terrain. In Trial 29, the gas source was a cylindrical container 14 m in diameter, 13 m in height with a total volume of about 2000 m³, made from flexible material, which was triggered to collapse to the ground at the beginning of the trial. This physically simulated an ‘instantaneous’ release. The composition of the released gas was 68.4% Nitrogen ($N_2$) and 31.6% Freon 12, with a relative density of 2.0. The complexity in the terrain consisted of an obstacle used to mimic a cubical building measuring 9 m × 9 m × 9 m. This was constructed of plastic sheets attached to a wooden frame. In Trial 29, the obstacle was placed upwind from the source, with a separation of 20 m from the rear face edge of the cube to the upwind surface edge of the cylindrical source, as shown schematically in Fig. 1.

![Fig. 1. Schematic diagram of Thorney Island Trial 29](image)

In Trial 29, the gas concentration was monitored on the leeward face at a height of 0.4 m. Fig. 3 shows the measured and predicted gas concentration time histories. Clearly, the numerical model showed good performance. The maximum concentration was successfully predicted with reasonable deviation. The time variations in the concentrations at the monitor point are also well captured by the simulation. This indicates that the adopted methods are capable of predicting the heavy gas dispersion in a relatively complex environment.
3. Terrain types investigated

CO₂ dispersions over seven types of terrain were investigated. Five of them were used to study the effects of basic topographical elements (ramp, ridge, trench) on the dispersion. As shown in Figs. 3 and 4, Terrain A features a short backward-facing ramp; Terrain B a short forward-facing ramp; Terrain C is a narrow ‘ridge’ consisting of a forward-facing ramp and a backward facing ramp; Terrain D is a narrow ‘trench’ consisting of a backward facing ramp and a forward-facing ramp; and Terrain E features a long slope. The terrain elements stretch laterally across the terrain and are assumed to be perpendicular to the release direction.
depth of the terrain element $d$ in Terrains A to D, and the inclination angle $\alpha$ in Terrain E can be varied to investigate their effects. For all these simulations, the release source was placed 50 m upwind from the terrain element. Also, for conservatism that maximises consequence distances, horizontal releases 2 m above ground level were assumed.

![Fig. 4. Terrain E simulating a long slope (distances in metres)](image)

Terrain F was used to simulate dispersion over an urban area. As shown in Fig. 5, to represent an urban area, regular arrays of ‘blocks’ were employed to mimic buildings and streets. Here, two subsidiary dispersion scenarios were considered, with Terrain F1 simulating a release directly facing a street canyon, and Terrain F2 simulating a release directly facing a building wall. All the buildings were modelled as cubes, with an edge length of 10 m. The space between two buildings in both the longitudinal and lateral directions is set as 10 m. In Terrain F1, the buildings were arranged in 4 rows and 4 columns (Fig. 5a), while in Terrain F2, the buildings were arranged in 5 rows and 4 columns (Fig. 5b). The release source was placed 50 m upwind from the first row of buildings.
Fig. 5. Terrain F mimicking urban landscapes (dimensions in metres)

Fig. 6 shows Terrain G, a real terrain located in Golspie, NSW, Australia. It covers an area of 1000 m × 850 m. The topographic data of Terrain G was obtained using Google Maps. The data was then imported into NX Unigraphics to generate the terrain surface. Based on this, the computational domain containing the undulating terrain could be set up. The maximum altitude difference over the terrain is about 90 m.

4. Computational domains and boundary conditions

The overall features of the computational domains used to simulate dispersion over Terrain A to Terrain F are shown in Fig. 7. For clarity, the terrain features (ramps, etc) are not shown in the figure. To minimise the
effects of boundaries, the computational domain was chosen as 1500 m in length (along the wind direction), 600 m in breadth and 200 m in height. As mentioned in Section 3, a horizontal release parallel to the wind direction was considered to account for the worst case (farthest downstream reach of the cloud).

In this study, the release rate corresponding to a ‘full-bore’ rupture of a 50 km long pipeline with 400 mm ID was used for the dispersion simulation. The fluid carried by the pipeline is a typical pre-combustion CO₂ mixture for Australian conditions (Liu et al., 2014a), with 95.7% CO₂, 2% Methane (CH₄), 1% Hydrogen (H₂), 0.43% N₂, Oxygen (O₂) & Argon (Ar), and 0.04% Carbon Monoxide (CO). The stagnation pressure and temperature were assumed to be 15 MPa and 20°C respectively. Thus the nominal release rate of a full-bore rupture for dispersion simulation can be assumed as 3833 kg s⁻¹ (Liu et al., 2014a). In the present study, the possible formation of solid CO₂ particles in the source was ignored. Thus in the subsequent simulations, the source fluid was assumed to be in a gaseous state.
The computational domain was discretised in the form of hexahedral cells as shown in Fig. 8, with refinement near the ground and the terrain element surfaces, and also around the CO$_2$ source. Before the final simulations, a grid independence study was carried out to ensure that the mesh has negligible impact on the results. For Terrain A to Terrain E, the grid contains about 2 million cells, while for Terrain F, the grid contains over 4 million cells due to the refinement near the building surfaces.

Typically, seven boundary conditions were required for the computational domain (Fig. 7): (1) CO$_2$ inlet, (2) top, (3) outlet, (4) left side, (5) right side, (6) wind inlet, and (7) ground and terrain element surface. The ‘CO$_2$ inlet’ was specified in terms of a mass flow rate. The ‘top’ and two ‘side’ boundaries were defined as impermeable ‘symmetry’ surfaces. The outlet was set as a pressure boundary with ambient pressure and temperature. The power law correlation described by Eq. (8) was used to define the wind inlet. The wind speed was assumed to be 2 m s$^{-1}$ at 10 m height. The ground and terrain element surface boundaries were defined as a no-slip, isothermal wall with temperature equal to the ambient temperature.

Fig. 9 shows the computational domain and surface mesh for Terrain G. To accommodate the 90 m elevation difference in the ground surface, the overall height of the computational domain was chosen to be 300 m. The computational domain was also discretised in the form of hexahedral cells, with refinement
5. Results and discussion

In the following analysis of the consequence distance for CO₂ releases, two CO₂ concentration levels were considered: 50,000 ppm and 80,000 ppm. According to the Australian Standard (Standards Australia, 2012), a CO₂ concentration level of 50,000 ppm will result in ‘very rapid breathing, confusion and vision impairment’, while that of 80,000 ppm will cause ‘loss of consciousness after 5–10 minutes’. The downstream consequence distance was determined as the maximum distance away from the pipe rupture contained by two concentration envelopes corresponding to these two concentration levels.

In order to evaluate the effects of terrain type on the consequence distance, CO₂ dispersion over a flat featureless terrain was simulated in advance. Fig. 10 shows the obtained CO₂ envelope for a CO₂ concentration of 50,000 ppm. The corresponding consequence distances for concentration levels of 80,000 ppm and 50,000 ppm are 230 m and 324 m respectively.

![50,000 ppm CO₂ envelope – flat terrain](image)

5.1 Dispersion over flat terrain with basic topographical elements (Terrains A to E)

Table 1 shows the consequence distances of the dispersion over Terrain A with a backward facing ramp. Two cases were simulated. One is with a ramp depth of 2 m and the other with ramp depth of 4 m. The consequence distances were compared with those of dispersion over a flat terrain. It was found that the backward facing ramp reduces the consequence distance. For the case with a ramp depth of 2 m, the consequence distances for 80,000 ppm and 50,000 ppm envelopes are reduced by 3% and 2.5% respectively. Larger ramp depth results in greater reduction in the consequence distance. For the case with a ramp depth of
4 m, the consequence distances for 80,000 ppm and 50,000 ppm envelopes are reduced by 6% and 5% respectively.

<table>
<thead>
<tr>
<th>Concentration (ppmv)</th>
<th>Flat terrain (m)</th>
<th>Terrain A - 2 m step (m)</th>
<th>Deviation</th>
<th>Terrain A - 4 m step (m)</th>
<th>Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>80,000</td>
<td>230</td>
<td>223</td>
<td>-3%</td>
<td>216</td>
<td>-6%</td>
</tr>
<tr>
<td>50,000</td>
<td>324</td>
<td>316</td>
<td>-2.5%</td>
<td>308</td>
<td>-5%</td>
</tr>
</tbody>
</table>

Fig. 11 shows the CO$_2$ envelope of 50,000 ppm concentration for dispersion over Terrain A. Compared to dispersion over flat terrain (Fig. 10), it is found that the envelope shape was changed due to the backward facing ramp. The main reason for the reduction in the consequence distance may be the expansion of downwind dispersion space due to the ramp, resulting in a higher rate of transport of CO$_2$ after passing the ramp. Also, the recirculation region caused by the ramp will contribute to curtail the downstream spread. In addition, the increase in the height of the envelope when the cloud passes the backward facing ramp may also contribute to the reduction in consequence distance.

Table 2 shows the consequence distances of the dispersion over Terrain B with a forward facing ramp. As in the earlier case, the ramp depths considered were 2 m and 4 m. It was found that the forward facing ramp results in more significant reduction in the consequence distance. For the case with a ramp depth of 2 m, the consequence distances for 80,000 ppm and 50,000 ppm envelopes are reduced by 5.7% and 3.7% respectively, while for the case with ramp depth of 4 m, the consequence distances for 80,000 ppm and 50,000 ppm envelopes are reduced by 13% and 9% respectively.
Table 2 Consequence distances – Terrain B vs flat terrain

<table>
<thead>
<tr>
<th>Concentration (ppmv)</th>
<th>Consequence distance</th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Flat terrain (m)</td>
<td>Terrain B - 2 m step (m)</td>
<td>Deviation</td>
<td>Terrain B - 4 m step (m)</td>
<td>Deviation</td>
</tr>
<tr>
<td>80,000</td>
<td>230</td>
<td>217</td>
<td>-5.7%</td>
<td>200</td>
<td>-13%</td>
</tr>
<tr>
<td>50,000</td>
<td>324</td>
<td>312</td>
<td>-3.7%</td>
<td>295</td>
<td>-9%</td>
</tr>
</tbody>
</table>

Fig. 12. 50,000 ppm CO\(_2\) envelope – Terrain B

Fig. 12 shows the CO\(_2\) envelope of 50,000 ppm concentration. Clearly, the reduction of consequence distance is because of the enhanced lateral spread of the CO\(_2\) cloud when it encounters the forward-facing ramp. It should be noted that the increase in the lateral spread may increase the dispersion area even though the maximum downstream length has decreased.

Table 3 shows the consequence distances of the dispersion over Terrain C with a narrow ridge that combines features of a forward-facing ramp and a backward facing ramp. The heights of the ridge considered were 2 m and 4 m.

Table 3 Consequence distances – Terrain C vs flat terrain

<table>
<thead>
<tr>
<th>Concentration (ppmv)</th>
<th>Consequence distance</th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Flat terrain (m)</td>
<td>Terrain C - 2 m step (m)</td>
<td>Deviation</td>
<td>Terrain C - 4 m step (m)</td>
<td>Deviation</td>
</tr>
<tr>
<td>80,000</td>
<td>230</td>
<td>218</td>
<td>-5.2%</td>
<td>204</td>
<td>-11.3%</td>
</tr>
<tr>
<td>50,000</td>
<td>324</td>
<td>312</td>
<td>-3.7%</td>
<td>297</td>
<td>-8.3%</td>
</tr>
</tbody>
</table>

As shown in Fig. 13, the forward-facing ramp in the protrusion also enhances the lateral spread of the cloud
and cause a reduction of the consequence distance. For the case with a ridge height of 2 m, the consequence distances for 80,000 ppm and 50,000 ppm envelopes are reduced by 5.2% and 3.7% respectively, while for the case with a ridge height of 4 m, the consequence distances for 80,000 ppm and 50,000 ppm envelopes are reduced by 11.3% and 8.3% respectively.

![a. Top view](image1)

![b. Side view](image2)

Fig. 13. 50,000 ppm CO\textsubscript{2} envelope – Terrain C

Table 4 shows the consequence distances of the dispersion over Terrain D with a narrow trench that is made up of a backward facing ramp and a forward-facing ramp. Two trench depths were considered: 2 m and 4 m. The trench also causes a reduction in the consequence distance. For the case with a trench depth of 2 m, the consequence distances for 80,000 ppm and 50,000 ppm envelopes are reduced by 3.5% and 2.5% respectively, while for the case with a trench depth of 4 m, the consequence distances for 80,000 ppm and 50,000 ppm envelopes are reduced by 7% and 5.9% respectively.

There is also a forward-facing ramp in Terrain D, but the magnitude of the consequence distance reduction is not as large as for Terrain B and Terrain C. This is because the CO\textsubscript{2} which encounters the forward-facing ramp is a small part of the cloud sinking into the cavity. Therefore, the enhancement of the lateral spread of the cloud is not as pronounced as in Terrain B and Terrain C, as shown in Fig. 14.

<table>
<thead>
<tr>
<th>Concentration (ppmv)</th>
<th>Consequence distance</th>
<th>Deviation</th>
<th>Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Flat terrain (m)</td>
<td>Terrain D - 2 m step (m)</td>
<td>Deviation</td>
</tr>
<tr>
<td>80,000</td>
<td>230</td>
<td>222</td>
<td>-3.5%</td>
</tr>
<tr>
<td>50,000</td>
<td>324</td>
<td>316</td>
<td>-2.5%</td>
</tr>
</tbody>
</table>
Table 5 shows the consequence of the dispersion over Terrain E, with the consequence distance measured along the slope. The inclination angle of the slope $\alpha$ was assumed as $15^\circ$ and $30^\circ$. It was found that the long slope mostly leads to a reduction in the consequence distance. Larger inclination angle results in larger reduction in the consequence distance. For the case with an inclination angle of $30^\circ$, the consequence distances for 80,000 ppm and 50,000 ppm envelopes are reduced by 36% and 17% respectively.

Table 5 Consequence distances – Terrain E vs flat terrain

<table>
<thead>
<tr>
<th>Concentration (ppmv)</th>
<th>Flat terrain (m)</th>
<th>Terrain E ($\alpha = 15^\circ$) (m)</th>
<th>Deviation</th>
<th>Terrain E ($\alpha = 30^\circ$) (m)</th>
<th>Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>80,000</td>
<td>230</td>
<td>231</td>
<td>0.4%</td>
<td>148</td>
<td>-36%</td>
</tr>
<tr>
<td>50,000</td>
<td>324</td>
<td>308</td>
<td>-5%</td>
<td>269</td>
<td>-17%</td>
</tr>
</tbody>
</table>

As shown in Fig. 15, the heavier-than-air CO$_2$ tends to sink due to gravity as it spreads. Compared to the dispersion over flat terrain, the envelope is thinner in the lateral direction. However, the increase in the space for downwind dispersion due to the slope is significant. Also, there is considerable increase in the height of the envelope. These effects may jointly lead to the reduction in the consequence distance.
Overall, the basic terrain types investigated in this section will mostly result in a reduction of the consequence distance, due to the enhanced lateral spread of the cloud, or an increase in the space for downwind dispersion.

5.2 Dispersion over more complicated terrains (Terrain F and Terrain G)

Table 6 shows the consequence distances of the dispersion over Terrains F1 and F2 representing urban landscapes. For Terrain F1 (source facing a street canyon), the consequence distance is increased by 16.5% and 8.6% for the 80,000 ppm and 50,000 ppm envelopes respectively. On the contrary, the consequence distance for dispersion over Terrain F2 (source facing a building) is reduced by 8% and 7% for 80,000 ppm and 50,000 ppm envelopes respectively.

<table>
<thead>
<tr>
<th>Concentration (ppmv)</th>
<th>Flat terrain (m)</th>
<th>Terrain F1 (m)</th>
<th>Deviation</th>
<th>Terrain F2 (m)</th>
<th>Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>80,000</td>
<td>230</td>
<td>268</td>
<td>16.5%</td>
<td>212</td>
<td>-8%</td>
</tr>
<tr>
<td>50,000</td>
<td>324</td>
<td>352</td>
<td>8.6%</td>
<td>301</td>
<td>-7%</td>
</tr>
</tbody>
</table>

The increase in the consequence distance for dispersion over Terrain F1 is due to the source facing a street canyon (see Fig. 16a). Along the dispersion path, the walls of the buildings form a partial channel, which confines the dispersing cloud and some CO$_2$ is reflected back by the walls. This leads to an increase in the
velocity. Consequently, the consequence distance is increased. On the contrary, for the dispersion over Terrain F2 (Fig. 16b), the release direction is facing the wall of the central building in the first row. The spread of the CO₂ cloud is impeded by the wall to a large extent and the lateral spread is enhanced. Also, the downwind velocity of the CO₂ cloud is reduced due to the buildings blocking the path of the dispersing cloud. These factors jointly lead to the reduction of the consequence distance.

Fig. 16. 50,000 ppm CO₂ envelopes (top view) – Terrain F

Fig. 17 shows the CO₂ concentration over a horizontal plane and a vertical plane for both Terrains F1 and F2. It also indicates that, in Terrain F2, the downwind dispersion of the cloud is blocked by buildings in the middle row and the lateral dispersion is enhanced. Higher concentrations are found near the buildings. Generally, the faces of buildings on the windward side experience higher concentrations than those on the leeward side, for both Terrains F1 and F2. This indicates that in an urban area, the region close to the windward wall is the most hazardous, even for buildings that do not face the source directly.
In the simulation of dispersion over the real terrain shown in Fig. 6, two cases were considered as shown in Fig. 18. In both cases, CO₂ was released downhill, with the wind in the same direction as the release. In case 1, the release is from the east side. In case 2, the release is from north side and the source point is located on a hilltop. Downstream from the source point, there is a valley (sloping trench) parallel to the release path.

Table 7 shows the predicted consequence distances for these two cases. In case 1, compared to dispersion over flat terrain, the consequence distances are increased by 9% and 4.9% for the 80,000 ppm and 50,000 ppm CO₂ levels.
ppm envelopes respectively. In case 2, the consequence distances are increased by 7.4% and 27.8% for the 80,000 ppm and 50,000 ppm envelopes respectively.

Table 7 Consequence distances – Terrain G vs flat terrain

<table>
<thead>
<tr>
<th>Concentration (ppmv)</th>
<th>Flat terrain (m)</th>
<th>Terrain G – case 1 (m)</th>
<th>Deviation</th>
<th>Terrain G – case 2 (m)</th>
<th>Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>80,000</td>
<td>230</td>
<td>251</td>
<td>9%</td>
<td>247</td>
<td>7.4%</td>
</tr>
<tr>
<td>50,000</td>
<td>324</td>
<td>340</td>
<td>4.9%</td>
<td>414</td>
<td>27.8%</td>
</tr>
</tbody>
</table>

In case 1, the increase in the consequence distance can be mainly attributed to the lateral slope, which constrains the spread of the cloud in +Y direction. In case 2, the valley confines the flow laterally on both sides, thus a much greater increase in the consequence distance of the 50,000 ppm envelope was observed. The higher wind velocity at the source location may also contribute to the increase in the consequence distance. In these two cases, the wind velocity at the lowest location was specified as zero. As the CO₂ release source was located at higher elevation, the resulting wind velocity at the source point is about 1 m s⁻¹ higher than that in the case using flat terrain.

In contrast with the results in the simulations with basic terrain elements, the dispersion in Terrain F1 and Terrain G showed increased consequence distance. The reason is that the lateral spread of the plume is constrained and the downstream dispersion is enhanced in these cases. The overall results suggest that a dispersion simulation using flat terrain can provide a conservative estimate of the consequence distance for most terrain types. However, if there are terrain features in the vicinity of the pipeline (source) which may possibly constrain the lateral spread of the cloud, the consequence distance may be increased. In this situation, it is recommended that dispersion simulations including the local topographic data should be performed to determine the appropriate impact area.

5.3 Dispersion of H₂S in CO₂ mixture – effect of terrain features

H₂S is a common component in typical CO₂ mixtures transported in pipelines and is harmful even at very low concentration levels. Exposure levels above 1000 ppm of H₂S will lead to ‘immediate death after as little as a single inhalation’ (Standards Australia, 2012). In general, the risk of H₂S at 200 ppm corresponding
to ‘sense of smell lost, and hence warning of danger lost; possible permanent eye damage’ (Standards
Australia, 2012) can be assumed to be equivalent to that of CO\textsubscript{2} at 50,000 ppm, while the risk of 500 ppm
H\textsubscript{2}S corresponding to ‘loss of consciousness after a few minutes, significant possibility of death’ (Standards
Australia, 2012) can be assumed to be equivalent to that of 80,000 ppm CO\textsubscript{2}.

Fig. 19 shows the predicted CO\textsubscript{2} and H\textsubscript{2}S envelopes for a full-bore rupture of a 400 mm ID pipeline carrying
CO\textsubscript{2} mixture with 0.9% H\textsubscript{2}S (flat terrain considered). As in the above studies, the stagnation pressure and
temperature were 15 MPa and 20°C respectively and a horizontal release was assumed. Clearly, for a
pipeline carrying a CO\textsubscript{2} mixture with 0.9% H\textsubscript{2}S, the H\textsubscript{2}S may pose a greater threat than the CO\textsubscript{2} itself.

Fig. 20 shows the consequence distances obtained through dispersion simulations over flat terrain with
different fraction levels of H\textsubscript{2}S, considering a full-bore rupture of a 400 mm ID pipeline. It is found that the
threshold source fraction of H\textsubscript{2}S is 0.6% for a 500 ppm H\textsubscript{2}S envelope, below which the 500 ppm H\textsubscript{2}S
envelope will be enclosed by the 80,000 ppm CO\textsubscript{2} envelope, while the threshold source fraction of H\textsubscript{2}S for a
200 ppm H$_2$S envelope is 0.4%.

To investigate whether the threshold value of H$_2$S fraction is affected by the complexity in the terrain, CFD dispersion simulations were also carried out for a full-bore rupture of a 400 mm ID pipeline, considering dispersion over complex terrains. Two terrain types were considered in this exercise: Terrain F1 and Terrain G.

Fig. 21. CO$_2$ and H$_2$S envelopes (top view, CO$_2$ source contains 0.3% H$_2$S)

Fig. 21 shows the dispersion envelopes for 50,000 ppm CO$_2$ and 200 ppm H$_2$S with 0.3% H$_2$S at source. In this case, the H$_2$S envelope is contained within CO$_2$ envelope. Fig. 22 shows the consequence distances for different H$_2$S levels. For the 200 ppm H$_2$S envelope the threshold source fraction of H$_2$S is 0.4% for both Terrain F1 and Terrain G, below which the 200 ppm H$_2$S envelope will be within the 50,000 ppm CO$_2$ envelope. This is the same as dispersion over flat terrain. For a 500 ppm H$_2$S envelope, the threshold source fraction of H$_2$S is 0.6% for Terrain F1, which is the same as dispersion over flat terrain. For Terrain G, the threshold source fraction of H$_2$S is 0.61%, which is slightly different from the dispersion over flat terrain.

The results show that terrain complexity has a very limited effect on the threshold value of H$_2$S fraction at the CO$_2$ source. As for dispersion over flat terrain, if the fraction of H$_2$S is less than 0.4% at the source, after rupture the 200 ppm H$_2$S envelope will be contained within the 50,000 ppm CO$_2$ envelope.
6. Conclusions

In this study, CFD models were developed for investigating the atmospheric dispersion of CO$_2$ over complex terrains. The numerical methods were validated through simulation of Trial 29 in the Thorney Island experiments. Seven terrain types were used for horizontal CO$_2$ releases to investigate the terrain effects on the consequence distance of CO$_2$ released from high-pressure pipelines. In addition, the terrain effects on the threshold value of H$_2$S volume fraction in the CO$_2$ mixture at the source were also studied. It can be concluded that:

1. CFD models are capable of predicting satisfactory CO$_2$ dispersion profiles over complex terrains. Simulations of the Thorney Island trials indicate that CFD models perform well not only in capturing the maximum concentration around the obstacle, but also the time evolution trend of the concentration during the dispersion.

2. Complex terrain features have a considerable effect on the consequence distance of CO$_2$ released from high-pressure pipelines. Relatively slender terrain elements (e.g. ramp, ridge, trench, slope) perpendicular to the release direction tend to reduce the consequence distance. In general, if the lateral spread of the dispersing cloud is enhanced due to the blockage of the terrain elements, the consequence distance will be reduced. On the other hand, if the lateral spread is confined, the consequence distance will be increased.
(3) For most terrain types, a dispersion simulation using a flat terrain may be able to provide a conservative estimate of the consequence distance. However, it is recommended to carefully determine if the terrain around the pipeline will constrain the lateral spread of the cloud. If this situation exists, dispersion simulations using the local topographic data should be performed.

(4) In an urban area, the CO$_2$ cloud is expected to be trapped in the street canyons between buildings. In the street canyons, higher CO$_2$ concentrations are likely near the windward face of the obstacle.

(5) Complex terrain features have limited effects on the threshold value of H$_2$S fraction at the CO$_2$ source. As in the case for dispersion over flat terrain, the threshold value of the fraction of H$_2$S is 0.4%. If the fraction of H$_2$S is less than 0.4% at the CO$_2$ source, it can be concluded that the consequence caused by H$_2$S will be less serious than that caused by CO$_2$ in any terrain conditions.

7. Acknowledgements

This work is being carried out under the aegis of the Energy Pipelines Cooperative Research Centre (EPCRC), supported through the Australian Government’s Cooperative Research Centre Program, and funded by the Department of Industry, Innovation and Science. Cash and in-kind support from the Australian Pipelines and Gas Association Research and Standards Committee (APGA RSC) is gratefully acknowledged.

References


ANSYS, 2011. ANSYS FLUENT theory guide. ANSYS Inc., USA.


