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Computational fluid dynamics simulation of carbon dioxide dispersion in a complex environment

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ABSTRACT

In order to quantitatively evaluate the risk associated with the Carbon Capture and Storage (CCS) technology, a deeper understanding of CO_2 dispersion resulting from accidental releases is essential. CO_2 is a heavier-than-air gas. Its dispersion patterns may vary according to local conditions. This study focuses on CO_2 dispersion over complex terrains. Computational Fluid Dynamics (CFD) models were developed to simulate the CO_2 dispersion over two hypothetical topographies: (1) a flat terrain with an axisymmetric hill and (2) a simplified model of an urban area with buildings. The source strength, wind velocity and height of the buildings were varied to investigate their effects on the dispersion profile. The study may offer a viable method for assessment of risks associated with CCS.

1. Introduction

The Carbon Capture and Storage (CCS) technique is widely seen as an effective and economical methodology to control what is perceived to be excessive concentration of Carbon Dioxide (CO_2) in the earth's atmosphere (Vianello et al., 2012). CO_2 is the main contributor to the 'greenhouse effect'. The CCS technique involves capturing waste CO_2 from large sources such as fossil fuel-powered electricity generation plants, transporting it to a storage site, and depositing it in underground sequestration sites (Liu et al., 2014; Tola and Pettinau, 2014). Commercial-scale transport of CO_2 uses tanks, ships, trains and pipelines. Pipelines are preferred when large quantities of CO_2 need to be transported over long distances (IPPC, 2005). When using pipelines to transport CO_2, safety issues must be considered (Lipponen et al., 2011). CO_2 pipeline failures or other releases associated with CCS are usually caused by third party interference, pipeline material corrosion, material defects, operator errors and ground movement (Gale and Davison, 2004). CO_2 is colourless and odourless under ambient conditions, and therefore escapes easy detection. It is also an asphyxiant which will lead to rapid loss of consciousness in humans if the exposure level exceeds 10% (OSHA, 1989). CO_2 released from pipelines can disperse downwind, potentially affecting populations and the environment. Therefore, obtaining a deeper understanding of the dispersion of CO_2 released from pipelines under different conditions is essential for assessing the safety of the technique.

In recent years, a number of models have been proposed to estimate the atmospheric dispersion of gases resulting from accidental or planned release. These can be classified into three categories: (a) "Gaussian-based" models, (b) "Similarity-profile" models, and (c) Computational fluid dynamics (CFD) models (Koopman et al., 1989). CFD models use more detailed mathematical descriptions of the conservation principles, allowing the simulation of complex physical processes involving heat and mass transport in complicated computational domains. Although time-consuming, CFD models are more appropriate for the modelling of dispersion over complex terrains and under different meteorological conditions. Using CFD for dispersion modelling in all its complexity (terrain topography, presence of obstacles, etc.) is a relatively recent development (Hsieh et al., 2013; Kiša and Jelemenský, 2009; Labovský and Jelemenský, 2010; Liu et al., 2014; Mazzoldi et al., 2008, 2011; Tauseef et al., 2011; Xing et al., 2013). In the past decades, a few researchers have used general-purpose CFD packages (such as Fluent or CFX) for atmospheric dispersion modelling (Hsieh et al., 2013; Labovský and Jelemenský, 2011; Mazzoldi et al., 2011; Xing et al., 2013), while others have relied on CFD software packages (such as fluidyn-PANACHE) designed specifically for atmospheric dispersion modelling (Hill

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et al., 2011; Mazzoldi et al., 2008).

Although numerical simulation of the atmospheric dispersion of hazardous gases over flat terrains using CFD is a relatively recent development, there have been some reports in the literature. Labovský and Jelemenský (2011) used theý CFD software Fluent to model the dispersion of ammonia in the 'Fladis' field experiments. They found that it was important to model the turbulence level appropriately. Mazzoldi et al. (2008) evaluated the suitability of the dispersion simulation tool fluidyn-PANACHE using data from the Prairie Grass and Kit Fox field experiments for validation. Xing et al. (2013) carried out a scaled experiment on a CO_2 release for the purpose of measuring the downwind concentration levels. In their experiment, the CO_2 was released vertically from a circular source at ground level at different flow rates. In addition, CFD simulations were carried out using different turbulence models. They concluded that the results of simulations using the $k-\varepsilon$ and the shear stress transport (SST) $k-\omega$ turbulence models were in acceptable agreement with the experimental data. Mazzoldi et al. (2011) compared two atmospheric dispersion models, the Gaussian model and a CFD model, taking representative input parameters for high-pressure CO_2 releases. Results showed a lowering of the risk involved in the transportation of CO_2 by up to one order of magnitude, when modelling the same releases with a CFD tool, compared to the more widespread Gaussian models. Mocellin et al. (2015) simulated the accident release of CO_2 from CCS pipelines and the consequences related to a sublimating dry ice bank. Results showed that serious risks were associated to the sublimating dry ice bank near the release point and that the hazard level increases with a decreasing mean wind speed and at higher ambient temperature. Liu et al. (2014) used CFD techniques to simulate the atmospheric dispersion of CO_2 released from a high-pressure pipeline. Two cases in the CO_2 dispersion experiments carried out by DNV BP (Trial DF1) were simulated for validation (Witlox, 2006), and DNV Phast was employed for comparative studies. The above studies suggested that realistic representations of the 'Atmospheric Boundary Layer' and turbulence levels are crucial in CFD modelling.

In recent years, the modelling of hazardous gas dispersion over complex terrains has attracted increasing attention. McBride et al. (2001) simulated the dispersion of chlorine and found that complex terrain and buildings affected not only the downwind hazard range, but also the width of the dispersion cloud and its direction of travel. Chow et al. (2009) proposed a model to simulate the atmospheric dispersion of CO_2 resulting from a leakage. The results demonstrated even small topographical features had a notable effect on the dispersion of the heavy gas. Scargiali et al. (2011) simulated the formation of toxic clouds of a heavy gas in an urban area using the CFD package ANSYS CFX. The simulation strategy involved a steady-state simulation to establish the pre-release wind velocity field, followed by a transient after-release simulation. The computational domain was modelled as a simple network of straight roads with regularly distributed blocks mimicking buildings. Results showed that the presence of buildings lowered the maximum concentration and enhanced the lateral spread of the cloud. Dispersion dynamics was also found to be strongly dependent on the quantity of the heavy gas released. Tauseef et al. (2011) applied CFD techniques in an assessment of heavy gas dispersion in the presence of a cubical obstacle downstream of the source. The performance of different turbulence models was investigated. They found that the realizable k-ε model is slightly superior. Hsieh et al. (2013) studied the dispersion of CO_2 from a CCS-related infrastructure in a complex hypothetical topography. The simulated concentration levels were found to be reasonable. Overall, the presence of an obstacle and/or complex terrain has a significant influence on heavy gas dispersion. However, generally speaking, the research associated with CO_2 dispersion over complex terrains is in its early stages. For quantification of the risks associated with CO_2 dispersion, an appropriate dispersion model especially over complex terrains is essential.

This study focuses on an investigation of CO_2 dispersion over complex terrains using CFD techniques. Two hypothetical topographies, a flat terrain with an axisymmetric hill, and a model urban area with buildings, were chosen to investigate the topographical effects on the dispersion. The influences of source strength and wind velocity on the dispersion were also taken into account. This study may contribute towards offering a reliable methodology for risk assessment related to CCS.

2. Numerical methods and experimental validation

2.1. Basic equations

The CFD software ANSYS-Fluent provides a method to solve three-dimensional conservation equations for the mean quantities in a turbulent flow field. The conservation equations of mass, momentum, energy and species concentration are solved. The standard $k-\varepsilon$ turbulence model is chosen in this simulation because it has been widely validated in dispersion simulations (Kiša and Jelemenský, 2009; Scargiali et al., 2011; Sini et al., 1996; Xing et al., 2013). The turbulent kinetic energy k and the turbulent kinetic energy dissipation rate ε are two key parameters in these equations. The basic equations are (Launder, 1972):

Continuity equation:

$$\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x_i}(\rho u_i)=0 \tag{1}$$

where ρ is the density, t the time, and u_i the velocity component along the x_i direction.

Momentum equation (Reynolds-Averaged Navier–Stokes equations):

$$\frac{\partial}{\partial t}(\rho u_i)+\frac{\partial}{\partial x_i}(\rho u_i u_j)=-\frac{\partial p}{\partial x_i}+\frac{\partial}{\partial x_j}\left(\mu\frac{\partial u_i}{\partial x_j}-\rho\overline{u_i^{'}u_j^{'}}\right) \tag{2}$$

where p is the pressure and μ is the dynamic viscosity of the fluid.

Energy equation:

$$\frac{\partial}{\partial t}(\rho E)+\nabla\cdot[\vec{v}(\rho E+p)]=\nabla\cdot\left(k_{eff}\nabla T-\sum_j h_j\vec{J_j}+\overline{\overline{\tau}}_{eff}\cdot\vec{v}\right)+S_h \tag{3}$$

where E is the total specific energy, k_{eff} the effective thermal conductivity, h_j the enthalpy of species j, $\vec{J}_j$ the diffusion flux of species j, and S_h the source term.

The parameters k and ε are defined as:

$$k=\frac{\overline{u'^2}+\overline{v'^2}+\overline{w'^2}}{2} \tag{4}$$

$$\varepsilon=\frac{\mu}{\rho}\overline{\left(\frac{\partial u_l^{'}}{\partial x_k}\right)\left(\frac{\partial u_l^{'}}{\partial x_k}\right)} \tag{5}$$

The turbulent viscosity μ_t is a function of k and ε:

$$\mu_t=\frac{C_u\rho\, k^2}{\varepsilon} \tag{6}$$

k and ε are both unknown variables which can be calculated from the differential 'conservation' equations for k and ε: