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Heavy gas concentration prediction on complex terrain using CFD with Monin-Obukhov similarity theory

Charles Glover[a], Delphine Laboureur[a,b], and Jiayong Zhu[a]*
a Mary Kay O'Connor Process Safety Center, Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, Texas, 77843-3122, USA
b Von Karman Institute for fluid Dynamics, 72, chaussée de Waterloo, Sint-Genesius-Rhode, Belgiumon
*Presenter E-mail: jychriszhu@tamu.edu

Abstract

Under stable atmospheric conditions (***i.e.,*** low wind speed and low heat radiation), once heavy gases (***e.g.,*** CO_2, H_2S, LNG) release to the atmosphere, the gas clouds tend to stay near the ground for long period of time, thereby causing high concentration zone and increasing the threats to the local population and the environment. Despite of the advanced development of computational fluid dynamic (CFD) modelling, or the Reynolds-Averaged Navier-Stokes (RANS) models with standard turbulence closures (***e.g.,*** standard $\kappa-\varepsilon$, RNG $\kappa-\varepsilon$ and $\kappa-\omega$), researchers have pointed out that these models are incompatible with the experimental data under stable atmospheric conditions. Therefore, there is an increasing interest in developing a robust mathematical model for heavy gas dispersion, especially in the field of turbulence modelling. This present study is to develop a CFD model with a two-equation turbulence model for heavy gas dispersion over complex geometry in stable atmospheric conditions. This two-equation turbulence model is a modified $\kappa-\varepsilon$ turbulence model based on the Monin-Obukhov similarity theory (MOST). The calculations from the modified turbulence model can maintain the homogeneity of the flow properties. The calculations from the CFD model with the modified $\kappa-\varepsilon$ model is compared with the experimental data collected from the Kit Fox experiment under stable atmospheric conditions (Class F). A robust and reliable model can provide potential guidelines for emergency mitigation planning for heavy gas leakage incidents.

Keywords: Risk, Risk assessment, Emergency, Dispersion model

1. Introduction

Hazardous gases leakage accidents are likely to cause serious injury to human health and to harm the local environment (Sklavounos and Rigas, 2004), especially for heavy gases (e.g., CO_2, H_2S, LNG), which possess larger density than air. When heavy gases release to the atmosphere, they tend to move towards the ground, thereby increasing the threat to the local population (Markiewicz, 2012).

A robust and reliable quantitative model is crucial for risk assessment which can provide quick predictions of downwind concentration and minimize the negative influences to the people and the environment (Markiewicz, 2012). As the advancement of the computational technologies, the numerical methods using the Computational Fluid Dynamics (CFD) models, which can predict fluid flow in complex geometries, are popular in both academic researches and industrial studies (Scargiali et al., 2008; Liu et al., 2016).

However, in recent years, many studies showed that the CFD models are incompatible with the experimental data. Studies showed that the calculations from CFD model using Reynolds-Averaged Navier-Stokes (RANS) with standard turbulence closures do not agree well with the large-scale experimental data, especially under stable atmospheric conditions (Pieterse and Harms, 2013). Furthermore, researchers pointed out that the potential issue for the discrepancies between the calculations and the experimental data are due to the ways that the standard turbulence closure calculate the pressure and the velocity. Therefore, homogeneous profiles are not maintained in the flow domain (Yasin and et. Al., 2019).

This present study incorporates the Monin-Obukhov Similarity Theory (MOST), a universal acceptable assumption for stable atmospheric conditions, in the RANS CFD model and validates the model with the experimental data. To apply the MOST to RANS CFD models, turbulence kinetic energy profiles, the turbulence dissipation rate profiles and the temperature profiles are modified based on the MOST. Also, the experimental data from the Kit Fox experiment were collected from literature and compared with the calculations from the modified RANS CFD model. The results showed that the modified RANS CFD model is able to maintain the homogeneity of the flow properties. Also, the calculations from the modified RANS CFD model agree well with the maximum concentration observed in the experiment.

With better confidence on the model by validating this model with other experimental data, this model can provide potential guidelines for emergency mitigation planning for heavy gas leakage incidents in a complex terrain, such as chemical plants and urban area.

2. Numerical approach

Numerical simulations with the standards and the modified turbulence closures are performed in the commercial Computational Fluid Dynamics (CFD) codes, ANSYS Fluent. The calculations are based on finite volume method for the discretisation of differential equations.

2.1. κ–ε turbulence model

The standard κ–ε turbulent model is a widely used to estimate the fluid flow momentum due to turbulence. The fluid flow considered in this work has high Reynolds number, which is classified as turbulence flow. Turbulence flow is described as the chaotic characteristics of the fluid motion due to pressure and flow velocity. The standard κ–ε turbulent closure, for example, uses turbulent kinetic energy [m^2/s^2] and dissipation rate of turbulence kinetic energy [m^2/s^3] as velocity and length scale related variables. The shear stress is defined as following:

$$u'w' = -\nu_t \frac{\partial \bar{u}}{\partial z} \; with \; \nu_t = c_\mu \frac{\kappa^2}{\varepsilon} \tag{1}$$

Here, c_μ is the turbulent viscosity coefficient. In the standard κ–ε turbulent closure, the value for c_μ is 0.09. The turbulent kinetic energy, κ, and the dissipation rate of the turbulent kinetic energy, ε, are estimated by solving the nonlinear partial differential equations shown below:

$$\mu_j \frac{\partial k}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\frac{\nu_t}{\sigma_k}\frac{\partial k}{\partial x_j}\right] + P - \in \tag{2}$$

$$\mu_j \frac{\partial \epsilon}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\frac{\nu_t}{\sigma_\epsilon}\frac{\partial \epsilon}{\partial x_j}\right] + C_1 \frac{\epsilon}{\kappa} P - C_2 \frac{\epsilon}{\kappa} \in \tag{3}$$

where P is the shear production term and ∈ is the shear dissipation term. In standard κ–ε turbulence model, the closure coefficients are given below:

$$(\sigma_k, \sigma_k, C_1, C_2) = (1.0, 1.3, 1.44, 1.92, 1.3).$$

2.2. Application of Monin-Obukhov Similarity Theory (MOST)

MOST is a universal accepted theory for determination of vertical profiles of mean flow within the surface layer. Stratification effects could be important near the ground (roughly within 2 meters above the ground), especially in stable atmospheric conditions. Monin and Obukhov (1954) developed the Monin-Obukhov similarity theory (MOST) which suggested that the vertical variation of mean flow and turbulence characteristics in the surface flow should depends on the height (z) and the friction velocity (u_*). In order to define the velocity and potential temperature profiles within the surface layer, dimensionless stability functions for momentum and heat, which are denoted by Φ_m and Φ_m.

$$\Phi_m\left(\frac{z}{L}\right) = \frac{kz}{u_*}\left(\frac{du}{dz}\right) \tag{4}$$

$$\Phi_h\left(\frac{z}{L}\right) = -\frac{kz}{\theta}\left(\frac{d\theta}{dz}\right) \tag{5}$$

Gradients of wind speed and potential temperature are given with the dimensionless stability functions based on full-scale observations from the 1968 KANSAS experiments.

$$u(z) = \frac{u_*}{\kappa}\left[\ln\left(\frac{z}{z_0}\right) + \Phi_m\left(\frac{z}{L}\right) - 1\right] \tag{6}$$

$$T(z) = T_o + \frac{T_*}{\kappa}\left[\ln\left(\frac{z}{z_0}\right) + \Phi_m\left(\frac{z}{L}\right) - 1\right] \tag{7}$$

where

$$\Phi_m\left(\frac{z}{L}\right) = 1 + 5\frac{z}{L}$$

$$\Phi_h\left(\frac{Z}{L}\right) = 1 + 4\frac{Z}{L}$$

$$T_* = \frac{u_*^2 T_o}{gL\kappa}$$

The turbulence kinetic energy and turbulence dissipation rate are estimated in following profiles based on the full-scale experiment.

$$\kappa(z) = \frac{u_*^2}{\sqrt{C_\mu}}\sqrt{\frac{\Phi_m\left(\frac{z}{L}\right)}{\Phi_h\left(\frac{z}{L}\right)}} \tag{8}$$

$$\varepsilon(z) = \frac{u_*^3}{\kappa z}\left[\Phi_h\left(\frac{z}{L}\right)\right] \tag{9}$$

3. Experimental data

The Desert Research Institute (DRI) and Western Research Institute (WRI) conducted the Kit Fox field tests at the Nevada test site on August and September 1995. These tests were designed to represent a heavy gas release in a typical refinery plant or chemical processing plant. Since it was not practical to construct a real plant or to test in a plant, arrays of obstacles were arranged in the field and all setups were scaled down to a ratio of 1:10 compared to a typical plant (Hanna and Chang, 2001). The dimension of the test field was 314 meters long and 120 meters wide. CO_2 gas was released vertically from a 1.5-meter-by-1.5-meter square area on the ground (shown in ***Figure 1***). Eighty-four fast-responding concentration monitors were arranged in four arrays, which were 25 m, 50 m, 100 m and 225 m away from the releasing source. 6600 rectangular plywood billboards (Uniform Roughness Array, or URA) with dimensions of 0.8-meter width and 0.2-meter height in 133 arrays were set within the test boundary (light blue area in ***Figure 1***). 75 square plywood billboards (Equivalent Roughness Pattern, or ERP) with sides of 2.4-meter in 13 arrays were installed in a 39m X 85m rectangular area near the releasing source (dark blue area in ***Figure 1***). Meteorological data were collected by instruments mounted on a tower (Met4).

The experimental data used in this study is the experiment KF0711. The meteorological conditions are summarized in Table 1.

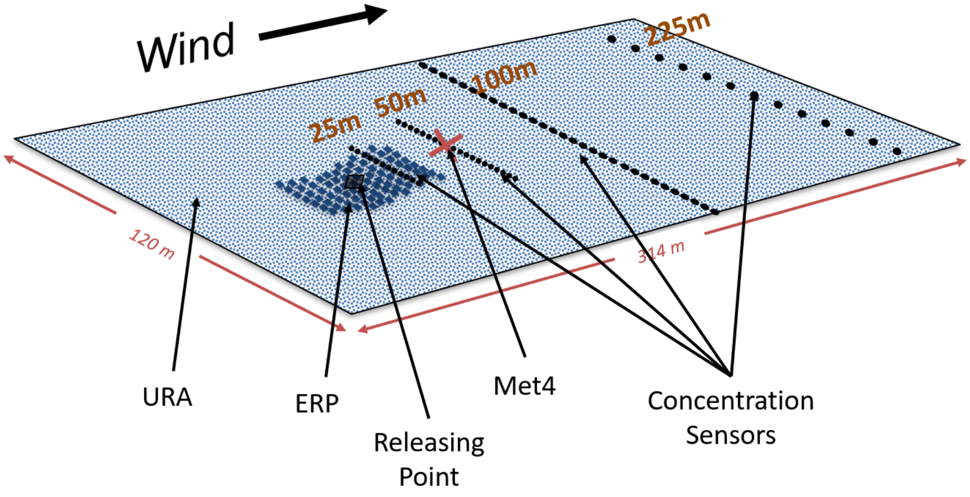

Figure 1. Layout of Kit Fox experiment showing locations of meteorological tower (Met4), concentration sensors, and releasing point.

Table 1. Summary of Experiment KF0711 including releasing source temperature (T_s), spill rate (Q), relative humidity (RH), duration (T_d) of the release, average wind speed (u) measured at 2m elevation, surface roughness values (z_o), inverse Monin-Obukhov length (1/L), and the atmospheric stability class (stab) during the tests.

	T_s (K)	**Q** (kg/s)	**RH** (%)	**T_d** (s)	**u** (m/s)	**z_o** (m)	**1/L** (m^{-1})	stab
0711	303	1.6	12	20	1.93	0.01	0.164	F

4. Parameterization in CFD simulation

In this section, detail descriptions of the 3-dimensional modelling setting in CFD code ANSYS Fluent are discussed. The boundary conditions for the top and the sides are symmetry boundaries, and bottom is ground boundary, the front is the wind inlet with velocity inlet boundary, the end is the wind outlet with pressure outlet boundary, and the gas inlet with velocity inlet boundary is located at the centreline on the ground and 1 meter away from the wind inlet boundary.

4.1. Equations solved

The equations solved in this study are the standard Reynolds Averaged Navier Stokes (RANS) equations with the assumptions that the fluids are not compressible and the Boussinesq assumption, which assumes the density is constant. Energy conservation equations are applied, and the potential temperature profile is considered with equation (7). The κ–ε turbulence closure was used in the form of equation (8) and (9).

4.2. Wind inlet condition

On the upwind boundary, vertical profile for wind velocity is given by equation (6), and the inlet turbulence condition for upwind boundary is given by equations (8) and (9).

4.3. Ground, top and side boundaries conditions

In order to preserve the momentum and heat fluxes through the domain, ground boundary is set to be zero heat flux. Also, a roughness constant of 0.01m represents the arrays of obstacles (0.8m width and 0.2m height) on the ground. Since the experiment is conducted in an open field, symmetry boundaries are set for top and sides boundaries. Symmetry boundaries represent zero normal velocity and zero normal gradients of all variables at the symmetry planes. Additionally, the symmetry plane has slip condition, which means zero shear stress at the symmetry plane.

4.4. Gas inlet condition

At the CO_2 inlet, vertical velocity profile modelled using User Defined Function (UDF) to represent the CO_2 gas flow at 0.21m/s for 20 seconds. The inlet turbulence conditions are given by equations (8) and (9).

4.5. Pressure outflow condition

Since the experimental setup is in a large-scale condition, fully developed flow is assumed in this modelling. Therefore, outflow boundary is utilized. Outflow boundary has zero diffusion flux for all variables at the exit direction.

5. CFD simulation results

Homogeneity of flow properties is examined in this study. This simulation domain used is a 3-dimensional of 250m length, 60m width and 100m height. In order to evaluate the homogeneity defined by equations (6), (7), (8) and (9), a model without CO_2 jet was simulated. Figure 1 illustrates that the equations (6), (7), (8) and (9) can well maintain the homogeneity of the flow properties in the domain. The average differences between the turbulence dissipation rate (ε), the turbulence kinetic energy (κ), and mean velocity profiles between the near-field (x=10m) and the far field (x=250m) are less than 18.50%, less than 29.02%, and less than 3.85%, respectively.

Additionally, the concentrations calculated from the CFD model with the modified turbulence closure are compared with the experimental data (shown in Figure 3). The results showed that the calculations were in good agreement with the experimental data. However, the results pointed out that the concentration peaks calculated from the CFD model generally arrived earlier than the ones that the experimental data showed. Also, the maximum concentration differences between the CFD model calculations and the experimental data were 16.49%, 24.70%, 20.99% and 16.92%, respectively. In other words, the maximum concentrations were within a factor of two of the observations.

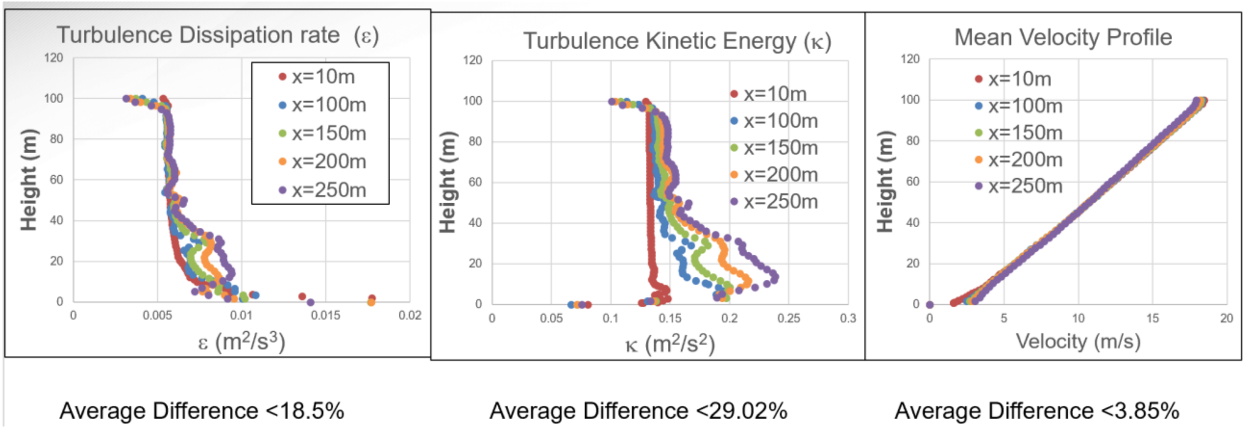

Figure 2. vertical profiles of turbulence dissipation rate, turbulence kinetic energy and mean velocity profile at different positions (10m, 100m, 150m, 200m, 250m)

6. Conclusion

In this work, we have investigated the application of RANS CFD approach with a modified κ–ε closure to the stable atmospheric condition. This modified κ–ε closure including modifications on turbulence kinetic energy equation, turbulence dissipation equation, velocity and temperature profiles were calculated with conservation equations in RANS. The results illustrate that the RANS CFD approach with modified κ–ε closure can maintain the homogeneity of the flow properties well. Also, the concentration profiles calculated from this modified model have good agreement with the experimental data.

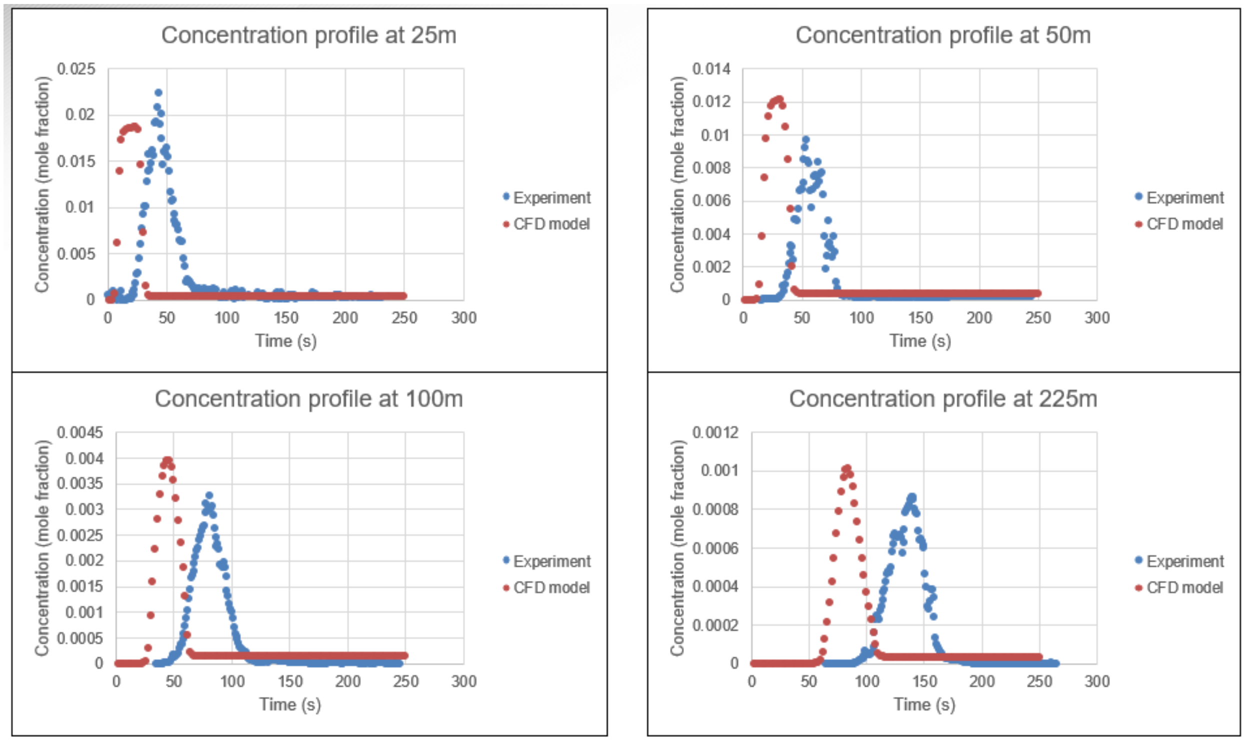

Figure 3. The concentration profiles of CFD calculations comparing with the experimental data at positions x=25m, x=50m, x=100m and x=225m.

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