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Temperature Gradient and Wind Profile Effects on Heavy Gas Dispersion in Build up Area

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Abstract: Dispersion of heavy gases is considered to be more hazardous than the passive ones. This is because it takes place more slowly. In this paper, based on the extensive experimental work of Hanna and Chang, the CFD model (Ansys-CFX) was tested compared with Kit Fox experiments. In order to accomplish this validation, the multiphase approach was employed as a new method in this area. In addition, the temperature gradient effects were investigated. The survey of wind speed was done taking factors such as time, height and direction into the consideration. To reduce the number of elements in computational domain, a combination of 2D and 3D geometries were utilized. Results showed that the wind inlet correction and temperature gradient had a significant influence on gas concentration records.

Key words: heavy gas dispersion, temperature gradient, wind profile, complex train, CFD

INTRODUCTION

Nowadays, large quantities of hazardous and toxic substances are produced, stored or transported. Many of these substances are gases that form clouds heavier than air when accidentally released into the atmosphere. These gases may have a density greater than that of the air for several reasons including the high molecular weight (like chlorine), low release temperature (like liquefied natural gas), high storage pressure (for example a failure of the container of ammonia and subsequent formation of aerosol) or chemical reactions of the released substances with water vapor in the atmosphere (the polymerization of hydrogen fluoride) (Markiewicz, 2006).

The heavy gas cloud has the negative buoyancy that affects its behavior compared to a positively or neutrally buoyant cloud. These effects include: the additional gravity driven flow, wind shear at the heavy gas cloud interfaces, turbulence dumping, and inertia of the released material. Some special models have been developed to describe the heavy gas clouds dispersion in the atmospheric air known as heavy gas dispersion models or dense gas dispersion models (Lees, 1996).

These models include: empirical, intermediate and fluid dynamic models. The empirical and intermediate models (used in PHAST, ALOHA,etc software) are important components of emergency response systems and also they are appropriate models commonly used in environmental impact assessment and risk assessment studies. The fluid dynamics models (applied in Ansys CFX, Fluent,etc codes) are usually used as a research tools in order to reach better results on heavy gas properties.

Computational Fluid Dynamics (CFD) allows the simulation of complex physical process describing heat and mass transport phenomena with fully developed mathematical models. Specific models integrated in CFD codes can predict the turbulent mixing behaviour between gas molecules and air particles (Sklavounos and Rigas (2004).

Dense gas dispersion modeling in the obstacle area, is very complicated, because of sensitivity to various parameters and conditions. For this reason, many researchers, both in safety and environmental fields, are interested in this subject. Recently, CFD works are more focused in the effects of obstacles on gas dispersion phenomena (Hanna *et al*. (2004), Mouilleau and Champassith (2009), Pontiggia *et al*. (2009), Mazzoldi *et al*. (2008), Yassin *et al*. (2005), Kovalets and Maderich (2006), Mavroidis *et al*. (2007), Wilkening and Baraldi

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(2007), Kashi *et al*. (2008) and effects of heat transfer on Liquefied Natural Gas (LNG) spills (Sklavounos and Rigas (2006), Hanlin *et al*. (2007), Gavelli *et al*. (2008).

In this paper, numerical simulation of the Kit Fox field experiments was performed using ANSYS CFX 11 code (ANSYS Company, 2006). CFD code is used for investigation of some essential parameters in dense gas dispersion modeling (e.g. obstacle effects, wind profile, heat transfer and CFD parameters like mesh type and size, various boundary conditions). The special aspects which have been taken into consideration in this paper are:

(a) Using and testing multiphase approach instead of additional variable model or multi-component model. A new method is used at the inlet boundary condition for wind inlet, that is time-dependent and local wind speed method, instead of usual wind speed profile.

(b) A buoyancy model (Boussinesq) is used instead of atmospheric stability models and its effects have been studied.

(b) Combination of 2D and 3D geometries is used in order to reduce the number of meshes and computational time.

2. Field experiment:

Field gas dispersion experiments are very expensive and can be set up in some large projects, so it is not the aim of this work and, consequently, we had to use standard experiments by permission.

2.1. Kit Fox field experiment:

A joint field experiment (named "Kit Fox") was conducted in August and September, 1995, at the Frenchman Flat area of the Nevada Test Site. The field operations, described in the Western Research Institute (1998) report, were carried out by Western Research Institute and Desert Research Institute. There were 52 independent Kit Fox data trials, with about 2/3 for "puff" or "finite duration" 20s releases, and about 1/3 for "continuous plume" 120-450s releases. A summary of the major characteristics of each of the 52 tests is given by Hanna and Chang (1999, 2001). Figure 1 shows the plot plan of the Kit Fox experiment. In this paper trial 3-7 (trial 3, release 7; an instantaneous release) is implemented for the simulation purposes.

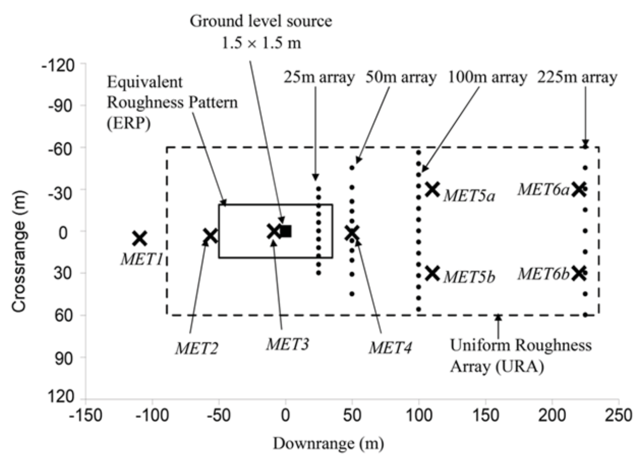


Fig. 1: Plot plan of the Kit Fox dispersion grid including meteorological towers, concentration monitoring arcs, gas source, Equivalent Roughness Pattern (ERP), and Uniform Roughness Array (URA) (Hanna and *et al*. (1999).

3. Mathematical formulation:

Gas dispersion in atmosphere can be studied in different methods using CFD codes. These methods include: studying a flow with an additional variable, a flow with multi-component fluid and a multiphase flow. Using additional variables can help in modeling the transport of a passive material in the fluid flow like smoke in the air. The presence of an additional variable does not affect the fluid flow, even though some fluid properties may be defined to be dependent on additional variables. In multi-component flow method it is assumed that different components of a fluid are mixed together at molecular level sharing the same mean velocity, pressure and temperature fields. Also in this approach mass transfer is considered to take place by convection and diffusion. In more complex situations where different components are mixed on larger scales and with separate velocity and temperature fields, multiphase flow method is used.

In this work the multiphase flow method was employed in order to model dense gas dispersion. ANSYS CFX was used as a computational code for simulation purposes. In ANSYS CFX, the equations of momentum, mass transfer, heat transfer, buoyancy and turbulence model for homogeneous multiphase flow are supposed to be solved using finite volume method.

4. Simulation conditions:

***4.1. Geometry and grid generation*:**

ANSYS workbench design modeler and CFX mesh tools were used to make the geometry of domain and meshing it. In this simulation, two-dimensional boards were used as ERP obstacles. The thickness of the obstacles is eliminated and as a result even the smallest mesh can be greater than billboard thickness. The model geometry is shown in figure 2.

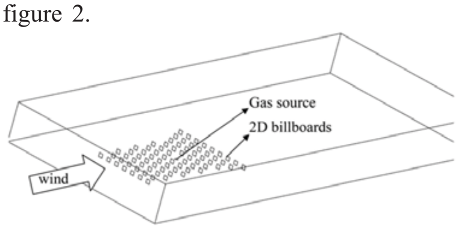


Fig. 2: Domain of simulation of Kit Fox experiment

Using line control techniques, cells were concentrated around the obstacles area. Also a fine resolution was implemented vertically from the ground up to a height of about 1m. In this study 20 inflation layers were used. The thickness of the first layer was determined at the beginning. Since the CFX code used wall function in its simulation and in which the near wall meshes are very important, the determination of the first layer was done using y^+ means. This can help us to get the better results from CFD code. Maximum distance of meshes in the area around the obstacles is 0.5m and normal maximum distance is 2m. Figure 3 shows the refinement of meshes near the surface and around the obstacles. The geometry of domain covered a volume of 25*110*300m (height*latitude*longitude). Computational grids consist of 3215092 cells.

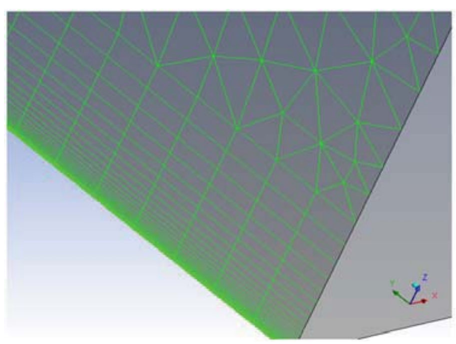


Fig. 3: Surface mesh of trial 3-7 from Kit Fox experiments

In order to investigate the grid performance, the problem was solved in a steady state condition. Flow vectors were studied on different planes. Figures 4 and 5 show the wakes that were shaped at the rear of the obstacles. As it was expected there was a flow recycle in these areas. After releasing the gas and its dispersion, there was a large amount of gas at the rear of the obstacles for a long time and this formed some new sources.

4.2. Boundary conditions:

4.2.1. Domain preparation:

Fluids under consideration were air and CO_2. Temperature was not fixed and varied vertically (in Z direction, see Fig. 6), therefore the computation was carried out using the thermal energy, and because of low temperature gradient, the Boussinesq buoyancy model was used for considering the free convection effects on gas dispersion. Since the flow was assumed to be turbulent the standard *k-ε* model was used.

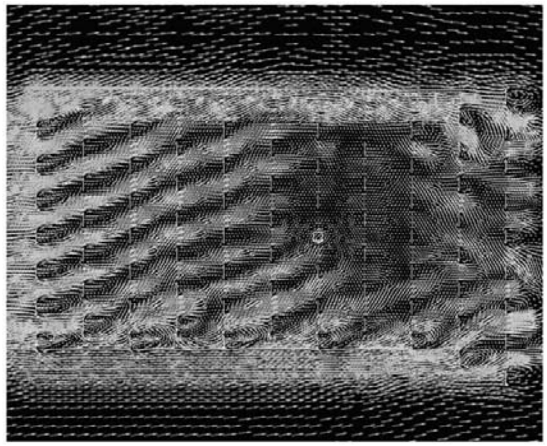


Fig. 4: Flow vectors on the 1m elevated plane

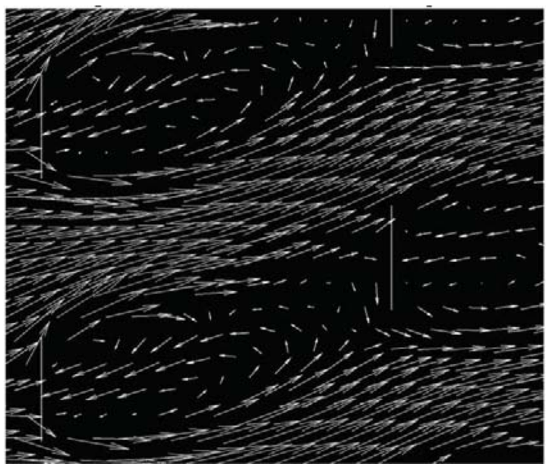


Fig. 5: Flow vectors rear of obstacles on the horizontal plane at 1m elevation

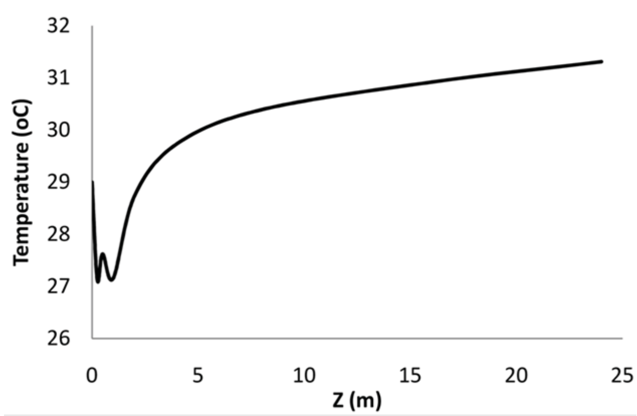


Fig. 6: Vertical temperature gradient in the EPA tower location

4.2.2. Wind inlet:

When there is low wind speed condition, wind direction can vary considerably within small periods of time. Low wind speeds are associated with a phenomenon called meander which is a horizontal oscillation of the local atmosphere. As the wind velocity decreases below a certain threshold, it is no longer possible to define a mean wind direction (see Fig. 7). These oscillations are independent to atmospheric stability and topography and are related to the equilibrium between the Coriolis force and the pressure gradient (Oettl *et al*. (2005). Therefore to get better results there wasn't use correlation in this simulation.

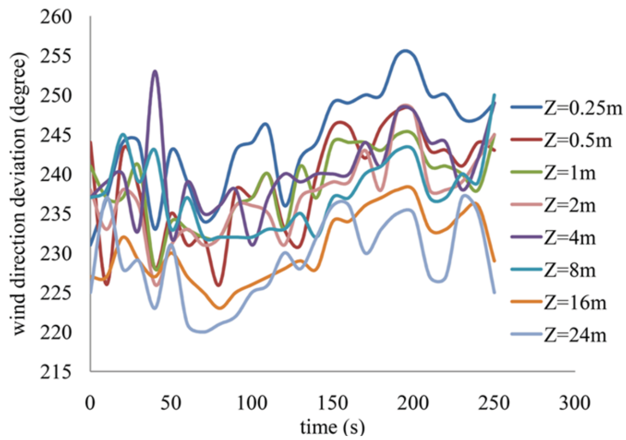


Fig. 7: Wind direction deviation with time at the EPA tower

Wind direction deviation with time and height at the EPA tower (front surface of the domain, wind boundary condition in the simulation) is shown in figure 7 (Hanna, *et al*. (1999). The EPA tower wind data was directly used as a wind inlet boundary condition. Cartesian velocity component was used for adding wind direction:

$$u = U\cos\theta \tag{1}$$

$$v = U\sin\theta \tag{2}$$

$$w=0 \tag{3}$$

where θ is a deviation of wind direction. For considering the time variation of the wind speed and its direction, step function applied to the simulation. Figures 8 and 9 show wind speed dependency on time and height at x direction in the inlet boundary.

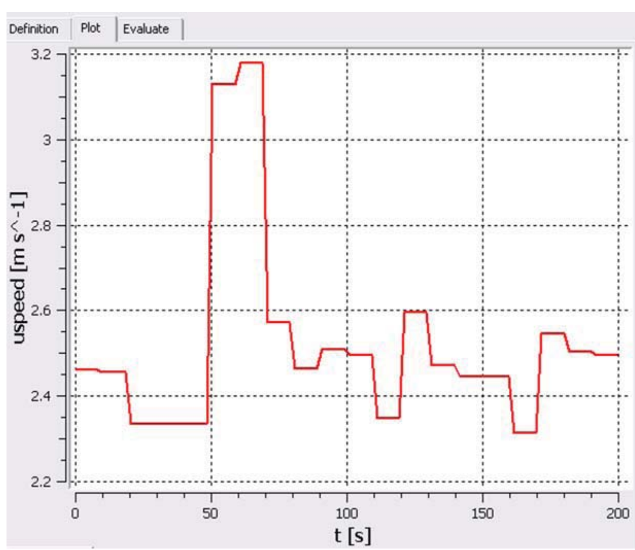


Fig. 8: u component of wind speed at the height of 2m in EPA tower location that included to the simulation

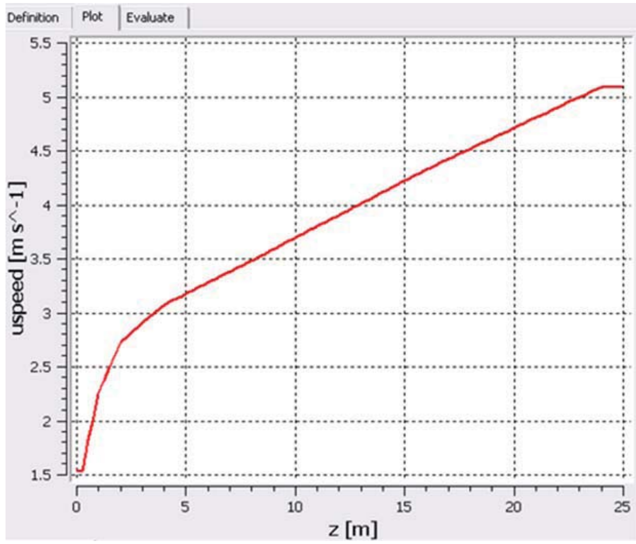


Fig. 9: u component of wind speed from 10 to 20 second after gas release in EPA tower location that included to the simulation

Since in this trial the normal wind direction has deviations from normal *x* line, both the front and right sides of the domain were defined as the wind inlets. *u* and *v* components were dominant at the front and right sides respectively.

The average velocity of air is 2.7m/s at the EPA tower and its distance to gas source is 90m, So the air particles need at least 50 seconds to reach the source of gas. In this simulation, the air velocity values were taken into consideration 50s before the gas release since the gas was discharged from the source 50s after introducing the air into the domain. This helped to maximize the effects of wind speed variations on gas dispersion in the domain.

4.2.3. Gas inlet:

In trial 3-7 of Kit Fox field experiment, carbon dioxide was released instantaneously into the atmosphere with 3.65kg/s rate for about 20s. In order to set the inflow boundary condition for the transient problem, released mixture mass inflow rate (Q_i) was given through a properly adapted step function:

$$Q_i = m_i \times step\left[-\frac{(t-t_0)(t-t_1)}{t_2^2} \right] \tag{4}$$

where m_i is equal to 3.65kg/s, t_0=50s, t_1=70s and t_2=1s.

To have a fully developed flow in the domain, the gas was released after 50s (t_0=50s) from the beginning of the wind inlet. Since the gas was released at the ground level and the ground surface temperature was 29°C during the experiment, the inlet gas temperature was set to 29°C in the simulation.

4.2.4. Ground surface roughness:

In the Kit Fox experiments 6600 obstacles implants in order to increase the surface roughness. The surface roughness length, Z_o, is a measure of mechanical mixing introduced by the surface roughness elements. As a rule of thumb, Z_0 is nearly equal to 0.1 times the average height of the roughness elements (Hanna and Britter (2002)). In this simulation the ground surface was defined as a rough wall with Z_0 equal to 0.01m.

4.2.5. Surfaces and planes temperature:

Temperature gradient data were used as the heat transfer boundary condition for all vertical boundary planes. Figure 6 shows the vertical temperature gradient in the domain. The ground surface temperature was 29°C at the time of the experiment. Therefore the ground surface temperature was set to 29°C.

RESULTS AND DISCUSSION

At first, the problem was solved in steady state condition and then its results were used as initial conditions in transient problem. Total time for transient simulation was set to be 250s with relatively short time steps (0.25s).

5.1. Wind profile effect:

Using our method, in comparison to the existing wind profiles like the logarithmic profile, the wind velocity inlet was more accurately modeled. In adition there is no need to extend the longitude and altitude of simulation domain.

In figures 10-13 gas concentration histories were compared with the values recorded on first arc (25m far from the source) in the x direction and at the heights of 0.6m, 1.2m. As it can be seen in our method, the results have the same trend compared to experimental data and cover it.

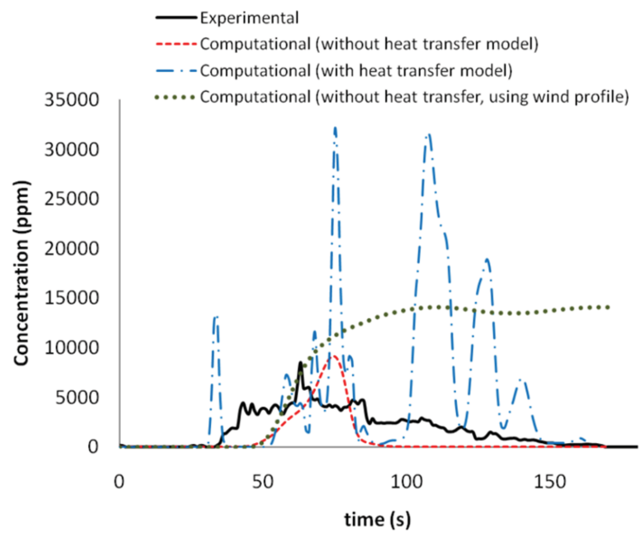


Fig. 10: Comparison of experimental and computational results in Kit Fox experiment (trial 3-7) on arc one, at height 0.3m.

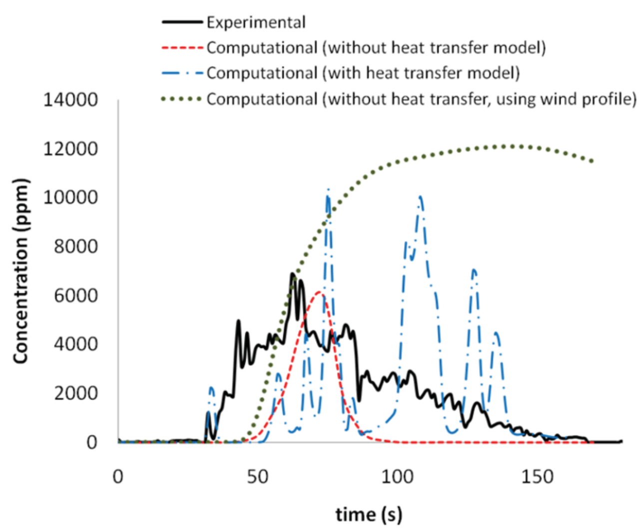


Fig. 11: Comparison of experimental and computational results in Kit Fox experiment (trial 3-7) on arc one, at height 0.6m.

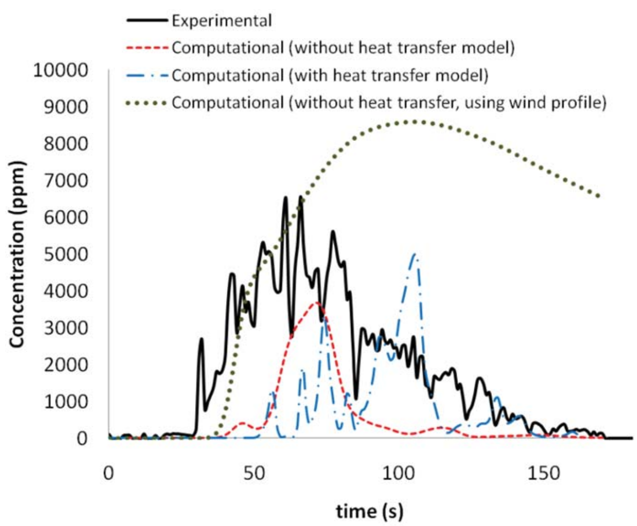


Fig. 12: Comparison of experimental and computational results in Kit Fox experiment (trial 3-7) on arc one, at height 1.2m.

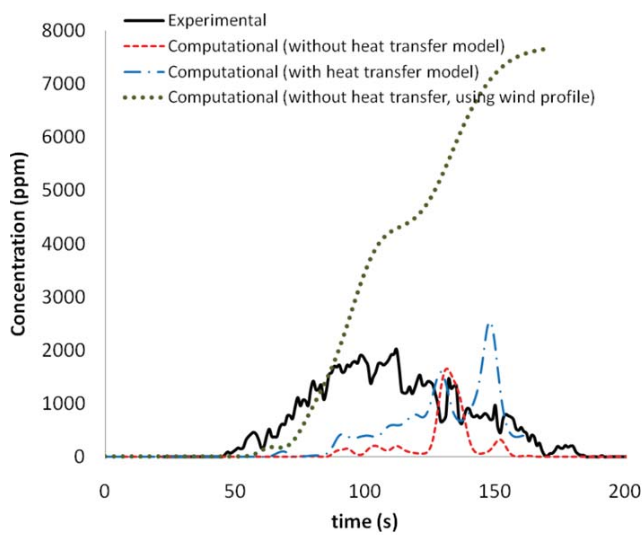
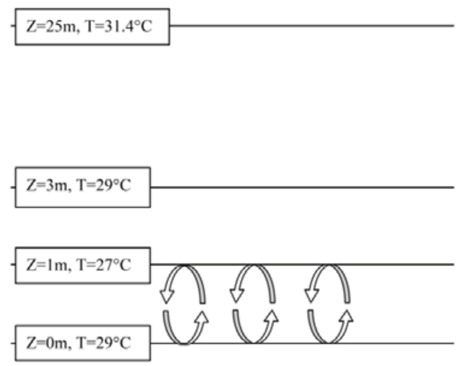


Fig. 13: Comparison of experimental and computational results in Kit Fox experiment (trial 3-7) on arc two, at height 0.5m.

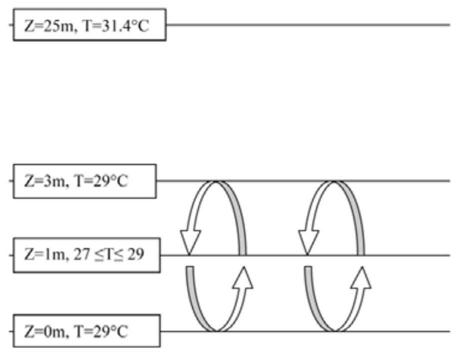
5.2. Free convection:

Multiphase and multi-component methods in the isothermal condition are similar but in the heat transfer condition, multi-component and buoyancy methods cannot be used at the same time. In the other word, multiphase method can be used with buoyancy methods such as Boussinesq and it can show free convection effects on gas dispersion process, while it cannot be done by multi-component method.

The ground surface temperature was 29°C during the experiment, while the adjacent air temperature was about 27°C, so air got warm near the surface and moved upward. Since the upper limit of the calculation domain had a temperature of 31.4°C, the warmed air cannot move upward and is forced to go down to the surface. This atmospheric condition happens in the afternoons because the earth is usually warmed by solar energy at noon and it's still warm, so it exchanges its heat with the adjacent air that is cooler now. This phenomenon can cause faster dispersion of gas however the prediction of gas concentration may become somehow difficult. It results buoyancy turbulence production and causes the gas to disperse with a more complex behavior. This is a dominant phenomenon in the obstacles area. This phenomenon is shown in Fig. 14. As it is shown, this event does not exist in the free obstacle areas. In fact, the flow has a little time to warm and goes up in this area; however there is plenty of time for the flow to be warmed with surface heat flux and moves upward in the obstacles area. This is a naturally expected important phenomenon that was ignored in the earlier CFD simulations of gas dispersion.



(A)



(B)

Fig. 14.a: Flow recycles in the flat area, b) Flow recycles in the obstacle area

When the heat transfer effect is included, the vertical fluctuation is produced in the flow pattern and consequently the gas dispersion is more complex and its concentration does not match very well with experimental results. However they have a same trend.

Comparing the vertical velocity component - it is produced by heat transfer between surface and adjacent air - in different cases (with heat transfer effect and without it) (Fig.15), we can show that in the second case vertical velocity does not exist. It means that, if we eliminate the heat transfer effect, the vertical velocity will be eliminated and gas dispersion is carried out in z direction only by molecular diffusion. Also this figure shows the negative speed of the flow in the z direction near the surface (with heat transfer effect). These findings illustrate the advantages of using heat transfer effect.

5.3. Safety consideration:

When the dense gas is released, unlike to the passive gas, it moves upwind and flows like a liquid. This phenomenon is clearly shown in Fig. 16. When the dense gas obstructs at the rear of the obstacles, it acts like secondary sources and therefore the gas dispersion process will continue for longer periods of time. Contrary to the old gas dispersion models, the CFD models can properly show this phenomenon.

CFD postprocessor also can help to figure out the volumes of flammable gas clouds whose concentration is more than their related Lower Flammable Limit (LFL).Moreover, tone can obtain the weight of the gas cloud which can be used in calculating the power of an explosion.

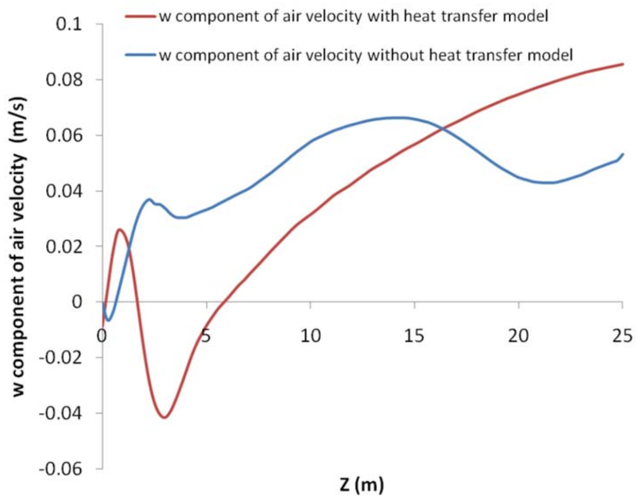


Fig. 15: Comparison of w component of air velocity in z direction at 25m far from source point

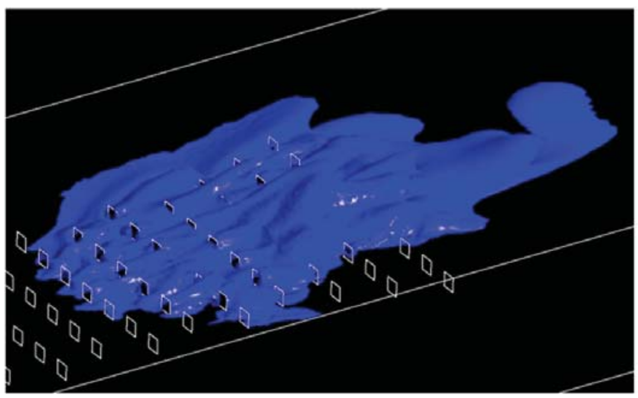


Fig. 16: Gas cloud with 150 ppm isosurface concentration, 100s after gas release. Its volume is equal to $2952.4m^3$ and its weight is 72kg.

Conclusion:

Computational simulations of atmospheric dispersion of the dense gas around an array of obstacles were conducted using the CFX11 code. The model was validated using results of Kit Fox experiments. The fluctuations of wind speed and its direction are the most important factors in an accidental gas release. The concentration results can be predicted more carefully by including experimental wind speed and direction data at different times and elevations in CFD code. In addition, the near wall mesh size is an important parameter that can affect gas dispersion. Using y^+ means at mesh generation stage helped in achieving acceptable and desirable results more easily. The vertical temperature gradient is an important phenomenon in gas dispersion modeling. It causes the vertical fluctuation in the flow pattern which leads to more complex gas dispersion.

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