Heavy Gas Dispersion Modeling Over a Complex Train with Computational Fluid Dynamic

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Abstract: In accidentally released gas at ground level or where the gas denser than the air or we have many obstructions, dispersion is much slower and hazard range maybe significant. Computational Fluid Dynamic (CFD) provides a potential means of improving the understanding of any effect on gas dispersion. In first stage commercial code must be validated with standard experimental results. In this paper used from Thorney Island and Kit Fox experiments to validate a CFX11 code. The results showed that CFX approximated gas concentration histories with a reasonably good agreement and predicted correctly the behavior of gas cloud during dispersion.

Keywords  Heavy Gas Dispersion, Computational Fluid Dynamic, Complex Train

1. Introduction

Large quantity of hazardous toxic substances are produced, stored or transported in a modern industry. Many of these gases form clouds heavier then air when accidentally released to the atmosphere. The gases may have a density greater than that of air for several reasons. These include the high molecular weight (for example chlorine), low release temperature (for example liquefied natural gas), high storage pressure (for example a failure of a containment of ammonia and subsequent formation of aerosol) or chemical reactions of the released substance with water vapor in the atmosphere (the polymerization of hydrogen fluoride) [1].

The heavy gas clouds have the negative buoyancy. It affects and modifies their behavior in relation to positively buoyant or neutrally pollution clouds. The differences include the additional gravity driven flow, wind shear at the heavy gas cloud interfaces, turbulence dumping, and inertia of the released material. Special models are developed to describe the heavy gas clouds dispersion in the atmospheric air. They are called heavy gas dispersion models or dense gas dispersion models.

There are many different types of heavy gas dispersion models developed. They include empirical models, intermediate models and fluid dynamic models. The empirical and intermediate models are important components of emergency response systems and valuable tools for environmental impact assessment and risk assessment. The fluid dynamics models are usually used as a research tool to get to know better the heavy gas properties.

Computational fluid dynamics allows the simulation of complex physical processes describing heat and mass transport phenomena with fully developed mathematical models. Specific models incorporated in CFD codes predict the turbulent mixing between gas molecules and air particles, in addition to cavity regions in the flow field (building wakes), which may result in entrapment of escaping gas at low heights for relatively long time with increased health effects.[2]

In this paper, numerical simulation of the Thorney Island trials and Kit Fox field experiments was performed via the use of CFX 11 code [3 ].

2. Computational Background

2.1. Turbulence Model

One of the most prominent turbulence models, the \( k - \varepsilon \) model, has been implemented in most general purpose CFD codes and is considered the industry standard model. The \( k - \varepsilon \) model use the gradient diffusion
hypothesis to relate the Reynolds stresses to the mean velocity gradients and the turbulent viscosity. \( k \) is the
turbulence kinetic energy and is defined as the variance of the fluctuations in velocity. \( \varepsilon \) is the turbulence eddy
dissipation (the rate at which the velocity fluctuations dissipate).

The \( k - \varepsilon \) model introduces two new variables into the system of equations. The momentum equation is then:
\[
\frac{\partial \rho \bar{u}}{\partial t} + \nabla \cdot (\rho \bar{u} \otimes \bar{u}) - \nabla \cdot (\mu_{eff} \nabla \bar{u}) = -\nabla p' + \nabla \cdot (\mu_{eff} \nabla \bar{u})^T + \mathbf{B}
\]  

(1)

Where \( \mathbf{B} \) is the sum of body forces, \( \mu_{eff} \) is the effective viscosity accounting for turbulence, and \( p' \) is the
modified pressure. The \( k - \varepsilon \) model is based on the eddy viscosity concept, so that:
\[
\mu_{eff} = \mu + \mu_t
\]

(2)

Where \( \mu_t \) is the turbulence viscosity. The \( k - \varepsilon \) model assumes that the turbulence viscosity is linked to
the turbulence kinetic energy and dissipation via the relation:
\[
\mu_t = C_{\mu} \frac{k^2}{\varepsilon}
\]

(3)

Where \( C_{\mu} \) is a constant. The values of \( k \) and \( \varepsilon \) come directly from the differential transport equations for
the turbulence kinetic energy and turbulence dissipation rate.

2.2. Scalar Transport Equation

The bulk motion of the fluid is modeled using single velocity, pressure, temperature and turbulence fields.
The influence of the multiple components is felt only through property variation by virtue of differing properties
for the various components. Each component has its’ own equation for conservation of mass. After Reynolds-
averaging this equation can be expressed in tensor notation as:
\[
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial (\bar{\rho} \bar{U}_i)}{\partial x_j} = -\frac{\partial}{\partial x_j} \left( \rho_i (\bar{U}_{ij} - \bar{U}_j) - \bar{\rho}_i \bar{U}_j \right) + S_i
\]

(4)

\( \bar{\rho}_i \) is the mass-average density of fluid component \( i \) in the mixture, i.e., the mass of the component per
unit volume, \( \bar{U}_j = \Sigma (\bar{\rho}_i \bar{U}_{ij})/\bar{\rho} \) is the mass-average velocity field, \( \bar{U}_{ij} \) is the mass-average velocity of fluid
component \( i \), \( \rho_i (\bar{U}_{ij} - \bar{U}_j) \) is the relative mass flux, \( S_i \) is the source term for component \( i \) which includes the
effects of chemical reactions.

Note that if all the equations (Equation 4) are summed over all components, the result is the standard
continuity equation,
\[
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial (\bar{\rho} \bar{U}_i)}{\partial x_j} = 0
\]

(5)

Since the reaction rates \( S_i \) must sum to zero.

The relative mass flux term accounts for differential motion of the individual components. This term may be
modeled in a number of ways to include effects of concentration gradients, a pressure gradient, external forces
or a temperature gradient. Of these possible sources of relative motion among the mixture components, the
primary effect is that of concentration gradient. The model for this effect gives rise to a diffusion-like term in
Equation 4.

\[
\rho_i (\bar{U}_{ij} - \bar{U}_j) = \frac{\Gamma_i}{\bar{\rho}} \frac{\partial {\bar{\rho}_i}}{\partial x_j}
\]

(6)

The molecular diffusion coefficient, \( \Gamma_i \), is assumed to be equal to \( \rho D_i \), where \( D_i \) is the Kinematic
Diffusivity. Now, define the mass fraction of component \( i \) to be:
\[
\bar{\gamma}_i = \frac{\bar{\rho}_i}{\bar{\rho}}
\]

(7)

Note that, by definition, the sum of component mass fractions over all components is 1. Substituting
Equation 7 and Equation 6 into Equation 4, we have:
\[
\frac{\partial (\bar{\rho} \bar{\gamma}_i)}{\partial t} + \frac{\partial (\bar{\rho} \bar{U}_i \bar{\gamma}_i)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \Gamma_i \frac{\partial \bar{\gamma}_i}{\partial x_j} \right) - \frac{\partial}{\partial x_j} (\rho \bar{U}_i \bar{\gamma}_i) + S_i
\]

(8)

The turbulent scalar fluxes are modeled using the eddy dissipation assumption as:
\[
\bar{\rho} \bar{U}_i \bar{\gamma}_i = \frac{\mu_t}{S_{Sc} \bar{\rho}_i \bar{U}_i}
\]

(9)

Where \( S_{Sc} \) is the turbulent Schmidt number. Substituting Equation 9 into Equation 8 and assuming now
that we have mass weighted averages of \( Y_i \):
\[
\frac{\partial (\bar{\rho} \bar{\gamma}_i)}{\partial t} + \frac{\partial (\bar{\rho} \bar{U}_i \bar{\gamma}_i)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \Gamma_{\nu eff} \frac{\partial \bar{\gamma}_i}{\partial x_j} \right) + S_i
\]

(10)

where:
\[ \Gamma_{\text{eff}} = \Gamma_i + \frac{\mu_i}{S_{\text{eff}}} \]  

Equation 10 is simply a general advection-diffusion equation of the form common to the equations solved for each of the other dependent variables in the fluid flow calculation. Thus, it is convenient to solve for the \( \Gamma_i \) in order to establish the composition of the fluid mixture.

### 2.3. Buoyancy

For buoyancy calculations, a source term is added to the momentum equations as follows:

\[ S_{\text{M, buoy}} = (\rho - \rho_{\text{ref}}) g \]  

The density difference \( \rho - \rho_{\text{ref}} \) is evaluated using either the Full Buoyancy model or the Boussinesq model, depending on the physics.

When buoyancy is activated, the pressure in the momentum equation excludes the hydrostatic gradient due to \( \rho_{\text{ref}} \). This pressure is related to the absolute pressure as follows:

\[ p_{\text{abs}} = p + p_{\text{ref}} + \rho_{\text{ref}} g (\vec{r} - \vec{r}_{\text{ref}}) \]  

Where \( \vec{r}_{\text{ref}} \) is a reference location. Absolute pressure is used to evaluate fluid properties which are functions of pressure.

#### 2.3.1. Full Buoyancy Model

For buoyancy calculations involving variable density, \( \rho - \rho_{\text{ref}} \) is evaluated directly. This option is set when the simulation involves multicomponent flow, multiphase flow, or a fluid having density set as a function of pressure, temperature, or other field variables.

### 2.4. Finite Volume Technique

In this technique, the region of interest is divided into small sub-regions, called control volumes. The equations are discretized and solved iteratively for each control volume. As a result, an approximation of the value of each variable at specific points throughout the domain can be obtained. In this way, one derives a full picture of the behavior of the flow.

### 3. Field experiments

#### 3.1. Thorney Island trial 26

The Thorney Island Heavy Gas Dispersion Trials were organized by the Health & Safety Executive, and detailed information about the trials program has been given by McQuaid and Roeback (1985) [4]. In the first phase, large instantaneous dense gas clouds were released in flat, unobstructed terrain. The second phase incorporated the effects of buildings and fenced.

Trial 26 from the phase II program include the obstacle was a cube 9m × 9m × 9m consisted of plastic sheets attached to a wooden frame. The complete structure was mounted on a trailer and was moved to the required position shortly before the release of gas, according to the wind direction record. The gas source was a cylindrical (actually 12-sided) tent of 14m diameter, 13m height and total volume capacity of 2000m³, made from flexible material, and at the start of the trial, the sides were allowed to collapse rapidly to the ground leaving a stationary cylinder of dense gas standing still. Within a few second, this gas cylinder completely collapsed resulting in a low level cloud front spreading radially outwards. In this trial, the mobile cubical building was situated 50m downwind from the cylindrical gas tent (Fig. 1) and the released gas was a mixture of Refrigerant-12 diluted with nitrogen. The percent gaseous mixture composition was 31.6% nitrogen and 68.4% Freon 12 (w/w). During the trial execution, wind speed was relatively low (1.9ms⁻¹) and the cloud was swept around the sides of the building without significant elevation at the front of the cube [2, 5].

#### 3.2. 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 (NTS). The field operations, described in the WRI (1998) report [6], were carried out by Western Research Institute (WRI) and Desert Research Institute (DRI). Dense gas (CO₂) was released from a 1.5 m by 1.5 m ground-level area source. The entire experimental set-up was intended to represent an industrial site at about 1/10 of full-scale. To simulate an oil refinery or chemical plant at about 1/10 scale, the flat desert lake bed at Frenchman Flat had thousands of “flat billboard” roughness elements installed over a 120m * 314 m area in order to increase the roughness to a value that was about 1/10 of the value typical of an industrial site and its surroundings (see Figure 2 and 3 for a plot plan of the experiment) [7-10].
The Kit Fox field experiment had the following geometric set up, gas release methodology, and concentration and meteorological observations (refer to Figures 2 and 3):

- The large Equivalent Roughness Pattern (ERP) (2.4 m squares) was installed on the inner 39m * 85m rectangle, with the dense gas source near the center. The roughness elements were staggered, with 6.1 m lateral spacing and 8.1 m along-wind spacing.
- The smaller Uniform Roughness Array (URA) (0.2 m high by 0.8 m wide rectangles) was installed on the outer 120m by 314 m rectangle. The roughness elements were staggered, with 2.4 m lateral spacing and 2.4 m longitudinal spacing. Irwin spires with height 4.9 m were set up on the upwind edge of the URA.
- 84 fast-response (one reading per second) concentration monitors were installed on 4 downwind arcs (25 m, 50 m, 100 m, and 225 m), with some mounted on towers. There were three towers on each of the 25 m, 50 m, and 100 m arcs. There were no towers located on the 225 m arc.
- Meteorological instruments (including nine sonic anemometers) were installed on five towers, plus wind vanes at six other locations.
- CO2 was released from a 1.5 m * 1.5 m area source near the middle of the ERP, with an emission rate of about 4 kg/s for 2 to 5 minute (continuous) and 20 second (finite duration) bursts when the ERP was in place. When the ERP was removed (leaving the URA), the CO2 release rate was decreased to 1.6 kg/s, since the rate of dispersion was expected to be less and the concentrations were therefore expected to be larger.
- Schedule: One week of field tests (trials 2-5) took place with the ERP and the URA roughness obstacles installed. One week of field tests (trials 6-8) took place with only the URA roughness obstacles in place.
- One week of test trials took place with the ERP and URA roughness obstacles removed (i.e., flat desert).
- There were 52 independent Kit Fox data trials, with about 2/3 for “puff” or “finite duration” 20 s releases, and about 1/3 for “continuous plume” 120-450 s releases. A summary of the major characteristics of each of the 52 tests is given by Hanna and Chang [7]. We use from trial 3-7 (trial 3, release 7 instantaneous release) for our simulation propose.

4. Simulations and Results

Using embedded meshing techniques, cells are concentrated around the initial position of the gas cloud, in order to capture the detailed shear and entrainment effects at the edge of the gas column. In addition, a fine resolution was used vertically from the ground up to a height of about 2m, since, during the initial stages before the cube is encountered, most of the gas cloud remains below this level. Cells were also concentrated close to the cube (in Thorney Island trial) and billboards (in the Kit Fox trial), to help resolve the interaction between the cloud and the obstacle. Computational grids consisted of 365599 and 987219 volume elements, in the Thorney Island and Kit Fox trials respectively. Since the aim was to compute concentration values at different times, the problem must be solved in transient form. Total simulation time was 200 s with relatively short time steps (1s). In both cases, each problem was firstly solved in steady state to obtain initial values for the transient simulations. Steady state runs terminated after approximately 140–200 iterations allowing a reasonable convergence to be achieved. The convergence criterion was the residual RMS (residual of root mean square) to be equal to or less than 10^{-4}. Transient runs needed 3–12 iterations per time step to reach the desirable residual value.

4.1. Thorney Island

For the present study, it was used symmetry plan. The model geometry is shown in Figure 1. The extent of the domain was 130m in the x-direction, 100m in the y-direction and 40m vertically.

4.1.1. Boundary conditions

Boundary conditions are specifications of properties or conditions on the surfaces of the domains and are required to fully define the flow simulation. Regarding the computational domains in Figure 1, the boundary conditions set the wind profile and gas inflow are demonstrated below.

4.1.1.1. Gas inlet

At Thorney Island no. 26 approximately 2000m³ of Freon 12/nitrogen mixture was released into the atmosphere instantaneously. In order to set the inflow boundary condition for the transient problem, released mixture mass inflow rate \( Q_1 \) was given through a properly adapted step function:

\[
Q_1 = m_1 \times \text{step} \left[ \frac{(t - t_0)(t - t_1)}{t_c^2} \right]
\]

\( m_1 \) is equal with 4780 kg s⁻¹.

Gas entered from surface level source to domain at 1s and its height reach to 13m in domain. With this way we can have one cylindrical cloud after 1s. This condition was same as the experimental condition and affect very much on the simulation.
4.1.1.2. Wind inlet
Wind speed is one of the most significant parameters in problem definition procedure, since it determines how quickly emitted gas will be diluted by passing volumes of air. The corresponding boundary condition should take into account the reduction of wind speed value near the ground level due to frictional effects. If wind speed at a fixed height is known (typical reference height 10 m), then wind velocity profile may be given through a power low correlation [11]:

\[ u_z = u_0 \left( \frac{Z}{Z_0} \right)^\lambda \]  

(15)

Where \( \lambda \) is a dimensionless parameter, whose value depends upon atmospheric stability category and surface roughness (\( Z_0 \)). Regarding the trial 26, the values of \( Z_0 \) is 0.005m; \( \lambda \) is 0.07and \( u_0 \) is 1.9m/s.

In addition to the above, the ground and the building faces were defined as fixed stable walls, where the fluid velocity is equal to zero according to the no slip condition, whereas the remaining planes of the domain were specified via a relative pressure value, which was set equal to zero and corresponds to the relative static pressure when outflow takes place (opening condition).

4.1.2. Results
In figure 4 computational results are compared with experimental concentration measurements recorded on the front face of building at the height of 6.4 m. As one can see, simulation yielded result that is found in good agreement with the experimental records.

4.2. Kit Fox
In this simulation, two dimensional board used as a billboard. With this way the roughness thickness eliminated and consequently minimum size of mesh were greater than the billboard thickness. The model geometry is shown in Figure 5.

4.2.1. Boundary conditions
4.2.1.1. Gas inlet
In trial 3-7 of Kit Fox field experiment, carbon dioxide was released in to the atmosphere with 3.65kg/s rate and for about 20s corresponding to an instantaneous release. In order to set the inflow boundary condition, like the Thorney Island case, the mass inflow rate from the surface level were defined (\( m_i=3.65\)kg/s, \( t_i=50s \)). For performing fully develop flow in domain, gas release begin after 50s.

4.2.1.2. Wind inlet
In this simulation didn’t used from any correlation. The EPA tower wind data imported directly as a boundary condition. This way helps to define the experimental wind speed and direction in any time and any height. The average value of wind speed and direction is given in table1. For inputting the wind direction, Cartesian velocity component is used:

\[ u = U \cos \theta \]  

(16)

\[ v = U \sin \theta \]  

(17)

\[ w = 0 \]  

(18)

Where \( \theta \) is a deviation of wind direction. For inputting the time dependency of wind speed and direction, step function is used.

4.2.1.3. Surface roughness
The surface roughness length, \( z_0 \), is a measure of the amount of mechanical mixing introduced by the surface roughness elements. The appropriate wind profile formula for nearly neutral conditions is:

\[ \frac{u}{u^*} = \frac{1}{\kappa} \ln \left( \frac{Z}{Z_0} \right) \]  

(19)

Where \( \kappa \) is the von Karman constant (assumed to equal 0.4), and \( u^* \) is the friction velocity. \( Z_0 \) can be given by this relation [12]:

\[ z_0 = \beta \frac{v}{u^*} \]  

(20)

\[ \ln \beta = \ln \frac{e u^*}{\nu} - 3.4 \]  

(21)

Where \( e \) is a real roughness element height, and \( \nu \) is a kinematic viscosity. As a rough rule of thumb, \( z_0 \) is equal to about 0.1 times the average height of the roughness elements[13]. In this simulation the ground surface were defined as rough wall with \( z_0 \) equal to 0.01m.
In figure 6 results are compared with measurements recorded at arc one (25m distance from source) at the height of 1.2 m.

4.2.2. Conclusion
Computational simulations of atmospheric dispersion around an isolated cubical obstacle and array of obstacles were conducted using the code CFX11 and the model predictions were validated using results from Thorney Island and Kit Fox experiments. Wind speed and direction fluctuation is most important factor in an accidental gas release. With importing the experimental wind speed and direction at any measurement time and height, to CFD code, it can be predicting the concentration carefully.

5. Acknowledgement
The authors wish to express their gratitude for the gratefully Kit Fox field experiment data provided by Dr Joseph Chang from George Mason university.

6. Reference
Fig. 1. Plot plan of the Kit Fox dispersion grid, showing the locations of the meteorological towers, the concentration monitoring arcs, the source, the Equivalent Roughness Pattern (ERP) array, and the Uniform Roughness Array (URA) array.

Fig. 2. Oblique view of the same Kit Fox dispersion grid shown in Fig. 1.

Fig. 3. Domain of simulation in Thorney Island experiment (half of the main domain)
Fig. 4. Gas concentration vs. time for trial no. 26, front face of building at height 6.4m.

Fig. 5. Domain of simulation of Kit Fox experiment

Fig. 6. Comparison of experimental and computational results in Kit Fox experiment (trial 3-7) at on arc one and height 1.2m.
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