Large Scale Outdoor Flammable & Toxic Gas Dispersion Modelling in Industrial Environments.

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Abstract: This paper presents and discusses HazRes' research and results associated with the simulation and modelling of large scale, outdoor flammable and toxic gas dispersion events in industrial environments using COMSOL Multi-Physics (COMSOL). HazRes has developed a gas discharge and dispersion model in COMSOL which takes into account the effects of localised wind profiles and turbulence generated by buildings, structures and terrain on the dispersion of gases in question. The main focus of this work is to develop & provide clients with more accurate prediction methods relative to industrial standard software tools in modelling potential Major Accidental Hazards (MAH), gas discharge and dispersion events in order understand the risks to people & assets both onsite and offsite. This research would be of particular interest to organisations that have to conform to the Control Of Major Accidental Hazards (COMAH) Directive in the UK and Seveso II Directive in Europe.

Keywords: Fluid-Dynamics, Dispersion, Safety, Risk, Toxic, Flammable.

1. Introduction

The prediction of an accidental gas release, whether toxic or flammable, in terms of people, assets and production of a facility is of paramount importance in terms of identifying, understanding, managing and reducing the impact from such a Major Accidental Hazard (MAH).

In safety case studies, for such regulations as COMAH in the UK and Seveso II in Europe, when conducting consequence analysis of gas releases, integral models are widely used in order to obtain calculated estimates of the extent and spread of the dispersed gas cloud [1]. Integral models tend to be easier to use and are economic in terms of time & computational resources, as discharge and dispersion prediction tools. However, integral models, which can account for a wide range of release and dispersion scenarios, do not account correctly for the effects of obstacles (e.g. buildings, structures, process units, towers etc) and non-flat terrain (e.g. hills, inclines, descents etc)[2].

Geometrically complex scenarios make integral models inaccurate and require more rigorous calculation methods such as Computational Fluid Dynamic (CFD) simulations in order to obtain more accurate estimates of the dispersed cloud extent and its effect.

HazRes' CFD Gas Dispersion Model, using COMSOL, is a three-dimensional (3D) model adapted to simulate atmospheric air flow and dispersion simulation. HazRes CFD solver is capable of handing complex large geometries and complex interconnected physical sub-models. The model and solver provide simulations based on the Eulerian approach, utilizing an un-structured grid, finite element method to model atmospheric air flow and dispersion at full scale and fine resolution. It also has the ability to model the interaction with complex terrain and obstacles using the k-ε turbulence closure model.

HazRes' CFD Gas Dispersion Model using COMSOL has been validated against both experimental results and against an industry standard integral model for which it is found to be in good agreement. A summary of this validation will be presented in this paper.

In order to show & demonstrate the capability of COMSOL and HazRes' CFD Gas Dispersion Model, the authors have conducted numerous different flammable & toxic gas discharge and dispersion simulations for a variety of industrial environments, some of which are presented in this paper.

2. Use of COMSOL Multi-Physics

HazRes' CFD Gas Dispersion Model, solved using COMSOL Multi-Physics, is a 3D model adapted to model atmospheric air flow and dispersion phenomena.

The model and solver provide simulations based on the Eulerian approach, utilising an unstructured grid, finite element method to model atmospheric air flow and dispersion at full scale and fine resolution. It also has the ability to simulate the interaction with complex terrain and obstacles using the k-ε turbulence closure model.

The gas dispersion process is governed by the general conservation equations, i.e. the momentum equation, the continuity equation and the mass species conservation equations. These governing equations of the model are well described in the COMSOL documentation and for turbulence modelling using the k-ε closure they can be expressed as:

$$\nabla.\mathrm{U} = 0$$

$$\rho\frac{\partial \mathrm{U}}{\partial t} - \nabla\left[\left(\eta + \rho C_\mu \frac{k^2}{\varepsilon}\right).\left(\nabla \mathrm{U} + (\nabla \mathrm{U})^T\right)\right] + \rho \mathrm{U}.\nabla \mathrm{U} + \nabla P = \mathrm{F}$$

$$\delta_{ts}\frac{\partial c_i}{\partial t} + \nabla\left(-D_i \nabla c_i\right) = R_i - \mathrm{U}\nabla c_i$$

where;

- $\mathbf{U}$ is the velocity vector (m/s)
- ρ is the density (kg/m^3)
- η is the dynamic viscosity (Pa.s)
- P is the pressure (Pa)
- $\mathbf{F}$ is the body force vector (N/m^3)
- c_i is the concentration of species i (mol/m^3)
- D_i denotes its diffusion coefficient (m^2/s)
- R_i is the reaction rate for species i (kg/m^3·s)
- δ_{ts} is a time-scaling coefficient
- t is the time (s)
- C_μ is a model constant
- k is the turbulent kinetic energy (m^2/s^2)
- ε is the turbulent dissipation rate (m^2/s^3)

The k-ε turbulence model uses a logarithmic form of the equations for k and ε. Further details about the k-ε equations can be found in the COMSOL documentation. The equations above are solved simultaneously for six (6) variables: u, v, p, $logk$, $log\varepsilon$ and c; fully coupled.

3. Industrial Integral Model Comparison

HazRes has conducted a comparison study between one of most popular, industry standard integral dispersion models and those obtained using HazRes CFD Gas Dispersion Model. For this particular comparison study, a toxic gas release which has a relatively high percentage of Carbon Monoxide (CO) was used where the release and weather conditions for each simulation method were identical.

This was achieved with HazRes' CFD Gas Dispersion model in COMSOL by using a very simple, rectangular box computational volume with no terrain (i.e. flat), buildings or obstacles, with footprint dimensions of 1,000 m by 800 m and 40m in height. The typical computational domain including a dispersion result represented by the concentration slice can be seen in Figure 1. The computational volume was modelled on an extremely fine mesh relative to the size of the computational volume used.

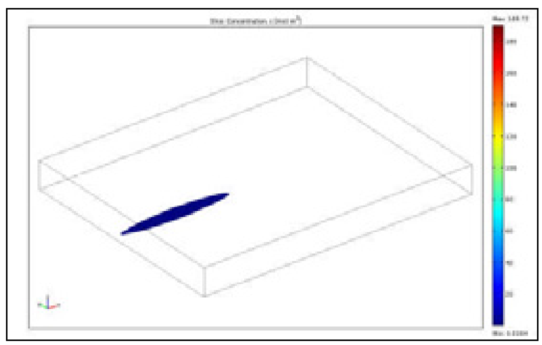

Figure 1. Computational Domain including dispersion result showing horizontal concentration slice at the same height of release.

HazRes analysed the toxic gas discharge and dispersion at a 12m release height as a static analysis with an infinite inventory volume to produce a static steady-state gas cloud. The wind was normal to one side of the rectangle computation volume as shown in Figure 1 and was logarithmically normalised to 2 m/s at a height of 10m, the same as the integral model computations.

The measurements taken of the length (extent) of the HazRes CFD Dispersion code generated gas clouds can be seen in Table 1, against the measurements taken from Integral model equivalent counterparts for all three (3) iso-concentration values for CO of 475, 670 and 1061 parts per million (ppm).

It can be seen from Table 1 that the length (i.e. extent) to each concentration value (i.e. 475, 670 and 1061ppm) is a consistent match and within 10% compared with the Integral Model results, except for the higher concentration value. For this higher concentration value of 1061 ppm, the length (or extent) is just over 23% more than that predicted using the Integral Model. Therefore this could be classed as increasingly more conservative, as the iso-concentration target (i.e. 475, 670 and 1061ppm) increases.

It must also be noted that neither HazRes' CFD Dispersion code nor the Integral Model used has been calibrated or verified against the toxic gas mixture released in real life experimental terms.

Table 1. Comparison Results between Integral Model & HazRes' CFD Dispersion Model relating to maximum cloud length (i.e. extent).

Cloud Characteristics	**Maximum Cloud Length (i.e. extent) (m)**		
Concentration Values	1061 ppm	670 ppm	475 ppm
Integral Model	180	316	403
HazRes' CFD Dispersion Model in COMSOL	221	305	409

4. MUST Validation

HazRes CFD Dispersion Model, solved using COMSOL Multi-Physics has been validated against the Mock Urban Setting Tests (MUST) [3][4]. The MUST tests were a series of nearly full-scale atmospheric dispersion tests conducted at the U.S. Army Dugway Proving Ground (Utah), conducted for the DTRA (Defence Thread Reduction Agency). The objectives of these tests were to acquire a meteorological and dispersion data set and overcome the scaling limitations of laboratory simulations in modelling urban environments.

The MUST tests used an array of 120 (12 by 10) shipping containers to simulate urban housing, where propylene gas was released at several different locations in the array and several different weather conditions. The surface mesh generated in COMSOL can be seen in Figure 2.

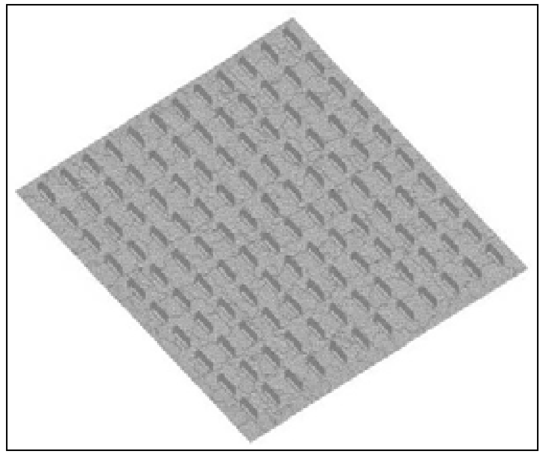

Figure 2. COMSOL MUST surface mesh.

The computational volume was constructed so that the length and width were both 200m and it was 35m high. The volume was meshed using a non-uniform triangular mesh with approximately 500,000 elements and 5,000,000 degrees of freedom.

Both flow fields and pollutant dispersal around a number of containers have been predicted using HazRes' CFD Gas Dispersion Model validated against the MUST experimental data and their wind speed profile and concentration profile against normalised height can be seen in Figure 3 and Figure 4, respectively. Figure 5 shows a 3D iso-surface concentration results display from HazRes; CFD Gas Dispersion Model.

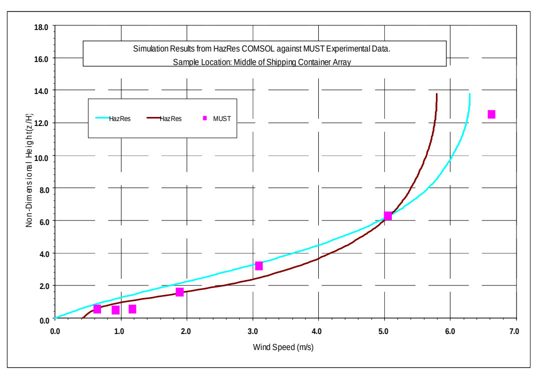

Figure 3. MUST Experimental Data versus HazRes' CFD Gas Dispersion Model for Wind Speed Profile with Normalised Height.

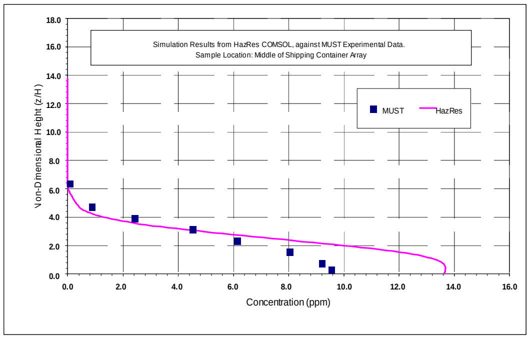

Figure 4. MUST Experimental Data versus HazRes' CFD Gas Dispersion Model for Concentration with Normalised Height.

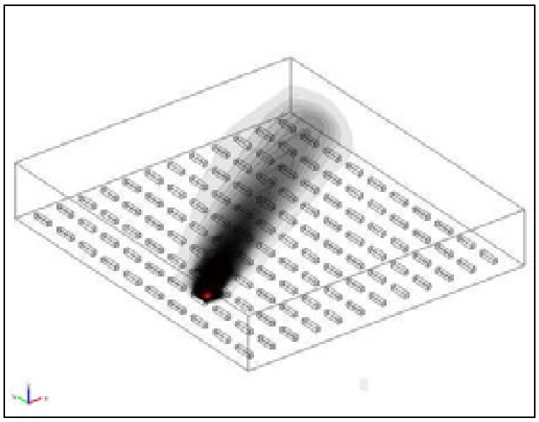

Figure 5. MUST Dispersion Iso-Surface Prediction using HazRes' CFD Dispersion Model in COMSOL.

The validation results obtained in this exercise demonstrate that the flow characteristics are captured well using the k-ε turbulent model. The pollutant concentrations were predicted at several target locations at a range of heights during stable conditions. The predicted propylene concentrations using HazRes' CFD Gas Dispersion model are in good agreement with the MUST experimental test data [3][4].

5. Industrial Example Cases

HazRes has conducted and presented three (3) different hypothetical industrial example cases to demonstrate the capability of HazRes' CFD Gas Dispersion model in COMSOL.

5.1 Case 1: Exhaust Stacks near a Hill

In this example demonstration, HazRes has used its CFD Dispersion model in COMSOL to model a Carbon Dioxide (CO_2) rich exhaust plume from three (3) different height and diameter exhaust stacks at the base of a hypothetical hill as seen in Figure 6. The three (3) exhaust stacks measure 25m, 50m and 100m in height.

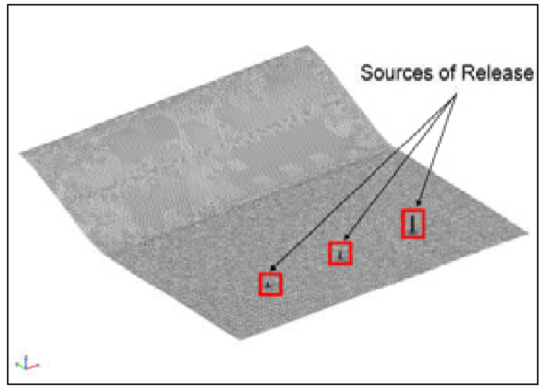

Figure 6. Exhaust Stack Model Surface Mesh

The computation volume has a footprint of 2km by 2km (i.e. 4km^2 in area) and the wind profile was logarithmic with height in a direction prevalent to the inclination of the hill. HazRes used its CFD Dispersion model in COMSOL to conduct a transient time-dependent analysis on the exhaust gas release in order to determine the cloud spread, extent and possible touchdown (cloud touches the ground) as a function of time.

In this particular demonstration, a CO_2 release could potentially cause displacement of oxygen and act as an asphyxiant hazard. However, it is worth mentioning that this analysis can be conducted for other flammable, toxic and asphyxiant gases as well as environmental pollutants and particulates.

The demonstration results are shown in Figure 7 of iso-concentration plots from the three (3) exhaust stack gas cloud dispersions from 10 seconds up to 500 seconds which is approximately where, in all three (3) exhaust stacks, a steady-state plume occurs.

It can be seen in Figure 7 that the highest exhaust stack provides the largest horizontal extent up to at 100 seconds and from approximately 250 seconds onwards establishes a steady-state dispersed cloud. Both the 25m and 50m height exhaust stacks both touch down at approximately 50 seconds, where the boundary layer effect aids in the dispersion at ground level and extends their extent significantly towards and up the hill.

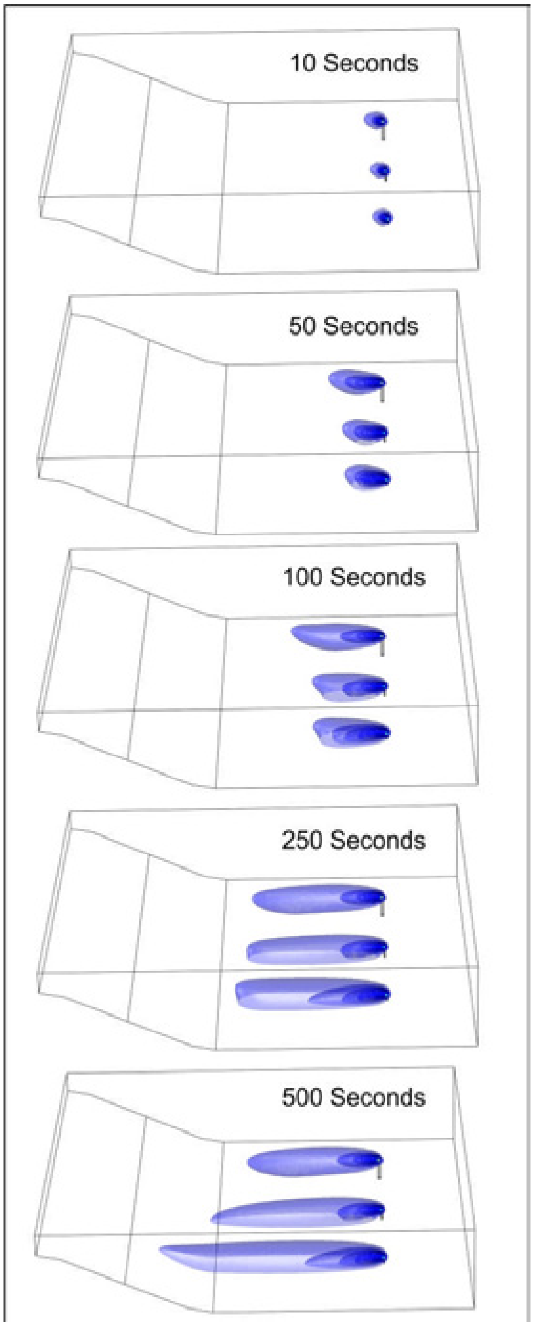

Figure 7. Iso-Concentration Plots showing Exhaust Stack Gas Dispersion with Time including Cloud Touchdown.

This demonstration shows the importance of stack height relative to wind speed in the dispersion process to improve dispersion and reduce the likelihood of touchdown.

5.2 Case 2: Onshore Facility Methane Release

HazRes, using its CFD Gas Dispersion model in COMSOL, has modelled a methane (CH_4) release in a hypothetical industrial onshore facility, as shown in Figure 8 in its surface meshed state. The aim of this particular exercise is to demonstrate how the model can be used to locate fixed stationary gas detection sensors on a facility. The source of the release is a 10m high vessel shown in Figure 8.

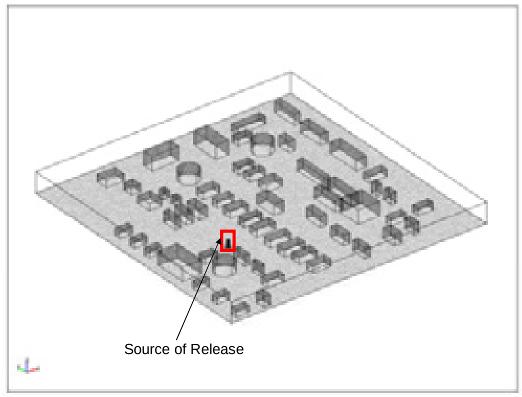

Figure 8. Computation Volume Model in COMSOL of Industrial Site and Source of Release

The computation volume has a footprint of 400m by 400m and the wind profile is logarithmic with height set at an angle of 30° from the X-axis anti-clockwise. HazRes used its CFD Dispersion model in COMSOL to conduct a transient time-dependent analysis on the methane release, in order to determine the concentration as a function of time on the fixed gas detector sensors.

In total, six (6) fixed gas detection sensors were located both upstream and downstream of the point of release as shown in Figure 9. From this plan view as shown in Figure 9, it can been seen that by using the wind direction of 30 anticlockwise from the X-axis, an integral model would automatically show higher concentrations in the downwind direction, namely at sensors No. 5 & 6. This is due to the fact no airflow (i.e. wind) interactions with structures or buildings are taken into consideration by an integral model or code.

In this particular example, the issue of concern is the concentration of methane in air that could provoke an explosion, if ignited. Therefore HazRes is interested in both the Lower Explosive Limit percentage for methane in air (LEL%) which is 5% (i.e. 50,000ppm) and 50% LEL which is 2.5% (i.e. 25,000ppm), purely as a safety factor. Figure 10 shows the predicted methane concentration levels as a function of time for each of the six (6) fixed gas detector sensors.

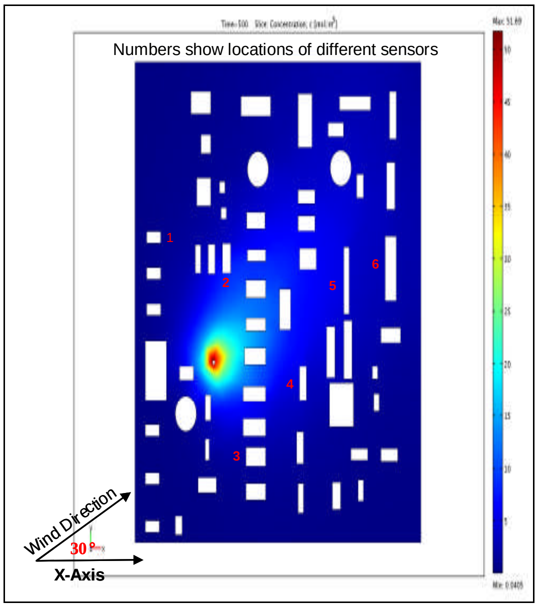

Figure 9. Plan View of Onshore Facility showing locations of the six (6) fixed gas detector sensors (Figure not to scale).

It can be seen from Figure 10 that it is predicted that fixed gas detector sensors No. 2, 4 and 3 could experience 50% LEL concentration level in less than 20 seconds, approximately 40 seconds and 50 seconds, respectively. However, fixed gas detector sensor No. 3 does not experience 100% LEL (i.e. 5% methane in air). Whereas fixed gas detector sensors No. 5 & 6 reach 50% LEL in approximately 100 & 200 seconds each and both obtain 100% LEL in approximately 140 & 290 seconds, respectively.
It can be seen from Figure 10 that the influence of the air-flow interactions with the buildings and structures in this example has a significant effect on the development and direction of the methane gas cloud dispersion in air from the gas sensor concentration rise times.

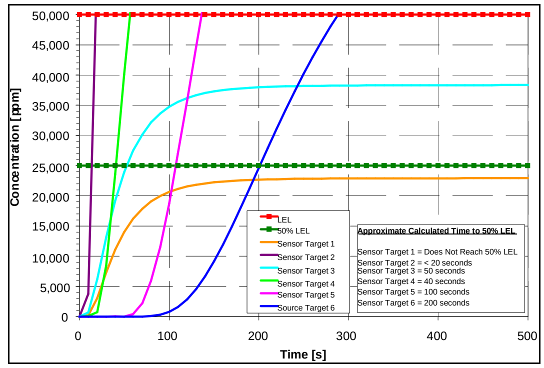

Figure 10. Predicted Methane Concentration Levels as a function of time for each of the six (6) fixed gas detector sensors.

Not only does this type of analysis provide significantly important information of where to place gas detector sensors within and external to a facility, but also provides the operators information with can directly assist them in developing their layers of protection methodology and emergency response procedures.

5.3 Case 3: Onshore Facility CO Release

Using the same computational model as shown in Figure 8, HazRes has used its CFD Gas Dispersion Model to model a release of Carbon Monoxide (CO) for the top of the same gas holder location. The purpose of this demonstration is that due to the cost and potential scarcity of fossil fuels, some industries are using low calorific process by-product gases for heating and energy production onsite. In this particular demonstration case, HazRes has modelled a CO rich by-product gas from a storage tank location.

The computation volume, wind direction and wind profile is identical as described in Case 2. HazRes used its CFD Gas Dispersion model in COMSOL to conduct a transient time-dependent analysis on the CO release relative to a target CO concentration which corresponds to significant Carboxyhemoglobin (COHb) level.

Some results of the transient CO gas discharge and dispersion analysis can be seen in Figure 11 for 10 to 100 seconds from start of release.

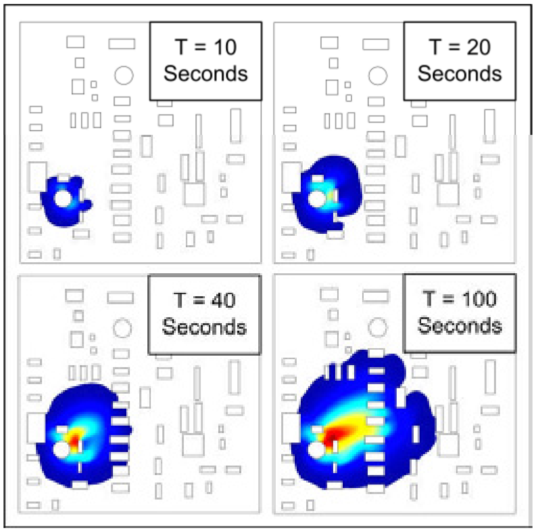

Figure 11. 2D Slice Plot at 3m Height Showing CO Dispersion as a Function of Time.

6. Discussion & Conclusions

It is believed that this paper and the results presented demonstrate the capability of HazRes' CFD Gas Dispersion model solved using COMSOL and its capability to perform both stationary and transient time-dependent analyses of flammable and toxic gas releases over large geographic areas and complex terrains and structures.

The validation work conducted with HazRes' CFD Gas Dispersion model using COMSOL is in good agreement with the MUST experimental data. When evaluated with an industry leading integral model, HazRes CFD Gas Dispersion model using COMSOL compared well, if not slightly more conservative.

In this paper, HazRes has given examples of both large scale flammable and toxic gas discharge and dispersion scenarios it has analysed in outdoor industrial environments to provide base information concerning consequential health, safety and environmental risks to people and assets onsite and offsite.

7. Future Work

As the localised air profile and turbulence (i.e. wind) is very important to conducting these types of CFD gas dispersion analysis it is imperative that good building, process, terrain and topological data is used as part of the simulations. HazRes has investigated other, more accurate geographical data sources which include all surface data including buildings, process and terrain data in one data source.

From initial investigations, LIDAR Digital Surface Maps (DSM) do show promise for this application. HazRes has found that the most recent LIDAR DSM data for the majority of the UK and has a longitude and latitude resolution of 2m with a height resolution of 0.15m.

HazRes is presently working on importing LIDAR DSM data into COMSOL to build and providing this level of accuracy to its clients relating to dispersion analysis for both safety and environmental cases.

8. References

[1] Bernatik, A., Libisova M., Loss Prevention in Heavy Industry: Risk Assessment of Large Gasholders, *Journal of Loss Prevention in the Process Industries*, 17, pp271-8, 2004.

[2] Fiorucci, A., Pontiggia, M., Derudi, M., Alba, M., Scanioni, M., Pendino, R., Uguccioni, G. & Rota, R., Risk Assessment of Dangerous Products Release and Dispersion: A Comparison between CFD and Integral Models, *3rd Int. Conf. on Safety & Envir. In Process Industry (CISAP3)*, Rome, Italy., 11th-14th May 2008.

[3] Biltoft, C.A., Customer report for Mock Urban Setting Test. *Report No. WDTC-FR-01-121*, U.S. Army Dugway Proving Ground, Dugway, UT., 2001.

[4] Biltoft, C.A., Yee, E. and Jones, C.D., Overview of the Mock Urban Setting Test (MUST), *Proceedings of the Fourth Symposium on the Urban Environment.*, Norfolk, VA., May 20-24 2002.

9. Acknowledgements

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