Hydrogen Vehicle Leak Modelling in Indoor Ventilated Environments.

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Abstract: This paper presents and discusses HazRes' research and results associated with the simulation and modelling of hydrogen (H_2) release and dispersion events in indoor enclosed environments, using COMSOL Multi-Physics (COMSOL). HazRes has developed a gas dispersion model in COMSOL, which takes into account the effects of buoyancy, localised ventilation effects and turbulence generated by obstacles on the dispersion of hydrogen in indoor environments. The authors analyse several hydrogen release scenarios to demonstrate the effectiveness and usefulness of this model for this application, using COMSOL. The main focus of this work is to continuously develop and provide more accurate prediction methods to assist "clean fuel" organisations with their hydrogen safety cases.

Keywords: CFD, Buoyancy, Dispersion, Hydrogen, Safety, Renewable, Vehicles

1. Introduction

In order to reduce carbon dioxide emissions, a number of international vehicle manufacturers are developing and building vehicles that use hydrogen as an alternative fuel source to conventional hydrocarbon-based fuels.

Unlike other fuels, hydrogen has a high diffusion coefficient and a relatively low density compared to air, which allows hydrogen to travel upwards without the need for any wind or ventilation. Thus, due to its natural buoyancy, hydrogen produces some interesting effects when consequence analyses are conducted for safety cases. One of these safety cases is the effect of a hydrogen leakage from a stationary vehicle in an indoor ventilated enclosure, such as a garage, where an accumulation of hydrogen could lead to fire or explosion in cases where no hydrogen detection or ventilation systems are installed.

In this paper, the effects and location of the indoor natural enclosure's ventilation system will be investigated to determine its effect on the extent and volume of the flammable hydrogen-air dispersed cloud, using HazRes' three-dimensional (3D) Gas Dispersion model based on COMSOL solver, which takes into account the effects of complex geometries, buoyancy and turbulence.

2. Experimental Description

Prior to using HazRes' gas dispersion model to simulate hydrogen leaks from a car, the model was first validated against hydrogen release and dispersion experimental results[1]. The experimental set-up is in the form of an indoor ventilated hallway measuring 2.90m by 0.74m, by 1.22m tall (i.e. volume = 2.62m^3). The hydrogen is released vertically, with a velocity 0.02m/s, from a 0.05m^2 area vent in the floor, whereby natural ventilation is provided by a wall vent and a roof vent, each of the same area, as shown in Figure 1.

The computational volume has been meshed with a tetrahedral mesh, as shown in Figure 2. The Number of Elements (NoE) equates to 43,565 and the associated Degrees of Freedom (DoF) equate to 385,477.

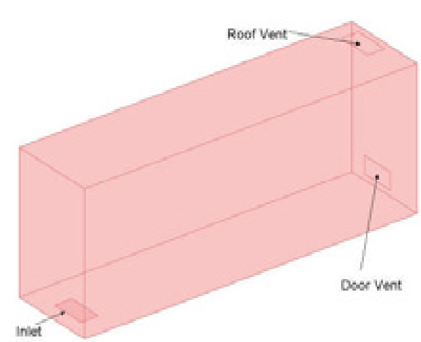

Figure 1. Geometry of the experimental facility

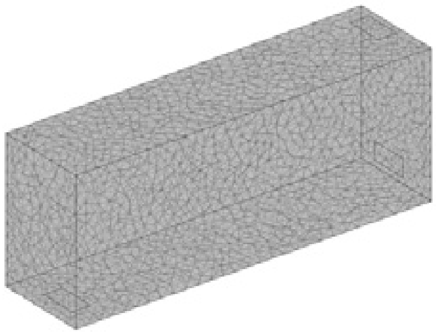

Figure 2. 3D mesh of the experimental facility

After validation, the model was applied to simulate the gas dispersion of hydrogen from a parked car in an enclosed volume measuring 10m by 6m, by 4m tall (i.e. volume = 240m^3). The hydrogen was released, with a velocity of 5m/s, from a circular hole located underneath the rear of the car, as shown in Figure3.

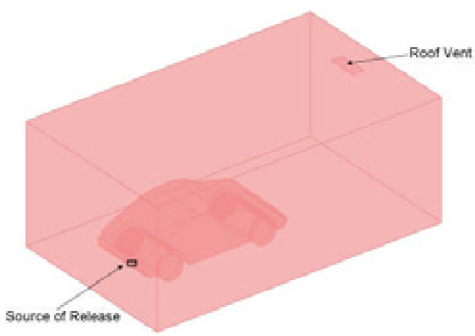

Figure 3. Geometry of the volume under study

The corresponding 3D computational domain is shown in Figure 4. This is a tetrahedral mesh, where the NoE is equal to 272,687 and the DoF is equal to 1,664,351.

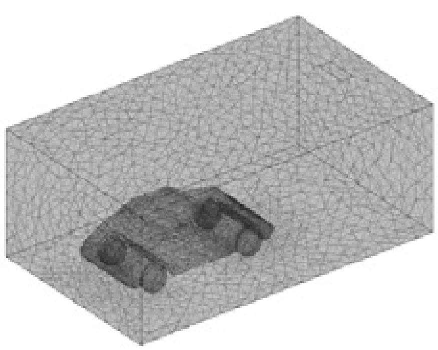

Figure 4. 3D mesh of the computational domain

3. Mathematical Model

HazRes' Gas Dispersion model, solved using COMSOL, is a 3D model adapted to simulate 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 conservation equations are well described in the COMSOL documentation, and for turbulence modelling using the *k-ε* closure, they could be expressed as:

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

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

$$\delta_{ts}\frac{\partial c_i}{\partial t} + \nabla.(-D_i\nabla c_i) = R_i - \mathbf{U}\nabla c_i$$

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.

The dispersion of hydrogen is driven by the buoyancy force caused by the density difference between the hydrogen gas and the air density. To include the effect of buoyancy, we expressed the density and the volume force in the sub-domain settings of the k-ε turbulence model as a function of the concentration c. We therefore had to solve the fully coupled system (turbulence model and convection and diffusion model equations).

The density is calculated using the following equation:

$$\rho = \frac{P_m}{(CR_{H_2} + (1-c)R_{air})T_m}$$

where:

P_m is the absolute pressure
T_m is the absolute temperature
R_{h2} is the hydrogen gas constant
R_{air} is the air gas constant

The buoyancy force was modelled using a formulation similar to the Boussinesq approximation, which is usually used for solving thermal convection problems and is defined as follows [1]:

$$F = -\beta c g$$

where c is the concentration, g is the gravity force and β a scalar value determined using the method described in [1].

The model developed was solved, both stationary and transiently, for both cases. While we did not encounter any convergence problems when solving the convection, diffusion and turbulence equations simultaneously, we did experience difficulties with convergence when attempting to solve the coupled turbulence and convection model simultaneously in transient mode. Therefore, we used a different approach which entailed first storing the stationary solution of the turbulence model then using the pre-calculated velocity profile as a basis for the calculation of the concentration profile with a time-dependant solver.

4. Results

Using the model developed, HazRes has conducted both stationary and time-dependent transient analyses of the hypothetical hydrogen leak and dispersion events simulated in order to determine how the dispersed flammable hydrogen-air gas cloud develops over time and how long a static steady-state dispersed gas plume takes to form, given the effect of ventilation and buoyancy.

In order to validate our model, the computed results are compared against hydrogen experimental tests that study the effects of buoyancy and ventilation on the hydrogen-gas cloud dispersion [1].

HazRes ran the simulation for 200 seconds, which means that the transient analysis ran up to, or very close to, the static steady-state.

Figures 5 and 6 show the variation of concentration with time at the sensor located in the ceiling directly above the inlet (Figure 5) and for the sensor located in the ceiling beside the roof vent (Figure 6).

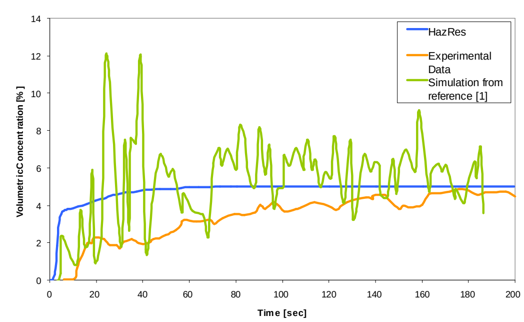

Figure 5. Variation of the concentration with time at the sensor located in the ceiling directly above the inlet

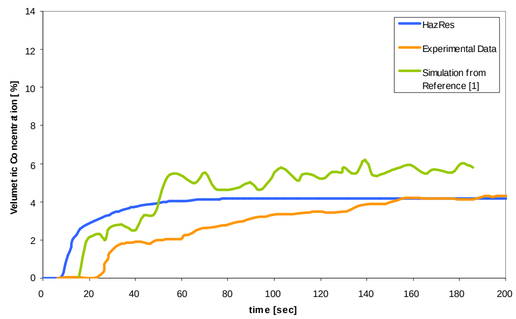

Figure 6. Variation of the concentration with time at the sensor located in the ceiling beside the roof vent

As can be seen, the results agree well with the experimental data, especially when the cloud reaches the steady-state where the volumetric concentration is about 5 % and 4% as shown in Figure 5 and Figure 6, respectively. The slight discrepancy that can be observed at the start of the simulation can be explained by the fact that we used a stationary solution for the air flow profile in order to make the solver converge and that we solved the concentration profile transiently.

The difference that can be noticed between our model and the model described in reference [1] can be attributed to the fact that different numerical models with different internal settings, as well as different boundary conditions settings, were used.

The transient time-dependent concentration results calculated for an iso-surface concentration, where hydrogen concentration is about 0~25 [volume %], can be observed in Figure 7. Snapshots at 1, 5, 15, 20, 30, 50 and 200 seconds after release have been presented in order to show the reader how the hydrogen-dispersed gas cloud develops over time and interacts with the hallway.

As can be seen, the initial development of the hydrogen cloud is strongly influenced by the buoyancy force and the inlet velocity. We should also note the influence of the geometry (ceiling) for the later development of the hydrogen gas cloud, making it extend more in the direction of the roof vent as a function of time.

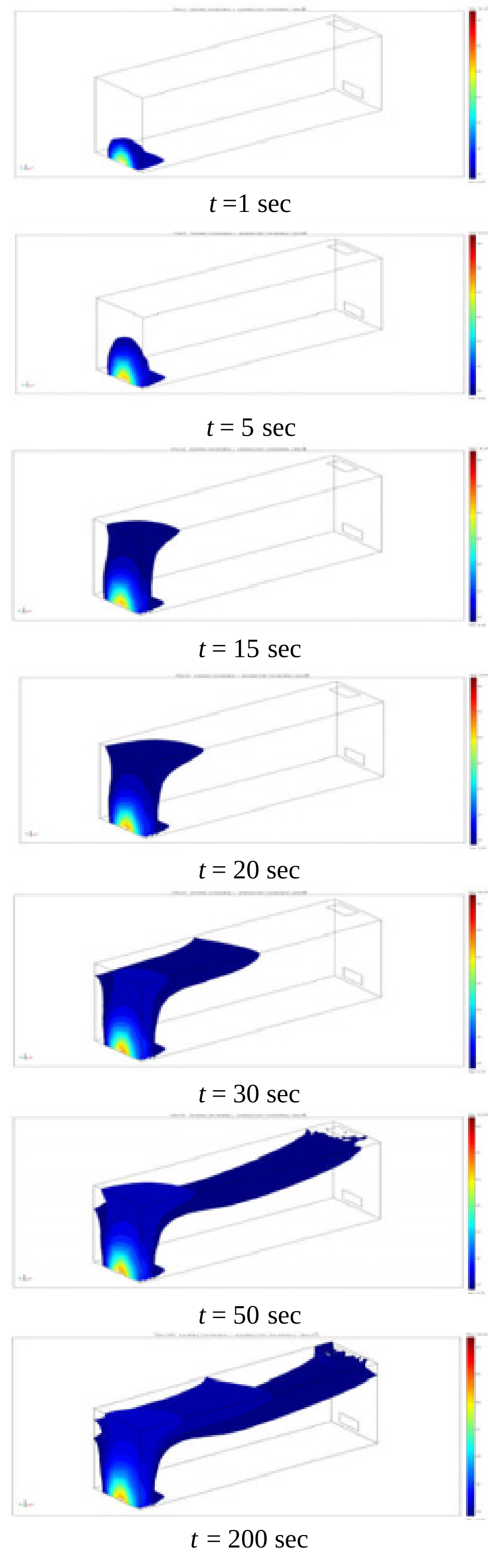

Figure 7. Transient hydrogen gas dispersion

HazRes has also conducted a steady-state concentration analysis for gas dispersion where hydrogen is released from the floor vent and natural ventilation is provided from both the roof and wall vent areas simultaneously. The steady-state concentration analysis simulates the effective static cloud formed after the release has occurred. Figure 8 shows the steady-state hydrogen gas cloud which is similar to the result obtained from transient analysis at later time stages.

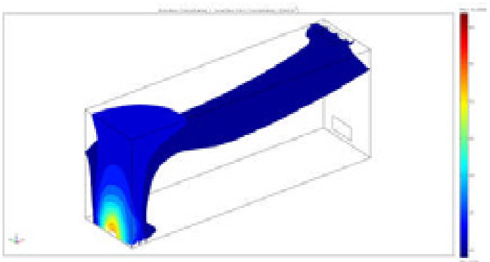

Figure 8. Steady state hydrogen gas dispersion in a hallway

Figure 9 shows the results of a hydrogen leakage from a stationary vehicle in an indoor ventilated enclosure. These results were obtained using a transient time-dependent analysis conducted in COMSOL. The influence of hydrogen buoyancy in the analysis, as well as the effects of natural ventilation on the development and extent of a flammable hydrogen-air gas cloud, is clearly shown in Figure 9.

As can be seen, the cloud rises vertically due to buoyancy effects, before moving forward to the roof vent. This kind of analysis is important for determining the location of gas detector sensors, whereby the location is linked to the ventilation system, in order to reduce the consequence of explosion, if ignition occurs.

It should be noted that in this analysis, the velocity field was calculated by first solving turbulence, convection and diffusion models simultaneously in stationary mode. The velocity field calculated as a result of the stationary analysis was used to start the transient analysis in order to calculate the concentration field; the main reason for this approach was to avoid convergence problems. In future works, we intend to try to improve the model and to solve all equations in transient mode.

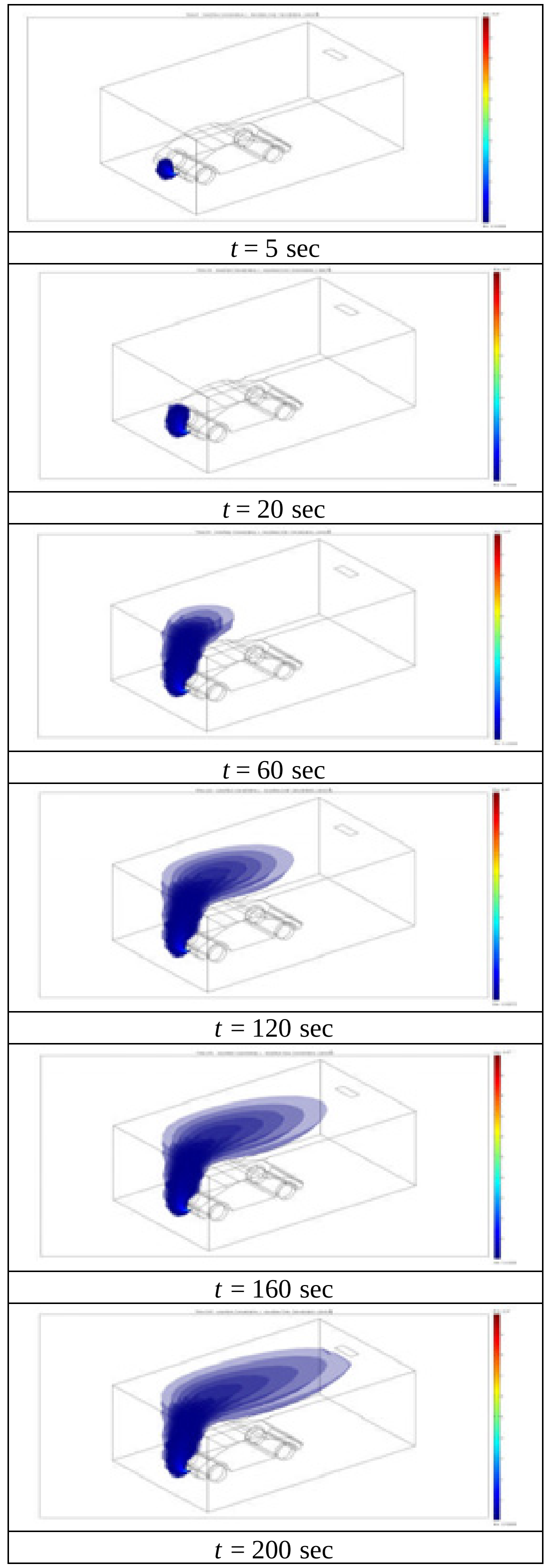

Figure 9. Transient analysis of the hydrogen gas dispersion from a car in a garage

5. Conclusions

HazRes has developed a CFD model, using the COMSOL solver, to simulate gas dispersion while taking into account the effects of buoyancy and ventilation. The model was validated against experimental data of gas hydrogen dispersion in a hallway. The model was also applied to simulate hydrogen gas leaks and dispersion from a car in a garage.

The computed results were in good agreement with the experimental data, especially when the cloud reached the steady state.

This analysis shows that HazRes' CFD Gas Dispersion model is a cost-effective tool for evaluating complex safety case problems, which involve hydrogen due to its unique characteristics, as a renewable fuel energy carrier.

6. References

[1] Kanayama Hiroshi, Tsukikawa Hisayoshi, Ndong-Mefane Stephane Boris, Sakuragi Osamu, Finite Element Simulation of Hydrogen Dispersion by the Analogy of the Boussinesq Approximation, *Journal of Computational Science and Technology*, **2(4)**, 643-654, (2008).

7. Acknowledgements

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