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Numerical modelling of gas dispersion using OpenFOAM

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ABSTRACT

In the current work the rhoReactingBuoyantFoam solver was customised for performing gas leak and gas dispersion modelling. Using experimental data from gas leaks the proposed modelling was investigated for subsonic and sonic releases. The gas molar fraction and velocity decay along the jet centreline were calculated using the modified reacting solver, and the numerical findings were compared with available experimental data. Different approaches for the turbulence closure problem were considered using standard two-equation models. The numerical stability of the solver was also investigated varying the CFL number for a set of simulations. The work also considered the modelling of gas cloud volume in a real engineering case. Standard computational setup for ANSYS-CFX was applied, and the same set of scenarios were modelled in OpenFOAM using the modified rhoReactingBuoyantFoam solver. The analysis considered 5 different leak directions and 4 wind directions in a typical industrial site.

For all scenarios simulated, very good agreement with experimental data and with the commercial CFD (computational fluid dynamics) tool considered in this study was observed. The results are within 10% tolerance intervals. Detailed information of the modelling is also provided, which enable any CFD user to reproduce the results and also apply it for future analysis.

1. Introduction

Accidental releases of flammable or toxic gas can significantly drive the risk level to workers and the environment.

Risk management relies on the proper understanding of the hazards and the risk gas releases pose to personnel. It is therefore crucial to perform a large amount of failure scenarios in order to estimate the measures of protection such as gas detectors location and reinforcement structures due to accidental explosions caused by gas releases.

There have been a large number of experiments concerning gas dispersion. Some of these experiments comprising jets (Birch et al., 1984, 1987; Chuech et al., 1989; Wakes et al., 2002; Rocco and Woods, 2015) and others dealing with large-scale field trials such as MUST, Kit Fox and Praine Grass (Hanna et al., 2004; Hanna and Chang, 2001). They provide data that enable the development of new mathematical dispersion models, and they also help the validation process of numerical tools.

On the other hand, the numerical modelling appears as an alternative approach to create dispersion scenarios. Computational fluid dynamics (CFD) simulation deals with complex geometries, and it is able to produce a wide range of accidental scenarios at low cost (Qiao and Zhang, 2010; Tauseef et al., 2011).

As far as CFD dispersion modelling is concerned, various commercial tools are extensively used as they present a friendly graphic interface and they are widely accepted in both academic and industrial sectors. Concerning the gas jet

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simulation, many turbulence models were tested and validated using commercial tools (e.g. CFX, Fluent) (Rigas and Sklavounos, 2004; Gant and Ivings, 2005; Wilkening et al., 2008). Far field gas plumes simulation were reported in Qiao and Zhang (2010) work where the authors create a method to quantify flammable gas cloud using FLACS. Hansen et al. (2010) also validated FLACS code against experimental data based on the procedure of the Model Evaluation Protocol (MEP). Cormier et al. (2009) analyzed the ANSYS-CFX code to perform consequence analysis for LNG releases. Initially, a validation of the tool against experimental data was considered and the numerical findings presented good agreement with experimental data. Additionally, key parameters of discharge source and dispersion variables such as LNG pool area, evaporation rate, wind velocity and obstacles effect also were simulated.

Currently, OpenFOAM has also been used to simulate gas dispersion. Mack and Spruijt (2013) applied OpenFOAM code to heavy gas dispersion calculation. For large scale simulation, OpenFOAM results were compared with ANSYS-Fluent code. For some cases, the modelling performed with OpenFOAM presented better results than ANSYS-Fluent when compared with experimental data. The comparison, however, was limited to gravity flows and it did not consider the jet release near-field region where the momentum is high.

Similarly, Dixon (2012) has applied PDRFoam solver for gas dispersion simulation. Several simulations were conducted and the flammable gas cloud volume was compared with experimental data. Most of OpenFOAM results fall within a 10% confidence interval.

Kumaresh et al. (2016) customised an OpenFOAM solver to deal with gas dispersion calculation. The solver, namely cloudIgnitionFoam, comprises a transient leak discharge model, gas dispersion and ignition probability models. Although some results are presented, the code has not been validated against existing experimental data.

There have also been attempts to use FDS (Fire Dynamics Simulator) for gas dispersion calculations. Mouilleau and Champassith (2009) report the evaluation of the code based on comparison with widely known experimental sets as Falcon and MUST. The code also was tested against PHAST (Process Hazard Analysis Software Tool) software. The modelling, however, considered only low momentum gas leaks, which are rare in accidental releases where the reservoir storage is kept at high pressure. On the other hand, since FDS relies on the LES (Large Eddy Simulation) approach to capture the fluctuations due to turbulence, Mouilleau and Champassith (2009) claim better results when the wind velocity fluctuations are considered in the modelling.

More recently Ferreira and Vianna (2014, 2016) developed a source model, namely DESQr (Diameter of Equivalent Simulation for Quicker Run) that was implemented in the framework of FDS (Fire Dynamics Simulator) to model high momentum jet release and gas dispersion. The results obtained with the modified FDS code agree well with experimental data and ANSYS-CFX for jet release and gas dispersion data. However, since the code relies on LES approach the computational time is an issue when compared with the computational time spent using RANS (Reynolds Averaged Navier Stokes) modelling.

In this work we explore the complementary application of OpenFOAM tool applied to gas dispersion using another solver, namely rhoReactingBuoyantFoam.

Firstly, we present the solver rhoReactingBuoyantFoam and the customisation executed. The modelling of the gas jet release is carefully investigated, and two different turbulence models are considered. The results are compared with experimental data alongside the mesh sensitivity analysis and optimised time step. A jet simulation performed by Gant and Ivings (2005) is reproduced and good agreement is observed. An engineering case study was developed based on a typical industrial facility. The analysis considered 5 leak directions and 4 wind directions. Numerical findings are compared with a commercial tool ANSYS-CFX and no significant difference is observed. We concluded with a discussion of our work with the implication for applying an alternative open source CFD tool on gas dispersion modelling considering the high momentum release. The Appendix A also provides detailed information of the modelling. It allows for the verification of the results obtained in this work, and it also serves as a guideline for future simulations.

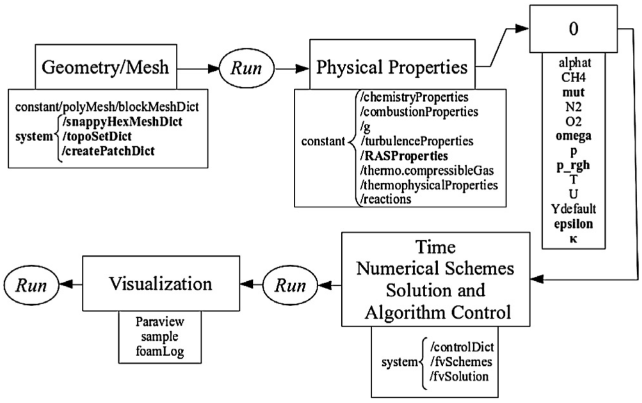

Fig. 1 – Flowchart with all steps of the gas dispersion modelling considered in the current research.

2. Gas dispersion modelling

As far as gas dispersion is concerned the large scale objects play a more significant role than the small scale parts of the geometry, such as piping and small bore fittings. The former, on the other hand, is very important in an accidental explosion. The current analysis is mainly focused on the influence of the large scale geometry. Therefore smaller scale objects have not been considered. Having said that, OpenFOAM has a native mesh generator (blockMesh) and it is able to deal with complex CAD geometries through the snappyHexMesh utility.

The gas dispersion was modelled using the solver rhoReactingBuoyantFoam. The conservation equations modelling the transport of chemical species were applied. The convective term was discretised using the upwind scheme. The diffusion term used central difference scheme. The time advancement was addressed using first order Euler. Pressure – velocity coupling is addressed via PIMPLE algorithm.

Although the solver was initially developed for reacting flows, the chemical reaction source term in the chemical species conservation equation was disabled. In order to accomplish the modelling of the gas dispersion, all physical properties concerning reactions were switched off. The chemical components were set as inert in the ChemistryProperties file located in the constant folder as listed in Fig. 1.

The density, rho, is selected as function of the solver and the reaction file (reactions) does not consider any reaction. In the current research, two turbulence closure models were investigated. The default set up for the $\kappa - \epsilon$ and SST $\kappa - \omega$ are found in the turbulenceProperties file.

Fig. 1 presents a detailed flow of information as considered in the current work.