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LNG Vapour Cloud Dispersion Modelling and Simulations with OpenFOAM

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Growth in demand for Liquefied Natural Gas (LNG) has increased calls for further research and development on LNG production and safer methods for its transportation. This paper presents the implementation of numerical models for dispersion of evaporated LNG in the open atmosphere. The developed model incorporates in its formulation LNG spill and pool formation into a source model. It is then coupled with a Computational Fluid Dynamics (CFD) approach in OpenFOAM for dispersion calculations. Atmospheric conditions such as average wind speed and direction were used to resolve wind boundary layers. The model also accounts for the humidity effect and its influence on air-density and buoyancy change. Verifications have been conducted using the experimental results from Maplin Sands series of tests by comparing the maximum evaporated gas concentration in every arc in relation to the release point. The results show good agreements between the model's predictions and experiments.

1. Introduction

The LNG industry involves 373 special ships with a combined capacity of about 55 million cubic meters carrying around 241.1 MT LNG to 30 major importers (International Gas Union, 2015). These countries are all of farthest from the resources. Transporting ships are exposed to hazards such as crash or terrorism attacks that could lead to LNG accidental spill and subsequent dispersion. The same risks exist for LNG liquefaction and regasification plants where accidental releases are credible scenarios. Researches have been conducted to model and simulate the hazards to remedy the risks and protect the general public.

LNG is a cryogenic liquid transported in highly well insulated storages under a temperature of about 110 Kelvin (-163.15 ºC). The boiling point depends on its composition, but typically is 111 K (-162 ºC). LNG is normally composed of a large share of 87-99% Methane (CH_4) together with 1-10% Ethane (C_2H_6), 1-5% Propane (C_3H_8) and less than 1% Butane (C_4H_{10}). Its density is less than half the water density that ranges from 430 kg/m^3 to 470 kg/m^3. Like any cryogenic liquid once it is exposed to ambient temperature it begins to evaporate immediately. LNG takes up about 1/600$_{th}$ of the volume of natural gas, therefore; once spill occurs it leads to release of a large volume of flammable natural gas in the atmosphere. LNG vapour is initially heavier than air and will remain near the ground, but it rapidly absorbs heat thus; starts to be buoyant. Buoyancy effect is more considerable when release occurs in less ventilated area (low wind). In this case the dominant dispersion force is buoyancy, however; in most cases wind is the main driving force of gas dispersion.

Experiments on spill and dispersion are large-scale and difficult to perform. Many of available datasets of experiment have not shed enough light on every aspect of the problem. Also in real incident the amount of LNG release is massive and small scale trials usually do not reproduce the reality. Therefore; numerical approach provides a better understanding of the phenomena..

Initial approaches to simulate cryogenic gas dispersion were based on integral models and solving ordinary differential equations (ODEs) with less flexibilities and resolution. Although some models such as developed by Raj & Kalenkar (1974) includes ice formation for LNG in water and both radial and linear one-dimensional spreading, the source models still provides limited information and are not capable to simulate the pool formation as well as gas dispersion in complex environment. FAY model is one of the latest updated integral

models (Fay, 2007), in which new aspects have been taken into consideration, such as the effect of ocean waves and their effect on spreading.

The recent approaches to LNG spills, spreading, evaporation and dispersion by CFD have shown more flexibility with reasonably better agreements with experimental results (Sklavounos and Rigas, 2005; Hansen et. al, 2010). But one of the remaining issues in applying the CFD approach is to simulate the evaporation and its rate, and couple this with the dispersion phenomenon. Reviewing the previous works there is still limited understanding over the type of the spill from a breach (Webber, 2010), and for spill onto/into water there is a large room to study the role of turbulence and ambient elements in accelerating the heat transfer and evaporation rate. The aim of the paper is to investigate a more accurate methodology that couples dynamically the LNG evaporation with the dispersion. This is achieved by imposing boundary conditions on the CFD model and using RANS turbulence model for resolving the flow in a relatively uncostly mesh. The open source CFD tool OpenFOAM is used for the study and results are verified with the Maplin Sands Experiments.

2. Methodology

This paper presents CFD based numerical approach to simulate dispersion of LNG-vapour in open atmosphere with OpenFOAM. The Maplin Sands (1980) series of experiment is used to verify the model. The model also was used to estimate the distances of flammable gas dispersion to far field. To impose an exact boundary conditions on the model the release process as well as the rate of evaporation were calculated by applying an integral model (Hissong, 2007). As OpenFOAM is an open source C++ toolbox for the development of numerical solvers, a multi-component reacting solver with inclusion of buoyancy was slightly modified and taken into account. Atmospheric boundary conditions (ABC) were specifically implemented in the way presented by Luketa-Hanlin (2007). The model accounts for turbulence by using a Reynolds Average Numerical Simulation (RANS) model, which applies to standard k-ε turbulence model. To improve the effect of buoyancy a term was added to the kinetic energy equation where the turbulence production or suppression through buoyancy is included (Luketa-Hanlin, 2007). Constant parameters inside the transport equations for k and ε were also changed recommended by Alinot and Masson (2005).

2.1 Numerical Equations

The model implements compressible continuity, momentum and energy equations. RANS model includes k, kinetic energy, and ε, the dissipation rate with the effect of buoyancy (Jaw & Chen, 1987):

$$\frac{\partial(\bar{\rho}k)}{\partial t} + \frac{\partial(\rho\tilde{u}_j k)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_k}\frac{\partial k}{\partial x_j}\right) + P_k + G_k - \bar{\rho}\varepsilon \tag{1}$$

$$\frac{\partial(\bar{\rho}\varepsilon)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\varepsilon)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x_j}\right) + \frac{\varepsilon}{k}\left(C_{\varepsilon 1}P_k + C_{\varepsilon 1}C_{\varepsilon 3}G_k - C_{\varepsilon 2}\varepsilon\right) \tag{2}$$

where

$$P_k = \mu_t\left(\frac{\partial\tilde{u}_i}{\partial x_j} + \frac{\partial\tilde{u}_j}{\partial x_i}\right)\frac{\partial\tilde{u}_i}{\partial x_j} - \frac{2}{3}\left(\bar{\rho}k + \mu_t\frac{\partial\tilde{u}_k}{\partial x_k}\right)\frac{\partial\tilde{u}_m}{\partial x_m} \tag{3}$$

$$\mu_t = C_\mu\bar{\rho}\frac{k^2}{\varepsilon} \tag{4}$$

$$C_\mu = 0.033\,, \quad C_{\varepsilon 1} = 1.17, \quad C_{\varepsilon 2} = 1.92$$

The term G_k is turbulence production or suppression through buoyancy, which is defined as follows:

$$G_k = \frac{\mu_t}{\bar{\rho}\sigma_k}\beta g_j\frac{\partial\tilde{T}}{\partial x_j} \tag{5}$$

where $\beta = 1/T$ is the thermal expansion coefficient. $C_{\epsilon 3}$ is varied from -0.8 for unstable atmospheric condition to 2.15 for stable conditions.

For ABC a reasonable representation of the surface layer is the Monin-Obukhov definition (Arya, 2005), from which the governing equation for velocity considered as follows:

$$\frac{\partial U}{\partial z} = \frac{u_*}{\kappa z}\phi_m\left(\frac{z}{L}\right) \tag{6}$$

where, $u_* = (\tau/\rho)^{1/2}$, is the shear velocity, $L = -u_*^3 \rho c_p T / \kappa g H$, is the Obukhov length that has units of length and represents the height at which buoyant destruction and shear production of turbulence is on the same order. This parameter is negative for unstable conditions, positive for stable and infinite for neutral conditions. The evaporation rate of LNG is determined by calculation of time varying change of LNG pool radius using the methodology suggested by Hissong (2007). It highly depends on the amount of heat that spilled materials absorbs from the ambient. Accordingly the pool radius changes in reference to the following relation:

$$\frac{dR}{dt} = K_s \sqrt{g\left(\frac{\rho_w - \rho_L}{\rho_w}\right)\delta} \tag{7}$$

where R is the pool radius, ρ_w the water density, ρ_L the LNG density, and δ the tickness of LNG layer. K_s is the spreading constant that chose to be 1.41. A series of similar models with different spreading constant for Maplin Sands test no. 35 did not show any remarkable change on the final results.

Relative humidity has been reported in every tests. Dry air is denser than humid air, so the more humid the air is the less buoyant the evaporated LNG is, as its relative density with respect to air density increases. The effect of humidity in the model is accounted for by adding the extra percentatge of water vapour, reported as relative humidity, to the atmosphere.

Table1: Tests parameters used in the numerical model (Colenbrander et al., 1980)

Trial name & no.	Maplin Sands 27	Maplin Sands 34	Maplin Sands 35
Cryogenic released	LNG	LNG	LNG
Spill type	Continues	Continues	Continues
Atmospheric Condition	F*	F	F
Cryogenic Molar Weight (g/mol)	17.2349	16.9123	16.4354
Volume discharged (m³)	12.6	10.2	18.3
Mean spill flow rate (m³/min)	3.2	3	3.9
Mean wind speed in z=10m (m/s)	5.5±0.8	8.6±0.6	9.8±1.2
Mean wind direction** in z=10m	-57±5	-96±3	-78±4
Air temperature in z=2m (ºC)	14.9	15.2	16.1
Relative humidity	53%	72%	63%

* F represents neutral atmospheric condition

** Wind direction is with respect to the layout shown in figure 1

2.2 Experiment Considered

Maplin Sands series of experiments were conducted in 1980 by Shell Research Ltd. at Maplin Sands in the south of England (Blackmore et al., 1984). A series of spills of up to 20 m³ of LNG and refrigerated liquid propane onto the sea were performed. Both instantaneous and continuous releases of croyogenics were made, and some were ignited. Dispersed gas concentration as well as temperature and atmospheric conditions were measured from an extensive array of floating pontoons up to 650 m downwind. Three spill trials were selected, as they were also mentioned in Model Evaluation Protocol (Ivings et al., 2007), and previously verified by others e.g. Hansen et al. (2010). An arcwise study has been done, where the maximum evaporated gas concentration in several arcs with respect to the release source is taken into account. Pointwise study by comparing gas concentration on the measurement points vs. time is not possible, as there is limited information about time varying change of wind speed and direction and spill rate in the report. Figure 1 shows the layout of the instrument pontoons as used in the experiments. In the three standard tests of Maplin Sands trials the spilled material was LNG in a continus rate. For each test a different LNG composition was used.

2.3 Numerical Details

For simplicity and avoid high computational time only dispersion zone was considered for computational mesh. The mesh was a rectangular domain throughout the length of dispersion path whose direction varied dependent upon the wind direction in every test (See Figure 1). The computational domain dimension was 1200x300x100, extended up to 300m upwind and 900m downwind and its height was 100m. Atmospheric open boundaries were arranged as typical inlet and outlet. The lateral and upper boundaries were set to slip.

The time varying pool radius was calculated by an extra code coupled to the solver. Here the LNG inlet BC updaes the time varying pool radius and incorporate it in the model. The pool temperature was initially set to 163.16 K (-110ºC) that is the buoyant LNG temperature. LNG-vapour rises from the bottom of the domain (sea surface) over the forming pool that considered as LNG-inlet. A Mesh Independent Solution Study was done, in which only the central core of the mesh as well as the wind boundary layer region were gradually refined. The optimum number of cells in entire domain at final stage reached to around 1.6 million cells. The Y+ value ranged from 7x103 to 2.5x103. At an optimum Y+ the Y value, distance of the first grid, was around 30 cm. Time step was adjusted automatically by the solver according to a pre-defined courant number of about 0.3, on which time step varied around 0.05 sec. Physical time was 200 seconds from the begining of release. An additional 50-100 seconds advance simulation was considered before LNG release in order to establish the wind boundary layers. The model implemented the equation of state for calculation of time varying gas density applying to the given molar weight.
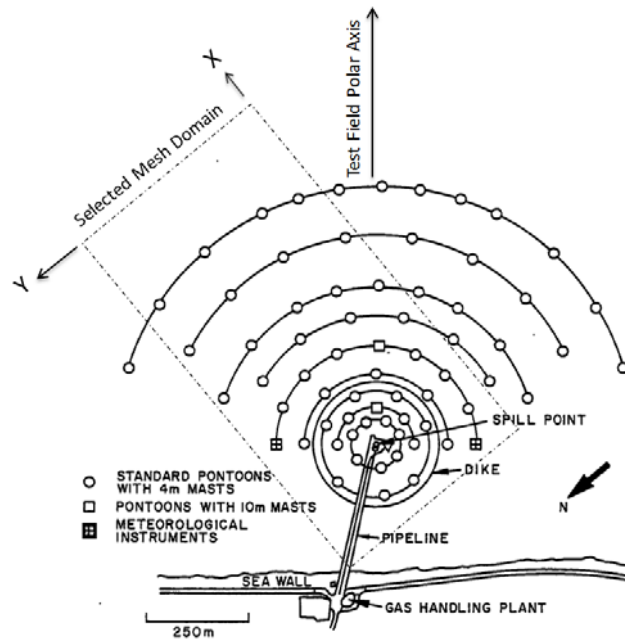

Figure1: The layout of the instrument pontoons as used for the trials including the selected mesh domain that meant to be aligned with wind direction varied in different trials, the layout has been taken from the Maplin Sands trial report (Blackmore et. al, 1984)

3. Results and Discussion

Figures 2(a-c) compare measured and model results on the reported stations. These values are the maximum concentration for the first 150 seconds of gas dispersion in each point at the same height measured in the experiment. In all three graphs a curve is fitted to the model data from which a 5% Low Flammability Limit distance has been detected, meaning that the flammable gas can be dispersed as far in 150 seconds. Figure 2.a shows results of trial 27, where the wind velocity was relatively low. Reported data were from quite a few available stations. Results show the model is in a good agreement with the measurements; discrepancies are less significant in farther points, however; both model and experiment show the same distance for 5% concentration. Figure 2.b compares the model with measured data obtained in trial 34. Measurements, especially at the beginning of the test, show of highly oscillatory wind speed and direction varied in different stations, as in a station, which was in the distance of 250m from the release point, wind speed ranged from 6.6 - 9.8 m/s. However; the average reported wind velocity is 8.6 m/s. In this test the humidity reported the highest. Model results are in good agreement in farther points where the concentration is almost 5%. Figure 2.c shows there is an excellent agreement between the model and the measured data at trial no. 35. In this test even though the wind velocity is relatively large, average wind velocity and direction were highly representative, because the amplitude of fluctuations was not so high. Measurements show that concentration increased unexpectedly at 129 m distance that was also detected by the model.
Figure 3 depicts differences between the test and model results. The solid line represents the reference measured data. The scattered points obtained from all models lie in a narrow region between the grey lines

below the factor of 2 showing of very small discrepancies between model and experiment for 90% of the results.
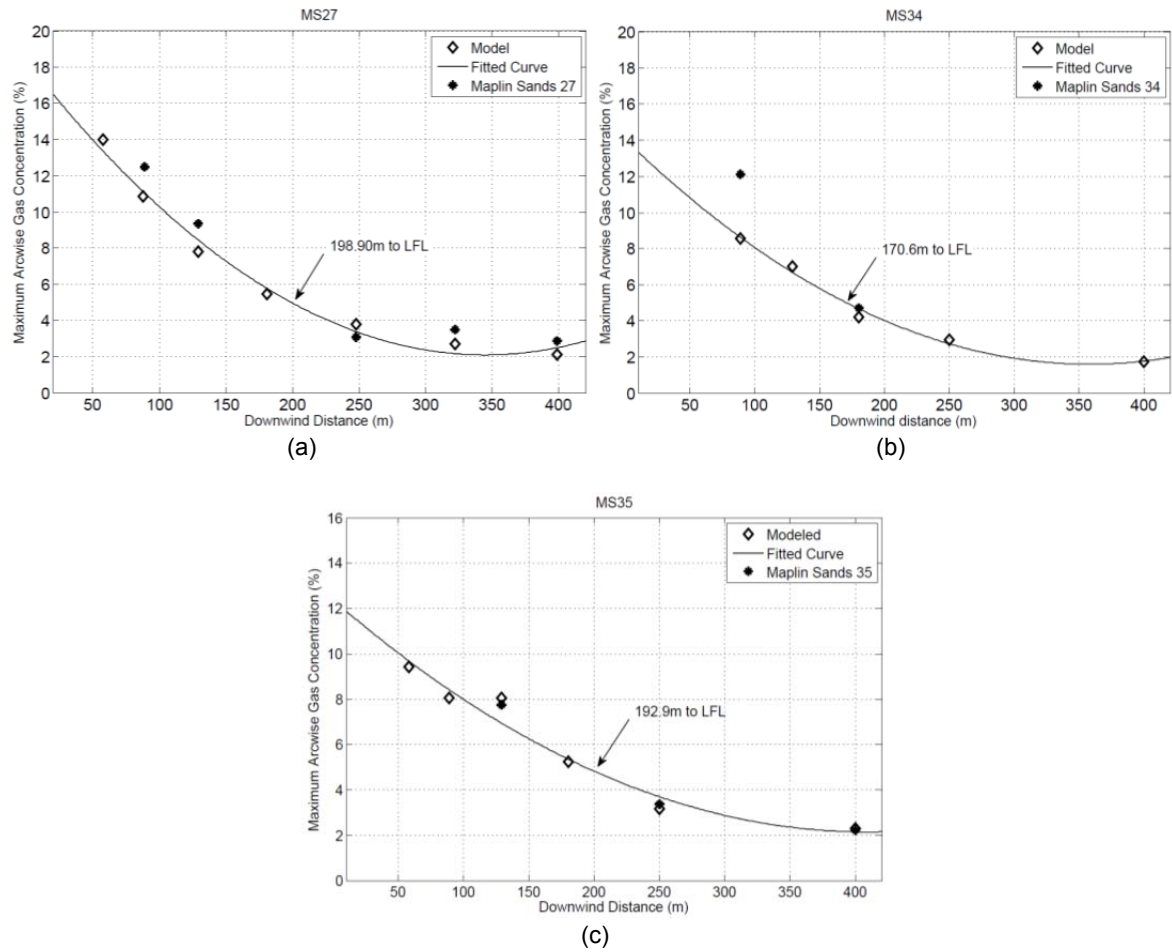

(a)

(b)

(c)

Figure 2: Comparison of measured and OpenFOAM model results. LFL represents Low Flammability Limit
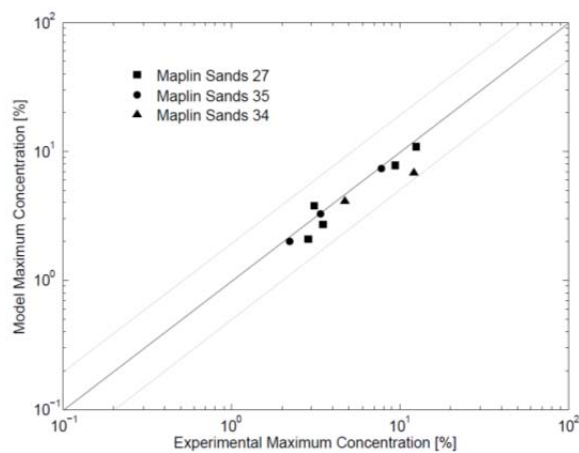

Figure 3: Correlation between the experiments and all model results located in a narrow region in the vicinity of measured data

4. Conclusion

A CFD approach, implemented in OpenFOAM is used to investigate LNG dispersion. A source model was used to define the pool radius as well as evaporation rate, which was then coupled to predict dispersion. To verify the model three standard trials of the Maplin Sands series of experiments were taken into account. The model is capable of incorporating the effect of humidity, and generates atmospheric boundary conditions over the domain. It also includes the buoyancy effect by modifying the constant parameters in the dissipation rate equation also by adding the turbulence production through buoyancy to the kinetic energy equation that both particularly enhanced the results. Mesh independent solution studies showed that mesh refinement especially around the release point and in the bottom vicinity had remarkable influence. Lack of enough information on time varying release rate and pool formation rate led investigations to an arcwise study, where verifications showed the model is in good agreement with the experiment, and the detection of low flammability limits is acceptable. The main advantage of the model is its high flexibility for additional modules and the capability of implementing different turbulence models. Further work will be undertaken to couple the spill and spreading process to the dispersion model.

Acknowledgments

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