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The Nature of Flammable Cloud Volumes in Semi-confined Environment under the Influence of Flow of Air

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Abstract

In the Explosion Risk Analysis (ERA), ventilation and dispersion calculations using Computational Fluid Dynamics (CFD) are usually considered when the level of confinement and congestion cannot be neglected. As far as the dispersion analysis is considered, alternative approaches are sought when a large number of simulations are required. Setting many scenarios and simulate them all is not always suitable within the timeframe of real engineering design. As a result, semi-empirical dispersion models and several procedures based on statistical approaches using CFD have been proposed to improve the robustness and the accuracy of prediction of the flammable gas cloud volume. In addition, notwithstanding the use of Response Surface Method (RSM) and Frozen Cloud Approach (FCA), it is convenient to address the problem on the basis of the physics underlying the dispersion of a scalar in the chemical process area. Following this line of reasoning, we propose a new dimensionless number balancing the transport of the flammable cloud and the accidental leak rate. Numerical experiments have shown that the dimensionless number is related to the angle of the wind direction as the angles in a circle are related to the phase angle in a sine wave, $V \sim \sin\left(k\frac{\phi}{\pi} + \beta\right)$, where $\hat{V}$ is the nondimensional flammable cloud volume and ϕ the phase angle. The numerical findings suggest a periodic function comprising harmonically sinusoids in the same fashion put forward by Fourier and observed in the analytical solutions of diffusive transport equations.

Keywords: dispersion modelling, CFD, dimensionless cloud volume.

1 Introduction

The estimation of flammable cloud volumes has been widely investigated in recent years in order to minimize the risk of accidental releases into the atmosphere. When a release is given, the jet flow acquires a high momentum which afterwards is diluted and dispersed by the influence of the atmospheric turbulence. The behaviour of this cloud is a complex phenomenon to analyse due to the different parameters involved in the flow dynamics. These parameters are the leak rate, the wind speed, the leak direction, release duration and other actions of mitigation [1, 2, 3, 4]. In the evaluation of the incidence of these affecting factors in the cloud behaviour have been done by numerous methodologies. These methods may be based on experimentation or by statistical concepts [1, 5], neural networks [4], numerical modelling by using Computational Fluid Dynamics (CFD) [3, 6], dense gas modelling [7], among others. However, the estimation of the physical understanding of the phenomena is still places a large burden on the researchers. Due to the complexity of the dispersion phenomena, this work makes use of dimensional analysis to identify the relationship of the affecting parameters with the flammable gas cloud volume. This dimensional analysis will be further used to develop a mathematical model by understanding the physical behaviour of the cloud after a release in the atmosphere.

This study is the result of an extensive evaluation of numerous cases, and the aim is to analyse the accuracy of the equations proposed to estimate flammable cloud volumes, that is, the dimensional volume and the mathematical model.

2 Methodology

The dispersion analysis was carried out in a semi-confined geometry designed in CFD-FLACS to calculate the equivalent stoichiometric gas cloud (Q9) at different case scenarios. The scenarios were set within four sets considering four main affecting parameters (leak rate, leak direction, wind speed, and wind direction). Each set comprised the variation of at least one of these parameters. To initiate the dispersion evaluation, it was assumed a single case (up-leak jet direction with a leak rate of 50 kg/s and a 6 m/s of wind speed varying the wind direction), afterwards, subsequent cases were performed to determine potential case scenarios after parameters were varied. The dispersion evaluation led to obtain the Q9 values for all the simulated cases, in which were only considered the largest cloud volumes for each group of scenarios. In total, 27 groups of scenarios and 17 different grids were performed within the four sets stablished in the entire analysis.

As the objective is to obtain a novel alternative in predicting the flammable cloud volume after accidental discharges, we sought to couple the affecting parameters with the Q9 outcome through dimensional analysis. The evaluation of this relationship generated a dimensionless volume that explains physically the dispersion phenomena. This dimensionless number $\hat{V}$, obtained by employing the Buckingham Pi theorem, evaluates the gas convective flow with the release momentum over time. The development of a dimensionless $\hat{V}$ allows to evaluate the parameters of leak rate, wind speed, density and the Q9 together. After Q9 results, $\hat{V}$ was calculated to have a physical understanding of the dispersion phenomena and being able to model it. With respect to the geometry, the wind rose was established as is shown in Figure 1.

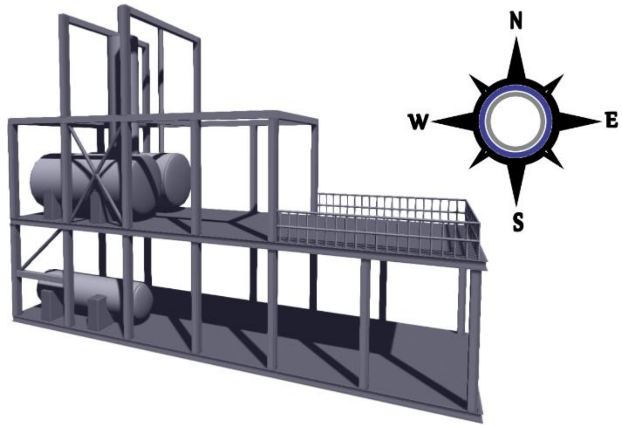

Figure 1. Geometry model and wind direction configuration

3 Results

The analysis led to observe that the flammable cloud volume (V_f) depends on different parameters. These parameters are related to the leak rate ($\dot{q}$), wind speed (u), fluid properties (ρ), leak direction (θ), geometry (L) and the wind direction (β). Considering this study, we obtain a non-dimensional number $\hat{V}$ that describe the dispersion phenomena given by:

$$\hat{V} = \frac{u^{3/2}\rho^{3/2}V_f}{\dot{q}^{3/2}} \tag{1}$$

Calculations showed that $\hat{V}$ ranged from 0.16 to 62.3 for cases simulated from 0.5 kg/s to 550 kg/s of leak rate, 1 m/s to 12 m/s of wind speed, with all wind directions (N, E, S, NE, NW, SE, SW, W), and for all leak jet directions (up, down, back, left, right, front).

In the evaluation of the cloud behaviour after accidental releases, we only considered the largest values of the flammable cloud volumes (Q9) for each group of dispersion scenarios. To develop a mathematical model, we analyse a specific group of simulated cases. This group was set with two parameters fixed (wind speed and leak rate) varying the wind direction for each leak jet direction. Based on the dimensional analysis, the proposed a model represented by the Equation 2, contains two functions, the cosine representing the sinusoidal behaviour and an exponential to the wake conditions. The model is also a function of two main angles, one referred to the wake angle (α) and the other to the wind direction (β). Both involving the influence of the wake volume (V_w), the mean (ϵ), amplitude (δ), and variables (A, B).

$$\hat{V}(\alpha,\beta) = \epsilon + \delta\cos(A\beta) + V_w \exp[-B\,(\beta - \alpha)^2] \tag{2}$$

After calculating $\hat{V}$, the sinusoidal form is seen in Figure 2 where group 8B and 8C (Table 1) are plotted. As we noticed, the curve tended to follow a periodical waveform, and then a slightly exponential behaviour is perceived as the wind direction varies.

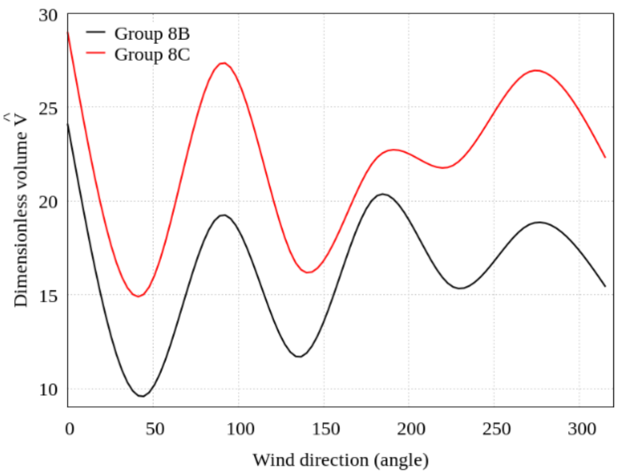

Figure 2. Representation of the waveform of the cloud volume based on the dimensional analysis for groups 8B and 8C.

In the non-dimensional flammable volume ($\hat{V}$) results, it was also identified some variations in wake angle in particular scenarios and conditions simulated. We found that in various cases, there were different values of wake angle representing the largest flammable cloud volume. Therefore, in order to see how this behaviour can affect the estimation of flammable cloud volumes, two different evaluations by using the proposed model were performed.

One first evaluation implied to plot four random cases (Table 1) at up leak direction divided into 12 groups and assuming that all the groups had the same wake angle (west wind direction or 270 degrees). The west wind direction according to the geometry (Figure 1) would be equivalent to the most likely to produce the largest cloud volume due to the re-circulation zone generated in the module when the flow encounters the objects (vessels). Based on this consideration, the CFD results are compared with the model (Figure 3) to see the agreement between the data.

Table 1. Group of scenarios used in the evaluation of the proposed model

Group	Parameters fixed*	Parameter varied
4A 4B 4C	5 kg/s leak rate	Wind direction
5A 5B 5C	25 kg/s leak rate	
7A 7B 7C	50 kg/s leak rate	
8A 8B 8C	100 kg/s leak rate	

* Each parameter fixed was measured at 2 m/s, 6 m/s, and 8 m/s of wind speed and up leak direction

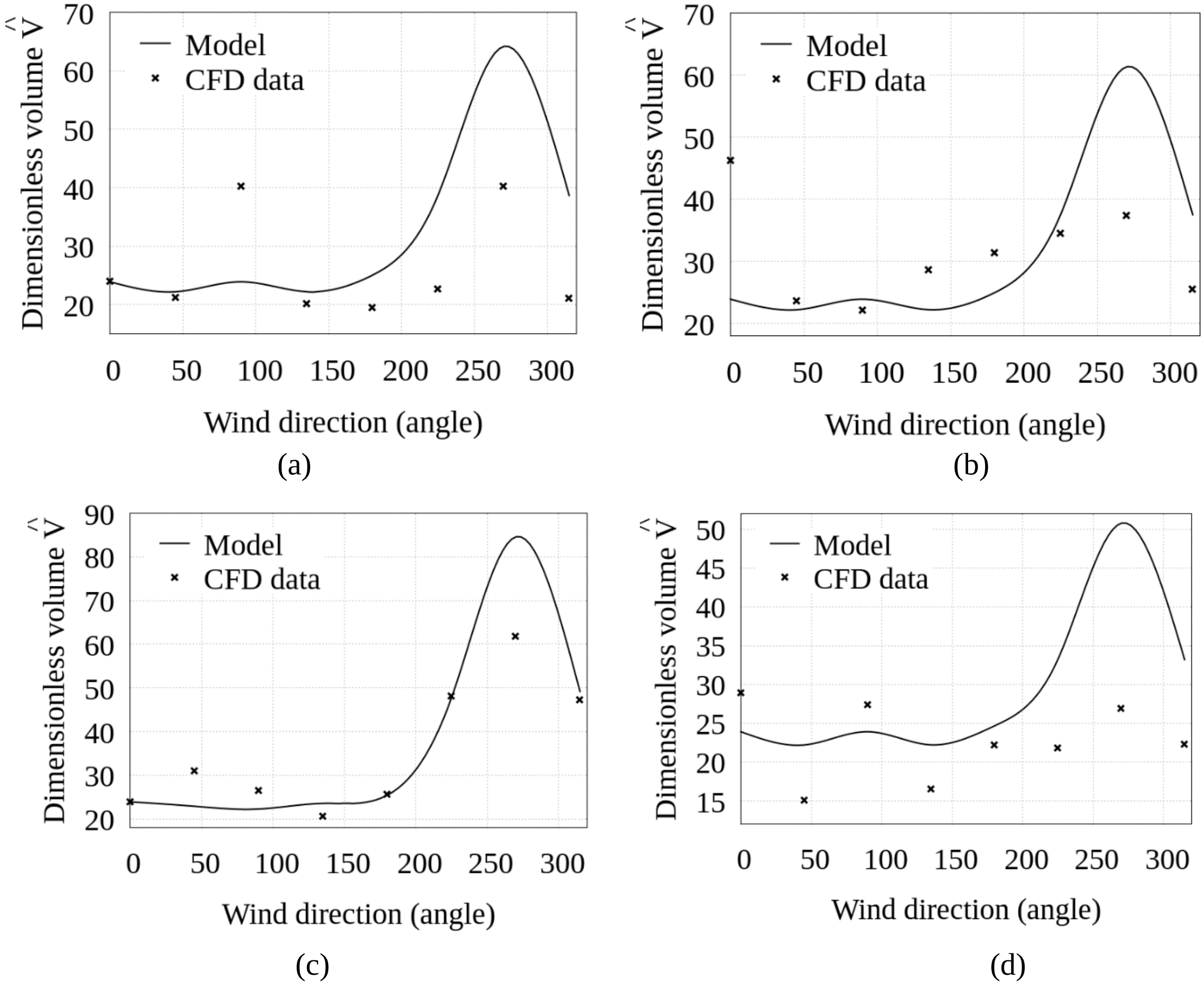

Figure 3. Comparison between the model and CFD data: (a) 5 kg/s at 8 m/s, (b) 25 kg/s at 8 m/s, (c) 50 kg/s at 6 m/s, and (d) 100 kg/s at 8 m/s.

Initially, Figure 3 shows four random groups from Table 1 considering the same wake angle (West). It is observed the model agreement after comparing it with CFD data for each wind direction. In this figure, the CFD data were the values obtained by using the Equation 1. It is also seen that the model begins estimating the sinusoidal behaviour, and then employs the exponential function to model the largest volume, which corresponds to the wake volume in the module at certain conditions.

Now, for all the cases in Table 1, Figure 4 represents the four leak rates (5 kg/s, 25 kg/s, 50 kg/s and 100 kg/s), with the same assumption of having the same wake angle. It is observed that for wind speed from 6 m/s to 8 m/s, the model presents a good agreement (Figure 4). However, even the scatter shows that the wind speed at 2 m/s is uncovered, the model can overpredict it. As in the entire dispersion analysis was identified that the highest Q9 changes were at leak rates going from 25 kg/s to 200 kg/s and wind speed from 2 m/s to 8 m/s, it is seen that the model may offer a good accuracy in the estimation of the cloud in these likely ranges.

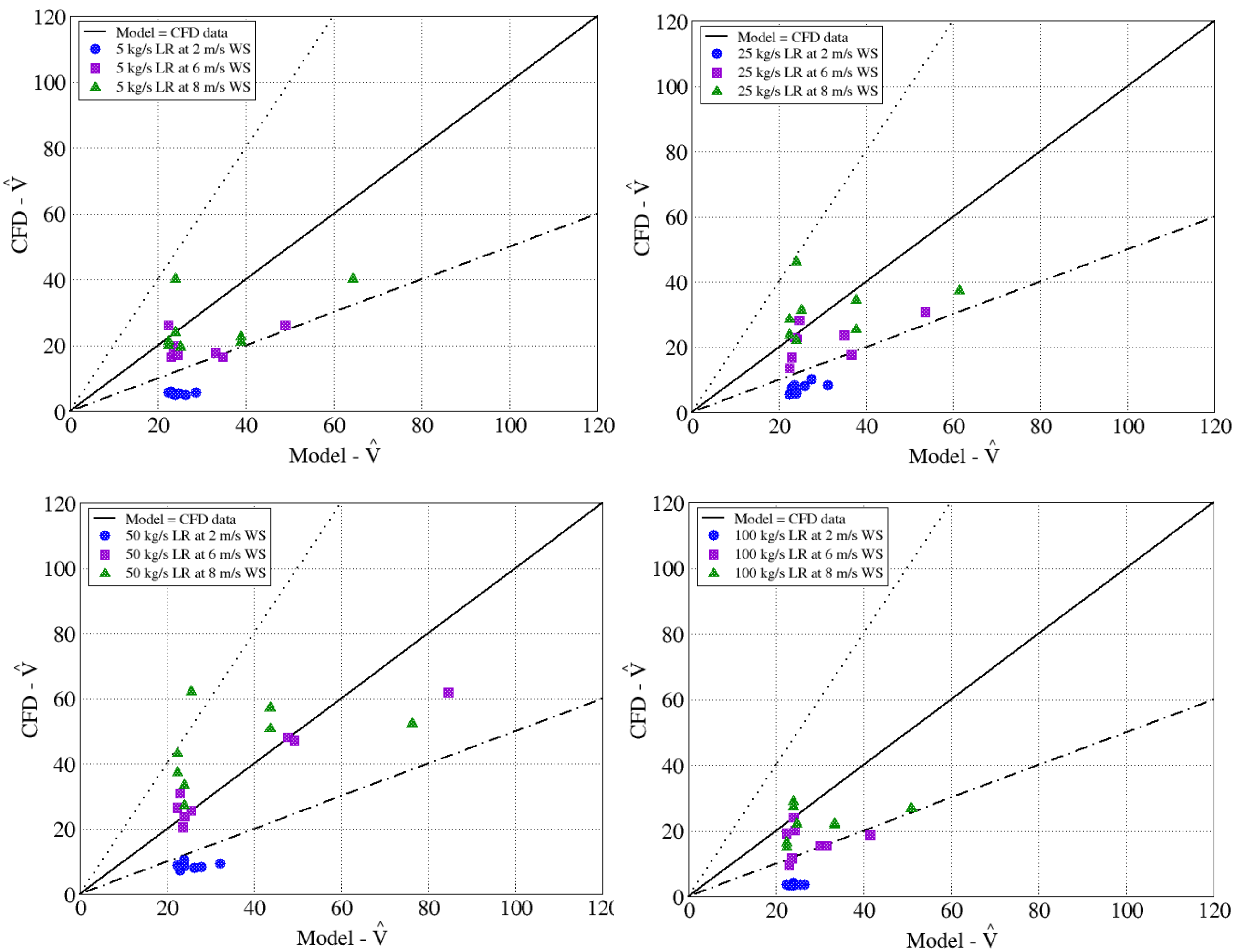

Figure 4. Comparison between CFD data, and the model at different values of leak rate (LR) and wind speed (WS).

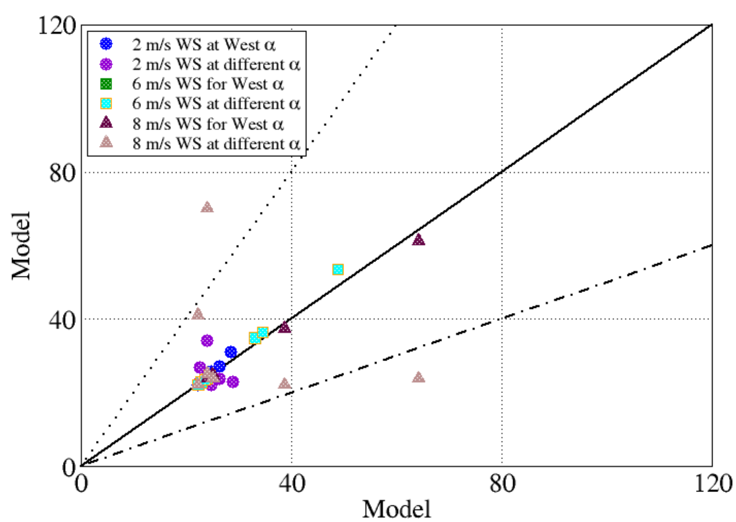

Figure 5. Comparison between data obtained by the proposed model at West wake angle with the data considering different wake angles (α).

The second evaluation comprised different values of wake angles as it was obtained during the analysis for each scenario. The variations of wake angle might be possible due to the geometry configuration and the association between variations of wind direction and leak direction. The representation of data obtained at different wake angles with the assumption of same wake angle is shown in Figure 5. From this figure, we can conclude that the discrepancies in evaluating the wake conditions aforementioned for all the cases are negligible. It suggests that the proposed model seems to be a good alternative in the estimation of flammable gas cloud volumes for both cases (different wake angles and same wake angle) without affecting the accuracy.

4 Conclusion and Future work

The current work evaluates the development of a dispersion model on the basis on the physics that may be used to estimate the flammable cloud volume after accidental releases. During the analysis, it was addressed two different evaluations to observe the reliability of the proposed model. It was determined that the proposed model seems to be accurate no matter the determination of fixed or a variable wake angle because the differences between the data calculated by the model at both conditions are minimal.

The dispersion analysis indicated that the flammable cloud volume follows a wavy pattern when it is related to the angle of the wind direction. The analysis also resulted in a dimensionless number that relates the leak rate, density and the wind speed with the flammable cloud volume leading to the development of a mathematical model that associate it with the wind direction. As future work, we will keep evaluating and improving the mathematical model to obtain better agreement for lower values of wind speeds.

5 References

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