Development of Cloud Exceedance Curves Employing Monte Carlo Simulations and Computational Fluid Dynamics

Pamella Palmeira de Araújo[1], Sávio S. V. Vianna[2]

ABSTRACT

The prediction of flammable cloud volumes in industrial sites is of paramount importance in risk analysis as well as in consequence analysis. Most chemical process areas comprise large equipment, and pipes which affect the air entrainment rate, the mixing, and dispersion of the cloud. Other than the influence of equipment on the fluid flow, the wind direction, the wind speed, the leak rate, and the leak direction are also important variables when calculating the cloud volume from accidental releases. These parameters are stochastic, which poses an additional burden on the modeling. In this work, we develop a novel model to calculate the volume of a gas cloud using Monte Carlo simulation. The various stochastic parameters are collapsed into two non-dimensional groups using the Pi Buckingham theorem. We show that the cloud volume increases rapidly at the early stages of the gas leak, and then it decays exponentially. The mathematical model is coded using a pseudorandom number generator (PRNG) algorithm to calculate the most likely cloud considering the wind rose data and the gas leak distribution. Numerical findings are used to generate the cloud exceedance curve, which can be used for gas detector optimization and explosion calculations.

1. INTRODUCTION

Accidental gas leaks are not desirable in chemical plants. As far as flammable gas clouds are concerned, the obstacles in the geometry of the industrial site plays an important role in the event of an unexpected discharge. Computational Fluid Dynamics (CFD) can model fluid flow taking into account the effects of obstacles in complicated geometries while also simulating real-world boundary conditions. However, these simulations are excessively expensive (from the computational point of view). The computation of tens of hundreds of CFD scenarios might be unfeasible during the course of the engineering project. As a result, some researchers had explored different routes to overcome this issue.

The application of models based on CFD data and experimental data have been explored. The main task is the development of mathematical expressions that can reduce the number of CFD simulations. Most of the approaches rely on the regression of numerical data [1,2].

On the other end of the modelling, the application of artificial intelligence emerges. CFD data has been used to train neural networks minimizing the weights in the entropy equation. The main concept relies on the optimization of the equation looking for the weights parameters that best fit the solution [3,4].

In both approaches, the main idea behind the analysis is the development of a model that can be used to calculate the most likely flammable cloud volume with minimal number of CFD runs.

Following this route, the model may be used to perform Monte Carlo simulations for probabilistic explosion analysis. The mathematical model is coupled with Monte Carlo sampling technique to calculate hundreds of thousands of scenarios that are applied to calculate the cumulative frequency of flammable cloud volumes or explosion overpressure [5]. Monte Carlo simulation becomes an attractive approach since it reduces the number of required CFD simulations and yet, leads to results with the same level of accuracy as long as the mathematical model of the physical effects mimics the real accidental scenario.

The exceedance curve can be thought of as a cumulative curve that identifies the consequences of flammable cloud volume. These outcomes are assessed sequentially, beginning with a maximum event and then accumulating subsequent occurrences that increase in accordance with the frequency [6]. It can also be combined with an overpressure database to enhance the calculations and to calculate the maximum explosion overpressure [7]. Taking into account the level of obstruction, the data can be utilized to calculate the overpressure exceedance curves using the CFD simulation as the starting inputs. [Qiao and Zhang] [6]

1 MS, Chemical Engineer – UNICAMP
2 PhD, Chemical Engineer – UNICAMP

applied the exceedance curve to identify potential explosion overpressures in offshore and onshore sites. The NORSOK requirements were followed as the reference standard for this type of analysis. Jin and Jang [8] also analyzed the explosion risk of selecting flammable cloud data from CFD simulations. The authors explored a new frequency distribution. The leak rate varied over time as well as the probability of ignition. Moreover, the authors claim that the accuracy of the analysis is enhanced without any significant increase in the computational time.

Although there has been considerable progress in the simulation of accidental scenarios using the Monte Carlo approach, particularly by employing statistical and artificial intelligence models, little research addressed the underlying physics of the phenomena, as far as the gas dispersion is concerned.

In this research, we introduced a new model for gas dispersion based on two non-dimensional numbers. The fundamentals of the model are based on the kinetic theory of gases for mixing. The model is used in the framework of Monte Carlo simulation where the pseudorandom number generator (PRNG) is applied. The paper is organized as follows: Section 2 describes the methodology, Section 3 discusses the results, and in Section 4 the conclusions are drawn.

2. DESCRIPTION

The Computational Fluid Dynamics (CFD) approach is a mathematical modeling procedure that solves numerically the equations that govern the physical fluid flow phenomena. Additionally, the technique also takes into account the hydrodynamics effects of the obstruction as well as the wake flow caused by the separation of the boundary layer on the obstacles.

In this research, we used the RANS (Reynolds Average Navier-Stokes) approach to solve the transport equations for mass, energy, and momentum. Additional two equations are solved for turbulent kinetic energy and its associated rate of dissipation. The turbulent fluxes are solved based on the hypothesis of Boussinesq.

2.1 Geometry

Figure 1 shows the geometry considered in the analysis. The geometry has a configuration typical of an offshore platform. The geometry is also composed of a semi-confined chemical process module. The module is 17.5 meters long, 7.5 meters wide and the height is 3 meters. The model comprises two vessels at the top deck and one vessel at the bottom. The vessels are expected to represent typical obstructions commonly found in industrial sites. We chose methane (CH_4) as the fluid to be released.

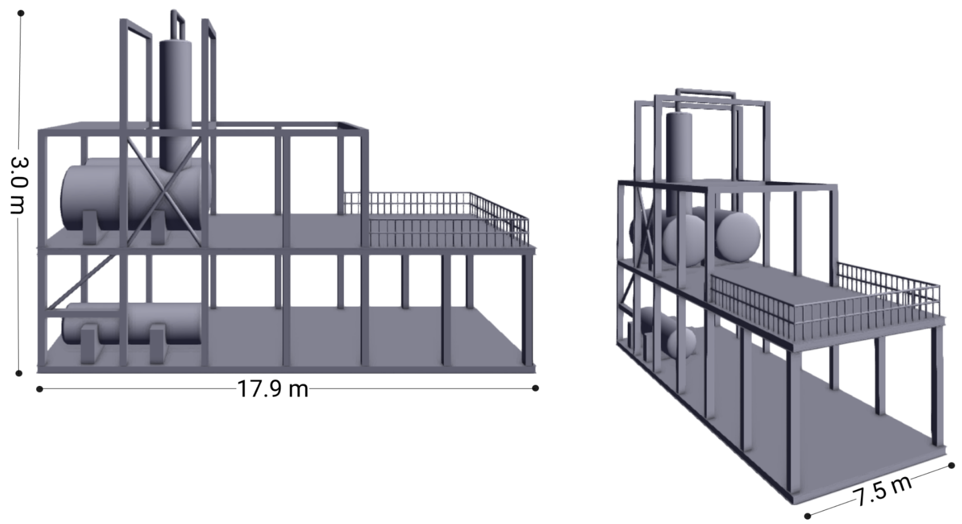

Fig.1 – Geometry for a semi-confined study platform

2.2 Review

This article is a continuation of a series of previous studies. Over the course of these studies, we performed 240 numerical simulations within the FLACS software. We developed two dimensionless mathematical equations for flammable cloud volume and discharge rate called respectively, as $\hat{V}$and R.

We developed this formula based on the assumption that when a leak occurs, there are stochastic parameters that will influence the formation of the volume of the flammable cloud. In this case, we consider as such factors the discharge rate, the study geometry, wind speed, specific mass of the released substance, wind direction, leak direction, and flammable cloud volume.

Next, we consider a correlation between five of these seven parameters by the theorem Π Buckingham. From this, we arrive at two dimensionless Π groups, which are R as Π_1 and $\hat{V}$ as Π_2. We followed the logic that if an equation is dimensionally homogeneous, it can represent a connection between non-dimensional groups [9].

The two parameters that we do not correlate are wind direction and leak direction. We brought these two parameters to analysis when we ran the FLACS simulations, as we simulated different scenarios with different wind and leak directions.

2.2.1 Non-dimensional Leak Rate - Π_1

Application of the Π theorem of Buckingham leads to:

$$R = \frac{m}{\rho Q \frac{u}{u_{ref}}} \qquad (1)$$

where m = leak rate $(kg.s^{-1})$; ρ = leak density $(kg.m^{-3})$; Q = volumetric fluid flow $(m^3.s^{-1})$; u = wind speed $(m.s^{-1})$; and u_{ref}= reference wind speed $(m.s^{-1})$.

2.2.1 Non-dimensional Flammable Cloud Volume - Π_2

The second Π the group is given by the non-dimensional flammable cloud volume. It was also derived using Buckingham's Π theorem, and it may be stated as follows:

$$\hat{V} = \frac{u^{1.5}\rho^{1.5}V_f}{m^{1.5}} \qquad (2)$$

where ρ = leak density $(kg.m^{-3})$; u = wind speed $(m.s^{-1})$; V_f= flammable cloud (m^3); and m =leak rate $(kg.s^{-1})$.

2.3 Model

We have the dimensionless flammable cloud volume (V) and dimensionless discharge rate (R) equations. Thus, we considered the potential of a connection between the two groups. Intuitively, we question if the two parameters should be related in any form. We knew that as the discharge rate increased, so did the amount of the flammable cloud inside that region. As a result, we developed a model that could demonstrate the connection between two dimensionless variables. The kinetic theory of gases and the

Maxwell velocity distribution provide our foundation. We used the physics of the situation to develop a mathematical model.

The model is divided into two parts. The model's first component (pre-exponential) considers the initial development of the cloud, while the second evaluates the decay of the cloud volume as the leak rate grows. The model is described as follows:

$$\hat{V} = A^{1.5} R^{1.5} exp\left(- B\ R^{0.8}\right) \tag{3}$$

Equation 3 presents a model that we assume will be applicable to all geometry. The model's variation is indicated by the values of constants A and B. These A and B values differ according to geometry and varied circumstances for wind and leak direction. As a result, the constant A is responsible for the model's exponential rise. While B is in charge of how quickly the exponential decays.

2.4 Monte Carlo Simulation (MCS)

In prior investigations, we compared the model to numerical CFD data. We observed that the two were in accord. Considering that these variables are stochastic, we presented a major study question as follows.

When compared to CFD, we have an acceptable model. We know that initial events, such as discharge rate, geometry, wind direction, leak direction, and wind speed, are random. These stochastic occurrences adapt relatively well to Monte Carlo simulation. Then brings the question of whether the constructed model is suitable for Monte Carlo simulations. Is it possible to calculate the flammable cloud most likely to develop in an industrial environment? In this line, given the probability distributions of the events, is the model sufficient for the Monte Carlo simulation? And what were the distributions? Wind direction, leak direction, wind speed, and hole size probability distribution.

From these questions, we generated 1000 random numbers by Monte Carlo simulation (MCS), following the formula:

$$MCS\ =\ (A\, Z_{i-1}\ +\ C)\, MOD_{M} \tag{4}$$

In which we consider $A\ =\ 7^5$, $MOD_{M}\ =\ 2^{31}\ -\ 1$, $Z_{0}\ =\ 19$, and $C\ =\ 0$.

We generate the Monte Carlo random numbers in a spreadsheet. From these numbers, we use some techniques that we will show below to obtain the discharge rate, wind direction, leak direction, and wind speed.

2.5 Leak Rate

Through some tests, we observed that the Rosin, Rammler, and Bennett (RRB) probability distribution effectively fit the data, and we used the following formula:

$$Y\ =\ 1\ -\ exp\left(\frac{-x}{D}\right)^{N} \tag{5}$$

where x was the possible discharge rates, $Y$was the probability distribution, and $N$and Dwere the parameters fitted to the experimental data.

After testing with varying values for $N$and Dacross a discharge rate range of $80\ -\ 280$, we discover that $N\ =\ 5$ and $D\ =\ 130$provide the optimum match. Knowing what the best fits were. We use this distribution in conjunction with random numbers. From there, we isolate the variable x.

$$x\ =\ exp\left(\frac{ln(ln\left(\frac{1}{1-Y}\right)+Nln\ D}{N}\right) \tag{6}$$

The corresponding values are then entered into the equation. As a result, we can calculate the leakage rates from the random numbers generated by the Monte Carlo simulation.

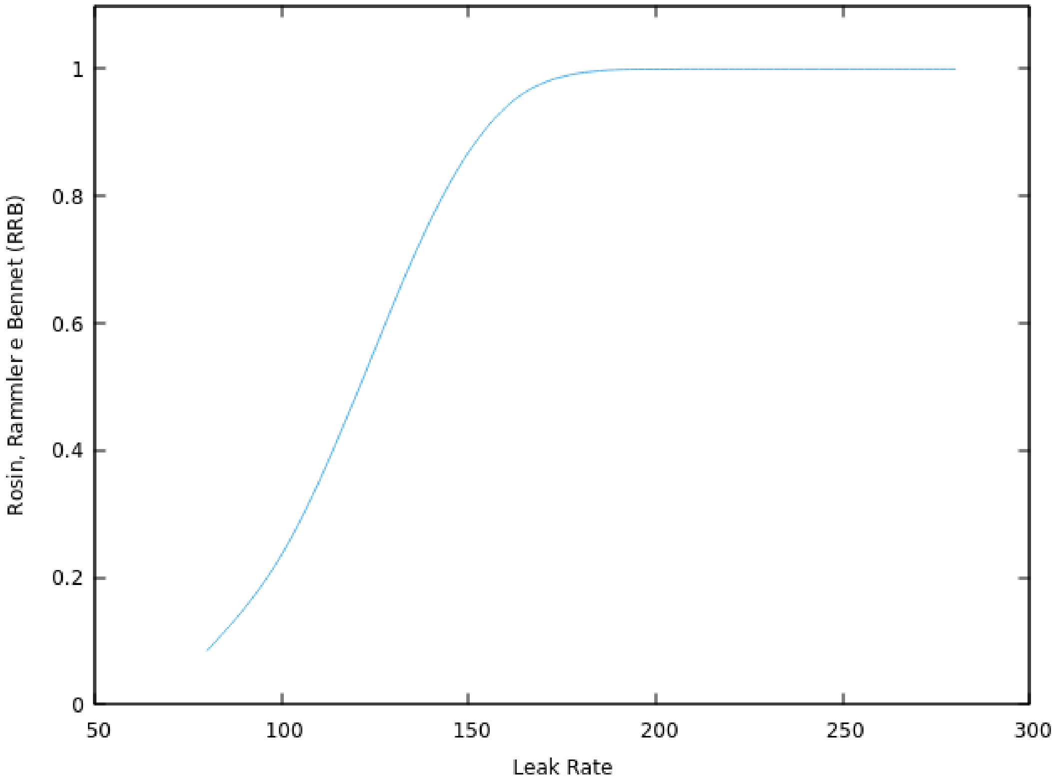

Fig.2 – Rosin, Rammler, and Bennett (RRB)

2.6 Wind Direction

We utilize data from prior research to determine the wind direction. In which we calculated the probability of each wind direction for the study of geometry. We leverage our previous knowledge and statistics. We use the closest neighbor theory, which is generated from the average distance between the locations of the nearest neighbors. Based on the theory's concept, we analyzed which random number was closest to the result acquired from the probability distribution of each direction of occurrence.

We use the following equation:

$$W_D = \frac{((MCS) - f(Wind))^2}{(MCS)^2} \quad (7)$$

where W_D is wind direction, MCS is Random number, and $f(Wind)$ is wind direction probability.

We approached it from eight different wind directions: North (N), Northeast (NE), Northwest (NW), South (S), Southeast (SE), Southwest (SW), East (E), and West (W) (W). However, we established that everything with the letters N, NE, or NO would be referred to as North, and anything with the letters S, SE, or SO would be referred to as South. We were able to determine which data had the lowest value as a result of this. In other words, we wanted to know how close the value created by the random number was to the probability distribution. To determine the most likely wind directions, we employed logical operators such as IF and AND.

2.7 Leak direction and Wind Speed

To determine the leak direction and wind speed, we utilize the same methods as the preceding item. We had a knowledge of literature on what were the most common wind speeds to occur. In terms of leak direction, we used the researchers' expertise and references from the literature to estimate the probability of occurrence to each leak direction. We use the same approach that we used to determine wind direction to determine leakage direction and wind speed, and we use the following equations:

$$L_D = \frac{((MCS) - f(Leak))^2}{(MCS)^2} \tag{8}$$

$$W_S = \frac{((MCS) - f(Speed))^2}{(MCS)^2} \tag{9}$$

where L_D is leak direction, W_S is wind speed, MCS is Random number, $f(Leak)$ is leak direction probability, and $f(Speed)$ is wind speed probability.

We evaluated which number was most similar to the distribution of leak direction and wind speed. We use the nearest neighbor theory and logical operators. As a result, we were able to extract the leak directions and wind speeds from the Monte Carlo Simulations' random values.

The leak rate, wind direction, leak direction, and wind speed are all calculated. So we found out what the volume of the flammable cloud was. This flammable cloud volume depended on constants A and B, whose values depended on geometry, leak direction Up, Down, East, West, North, and South), and wind direction (East, West, North, and South).

So we have several scenarios with 24 A and B values. So, in a spreadsheet, we utilized logical operators like IF and AND to determine which values of A and B should be used. We input the information about the leak direction, wind speed, wind direction, and leak rate into the model. We were able to determine the volume value of the flammable cloud in this manner.

3. DISCUSSION

We performed Monte Carlo simulations to determine the final volume of the flammable cloud. Figure 2 shows the distribution of random numbers generated from the Monte Carlo simulation. In which the flammable cloud volume value ranges between 0 and 25. The distribution of the numbers on the figure indicates that they are random.

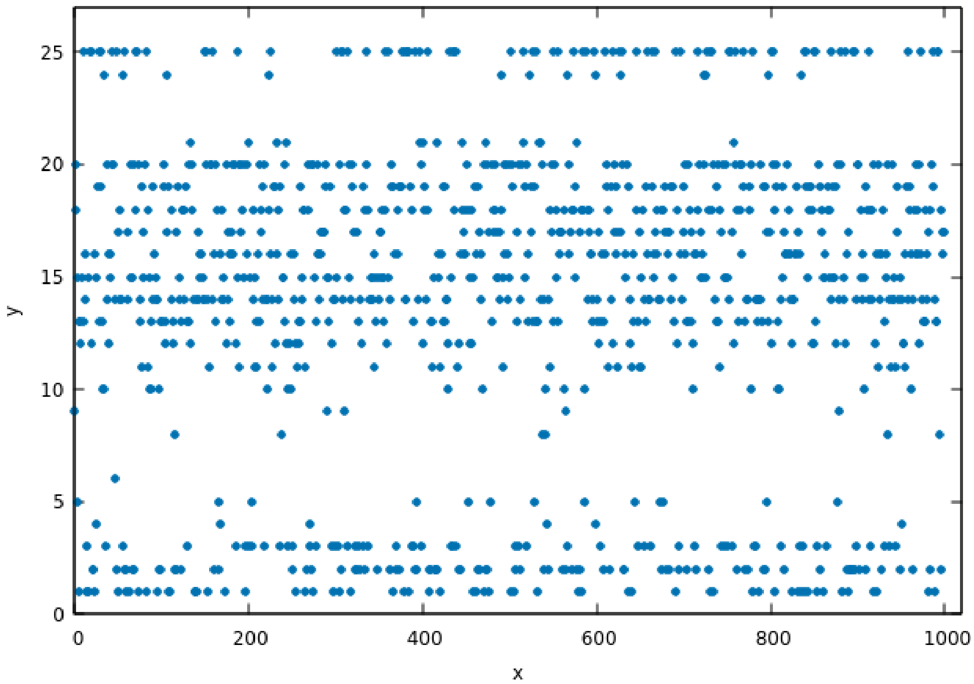

Fig.3 – Monte Carlo Simulation with 1000 random number generation

Table 1 shows a selection of the 1000 outcomes acquired by the Monte Carlo simulation. This table also provides the model's wind direction, leak direction, wind speed, R (dimensionless leak rate), and $\widehat{V}$ value.

Tab.1 – Monte Carlo Spreadsheet

Numbers	Leak Rate	Wind Speed	Wind Direction	Leak Direction	R	Model – $\widehat{V}$
1	22	21	NORTH	EAST	0.019	9.43
2	121	6	NORTH	UP	0.029	18.29
3	87	12	EAST	DOWN	0.041	5.12
4	153	6	NORTH	UP	0.036	12.74
5	76	16	SOUTH	EAST	0.048	1.37
6	91	12	EAST	WEST	0.043	1.45
7	67	16	WEST	EAST	0.042	2.50
8	76	16	SOUTH	EAST	0.048	1.36
9	98	2	NORTH	SOUTH	0.008	13.98
10	91	12	EAST	WEST	0.043	1.44
11	98	2	NORTH	SOUTH	0.008	14.00
12	115	6	NORTH	UP	0.027	19.32
13	82	12	SOUTH	DOWN	0.039	2.60
14	100	2	NORTH	UP	0.008	24.39
15	125	6	NORTH	UP	0.030	17.56

3.1 Case Study

We conducted a case study analysis to see whether the results were acceptable. The leak would be to the east, while the wind would be to the north and south. We examined the values acquired from the $\widehat{V}$ within the spreadsheet and compared them to an abacus generated in prior investigations for the East direction.

In the first scenario, we utilized spreadsheet simulation number 1, with the leak direction set to east, the wind direction set to north, the eak rate as 22 $kg.s^{-1}$, the R-value set to 0.019, and the wind speed set to 21 m.s-1 as initial conditions. In this scenario, the flammable cloud volume was calculated to be 9.43 m^3. As a result, we compared this table value to the abacus, which produced about 9.5 m^3.

In the second scenario, we selected simulation number 8, with the leak direction east and the wind direction south, the R-value of 0.048, the leak rate of 76 $kg.s^{-1}$, and the wind speed of 16$m.s^{-1}$. The volume of the flammable cloud volume in the table was 1.36 m^3. We compare the value from the table to the abacus and get a result of roughly 1.5 m^3.

We noticed that both the first and second cases analyzed had similar values when comparing the abacus and table values. In other words, the level of agreement was great.

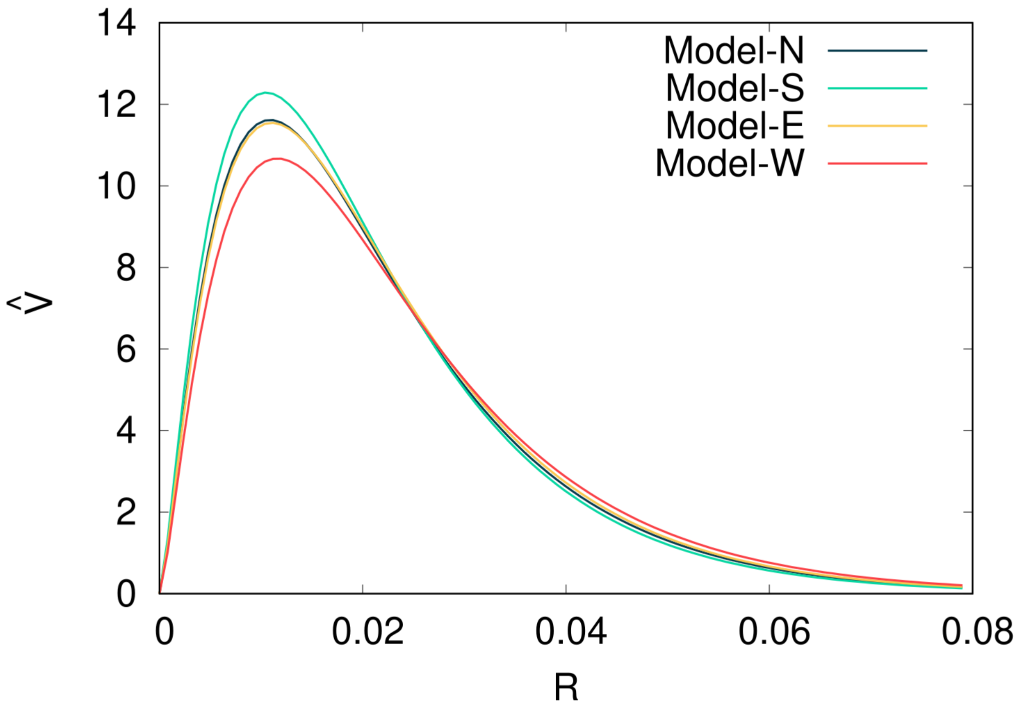

Fig.4 – Non-dimensional flammable cloud as a function of the non-dimensional leak rate for the four simulations of the leak direction to East. Four wind directions are considered.

In addition to the case study, we investigated which wind direction was predominant for the geometry under discussion. The most frequent leak direction that we observed in the Monte Carlo Simulations was for Up with a wind speed of 6 $m.s^{-1}$, a wind direction of north, a leak rate of 150 $kg.s^{-1}$, and an R-value of 0.03. As a result of evaluating the data for up leakage direction, it is possible to predict that the cloud most likely to occur is in the range of 16-19 m^3over the study platform. Knowing that the model works, if a leak develops in the study geometry, it will quickly be possible to predict the value of the flammable cloud most likely to occur, as in the case study.

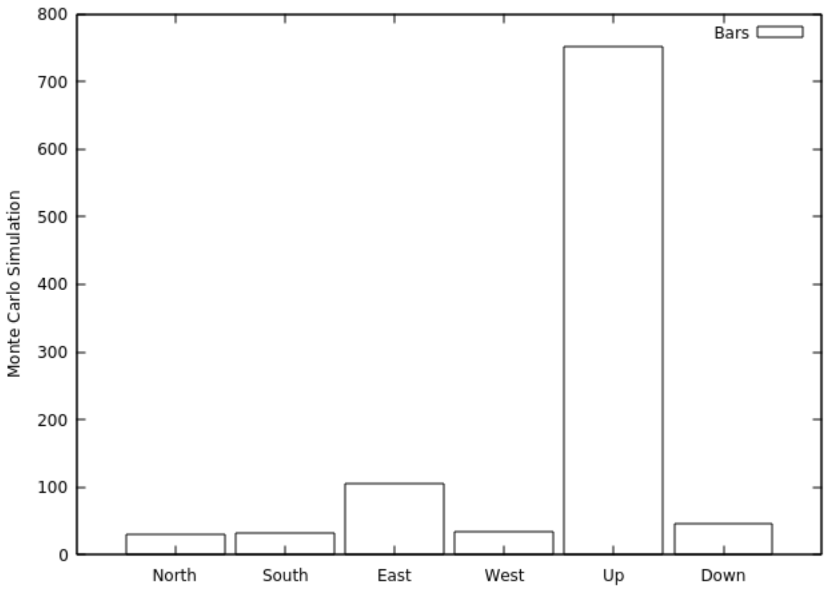

Fig.5 – Bar representation of the leak directions that appeared in the Monte Carlo simulation.

We show in figure 6 the exceedance curve. In this figure, we demonstrate the connection between the cumulative probability of a leak event occurring and the consequence (flammable cloud volume). In the accidental scenario, there is a 100% chance that the cloud will be $5m^3$ or greater. Similarly, we have a 75% probability of having a 12 - 16 m^3cloud. At 50%, we have a possibility of 18 m^3 clouds, and so on.

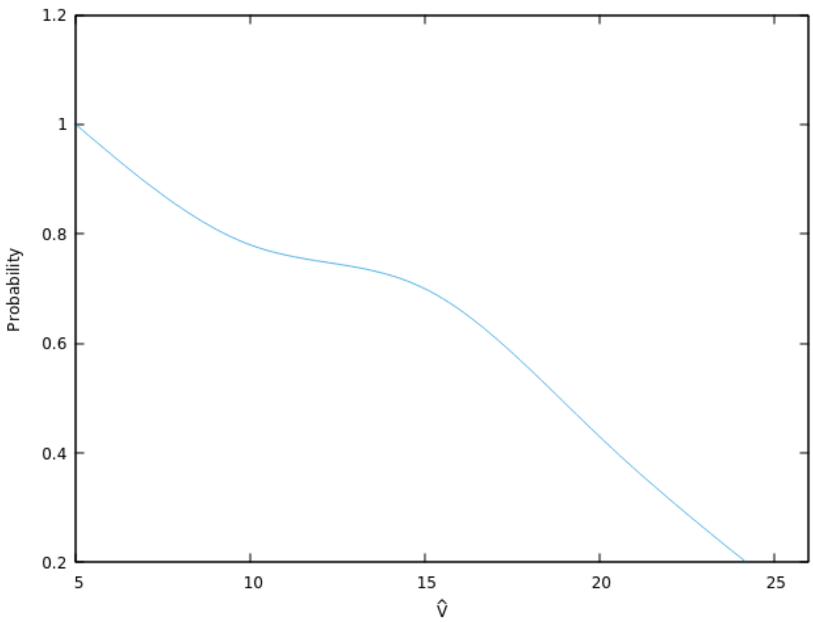

Fig.6 – Exceedance curve showing the cumulative probability and consequence of a leak event.

In figures 7, 8, and 9, we have the cumulative probability multiplied by the leak frequency, generating the cumulative frequency. Analyzing the cumulative frequencies for small, medium, and large leaks, we see that the highest frequency is for small leaks. Small leaks are more likely to occur because a small hole within an offshore platform is far more likely to occur than large holes. Furthermore, in Figure 10 we show a general graph for all accumulated frequencies and also a curve with the sum total of frequencies.

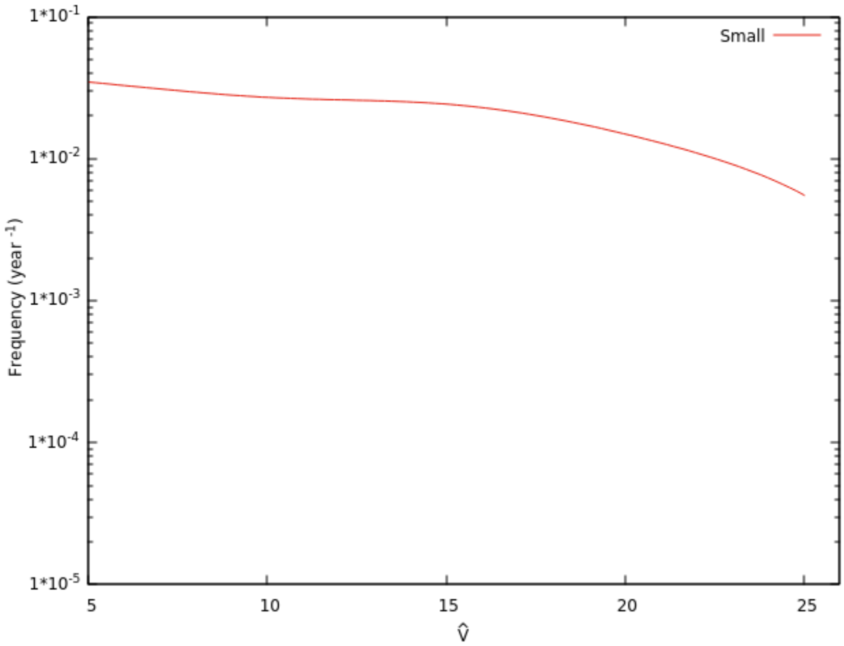

Fig.7 – In figure represents the cumulative frequency for small leaks.

A medium leak will have a lower frequency than a tiny leak and a greater frequency than a large leak.

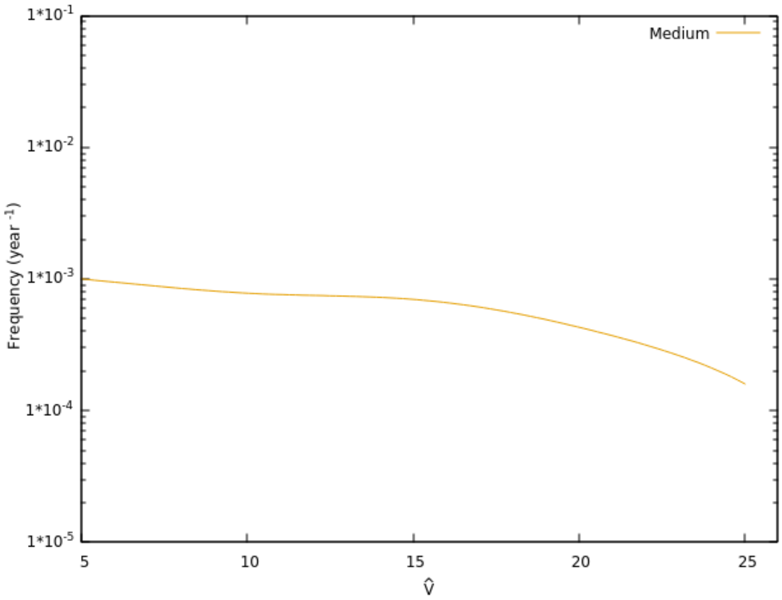

Fig.8 – In figure represents the cumulative frequency for medium leaks.

Interestingly, the frequency of a big leak is the lowest of all. This is due to the fact that most leaks originate through exceptionally small openings.

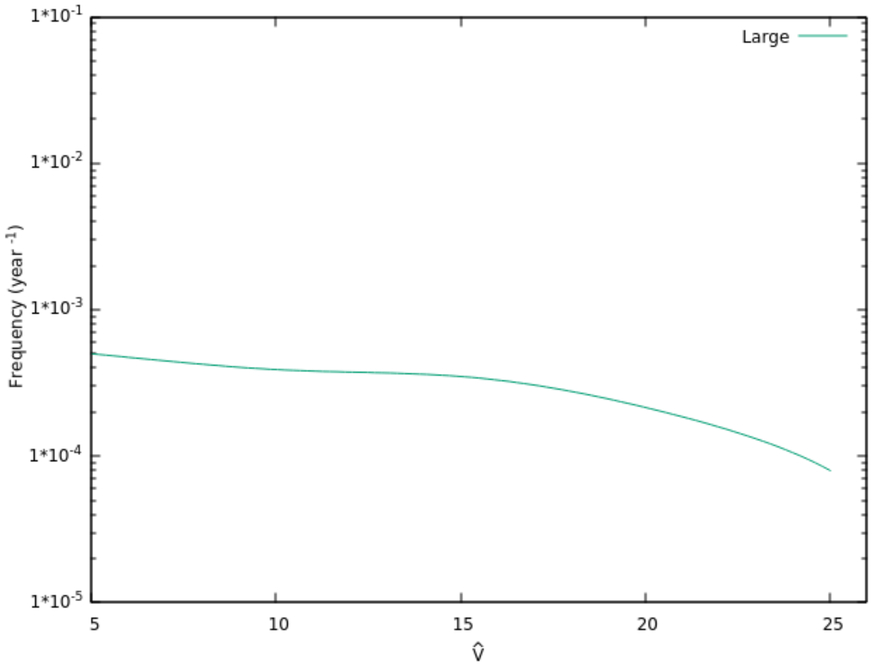

Fig.9 – In figure represents the cumulative frequency for large leaks.

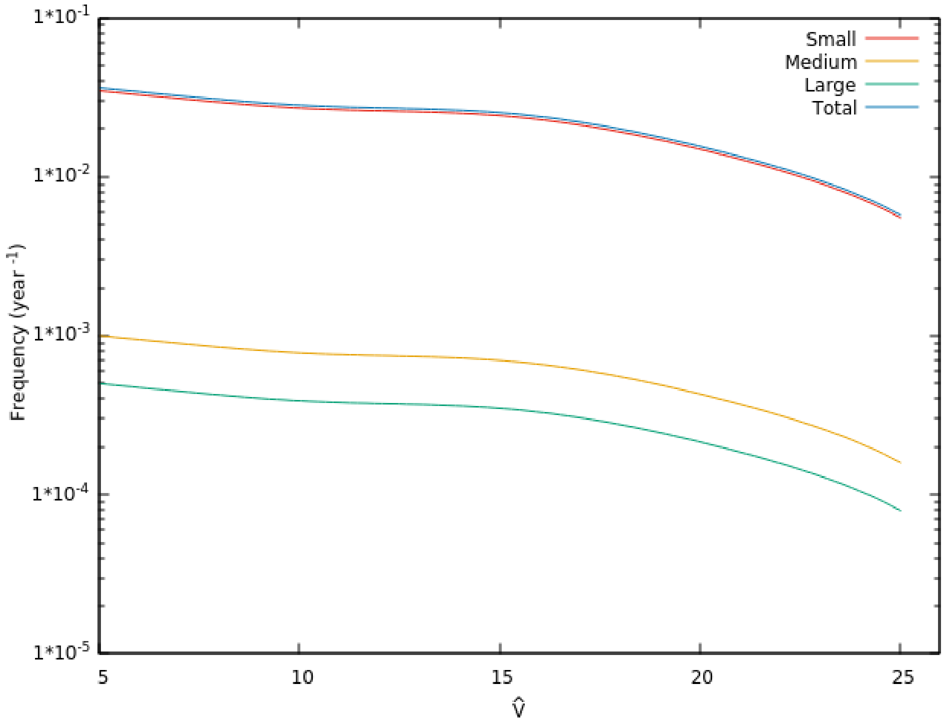

Fig.10 – In this figure, we have the cumulative frequency for small, medium, large leaks and also the sum of all these events together.

4. CONCLUSION

In comparison to CFD data, the model performs admirably. Monte Carlo is an excellent method for forecasting thousands of different situations. This ability to forecast hundreds of geometric situations opens new opportunities for explosion risk assessments and has the potential to transform what we know in the literature. The cumulative exceedance curve supplied the knowledge that a small hole had a one hundred percent chance of happening; in this situation, the curve is consistent with the literature. We discovered from the case study that for 1000 simulations, the most probable cloud to arise has a leak direction of UP, a wind direction of North, a wind speed of $6\ m.s^{-1}$, and a flammable cloud size ranging from 16-19 m^3. With this information, a decision-maker could prepare the whole structure of the chemical plant for this eventuality, allowing for escape routes, safety protocols, and the protection of human lives.

5. REFERENCES:

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