

**HAZARDOUS RELEASE SCENARIO ANALYSIS VIA
COMPUTATIONAL FLUID DYNAMICS**

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CHAPTER 1

EXECUTIVE SUMMARY

Computational Fluid Dynamics (CFD) has two major roles in risk management:

- (a) **Before building a facility:** risk assessment and analysis of potential fires and toxic releases; to identify optimal placement of detectors, alarms, sprinklers; mitigate what might happen.
- (b) **After a release has occurred:** root cause analysis of the situation; prediction of the release path; identify areas of high chemical concentration(s); preventive action against similar future releases.

The Chemical Process Industry has started to incorporate CFD into hazardous release scenario analysis. As part of this integration, it is essential to determine how accurately the existing methods for CFD modeling can predict an actual release so that it can be effectively used for risk management in such cases (risk analysis and assessment). The core of this project was to perform a Root Cause Analysis (RCA), simulate an actual release using CFD, and validate the developed models using first hand data from the release [1]. RCA is the very foundation of risk management and is used to determine why an incident occurred and to form as basis for actions can be taken to prevent future occurrences of similar situations. This project was suggested by the Purdue Process Safety & Assurance Center (PPSAC) steering team. The details of the leak are mentioned below.

A far-reaching propane release occurred at a Natural Gas Liquid (NGL) facilities' sales gas metering skid used for analysis of the quantity and quality of propane transferred through the pipelines. The leak which lasted for about 47 minutes released large quantities of highly flammable propane into the atmosphere. The propane liquid pool boils vigorously while also spreading on the ground due to the massive difference between the ground temperature and its normal boiling point. Any ignition source near the leak has a potential for a fire or Vapor Cloud Explosion (VCE) and hence an accurate CFD model is important for RCA and risk management of such situations.

The computational work in this project was carried out in Fire Dynamics Simulator (FDS) version 6.5.3 and Smokeview version 6.4.4 was used to visually represent the models. 65 simulations were carried out in total, and the 65th model closely resembled the actual leak for the first 200 seconds in terms of the propane cloud width and dispersion, velocity of the release, height of the release, direction of dispersion, etc.

CHAPTER 2

SCIENTIFIC ASSESSMENT

2.1 FDS and Smokeview

Fire Dynamics Simulator is an open source Computational Fluid Dynamics (CFD) software developed by the National Institute of Standards and Technology (NIST). It uses a low Mach number approximation appropriate for low speed applications like fire, vapor dispersion, etc. to numerically solve the Navier-Stokes equations [2].

Smokeview is a software tool which is designed to visualize the results of an FDS simulation. It is an essential tool which assists FDS users to monitor and visualize a simulation's progress [3].

2.2 Source Term Methodology

Defining the source term is the first step towards modelling a hazardous release scenario (Fig 1). First, an incident such as the rupture of a pipeline, a hole in a tank or a pipe, etc. is defined and then subsequent source models are employed to describe the release. The source model is used to determine the rate of discharge, the total amount discharged and the state of the discharge (solid, liquid, vapor or a mixed fraction). Next, a dispersion model is used to predict the downwind movement and concentration(s) of the released material(s) [4].

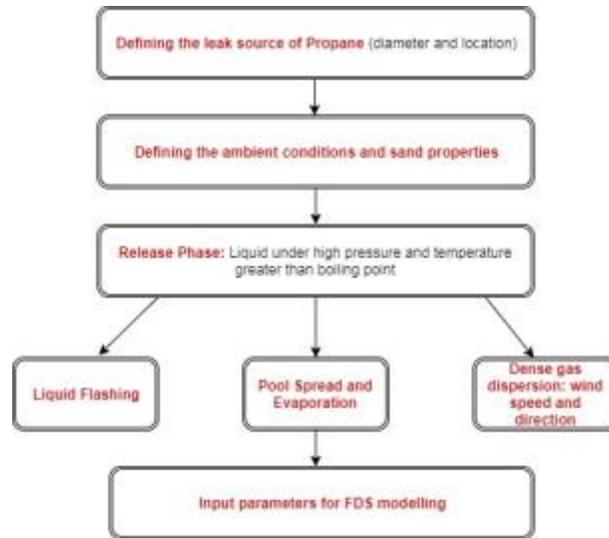


Fig 1 Flow of source term methodology for the Project

2.2.1 Source Model

Mechanical energy balance associated with fluids in motion, [5]:

$$\int \frac{dP}{\rho} + \Delta \left(\frac{\bar{u}^2}{2\alpha g_c} \right) + \frac{g}{g_c} \Delta Z + F = - \frac{W_s}{\dot{m}} \quad (1)$$

P Pressure (force/area)

ρ Density of the fluid (mass/volume)

\bar{u} Average instantaneous velocity of the fluid (length/time)

g_c Gravitational constant (length mass/force time²)

$\alpha = 0.5$ for laminar flow, $\alpha = 1.0$ for plug flow, and $\alpha \rightarrow 1.0$ for turbulent flow,

g Acceleration due to gravity (length/time²)

z Height above datum (length)

F Net frictional loss term (length force/mass)

W_s Shaft work (force length/time)

\dot{m} Liquid discharge rate (mass/time)

For our model, pure propane discharged from the leak source, which was an orifice in one of the pipe fittings of the plant. Hence, the energy balance can be simplified to:

$$\dot{m} = AC_D \sqrt{2\rho g_c (P_1 - P_2)} \quad (2)$$

\dot{m} Liquid discharge rate (mass/time)

A Area of the hole (length²)

C_D Discharge coefficient (dimensionless)

P_1 Upstream pressure (force/area)

P_2 Downstream pressure (force/area)

The coefficient of discharge was determined using the 2-K method [5]:

$$C_D = \frac{1}{\sqrt{1 + \sum K_f}} \quad (3)$$

$\sum K_f$ is the sum of all excess head loss terms, for Reynolds numbers greater than 10,000,

$K_f = 0.5$ for entrance and 1.0 for exit, and thus $C_D = 0.63$

2.2.2 Flash Evaporation:

When superheated propane comes in contact with atmospheric pressure and temperature at the point of the leak, it breakdowns into small droplets which is called flashing or flash evaporation. The fraction of propane that flashes is calculated assuming that the sensible heat contained within the superheated liquid is used to vaporize a fraction of the liquid [4].

$$F_v = C_p \frac{(T - T_b)}{h_{fg}} \quad (4)$$

C_p Heat capacity of the liquid, averaged over T to T_b (energy/mass deg)

T Initial temperature of the liquid (deg)

T_b Atmospheric boiling point of the liquid (deg)

h_{fg} Latent heat of vaporization of the liquid (energy/mass)

F_v Mass fraction of released liquid vaporized

FDS does not include any sub-models to determine flashing from the release of a superheated liquid and hence the above model is used to input the resultant terms into FDS [6].

2.2.3 Pool Vaporization:

At steady state, the vaporization rate is given as [4]:

$$\dot{m} = \frac{H}{L} \quad (5)$$

- \dot{m} Vaporization rate (mass/time)
- H Total heat flux to the pool (energy/time)
- L Heat of vaporization of the pool (energy/mass)

For a spill of liquid with normal boiling point below ambient temperature (231K for propane), the initial stage of vaporization is assumed to be due to the heat transfer from the ground. Hence, the heat flux from the ground to the pool can be expressed in terms of a simple one-dimensional heat conduction equation [4]:

$$q_g = \frac{k_s(T_g - T)}{(\pi\alpha_s t)^{1/2}} \quad (6)$$

- q_g Heat flux from the ground (energy/area)
- k_s Thermal conductivity of the soil (energy/length deg)
- T_g Temperature of the ground (deg)
- T Temperature of liquid pool (deg)
- α_s Thermal diffusivity of the ground (area/time)
- t Time after spill

2.2.4 Pool Spreading:

The radius of the pool is an important parameter for the evaporation model as it is directly proportional to total rate of vapor released into the atmosphere and subsequent dispersion by wind. The pool spread was calculated using Wu and Schroy's (1979) model which assumes that the pool growth is radial and uniform from the point of spill, unconstrained and on a flat surface. [4].

$$r = \left[\frac{t^3}{C^3 \pi^2 / 6g} \times \frac{\rho Q_{AF}^2}{\mu} \times \cos \beta \sin \beta \right]^{1/5} \quad (7)$$

- r Pool radius (length)
- t Time after the spill (time)
- C Constant developed from experimental data, see below (dimensionless)
- g Acceleration due to gravity (length/time²)
- ρ Density of the liquid (mass/volume)
- Q_{AF} Volumetric spill rate after flashing (volume/time)

- μ Viscosity of the liquid (mass/length time)
- β Angle between the pool surface and the vertical axis perpendicular to the ground, see below (degrees)

The Reynolds number for the pool spread is given by [4]

$$N_{Re} = \frac{2Q_{AF}\rho}{\pi r \mu} \quad (8)$$

$C = 2$ for $N_{Re} > 25$, and $C = 5$ for $N_{Re} \leq 25$

$$\beta = \tan^{-1}[(0.25 + B)^{0.5} - 0.5]^{0.5} \quad (9)$$

$$B = \frac{22.489r^4\rho}{Q_{AF}\mu} \quad (10)$$

The pool radius is iteratively determined using the above equations. As FDS does not include any sub-models for the pool spread, pool dimensions and corresponding vaporization rate(s) are used as inputs for FDS modelling [6].

2.2.5 Dispersion Model

As the density of propane vapor is greater than that of ambient air, a dense gas dispersion model should be used for our model. However, dispersion effects can be directly modelled in FDS by specifying certain parameters including wind speed, atmospheric stability, surface roughness etc.

CHAPTER 3

RESULTS AND DATA INTERPRETATION

3.1 Mathematical Modelling:

Pure propane was released through a 0.5-inch hole, at a line pressure of 450 psig and temperature ranging from 60-100F. The details of the release are mentioned in Table 1. Additional details such as the physical properties of propane and sand have been included in Appendix A.

Table 1 Parameters defining the leak

Parameter	Value
Mass flow rate	4.78 kg/s
Total mass of propane released	13500 kg
Fraction of propane flashed, F_p	0.4569
Mass flow of propane flashed	2.187 kg/s
Mass flow of propane into pool	2.6 kg/s

Using the mass flow rate of propane going into the pool i.e. 2.6 kg/s and the equations described in 2.2.3 and 2.2.4, the pool spread and evaporation models were calculated. Based on the location of the release, dry medium sand was assumed as the ground (Appendix A). The pool evaporation rate is directly proportional to the surface area (radius) of the pool as is evident in Fig 2 and Fig 3. As time progresses, the change in evaporation rate gradually decreases as the surface cools. When the leak is contained after 2820s, the pool reaches a radius of 37.5 m.

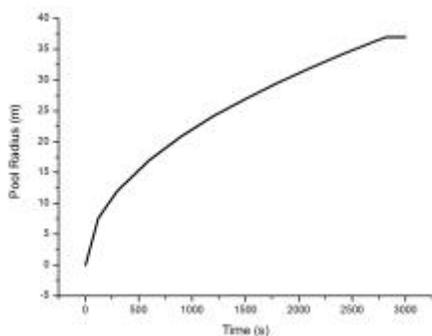


Fig 2. Increase in pool radius with time

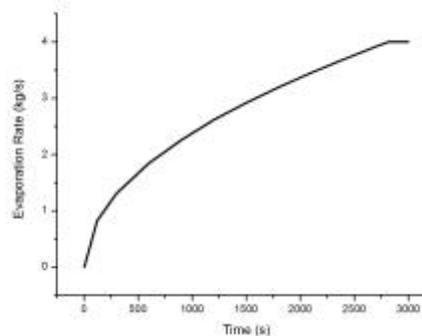


Fig 3. Increase in pool evaporation rate with time

According to the data collected [1], an average wind speed of 3.6 m/s was reported blowing from the North South direction (Appendix C). The atmospheric stability was assumed to be class A due to the low wind speed, strong-moderate insolation and as the release was during the day. Wind Class is shown in Fig 4. The credibility of the wind data was initially questioned as the weathering station was located far from the area of the leak. After running

the FDS simulations we concluded that the wind data was inaccurate, further details of which have been included in Chapter 4.

Surface wind speed, m/s	Daytime insolation			Nighttime conditions		Anytime
	Strong	Moderate	Slight	Thin overcast or >4/8 low cloud	≥3/8 cloudiness	Heavy overcast
<2	A	A-B	B	F	F	D
2-3	A-B	B	C	E	F	D
3-4	B	B-C	C	D	E	D
4-6	C	C-D	D	D	D	D
>6	C	D	D	D	D	D

A: Extremely unstable conditions

B: Moderately unstable conditions

C: Slightly unstable conditions

D: Neutral conditions

E: Slightly stable conditions

F: Moderately stable conditions

Daniel A. Crowl, Joseph F. Louvar. *Chemical Process Safety Fundamentals with Applications, 3rd Edition*. Prentice Hall Publication 2011

Fig 4. Wind Class

3.2 FDS Simulation

3.2.1 Defining the Mesh

All FDS computations are executed within a region made up of rectilinear volumes called meshes. Each mesh is divided into several rectangular cells which depend on the desired resolution of the flow dynamics [7]. The area of concern was determined to be 150m by 104m from the plot overview [1]. For our simulations, we assumed a mesh size of 200m*200m*10m with cell dimensions of 1m*1m. The following line is used to initialize the mesh.

```
&MESH ID='mesh', XB=-100.0, 100.0, -100.0, 100.0, 0, 10.0, IJK=200, 200, 10 /
```

By default, FDS assumes that the exterior boundaries of the computational domain are solid walls [7]. For outdoor simulations, each boundary must be explicitly defined **OPEN** as shown below.

```
&VENT PBX=-100, SURF_ID='OPEN' /
&VENT PBX=100, SURF_ID='OPEN' /
&VENT PBZ= 10, SURF_ID='OPEN', COLOR='SKY BLUE' /
&VENT PBY=-100, SURF_ID='OPEN' /
&VENT PBY= 100, SURF_ID='OPEN' /
&VENT PBZ= 0, SURF_ID='GROUND' /
```

3.2.2 Specifying the Ambient Conditions and Wind Speed

The release occurred on the 6th of December 2013 in the Middle East, and hence an ambient condition of 20°C and 1 bar were assumed for the simulations. The MISC namelist is used to specify these conditions in FDS.

```
&MISC RESTART=.FALSE., TMPA=20.0, P_INF=101325,RADIATION=.FALSE. /
```

There are a couple of methods available in FDS to specify a wind field, the one used in our simulations is the one recommended in the FDS user guide [7]. For this method, each component of the wind velocity vector is explicitly defined using U0, V0 and W0. Each velocity component can be individually varied with time and height. The following code,

```
&MISC U0=-3.6,v0=0,w0=0,MEAN_FORCING(1:3)=.TRUE.,DT_MEAN_FORCING=0.1 /
```

points a wind of 3.6 m/s in the negative x direction, i.e. from the right to the left of the mesh.

3.2.3 Defining the Sources of Propane Release

There are two sources for the propane release into the atmosphere: propane flashing from the leak point and propane evaporating from the liquid pool on the ground. In FDS we have to specify separate models for both these sources. Defining a source of release in FDS is a three steps process:

1. Defining the leak in terms of the species released with **SPEC** namelist; the mass flux of the release etc. using the **SURF** namelist.
2. Include rectangular obstructions into the domain using **OBST** namelist.
3. Use **VENT** namelist to inject propane into the computational domain.

The physical properties of propane gas are tabulated within FDS and need not be explicitly specified. An example of defining the source(s) is include below.

```

&SPEC ID='PROPANE' /
///leak from pipe\\
&SURF ID='LEAK SOURCE', SPEC_ID='PROPANE', MASS_FLUX(1)=2.187, RAMP_MF(1)='leak_ramp' /
&OBST XB=-1.0,0.0,-0.5,0.5,2.0,3.0,
SURF_ID6='INERT','INERT','INERT','INERT','INERT','INERT', COLOR='BLUE' /
&VENT XB=0.0,0.0,-0.5,0.5,2.0,3.0, SURF_ID='LEAK SOURCE', COLOR='RED' /
///pool evaporation \\
&SURF ID='Pool_1', SPEC_ID='PROPANE', MASS_FLUX(1)=0.00435 ,
RAMP_MF(1)='pool_ramp_1', TMP_BACK=-42, TMP_INNER=-42, TMP_FRONT=-42 /
&OBST XB=-79.0,71.0,-47.0,57.0,0.0,1.0,
SURF_ID6='INERT','INERT','INERT','INERT','INERT','GROUND', COLOR='TAN' /
&VENT XB= -6.89, 6.89, -6.89, 6.89, 1.0, 1.0, SURF_ID='Pool_1' /

```

3.2.4 Gas Detectors and Obstructions

There were 15 propane gas sensors located around the area of the release, Fig 5. The detectors were calibrated to alarm if the concentration of propane (vol %) increased above 25% of its Lower Flammable Limit (LFL) i.e. 2.1% (vol /vol). **DEVC** namelist is used to define the gas sensors in FDS. Each gas sensor has a time dependent output associated with it, which is stored in a comma-delimited ASCII file (.csv). At the end of the simulation, the .csv file was analyzed to note the time at which each sensor first reported a concentration greater than or equal to 0.00525 (Appendix C).

```

&DEVC XYZ=3.33,3.16,2.0 ,ID='2605',
QUANTITY='VOLUME FRACTION', SPEC_ID='PROPANE' /

```

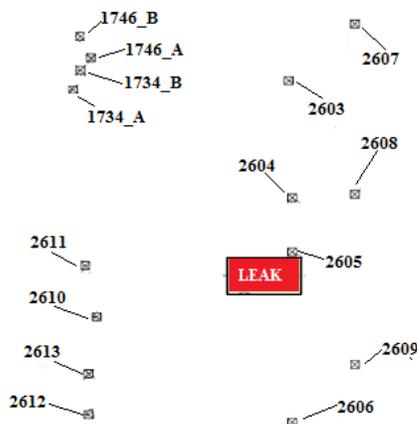


Fig 5 Location of the gas detectors (not to scale)

Any notable obstructions which might affect the flow path of propane vapors and the pool were included in the simulations using the **OBST** namelist.

```
&OBST XB=-4.67, 4.67, -2.17,2.17,1.0,2.0, SURF ID='INERT', COLOR='WHITE' /
```

3.2.5 Smokeview Representation and Analysis

For the base model of our project, we decided to exclude any wind as we didn't have accurate data. Further models with different wind profiles were developed to validate the model(s) with the actual alarm summary included in Chapter 4. All the data included in this Chapter are for the no wind condition.

The dispersion path of the propane vapors can be visually represented by using the **ISO**F namelist. The concentrations (mol/mol) to be displayed in Smokeview must be explicitly specified. For our models, we selected concentrations of 2.1 % propane in the atmosphere, which is its LFL and 0.525% which is the concentration above which the detectors go off. Figure 6 shows the direction of the release from 14 secs to 452 secs.

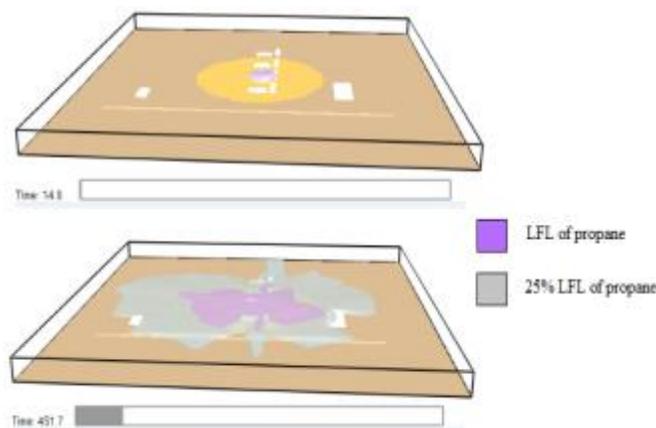


Fig 6 Spread of Propane Vapor

As propane vapor is heavier than air, the height to which it is dispersed is limited. To determine the maximum height of the dispersed gas, we studied the propane concentrations at various planes and concluded that it is essentially zero above 9 m.

Further analysis of the leak was done by examining the variation of propane volume fraction at different planes within the domain, using the **SLCF** namelist. Fig 7 shows the distribution of propane mole fraction, 10 minutes into the release, at the plane $Z=1$, which is the ground (sand) for our simulation.

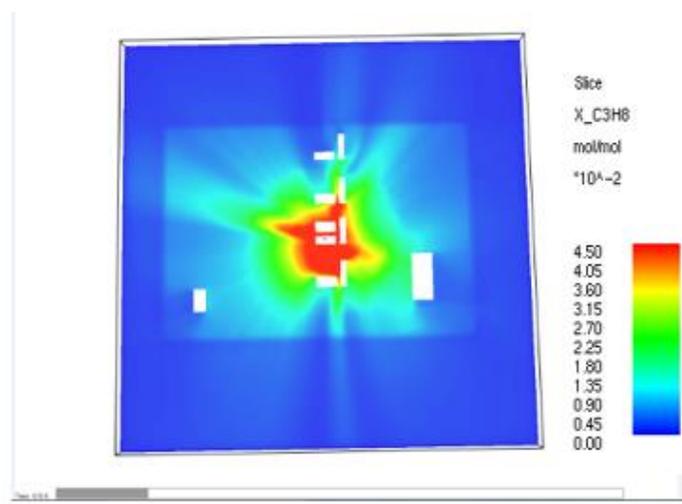


Fig 7 Smokeview rendering of the propane fraction at Z=1

In the absence of any wind, the sequence in which the detectors alarm (i.e. reach a concentration above 25% LFL) is different from the detector alarm sequence collected from the release location as shown in Fig 8. Also, the total time required for all the detectors to sound is much greater as there is no external driving force to speed up the dispersion of propane vapors.

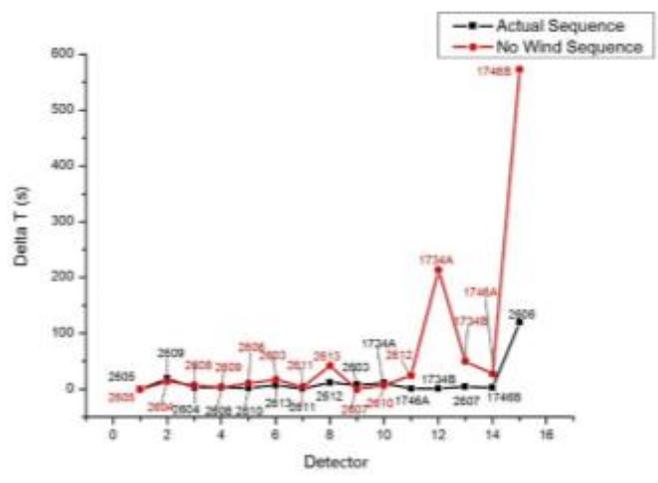


Fig 8 Detector alarm summary

Table 2 Detector alarm summaries (No Wind)

Actual Sequence	Time between each detector	FDS Sequence	Time between each detector
2605	0	2605	0
2609	19	2604	14
2604	3	2608	7
2608	3	2609	3.5
2610	2	2606	10.5
2613	7	2603	17.5
2611	1	2611	3.5
2612	12	2613	42
2603	8	2607	0
1734_A	11	2610	7
1746_A	1	2612	24.5
1734_B	1	1734_A	213.5
2607	4	1734_B	50
1746_B	3	1746_A	27
2606	120	1746_B	573

3.2.6 3.6m/s from NE to SW

For this case, we assumed a wind blowing at an average speed of 3.6 m/s from the NNE direction for the entire duration of the leak in accordance to the data provided (Appendix C). The North in the plot overview was in the negative x direction and hence the wind direction input into the FDS simulation was adjusted accordingly. Fig 9 depicts how the mole fraction of propane on the ground varied throughout the leak.

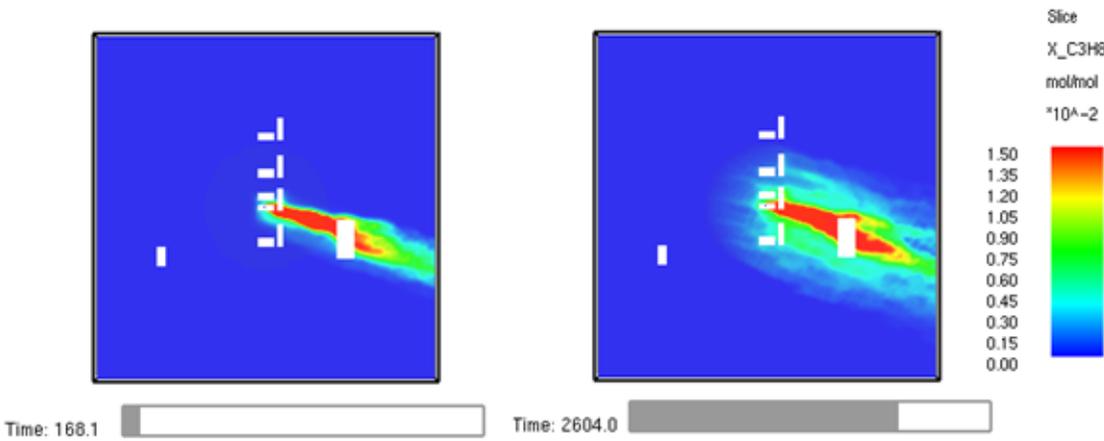


Fig 9 Variation of propane mole fraction on the ground (Case 1)

A comparison of the detector alarm summaries in Fig 10, shows the inaccuracy of the wind data. Only five detectors marked in red reached a concentration above 25% LFL propane which is not consistent with the actual detector alarm summary. The unalarmed detectors were located opposite to the direction of the wind.

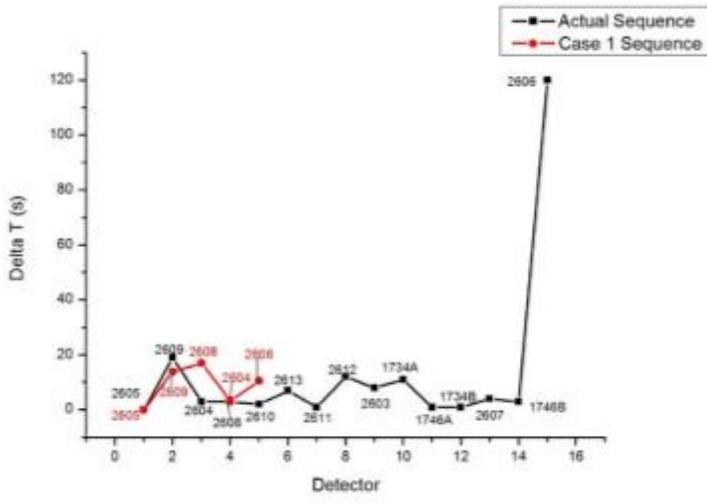


Fig 10 Detector alarm summaries (Case 1)

Table 3 Detector alarm summaries (Case 1)

Actual Sequence	Time between each detector	FDS Sequence	Time between each detector
2605	0	2605	0
2609	19	2609	14
2604	3	2608	7
2608	3	2604	3.5
2610	2	2606	10.5
2613	7	2610	Did not alarm
2611	1	2613	Did not alarm
2612	12	2611	Did not alarm
2603	8	2612	Did not alarm
1734_A	11	2603	Did not alarm
1746_A	1	1734_A	Did not alarm
1734_B	1	1746_A	Did not alarm
2607	4	1734_B	Did not alarm
1746_B	3	2607	Did not alarm
2606	120	1746_B	Did not alarm

CHAPTER 4

DISCUSSION AND CONCLUSIONS

4.1 Validation Studies

4.1.1 FDS Validation Model

Several simulations were carried out varying the wind speed and direction, and the following wind profile gave the most satisfactory results:

- A strong gush of wind (3m/s) lasting for a very short duration of time (5 sec) blowing from south to north which may be attributed to the unstable atmospheric conditions of the region.
- A relatively benign but persistent wind of 0.5 m/s blowing from west to east.

The following table summarizes the wind for this model.

Table 4 Wind Profile (Case 2)

Wind Profile	Duration
No wind	35 s
3 m/s South to North	5 s
0.5 m/s West to East	150 s

Fig 11_A and 11_B show the effect of change in the wind speed and direction on the mole fraction of propane.

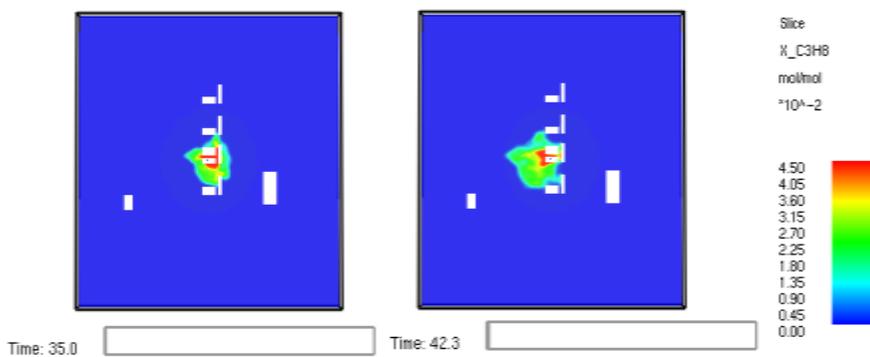


Fig 11_A Variation of propane mole fraction on the ground (Case 2)

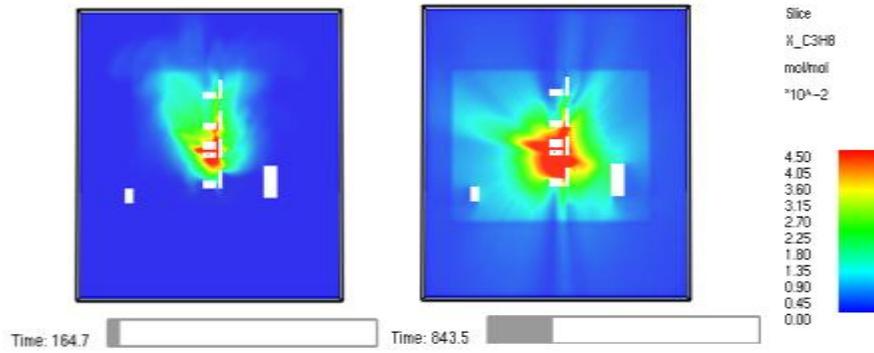


Fig 11_B Variation of propane mole fraction on the ground (Case 2)

As shown in Table 5 and Fig 12, the detector alarm summary of our model closely resembled the actual sequence. Baring detector 2609, all the others were in sequence and the time differences between activation of each detector were also accurate, within a few seconds of the actual scenario.

Table 5 Detector alarm summaries (Case 2)

Actual Sequence	Time between each detector	FDS Sequence	Time between each detector	Difference between Case 2 and actual sequence (sec)
2605	0	2605	0	0
2609	19	2604	13	7
2604	3	2608	7	4
2608	3	2609	4	1
2610	2	2610	7	5
2613	7	2613	1	6
2611	1	2611	1	0
2612	12	2612	10	2
2603	8	2603	20	12
1734_A	11	1734A	11	0
1746_A	1	1746A	3	2
1734_B	1	1734B	1	0

2607	4	2607	1	3
1746_B	3	1746B	3	0
2606	120	2606	116	4

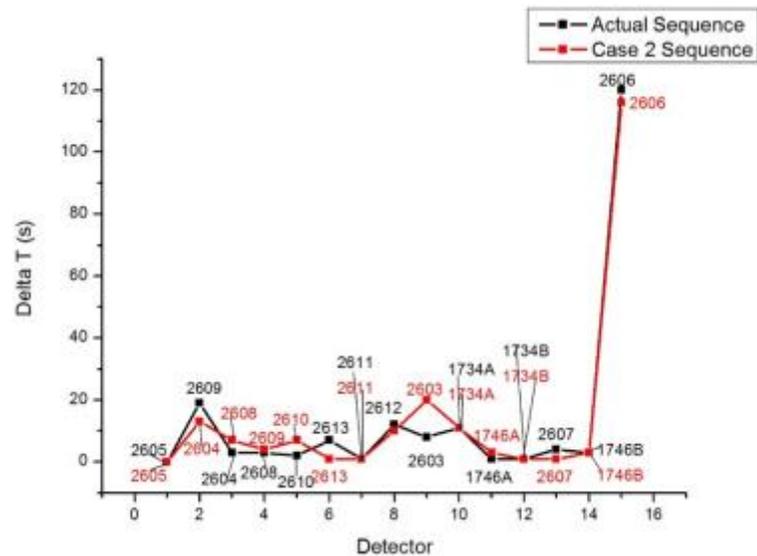


Fig 12 detector alarm summaries (case 2)

4.1.2 Iterative Nature of FDS

FDS and CFD modelling is an exercise in iteration. We started with a simplistic model and gradually increased the complexity of our models to match what happened at the release. Table 6 provides a summary of some of our model iterations.

Table 6 Iterations in FDS modelling

Model no	Description
1-9	Simple models incorporating flashing and pool evaporation separately (indoor simulation)
10-15	Introduction of wind into the system
16-18	Increasing complexity of models to represent the leak in the absence of wind (indoor + outdoor simulation).

18	Model for a no wind condition
19-39	Models trying to fit the given wind profile with simulation data.
39	Model verifying the inaccuracy of the wind data.
40-65	Predictive models to determine the wind data representative of the location.
65	Validated model representing the leak for the first 200 seconds.

4.2 Conclusion

FDS was effectively used to model the propane release from the metering skid which helped in understanding the direction of the release, the cloud width and dispersion and variation of propane volume fraction with time and space.

Despite the inaccuracy of the wind data, our final model could predict the actual path of the release for the first 200 secs (Fig 13) by assuming a wind profile which was representative of the region where the leak occurred (Section 4.1.1). Thus, we can conclude that our model can be effectively used in the prediction of similar release scenarios and as a tool for Root Cause Analysis.

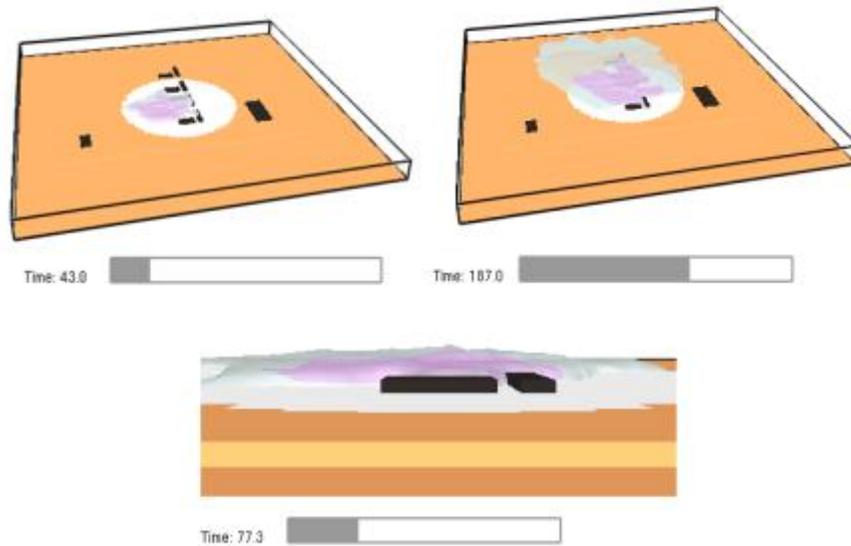


Fig 13 Propane cloud dispersion during the first 200s of the leak

CHAPTER 5

PROPOSED STEPS FORWARD

5.1 Improvement of results

- More demanding and complex equations to calculate the source terms to be entered into FDS that takes into account variables such as the actual size of the release, reduction in discharge pressure, etc.
- Add internal models to FDS to represent the vapor-liquid thermodynamics of flashing, pool spreading and evaporation.
- Use varying wind profiles across a year to form a coverage map.

5.2 In General

- Utilize CFD modelling to understand such releases in terms of the direction of release, vapor cloud width and dispersion etc.
- Use the results obtained from the models to assess risk mitigation steps for new developments and for Root Cause Analysis of incidents.
- Compare results with those from other CFD software.
- Collection of on-site wind data for sound release & dispersion analysis during risk management modeling, since CFD models are very sensitive to the wind profile.

References:

- [1] Confidential Data. Kenexis, May 2017
- [2] McGrattan K., Hostikka S., McDermott R., Floyd J., Weinschenk C., Overholt K. . *Fire Dynamics Simulator Technical Reference Guide 6th Edition, Volume 1*. NIST Special Publication 1018-1, 2017
- [3] Glenn P. Forney. *Smokeview, A Tool for Visualizing Fire Dynamics Simulation Data, Volume 1*. NIST Special Publication 1017-1, 2017
- [4] Center of Chemical Process Safety of the American Institute of Chemical Engineers. *Guidelines for Chemical Process Quantitative Risk Analysis, 2nd Edition*. Wiley Interscience Publication, 2000
- [5] Daniel A. Crowl, Joseph F. Louvar. *Chemical Process Safety Fundamentals with Applications, 3rd Edition*. Prentice Hall Publication 2011
- [6] Andrew Joseph Kohout. *Evaluation of Fire Dynamics Simulator for Liquefied Natural Gas Vapor Dispersion Hazards*. University of Maryland, College Park 2011
- [7] McGrattan K., Hostikka S., McDermott R., Floyd J., Weinschenk C., Overholt K. . *Fire Dynamics Simulator User's Guide 6th Edition*. NIST Special Publication 1019, 2017

APPENDIX A**PHYSICAL PROPERTIES AND PLANT PLOT**

Table 1 Propane properties

Parameter	Value	Unit
Liquid density	580	kg/m ³
Initial liquid temp	311	K
Boiling temp	231	K
Heat of Vaporization, h_{fg}	429	KJ/kg
Heat capacity	2.45	KJ/kgK

Table 2 Sand properties

Parameter	Value	Unit
Thermal conductivity	0.27	W/mK
Thermal diffusivity	1.98×10^{-7}	m ² /s
Temperature	293	K
Specific heat	0.8	KJ/kgK

APPENDIX B

INPUT FILE FOR CASE 2

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&OBST XB=42,51.67, -30,-6.67,1.0,2.0,
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&OBST XB=-65.33,-59, -34,-23.33,1.0,2.0,
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/// sensors \\

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&DEVC XYZ=-20.33,-5.2,2.0 ,ID='2610',
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QUANTITY='VOLUME FRACTION', SPEC_ID='PROPANE' /

\\ \ slice files \\ \

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&SLCF PBZ= 2.0, QUANTITY='VELOCITY', VECTOR=.TRUE.,SPEC_ID='PROPANE' /

&SLCF PBX= 0.0, QUANTITY='VOLUME FRACTION', SPEC_ID='PROPANE' /
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&ISOF QUANTITY='VOLUME FRACTION', SPEC_ID='PROPANE',
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&TAIL /
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APPENDIX C

• Pool Vaporization:

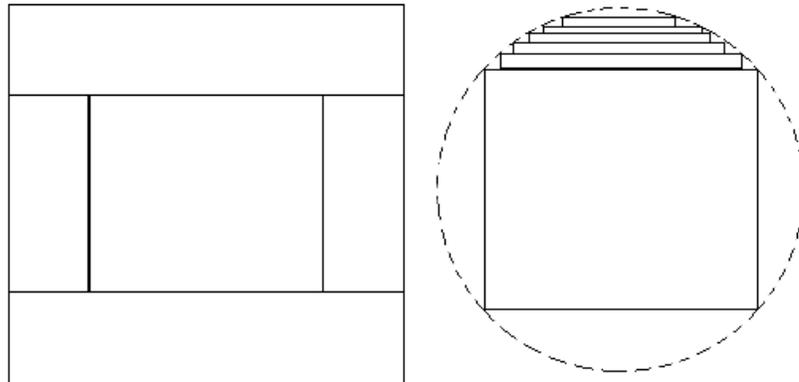
The total vapor loading into the atmosphere is due to the combined effect of flash evaporation and vaporization from the liquid pool formed on the ground which is governed by the equation [3]:

$$mC_p \frac{dT}{dt} = H - L\dot{m} \quad (1)$$

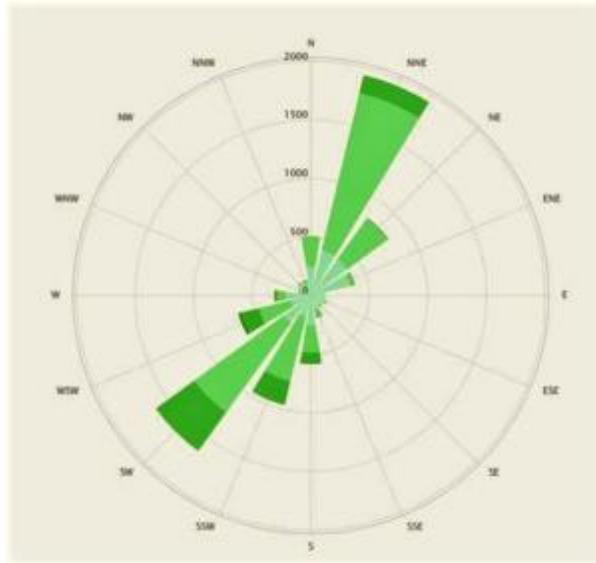
For a highly volatile liquid such as propane at steady state, heat transfer by conduction controls the vaporization rate. H, as the total heat flux in equation (1), can be simplified as heat transfer from the ground. The above equation can be simplified as [3]:

$$\dot{m} = \frac{H}{L} \quad (2)$$

• Simulating the increase in pool radius with time in FDS and Smokeview



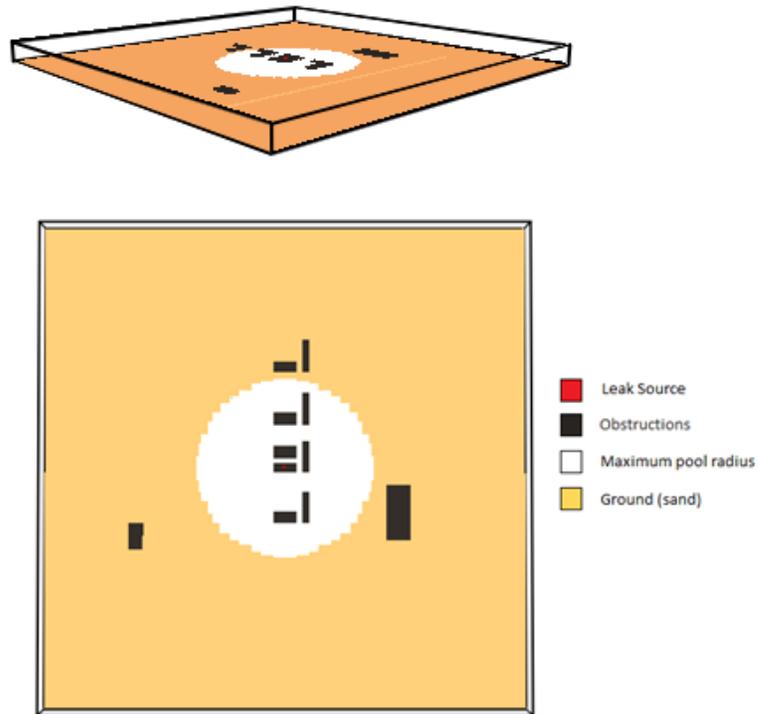
- Wind rose



- Csv output file of case 2

	A	B	C	D	E	F	G	H
1	s	mol/mol						
2	Time	2605	2609	2604	2608	2610	2613	2611
3	0.00E+00							
4	3.67E+00	4.14E-07	4.48E-23	4.51E-17	4.78E-21	7.54E-53	0.00E+00	6.59E-56
5	7.00E+00	4.05E-03	1.03E-20	4.01E-14	1.06E-18	1.19E-46	2.52E-55	9.63E-49
6	1.07E+01	7.03E-02	3.25E-19	1.77E-12	9.88E-18	1.64E-43	9.67E-51	2.48E-45
7	1.40E+01	6.48E-02	4.19E-18	3.53E-09	3.95E-17	3.61E-41	9.80E-48	1.48E-42
8	1.77E+01	5.81E-02	4.79E-17	2.25E-05	2.05E-16	3.04E-38	5.73E-45	2.43E-39
9	2.10E+01	7.01E-02	1.40E-14	5.05E-03	2.78E-13	3.61E-35	1.78E-42	2.77E-36
10	2.47E+01	7.30E-02	9.18E-09	2.41E-02	6.55E-08	3.79E-32	5.61E-40	1.04E-31
11	2.80E+01	7.57E-02	2.22E-04	2.46E-02	9.76E-04	1.71E-29	2.78E-37	4.34E-26
12	3.17E+01	7.55E-02	5.02E-03	1.93E-02	1.86E-02	1.06E-26	3.66E-34	5.46E-21
13	3.50E+01	7.45E-02	1.25E-02	1.94E-02	1.87E-02	6.19E-24	9.40E-31	9.82E-17
14	3.85E+01	4.38E-02	1.37E-02	1.49E-02	7.01E-03	6.10E-07	2.41E-11	2.54E-03
15	4.23E+01	1.65E-02	5.63E-04	6.70E-03	2.20E-05	1.19E-02	8.06E-03	1.17E-02

- Computational domain in Smokeview



- Maximum height of the propane vapors at the release source

