HAZARDOUS AREA CLASSIFICATION OF LOW PRESSURE NATURAL GAS SYSTEMS USING CFD PREDICTIONS

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Whilst area classification has been applied in the past to high pressure natural gas installations, with the implementation of DSEAR it has been necessary to consider it for all pressures, including the relatively low pressures used for distribution and supply.

BS EN 60079-10:2003 defines 'High Ventilation' as that required to ensure that the volume (Vz) of a flammable gas cloud is maintained below 0.1 m^3 for foreseeable gas leaks. Demonstrating that this criterion is met implies that a zone of "Negligible Extent" (NE) can be applied. However, the methodology given in the standard for the estimation of this cloud size makes it very difficult to achieve even for outdoor low pressure systems.

This paper presents the results of a study that uses Computational Fluid Dynamics (CFD) modelling to estimate the gas cloud volume, Vz, as defined in BS EN 60079-10:2003. Leaks are considered over a range of pressures (0.5 to 5.0 barg) and hole sizes (0.25 to 5.0 mm^2). The size of the gas clouds obtained from these simulations is compared to those obtained from using the methodology in BS EN 60079-10, which presents simple formulae for estimating gas cloud volumes. The results from the CFD simulations, based on conservative assumptions, indicate that the gas cloud volumes according to the "Vz" criteria may be overestimated for low pressure releases by two to three orders of magnitude using the BS EN 60079-10:2003 formulae for outdoor unobstructed release sources. This clearly has implications for hazardous area classification practice in these circumstances.

INTRODUCTION

The Dangerous Substances and Explosive Atmospheres Regulations 2002 (DSEAR) place duties on employers to control or eliminate the risks from explosive atmospheres in the workplace. The regulations put into effect the European Directive 99/92/EC, otherwise known as the ATEX Workplace Directive. DSEAR requires employers to identify areas where explosive atmospheres may occur, to classify these areas according to the likely occurrence and duration of explosive atmospheres, and to adopt appropriate measures to control or minimize the risks of an explosion.

Classification of hazardous areas under DSEAR uses the well-established concepts of hazardous zones. In a Zone 0 area, explosive atmospheres are present continuously or

frequently for long periods. In Zone 1 areas, explosive atmospheres may occur occasionally under normal operating conditions and in Zone 2 areas explosive atmospheres are unlikely to occur and will persist for only a short time. As part of a risk assessment, employers must take control measures to minimize the risks of explosions occurring in zoned areas. This may involve, for example, ensuring adequate ventilation. Mitigation measures must also be put in place, which may include installing equipment and protective systems of an appropriate category to comply with the Equipment and Protective Systems for Use in Potentially Explosive Atmospheres Regulations, 1996. Compliance with these regulations can have significant cost implications for businesses.

In a significant change to previous regulations, DSEAR applies to all workplaces where dangerous substances are present, used, or produced. This includes industrial and commercial premises, land-based and offshore installations, private roads and paths on industrial estates, road works on public roads, and houses or other domestic premises where people are at work. It excludes domestic premises where people are not at work. Considering solely the fact that leaks from natural gas supply pipework have the potential to cause explosive atmospheres, DSEAR affects around 600,000 businesses. The regulations came into force for all new workplaces in July 2003 and all workplaces, old or new, must meet the requirements by July 2006.

The DSEAR ACOP suggests that BS EN 60079-10:2003 can be used to assess the classification of hazardous areas. This standard introduces the concept of 'negligible extent' (NE): a volume of explosive gas that is so small that even if it were ignited would cause no significant damage. The definition of NE is a gas cloud of volume 0.1 m^3 in which the mean concentration is a quarter or half the lower explosive limit (25% or 50% LEL). For Zone 1 areas the 25% LEL figure should be adopted and 50% LEL for Zone 2 areas. If it can be demonstrated for a nominally Zone 2 area that there is sufficient ventilation so that a foreseeable flammable gas release will only form a cloud smaller than this 0.1 m^3 volume, the area may be classified as 'Zone 2 NE'. Such areas should not be subject to the control and mitigation measures specified in DSEAR, provided that this is in agreement with the risk assessment. Clearly, classification of areas as Zone 2 NE has significant financial implications for businesses seeking DSEAR compliance.

ESTIMATION OF VZ

Section B.4.2 of BS EN 60079-10:2003 presents the following method to calculate the gas cloud volume in which the mean concentration is 25% or 50% LEL, which it calls the 'Vz' volume. Firstly the theoretical minimum ventilation flow rate of fresh air necessary to dilute a given release of flammable material to the LEL condition is calculated from:

$$\left(\frac{dV}{dt}\right)_{\min} = \frac{(dG/dt)_{\max}}{k.LEL_m}\frac{T}{293} \tag{1}$$

where, using the same notation as BS EN 60079-10:2003:

$(dV/dt)_{min}$ = Minimum volumetric flowrate of fresh air (m³/s)
$(dG/dt)_{max}$ = Maximum release rate at source (kg/s)
LEL_m = Lower explosive limit (kg/m³)
k = Safety factor ($k = 0.25$ for continuous or primary grades of release, $k = 0.5$ for secondary grades of release)
T = Ambient temperature (K)

The mass-based LEL_m is calculated from:

$$LEL_m = 0.416 \times 10^{-3} \times M \times LEL_v \qquad (2)$$

where M is the relative molecular mass in kg/kmol.

For open air situations, the standard presents what it terms a "conservative approximation" for the air exchange rate. Based on a hypothetical cube with 15 metre sides and a 0.5 m/s wind speed, the air exchange rate is 0.03 air-changes per second. Using this value, the Vz volume is calculated from:

$$Vz = \frac{f(dv/dt)_{min}}{0.03} \qquad (3)$$

where f is a factor varying from 1 to 5 that accounts for impeded air flow.

The origin of the above calculation method is unknown. To investigate its accuracy, the present paper compares its predictions for a number of secondary releases in open air environments to those obtained using Computational Fluid Dynamics (CFD). Details of this alternative technique are presented in the following section.

COMPUTATIONAL METHODOLOGY

Computational Fluid Dynamics (CFD) involves the numerical solution of the conservation equations for mass, momentum and energy, which govern fluid flow. The CFD method involves subdividing the flow domain into a large number of small cells, where the gas velocity, pressure and temperature are calculated at nodes in each cell. The gas releases considered in the present work are turbulent. To account for the effect of unsteady turbulent fluctuations on the mean flow behaviour, the Reynolds-Averaged Navier-Stokes (RANS) approach is used in conjunction with the industry-standard k-ε model.

The gas leak is simulated as a free jet issuing from a circular hole into an unconfined space. A mass-fraction equation is solved in the CFD model for the transported gas. Three hole sizes and three leak pressures are considered:

- Hole size: 0.25 mm², 2.5 mm² and 5 mm². The two smaller hole sizes (0.25 and 2.5 mm²) are often used for area classification

- Pressure: 500 mbarg, 2.5 barg, and 5 barg. These are cut-off values in use for standards development in Europe.

All of the above combinations of pressures and hole sizes are simulated with methane as the released gas. Some sensitivity studies are also made using propane (at 5 barg), butane (at 2 barg) and a more accurate natural gas composition. The composition of natural gas is taken from Institution of Gas Engineers Safety Recommendations, IGE/SR/25, for the Lupton gas terminal.

For cases with pressures of approximately 2 barg or over, the gas jet exits at the local speed of sound and the flow is described as 'choked'. Rather than try to resolve the complex shock structures immediately downstream of the leak using CFD, a "resolved sonic source" approach is adopted. This involves modelling the flow downstream of the sonic point (see Ewan & Moodie, 1986, and Ivings et al., 2004, for details). Mass flow rates are calculated based on an assumed isentropic expansion. An alternative approach for determining the mass flow rate is given in IGE/SR/25. The conditions at the inlet to the CFD model are given in Tables 1 to 4. Mass flow rates calculated using the IGE/SR/25 methodology are shown for comparison.

The IGE/SR/25 values are around 20–30% lower than those predicted from assuming an isentropic expansion. In the CFD simulations, the higher, more conservative, mass flow rates are adopted.

For well-ventilated or outdoor applications, it is known from previous CFD work at higher pressures that a modest ventilation rate, or wind velocity, can affect the cloud size, depending on its direction. Cross or counter-current flow significantly reduces cloud size, whilst co-current flow generally leads to the largest gas cloud volumes. To take into account the effect of ventilation and study the worst-case scenario, the CFD model uses

Table 1. Methane inlet boundary conditions

	Leak conditions		CFD model boundary conditions				
Case	Pressure (barg)	Area (mm^2)	Temp. (K)	Area (mm^2)	Velocity (m/s)	Mass flux (kg/s)	IGE/SR/25 Mass flux (kg/s)
1	5.0	5.0	246.2	16.2	393.6	5.42E-3	4.37E-03
2	5.0	2.5	246.2	8.11	393.6	2.71E-3	2.19E-03
3	5.0	0.25	246.2	0.811	393.6	2.71E-4	2.19E-04
4	2.5	5.0	246.2	9.47	393.6	3.17E-3	2.49E-03
5	2.5	2.5	246.2	4.73	393.6	1.58E-3	1.24E-03
6	2.5	0.25	246.2	0.473	393.6	1.58E-4	1.24E-04
7	0.5	5.0	258.1	5.0	324.2	1.31E-3	1.05E-03
8	0.5	2.5	258.1	2.5	324.2	6.57E-4	5.23E-04
9	0.5	0.25	258.1	0.25	324.2	6.57E-5	5.23E-05

Table 2. Propane inlet boundary conditions

	Leak conditions		CFD model boundary conditions				
Case	Pressure (barg)	Area (mm^2)	Temp. (K)	Area (mm^2)	Velocity (m/s)	Mass flux (kg/s)	IGE/SR/25 Mass flux (kg/s)
1	5.0	2.5	266.4	8.60	237.8	4.12E-3	3.50E-3
2	5.0	0.25	266.4	0.860	237.8	4.12E-4	3.50E-4

a co-flow velocity of 0.5 m/s. For three of the methane cases studied, calculations are also made using co-flow velocities of 0.1 and 1.0 m/s to assess the sensitivity of Vz to this parameter. A three-dimensional view of the CFD model and its boundary conditions are shown in Figure 1.

Calculations were performed using the commercial code CFX. More details of the computational techniques employed in this study can be found in Gant & Ivings, 2005. For general information on CFD, see for example Anderson, 1995, or Versteeg & Malalasekera, 1995.

RESULTS

Figure 2 shows a typical result from the CFD of a cross-section through the domain. Cells boundaries are outlined in black and contours display the predicted gas concentration in terms of molar fraction. Tables 5 to 8 summarize the results of the test cases for methane, propane, butane and Lupton natural gas. Values in the columns marked 'CFD Vz' are the volume of the cloud in which the average gas concentration is 50% LEL. These results can be compared to the range of values calculated by the formulae given in BS EN 60079-10:2003 for estimating the Vz volume (the range is due to a correction factor varying from 1 to 5 to account for impeded air flow). The methane data is also plotted in Figures 3 and 4 using different axes scales.

Table 3. Butane inlet boundary conditions

	Leak conditions		CFD model boundary conditions				
Case	Pressure (barg)	Area (mm^2)	Temp. (K)	Area (mm^2)	Velocity (m/s)	Mass flux (kg/s)	IGE/SR/25 Mass flux (kg/s)
1	2.0	2.5	270.8	4.36	205.6	2.34E-3	1.95E-3
2	2.0	0.25	270.8	0.436	205.6	2.34E-4	1.95E-4

Table 4. Lupton natural gas inlet boundary conditions

	Leak conditions			CFD model boundary conditions			
Case	Pressure (barg)	Area (mm^2)	Temp. (K)	Area (mm^2)	Velocity (m/s)	Mass flux (kg/s)	IGE/SR/25 Mass flux (kg/s)
1	5.0	2.5	250.0	8.20	375.0	2.80E-3	2.28E-3
2	5.0	0.25	250.0	0.820	375.0	2.80E-4	2.28E-4
3	2.5	2.5	250.0	4.79	375.0	1.64E-3	1.298E-3

There are significant differences between the CFD results and those of the BS EN 60079-10:2003 formulae. In all of the methane cases considered, the CFD cloud volume is lower than the 'negligible extent' cutoff of $0.1 \, \text{m}^3$ whereas the BS EN 60079-10:2003 values are between 100 and 3000 times larger than the CFD values. Figures 3 and 4 show that BS EN 60079 predicts Vz to increase linearly with mass flow rate whereas the trend shown by the CFD results is non-linear, the Vz showing some tendency to increase faster at higher mass flow rates. Closer inspection of the CFD data reveals that the results are in fact composed of a family of curves, one for each release pressure, rather than a single trend line. This reflects the fact that the size of the gas cloud is a function of the hole size and jet velocity (and whether the flow is choked or not) rather than a simple function of the mass flux.
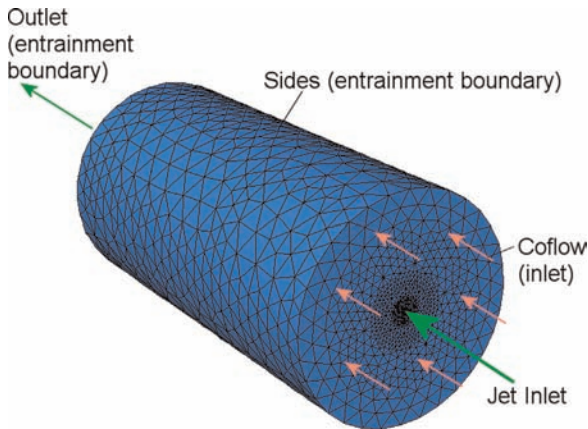

Figure 1. Three-dimensional view of the domain showing surface mesh and boundary conditions
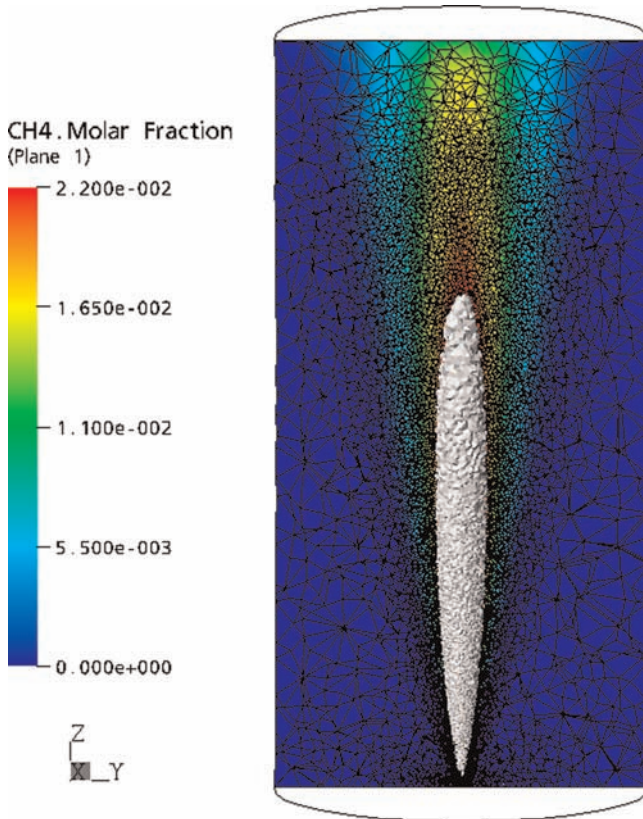
Figure 2. Two-dimensional slice through a typical simulation showing the computational mesh, contours of the methane molar fraction with the Vz volume highlighted in grey

Comparing Tables 5 and 8, the CFD Vz volumes calculated using methane are approximately 15 to 20% larger than those of natural gas, which itself is composed of 87% methane. Both propane and butane give higher Vz volumes than for methane releases at comparable pressures and hole sizes. This is mainly due to the higher mass flow rates with propane and butane.

All of the CFD results presented in Tables 5 to 8 were obtained using a co-flow velocity of 0.5 m/s. Table 9 presents the results for three methane cases in which the co-flow velocity is set to 0.1, 0.5 and 1.0 m/s. Differences in the calculated Vz volumes due to changes in the co-flow velocity are relatively small. Typically, the Vz decreases by around 10% as the co-flow velocity is decreased from 1.0 m/s to 0.1 m/s.

Table 5. Summary of methane results

Case	Leak conditions		50% LEL volumes (m^3)	
	Pressure (barg)	Area (mm^2)	CFD Vz	BS EN 60079-10:2003 Vz
1	5.0	5.0	0.0936	12.3 – 61.7
2	5.0	2.5	0.0326	6.17 – 30.8
3	5.0	0.25	0.0012	0.62 – 3.08
4	2.5	5.0	0.0433	7.22 – 36.1
5	2.5	2.5	0.0148	3.60 – 18.0
6	2.5	0.25	0.0005	0.36 – 1.80
7	0.5	5.0	0.0147	2.98 – 14.9
8	0.5	2.5	0.0054	1.50 – 7.48
9	0.5	0.25	0.0002	0.15 – 0.75

A number of assumptions and approximations are made to create the CFD model of the gas jet, such as turbulence modelling simplifications and discretization approximations. However, these factors do not account for the two to three orders of magnitude differences between the CFD and the BS EN 60079-10:2003 formulae results.

DISCUSSION & CONCLUSIONS
The aim of this work has been to examine the validity of the BS EN 60079-10:2003 method for calculating the extent of gas clouds due to leaks in low-pressure natural gas systems. For pressures of 5.0, 2.5 and 0.5 barg and leak areas of 5.0, 2.5 and 0.25 mm^2, the Vz gas cloud volumes calculated using CFD are two to three orders of magnitude smaller than those estimated using the BS EN 60079-10:2003 formulae. For the methane cases considered, all of the gas cloud volumes calculated using CFD are

Table 6. Summary of propane results

Case	Leak conditions		50% LEL volumes (m^3)	
	Pressure (barg)	Area (mm^2)	CFD Vz	BS EN 60079-10:2003 Vz
1	5.0	2.5	0.0579	6.82 – 34.1
2	5.0	0.25	0.00187	0.68 – 3.41

Table 7. Summary of butane results

	Leak Conditions		50% LEL Volumes (m³)	
Case	Pressure (barg)	Area (mm²)	CFD Vz	BS EN 60079-10:2003 Vz
1	2.0	2.5	0.0417	4.32 – 21.6
2	2.0	0.25	0.00137	0.432 – 2.16

Table 8. Summary of Lupton natural gas results

	Leak Conditions		50% LEL Volumes (m³)	
Case	Pressure (barg)	Area (mm²)	CFD Vz	BS EN 60079-10:2003 Vz
1	5.0	2.5	0.0275	5.54 – 27.7
2	5.0	0.25	0.0009	0.55 – 2.77
3	2.5	2.5	0.0124	3.25 – 16.2

smaller than those defined as being of 'negligible extent', i.e. 0.1 m³. These results suggest that there is a very high level of conservatism in the method for calculating Vz in BS EN 60079-10:2003 for low pressure jets. The results in this study are relevant to open unobstructed areas, where we have assumed a worst case scenario of a co-flow velocity
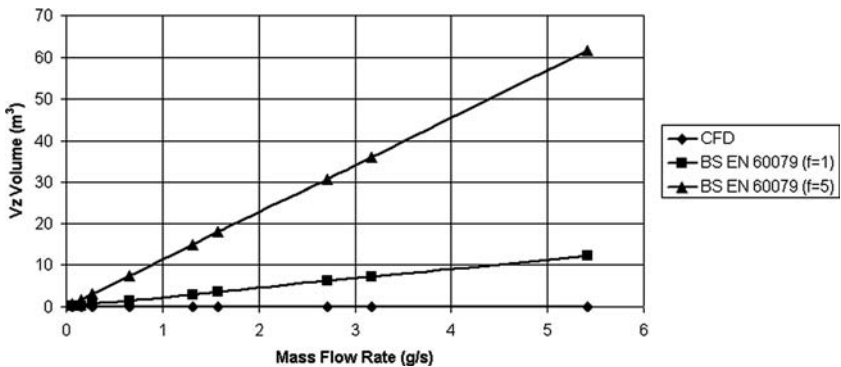

Figure 3. Comparison of methane Vz volumes predicted by CFD and the BS EN 60079 formulae using correction factors, f = 1 and f = 5
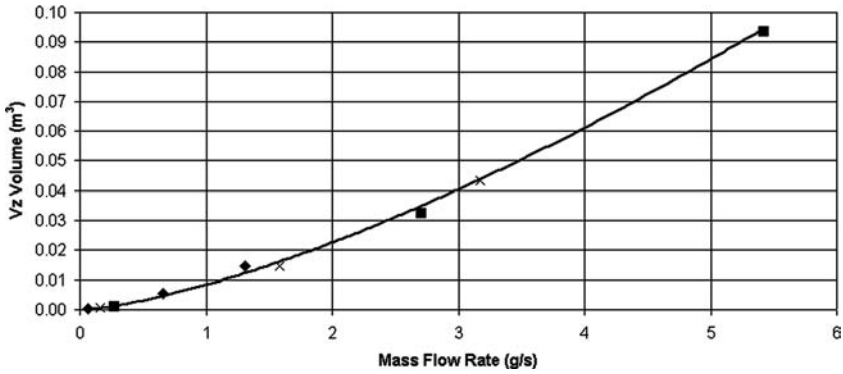
Figure 4. Predicted methane Vz volumes using CFD. Symbols: ■ 5.0 barg; ×: 2.5 barg; ◆: 0.25 barg. Line: best fit through points

Table 9. Effects of co-flow velocity on calculated Vz volume

Case	Leak conditions		50% LEL volumes from CFD (m^3)		
	Pressure (barg)	Area (mm^2)	0.1 m/s	0.5 m/s	1.0 m/s
1	5.0	2.5	0.0342	0.0330	0.0308
2	5.0	0.25	0.0012	0.0012	0.0011
3	2.5	2.5	0.0156	0.0148	0.0138

and a discharge coefficient of unity. It is expected that the results will be of value to those preparing risk assessments and area classification under DSEAR.

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