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CFD Modelling of Low Pressure Jets for Area Classification

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EXECUTIVE SUMMARY

The objective of this work was to perform a number of CFD simulations of low pressure gas leaks 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 was compared to those obtained from the British Standard BS EN 60079-10:2003, which presents simple formulae for estimating gas cloud volumes. The results from the CFD simulations indicate that the gas cloud volumes specified 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. This clearly has implications in terms of the current practice of hazardous area classification.

1 INTRODUCTION

1.1 BACKGROUND

Whilst area classification has been applied in the past to high pressure natural gas installations, with the implementation of DSEAR[1] it has been necessary to consider it for all pressures, including the pressures used for distribution and supply. In the UK, the principal source of guidance on area classification is the Institute of Gas Engineers & Managers (IGEM) safety regulations IGE/SR/25 [1], which is based on a British Gas document SHA 1, originally drafted some 10 years ago. Whilst most of the guidance therein is based on experimental or sound theory, the recommendations have been increasingly regarded as possibly excessive at lower pressures. The gas industry has maintained that the incidence of fires or explosions following small leaks from flanges, fittings, joints etc. is so low that area classification is inappropriate. Little firm evidence has been put forward and discussions with HSE based on experience and qualitative risk assessment continue.

Small leaks are defined in the BS EN 60079-10:2003 standard [2] as giving rise to flammable clouds of "negligible extent" (NE). This NE criteria is based on the concept of a gas cloud volume, denoted "Vz", which has a mean concentration of 50% of the lower explosive limit (LEL). In cases where the Vz is less than 0.1m^3, for secondary sources, the releases are classified as being of negligible extent. The British Standard contains a methodology for the estimation of this cloud size which is of unknown origin and dubious accuracy, but the essential concept of NE is clear.

During a recent review of area classification in well ventilated or open air situations at a steel works, it was shown that leaks from hole sizes typically used for area classification at lower gas pressure produced gas clouds that fall within the NE criterion. These findings need to be evaluated since, if fully validated, they would have a significant impact on the gas industry, and potentially for other applications. The study of the steel works used GaJet, a one dimensional model and spreadsheet developed by HSL for gas turbine ventilation evaluation. The theory underlying this model was taken from a paper by Ewan & Moodie [3] where the gas cloud size is estimated from a given value of LEL and its axial extent for sonic releases. Whilst the GaJet model provides useful information on gas cloud volumes, it only identifies the volume enclosed by a 50% LEL *iso-surface* and does not identify Vz volumes where the *mean* concentration is 50% LEL. At pressures of around 30 barg, HSL demonstrated using previous CFD simulations that the difference in the gas cloud volume from using the 50% LEL iso-surface and the Vz criterion was a factor of 6. The variation of this factor with pressure and hole sizes is, however, unknown.

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[1] Dangerous Substances and Explosives Atmospheres Regulations, 2002.

1.2 OBJECTIVES

The purpose of the present work is to evaluate the Vz cloud volume as defined by BS EN 60079-10:2003 over a range of relevant pressures and hole sizes using CFD. The proposed ranges are:

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

- Hole size: 0.25mm^2, 2.5mm^2 and 5mm^2 . The two smaller hole sizes (0.25 and 2.5 mm^2) are often used for area classification.

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 direction. Cross or counter-current flow significantly reduces cloud size, whilst co-current flow leads to the largest gas cloud volumes. To take into account the effect of ventilation and study the worst-case scenarios, three coflow velocities will be investigated: 0.1, 0.5 and 1.0 m/s.

The main focus of this study is jets of natural gas. Some sensitivity studies will also be made, however, using propane (at 5 barg) and butane (at 2 barg).

2 DESCRIPTION OF CFD MODELLING

2.1 INTRODUCTION

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. For turbulent flows, it is not computationally feasible to directly resolve all of the fine eddy structures in the flow. Instead, the flow is time-averaged and the *mean* conservation equations are solved. As a consequence of this averaging, additional terms are introduced into the equations to account for the unresolved eddy motions. These terms are approximated using a turbulence model. In the present work, the industry-standard k-ε model has been applied.

2.2 MODELLED GAS COMPOSITION

Rather than use a complete natural gas composition, initial CFD tests have been performed using methane. To confirm that the results using methane are sufficiently accurate, selected cases have been re-run using a more complete natural gas model which accounts for 99.93% of a typical natural gas composition. This typical natural gas composition was taken from Appendix 4 of the IGE procedures document, UP/9, for the Lupton gas terminal [4]. Table 1 shows the full list of components, with the simplified natural gas composition used in the CFD shown unshaded. A summary of the properties of all the gases tested in the present work, including propane and butane, is given in Table 2. The methods used to calculate the specific heat ratio and LEL for the natural gas mixture are described in Appendix A.

In the CFD model, the two component mixture of methane-air, propane-air etc. is handled by solving a transport equation for the mass fraction of methane or propane etc.. Fluid entering at the jet inlet is assigned a mass fraction of 1.0, whilst the mass fraction of the coflow air and any entrained fluid is given a value of zero.

Table 1 Lupton natural gas composition (from Appendix 4 of IGE/UP/9)

Molecule	*Composition*	*Molar fraction (%)*
Carbon Dioxide	CO_2	2.45
Nitrogen	N_2	1.69
Methane	CH_4	87.21
Ethane	C_2H_6	6.18
Propane	C_3H_8	1.74
Isobutane	C_4H_{10}	0.19
Pentane	C_5H_{12}	0.33
Hexane	C_6H_{14}	0.14
Heptane	C_7H_{16}	0.05
Octane	C_8H_{18}	0.01
Nonane	C_9H_{20}	0.003
Benzene	C_6H_6	0.001
Toluene	C_7H_8	0.003

Note: molecules highlighted in grey were not used in the CFD study.

Table 2 Summary of the properties of gases used in the CFD study

Gas	*Relative Molecular Mass (kg/kmol)*	*Specific Heat Ratio, γ*	*Gas Constant, R (kJ/kg·K)*	*LEL (% molar fraction)*
Methane	16.0	1.299	518.23	4.4
Butane	58.1	1.091	143.0	1.5
Propane	44.1	1.126	188.6	2.2
Lupton Natural Gas	18.7	1.265	444.6	4.3

2.3 INLET CONDITIONS

Where there is a significant reduction in pressure from the stagnation conditions to the ambient pressure, the gas exits the pipe at the local speed of sound and the flow is described as ‘choked’. The initial structure of the jet contains a series of oblique and normal shock waves, the number of which depends on the pressure ratio. Further downstream, the jet equilibrates into a sonic stream and undergoes transition into a fully-developed region in which the radial variation of axial velocity is approximately Gaussian. This behaviour is shown schematically in Figure 1, where the subscript ‘0’ denotes the stagnation conditions, the subscript ‘1’ denotes the exit conditions and the subscript ‘2’ denotes the conditions at the sonic point.

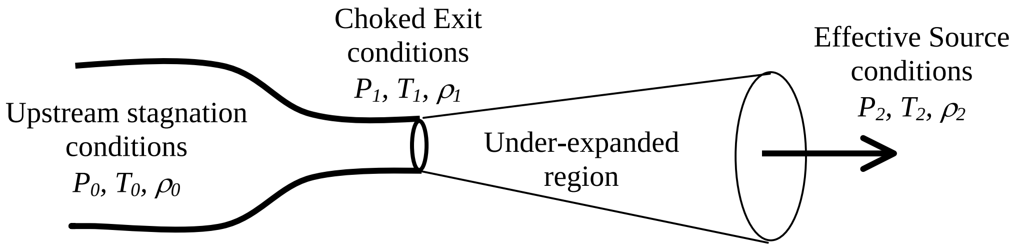

Figure 1 Schematic of jet development under choked flow conditions

Whether the flow is choked or not, the conditions at the exit can be computed from the isentropic flow equations:

$$\frac{T_0}{T_1} = 1 + \frac{\gamma - 1}{2} M_1^2 \tag{1}$$

$$\frac{P_0}{P_1} = \left(\frac{T_0}{T_1} \right)^{\gamma/(\gamma-1)} \tag{2}$$

$$\frac{\rho_0}{\rho_1} = \left(\frac{T_0}{T_1} \right)^{1/(\gamma-1)} \tag{3}$$

where M is the Mach number, P is the pressure, T is the temperature and γ is the specific heat ratio.

In the present study, all the cases with pressures of 2 barg or over are choked. Rather than try to resolve the complex shockwave structure using CFD in the early stages of the jet flow, the "resolved sonic source" approach (see Ivings *et al*. [5]) is adopted. This involves only modelling the flow downstream of the sonic point. Following Ewan & Moodie [3], it is assumed that there is no entrainment of air between the jet exit and the sonic point. Conditions at the sonic point are then calculated from:

$$\rho_1 A_1 V_1 = \rho_2 A_2 V_2 \tag{4}$$

where the velocities V_1 and V_2 can both be assumed to be the speed of sound (i.e. $V_1 = V_2$) and the cross-sectional area of the jet at the sonic point can be estimated from:

$$A_2 = \frac{A_1 P_1}{P_2} \tag{5}$$

where P_2 is the ambient pressure. A summary of the resulting inlet conditions for the CFD simulations is given in Tables 3a-d for methane, propane, butane and the Lupton natural gas mixture. In all cases, an ambient temperature of 10°C was assumed. For methane, inlet conditions were calculated using an assumed relative molecular mass and gas constant of 17.18 kg/kmol and 483.9 kJ/kg·K, respectively. These values were based on natural gas, to make the calculated inlet mass flow rate of methane closer to that one would expect for natural gas.

The IGE safety recommendations, SR/25, provide an alternative method of approximating mass flow rates for outdoors or freely ventilated spaces. The calculation of these flow rates is presented in Appendix B and values are shown in Tables 3a-d. The IGE/SR/25 values are around 20 – 30% lower than those predicted assuming an isentropic expansion. In the CFD simulations, the higher, more conservative, figures from the Ewan & Moodie calculation have been adopted.

Table 3a Methane inlet boundary conditions

Case	*Leak Conditions*		*CFD Model Boundary Conditions*				*IGE/SR/25*
	Pressure (barg)	*Area (mm^2)*	*Temp. (K)*	*Area (mm^2)*	*Velocity (m/s)*	*Mass Flux (kg/s)*	*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 3b Propane inlet boundary conditions

Case	*Leak Conditions*		*CFD Model Boundary Conditions*				*IGE/SR/25*
	Pressure (barg)	*Area (mm^2)*	*Temp. (K)*	*Area (mm^2)*	*Velocity (m/s)*	*Mass Flux (kg/s)*	*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

Table 3c Butane inlet boundary conditions

Case	*Leak Conditions*		*CFD Model Boundary Conditions*				*IGE/SR/25*
	Pressure (barg)	*Area (mm^2)*	*Temp. (K)*	*Area (mm^2)*	*Velocity (m/s)*	*Mass Flux (kg/s)*	*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 3d Lupton natural gas inlet boundary conditions

Case	*Leak Conditions*		*CFD Model Boundary Conditions*				*IGE/SR/25*
	Pressure (barg)	*Area (mm^2)*	*Temp. (K)*	*Area (mm^2)*	*Velocity (m/s)*	*Mass Flux (kg/s)*	*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

2.4 CFD SIMULATIONS

An example of the three-dimensional domain used in the CFD simulations is shown in Figure 2. In the majority of cases, the domain used was 2.0 metres long and 1.0 metre in diameter. For a few cases where the inlet mass flux was large (at 2.5 and 5.0 barg with an inlet area of 5.0 mm^2) the domain was extended to 3.5 metres. In some cases with smaller diameter inlets, shorter domains were also tested to create a more efficient computational grid. In all cases the gas cloud specified by the Vz criterion was accommodated easily within the domain boundaries.

Specified inlet velocity and temperature conditions, given in Tables 3a-d, were prescribed on a circular area comprising a number of cell faces (a minimum of 30) at one end of the cylindrical domain (see Figure 3). A coflow velocity inlet condition of air at 20 °C was imposed on the surrounding annular surface. Entrainment boundary conditions were applied on all remaining boundaries.

A non-uniform arrangement of cells was used to maximize the number of nodes near the inlet and along the anticipated path of the free jet (see Figure 4). The mesh was comprised of tetrahedral cells and the number of computational nodes was typically around 220,000. For four of the test cases, two simulations were run: with a standard mesh and with an increased number of nodes. The size of the gas clouds in the repeated runs was monitored to see how Vz changed as a function of the grid quality. In addition, the mass flux through the inlet was compared to the value given in the original isentropic expansion calculations[2]. For a stagnation pressure of 5 barg and hole area of 2.5 mm^2, increasing the number of nodes by a factor of four led to a change in the calculated Vz of only 1.2% and a decrease in the inlet mass flux error from 2.4% to 0.3%. The results were therefore considered adequately grid-independent. It should be noted, however, that these grid-refinement tests were not undertaken for every case considered.

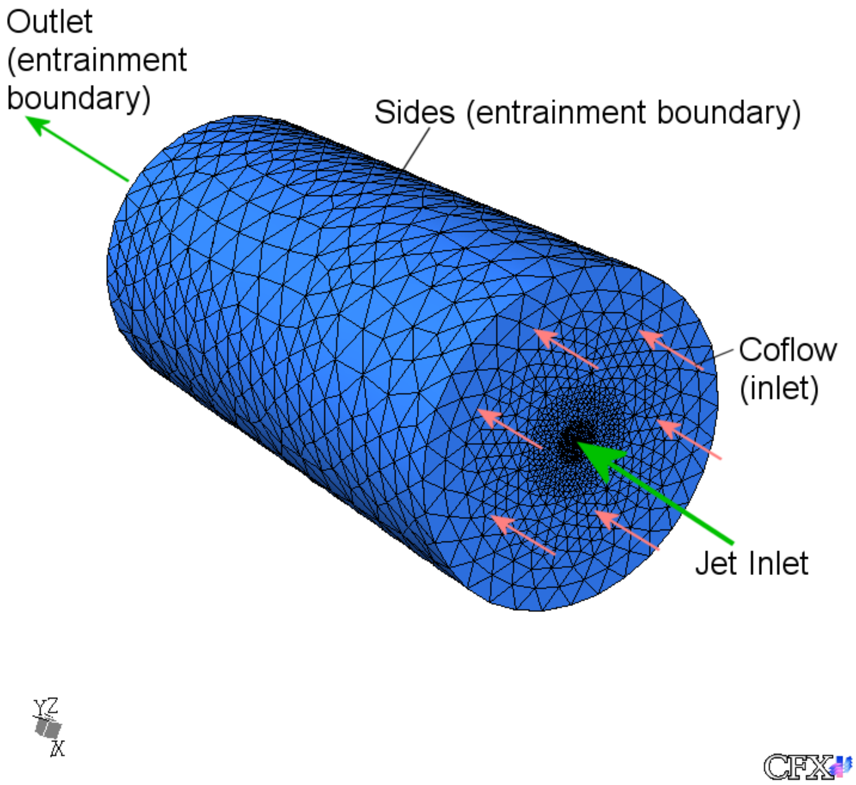

Figure 2 Three-dimensional view of the domain showing surface mesh and boundary conditions

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[2] Inlet conditions are specified in the CFD model by a velocity and a temperature. Differences between the mass flux calculated from the CFD model and that given by the isentropic expansion calculation are a consequence of an error in the surface area of the inlet, due to the approximation of the circular inlet face with triangular elements. By using a greater number of smaller triangles one should be able to approximate a circle more accurately and hence reduce any error in the mass flux value.

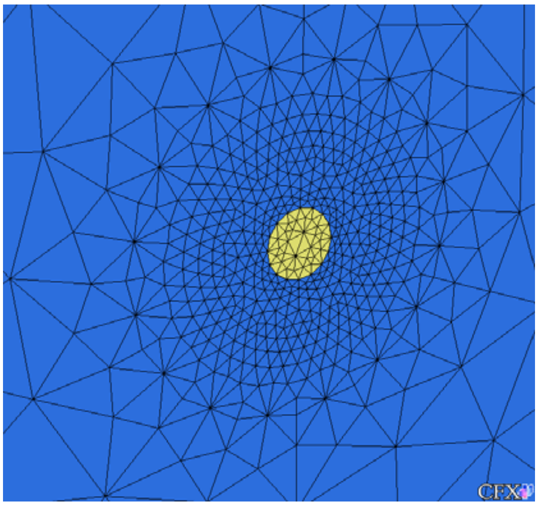

Figure 3 Close up view of the mesh around the jet inlet (shown in yellow)

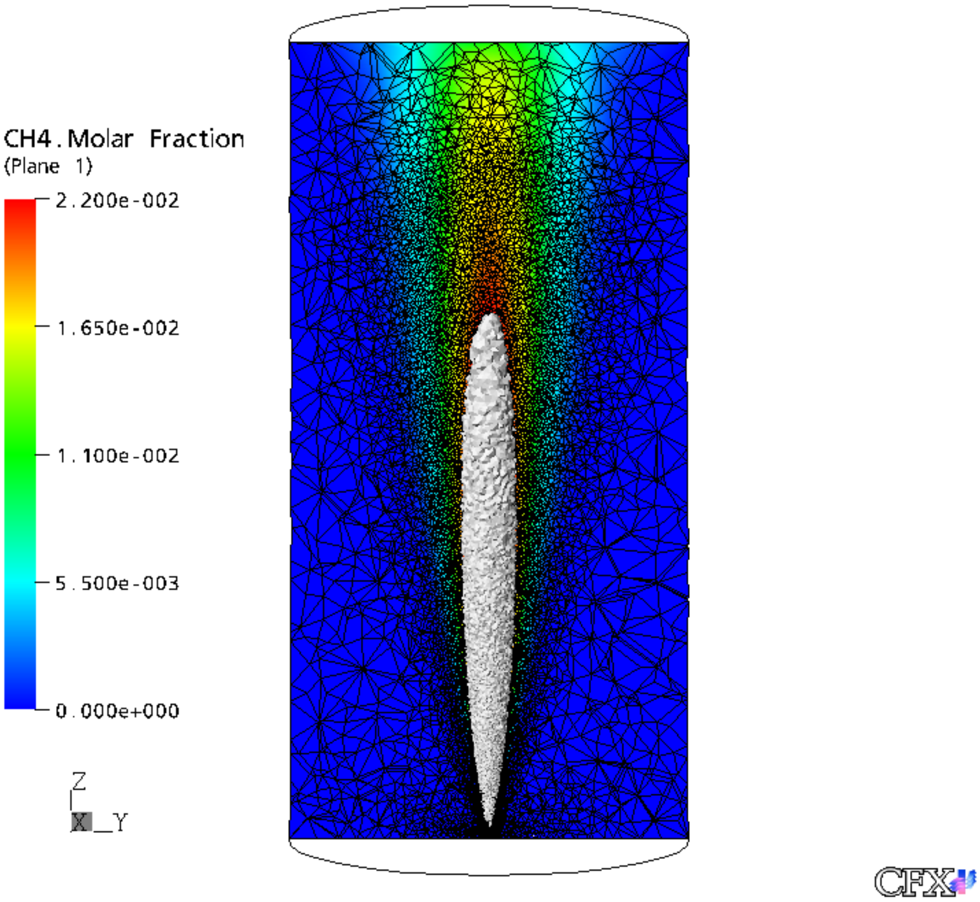

Figure 4 Two-dimensional slice through a typical simulation showing the computational mesh, contours of the methane molar fraction with the Vz volume highlighted in grey

3 RESULTS AND DISCUSSION

Tables 4a-d summarize the results of the test cases for methane, propane, butane and Lupton natural gas, respectively. Values in the columns marked 'CFD Vz' are the volume of the cloud in which the average gas concentration was 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, see Appendix C for details). The methane results (Table 4a) include two additional columns of data: the GaJet results and a column marked “CFD Iso-surface”. Both these sets of results calculate the gas cloud volume enclosed by a 50% LEL iso-surface, which one would expect to be smaller than that defined by the Vz criterion. These results show that the CFD model over-predicts the 50% LEL gas cloud volume by a factor of approximately 2.5 compared to the one-dimensional integral model GaJet. Although this difference is greater than in previous studies [5], the method that has been used here to calculate (‘post-process’) the gas cloud volume is conservative, i.e. it leads to larger gas clouds. This accounts for, at least some, of this discrepancy.

There are far more 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 was lower than the 'negligible extent' cutoff of 0.1 m^3 whereas the BS EN 60079-10:2003 values were between 100 and 3000 times larger than the CFD values. Comparing Tables 4a and 4d, the CFD Vz volumes calculated using methane were approximately 15 to 20% larger than those of natural gas.

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.

Previous simulations at higher pressures (30 barg) found that the gas cloud volume enclosed by a 50% LEL iso-surface was approximately 6 times smaller than that defined by the Vz criterion. In the present study, at pressures between 0.5 and 2.5 barg, the 50% LEL iso-surface volumes were around 2.7 to 3.0 times smaller than those defined by the Vz criterion.

All of the CFD results presented in Tables 4a-d were undertaken using a coflow velocity of 0.5 m/s. Table 5 presents the results for three methane cases in which the coflow velocity is set to 0.1, 0.5 and 1.0 m/s. The difference in the calculated Vz volume due to changes in the coflow velocity are relatively small. Typically, the Vz decreases by around 10% as the coflow velocity is decreased from 1.0 m/s to 0.1 m/s.

Table 4a Summary of methane results

Case	Leak Conditions		50% LEL Volumes (m^3)			
	Pressure (barg)	Area (mm^2)	GaJet	CFD Iso-surface	CFD Vz	BS EN 60079-10:2003 Vz
1	5.0	5.0	0.0140	0.0313	0.0936	12.3 – 61.7
2	5.0	2.5	0.00495	0.0107	0.0326	6.17 – 30.8
3	5.0	0.25	0.000156	0.00044	0.0012	0.62 – 3.08
4	2.5	5.0	0.00625	0.0154	0.0433	7.22 – 36.1
5	2.5	2.5	0.00221	0.0053	0.0148	3.60 – 18.0
6	2.5	0.25	0.00007	0.00019	0.0005	0.36 – 1.80
7	0.5	5.0	n/a	0.0053	0.0147	3.46 – 17.3
8	0.5	2.5	n/a	0.0019	0.0054	1.73 – 8.63
9	0.5	0.25	n/a	0.00007	0.0002	0.17 – 0.86

Table 4b 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 4c Summary of butane results

Case	Leak Conditions		50% LEL Volumes (m^3)	
	Pressure (barg)	Area (mm^2)	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 4d Summary of Lupton natural gas 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	0.0275	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

Table 5 Effects of coflow 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

4 CONCLUSIONS

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 are smaller than those defined as being of 'negligible extent', i.e. 0.1 m^3. These results suggest that there may be scope for modifying the BS EN 60079-10:2003 formulae and/or relaxation of the guidance on hazardous area classification for low pressure jets. The results in this study are relevant to open areas, where we have assumed a worst case scenario of a coflow velocity and a discharge coefficient of unity. Any further study on low pressure jets in enclosed spaces would need further CFD modelling to be carried out preferably supported by experimental data.

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APPENDIX A – NATURAL GAS COMPOSITION

The LEL for a gas mixture is calculated from Le Chatelier's law:

$$x_{LEL,mixture} = \frac{100}{\sum_{i=1}^{n} \frac{x_i}{x_{LEL,i}}}$$

where n is the number of species in the gas mixture, x_i is the molar or volume fraction and $x_{LEL,i}$ is the LEL of species "*i*". Molecules in the mixture which are inert (i.e. not flammable) are linked in arbitrary proportions with methane. The LEL of the combined (inert gas + methane) components, obtained from reference [7], and the remaining flammable components are then used in the above equation. Further details of the method can be found in [8]. A spreadsheet was designed to perform the calculation (shown below as Table A1). All of the molecules present in Lupton natural gas as specified in IGE/UP/9 [4] have been used to calculate its LEL. The resulting values are 4.33% and 2.17% for the 100% LEL and 50% LEL conditions.

Table A1 Calculation of Lupton natural gas LEL

Combustible Components			*Inert Components (mol %)*		*Net Molar*	*LEL*	*Ratio of*
Molecule	*Composition*	*Molar Fraction (mol %)*	*Nitrogen (N2)*	*Carbon Dioxide (CO2)*	*Fractions (mol %)*	*(vol %)*	*MF / LEL*
Methane	CH4	60.00	1.69	-	61.69	4.5	13.6
Methane	CH4	27.21	-	2.45	29.66	4.9	6.08
Ethane	C2H6	6.18	-	-	6.18	3.0	2.06
Propane	C3H8	1.74	-	-	1.74	2.2	0.791
Isobutane	C4H10	0.19	-	-	0.19	1.5	0.127
Pentane	C5H12	0.33	-	-	0.33	1.5	0.220
Hexane	C6H14	0.14	-	-	0.14	1.2	0.117
Heptane	C7H16	0.05	-	-	0.05	1.2	0.0417
Octane	C8H18	0.01	-	-	0.01	1.0	0.0100
Nonane	C9H20	0.003	-	-	0.003	0.8	0.0038
Benzene	C6H6	0.001	-	-	0.001	1.4	0.0007
Toluene	C7H8	0.003	-	-	0.003	1.1	0.0027
						Total	23.1
				Combined LEL (100%)			**4.33**
				Combined LEL (50%)			**2.17**

The specific heat ratio, γ, was calculated based on a mass-weighted average of each of the natural gas components. Table A2 shows how this was calculated. The mass fraction, y_i, for each component was calculated from:

$$y_i = \frac{M_i x_i}{\sum_{i=1}^{n} M_i x_i}$$

where x_i is the molar fraction and M_i the relative molecular mass. The combined mass-weighted specific heat ratio for Lupton natural gas, with a value of $\gamma_{LuptonNG} = 1.265$, was calculated from:

$$\gamma_{mixture} = \sum_{i=1}^{n} \gamma_i y_i$$

Values of the specific heat ratios for each of the molecules were taken from the National Institute of Standards & Technology (http://webbook.nist.gov) and from standard thermodynamics text books such as Van Wylen & Sonntag [6], making use of the following formulae:

$$c_p = c_v + R_u$$

$$k = \frac{c_p}{c_v}$$

where c_p and c_v are the constant pressure and constant volume specific heats, respectively, and R_u is the universal gas constant. The parameters c_p, c_v and R_u in the above two equations are in units of kJ/kmol·K and the universal gas constant is $R_u = 8.314$ kJ/kmol·K.

Table A2 Calculation of the mass-weighted specific heat ratio for Lupton natural gas

Molecule	*Composition*	*Specific Heat Ratio, γ*	*Molar Fraction (mol %)*	*Mass Fraction (%)*	*Mass-Weighted Specific Heat Ratio*
Carbon Dioxide	**CO2**	1.091	2.45	0.05777	0.06302
Nitrogen	**N2**	1.4	1.69	0.02536	0.03550
Methane	**CH4**	1.299	87.21	0.74773	0.97130
Ethane	**C2H6**	1.186	6.18	0.09935	0.11783
Propane	**C3H8**	1.126	1.74	0.04103	0.04620
Isobutane	**C4H10**	1.091	0.19	0.00591	0.00644
Pentane	**C5H12**	1.07	0.33	0.01273	0.01367
Hexane	**C6H14**	1.06	0.14	0.00645	0.00685
Heptane	**C7H16**	1.05	0.05	0.00268	0.00282
Octane	**C8H18**	1.044	0.01	0.00061	0.00064
Nonane	**C9H20**	1.04	0.003	0.00021	0.00021
Benzene	**C6H6**	1.11	0.001	0.00004	0.00005
Toluene	**C7H8**	1.09	0.003	0.00015	0.00016
		Total	99.997	1.000	**1.265**

The gas constant for Lupton natural gas, $R_{mixture}$, is calculated from:

$$R_{mixture} = \frac{R_u}{M_{mixture}}$$

where the relative molecular mass for the mixture, $M_{mixture}$ is given by:

$$M_{mixture} = \sum_{i=1}^{n} M_i x_i$$

APPENDIX B – IGE/SR/25 MASS FLUX CALCULATIONS

In section 5.2.3.2 of the IGE/SR/25 document, the following formulae are presented for estimating mass flowrates from orifices for outdoors or freely ventilated spaces:

For pressures ≥ 0.85 bar,

$$g = 675 C_d A M^{0.5} T^{-0.5} (P + 1.013)^{1.05}$$

and for pressures < 0.85 bar,

$$g = 1500 C_d A M^{0.5} T^{-0.5} P^{0.5}$$

where:

g = Mass flowrate (kg/s)
M = Relative molecular mass (kg/kmol)
T = Gas temperature upstream of orifice (K)
P = Gas pressure (barg)
C_d = Coefficient of discharge of orifice (assumed $C_d = 0.8$)
A = Cross-sectional area of orifice (m^2)

An example of the spreadsheet used to calculate the mass flux for methane is given below in Table B1.

Table B1 IGE/SR/25 mass flux calculation for methane

Case	***Coefficient of Discharge, C_d***	***Orifice Area, A (mm^2)***	***M (kg/kmol)***	***Gas Temperature Upstream, T (K)***	***Gas Pressure, P (bar)***	***Mass Flowrate g (kg/s)***
1	0.8	5	17.18	283.15	5	0.004374
2	0.8	2.5	17.18	283.15	5	0.002187
3	0.8	0.25	17.18	283.15	5	0.000219
4	0.8	5	17.18	283.15	2.5	0.002488
5	0.8	2.5	17.18	283.15	2.5	0.001244
6	0.8	0.25	17.18	283.15	2.5	0.000124
7	0.8	5	17.18	283.15	0.5	0.001045
8	0.8	2.5	17.18	283.15	0.5	0.000523
9	0.8	0.25	17.18	283.15	0.5	0.000052

N.B. The relative molecular mass, *M*, used here is the value assumed for natural gas ($M = 17.18$ kg/kmol) rather than that of methane ($M = 16.04$ kg/kmol). For the reasoning behind this choice, see Section 2.3.

APPENDIX C – BS EN 60079-10:2003 ESTIMATION OF VZ

Section B.4.2 of the British Standard BS EN 60079-10:2003 on “Electrical apparatus for explosive gas atmospheres” presents the following formulae to be used to estimate the hypothetical volume, Vz:

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

where:

$(dV/dt)_{\min}$ = Minimum volumetric flowrate of fresh air (m^3/s)
$(dG/dt)_{\max}$ = Maximum release rate at source (kg/s)
LEL_m = Lower explosive limit (kg/m^3)
k = Safety factor (k = 0.5 for secondary grades of release)
T = Ambient temperature (K)

The mass-based LEL_m is calculated from:

$$LEL_m = 0.416 \times 10^{-3} \times M \times LEL_v$$

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 with a 0.5 m/s wind speed, the air exchange rate works out as 0.03 air-changes per second. Using this value, the Vz volume is calculated from:

$$Vz = \frac{f(dV/dt)_{\min}}{0.03}$$

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

The above equations have been coded into a series of spreadsheets for methane, butane, propane and Lupton natural gas, which are presented below in Tables C1 – C4.

Table C1 Vz Calculation for methane

Case	*LEL (vol %)*	*M (kg/kmol)*	*LEL (kg/m^3)*	*Release Rate (g/s)*	*Safety Factor, k*	*Ambient Temp. (K)*	$(dV/dt)_{\min}$ *(m^3/s)*	*Volume, Vz (m^3) (f = 1)*	*(f = 5)*
1	4.4	16	0.0293	5.42	0.5	293	0.370	12.34	61.69
2	4.4	16	0.0293	2.71	0.5	293	0.185	6.17	30.84
3	4.4	16	0.0293	0.271	0.5	293	0.019	0.62	3.08
4	4.4	16	0.0293	3.17	0.5	293	0.216	7.22	36.08
5	4.4	16	0.0293	1.58	0.5	293	0.108	3.60	17.98
6	4.4	16	0.0293	0.158	0.5	293	0.011	0.36	1.80
7	4.4	16	0.0293	1.52	0.5	293	0.104	3.46	17.30
8	4.4	16	0.0293	0.758	0.5	293	0.052	1.73	8.63
9	4.4	16	0.0293	0.0758	0.5	293	0.005	0.17	0.86

Table C2 Vz Calculation for propane

Case	*LEL (vol %)*	*M (kg/kmol)*	*LEL (kg/m^3)*	*Release Rate (g/s)*	*Safety Factor, k*	*Ambient Temp. (K)*	$(dV/dt)_{\min}$ *(m^3/s)*	*Volume, Vz (m^3) (f = 1)*	*(f = 5)*
1	2.2	44	0.0403	4.12	0.5	293	0.205	6.82	34.12
2	2.2	44	0.0403	0.41	0.5	293	0.020	0.68	3.41

Table C3 Vz Calculation for butane

Case	*LEL (vol %)*	*M (kg/kmol)*	*LEL (kg/m^3)*	*Release Rate (g/s)*	*Safety Factor, k*	*Ambient Temp. (K)*	$(dV/dt)_{\min}$ *(m^3/s)*	*Volume, Vz (m^3) (f = 1)*	*(f = 5)*
1	1.5	58	0.0362	2.34	0.5	293	0.130	4.32	21.59
2	1.5	58	0.0362	0.23	0.5	293	0.013	0.43	2.16

Table C4 Vz Calculation for Lupton natural gas

Case	*LEL (vol %)*	*M (kg/kmol)*	*LEL (kg/m^3)*	*Release Rate (g/s)*	*Safety Factor , k*	*Ambient Temp., K*	$(dV/dt)_{\min}$ *(m^3/s)*	*Volume, Vz (m^3) (f = 1)*	*(f = 5)*
1	4.33	18.7	0.0337	2.80	0.5	293	0.166	5.54	27.71
2	4.33	18.7	0.0337	0.28	0.5	293	0.017	0.55	2.77
3	4.33	18.7	0.0337	1.64	0.5	293	0.097	3.25	16.23