METHODS OF PREDICTING THE DISPERSAL OF NATURAL GAS RELEASES IN VENTILATED DUCTS

P.S. Cumber and R.P. Cleaver

British Gas plc, Research & Technology, Gas Research Centre, Ashby Road, Loughborough, Leicestershire LE11 3QU

In this paper, a combination of small-scale physical modelling, full-scale experiments, simple mathematical models and a computational fluid dynamic (CFD) model have been used to investigate the flow produced by a high pressure leak of natural gas in a duct. From these analyses a simple mathematical model has been developed for predicting the bulk gas concentration and validated. The accuracy of the model suggests that it can be used to supplement existing guidelines on the minimum vent area and frequency of vents necessary to maintain a safe environment.

Key Words: Ducts, high pressure natural gas releases, dispersion, explosion, ventilation, mitigation, mathematical modelling, computational fluid dynamic modelling.

BACKGROUND

On industrial sites, pipework carrying natural gas is often sited within underground ducts. This may be to protect the pipework from possible accidental interference damage or to improve access within the site. A consequence of enclosing the pipework within a duct is that it is necessary to consider the consequences of a leak from the pipe into the duct.

The primary concern from the safety perspective is the possible explosion hazard following the accumulation of a gas-air mixture within the duct due to a leak. Whilst it is possible to mitigate the consequences of explosions in enclosures using pressure relief panels, a safer and cheaper alternative is to have sufficient vents to prevent the gas concentration reaching the lower flammability limit in the first place. However, in order to achieve this, it is necessary to be able to define the frequency and area of vents required to prevent gas build up to dangerous levels within the duct.

Experimental work was carried out by Barnett (1) to address this issue. The latter author carried out experiments at small-scale, and used standard scaling arguments to simulate natural gas releases in air with brine into a water-filled duct. Barnett also postulated a simple mathematical model to predict the dispersal of the gas in the duct. This model was derived from insight gained from the small-scale experimental work.

Subsequently, British Gas carried out a series of full-scale experiments, releasing natural gas at high pressure into horizontal ducts. Cumber et al(2) showed how the model of Barnett may be adapted to predict high pressure natural gas releases, as well as the original small-scale experiments of Barnett. The purpose of this paper is to show how a computational fluid dynamic model may also be used to support the use of this earlier model and to gain further insight into the flow patterns produced in the large-scale experiments.

The practical significance of this work is highlighted by applications of the simple model. This work supports the use of existing guidelines on ventilation requirements for ducts.

PREVIOUS EXPERIMENTAL WORK

Small-scale physical modelling

In the small scale physical modelling study of Barnett (1), a 1/6th scale model of a typical duct was used. The gas leak was simulated by injecting a salt solution of an appropriate density, into a water filled duct. The salt solution density and release rate were specified to conserve the dimensionless jet length between the physical model and the full scale flow. The flow patterns in the duct were visualised by introducing a small amount of dye to the salt solution. In the small-scale physical model the parameters investigated were the leak orientation, leak flow rate, area of vents and frequency of vents.

Figure 1 is a schematic of the flow field obtained for a vertical release with high initial momentum into a duct in the case when the vents are remote from the release point. It shows the physical characteristics found in the small scale experiments. The nomenclature used is listed at the end of the paper.

The buoyant jet is driven predominantly by its initial momentum, spreading out horizontally on impingement on the roof of the duct. The jet entrainment velocities are sufficiently high to drive a circulation cell (region 1) near to the source. The centre of the circulation is approximately 1.5d from the source axis. The buoyancy of the jet is sufficient to inhibit the formation of a second circulation cell. Turbulent momentum transfer excites the fluid adjacent to the primary cell (region 2), entraining ambient fluid and releasing buoyant fluid to the two layer flow (region 3). The fluid released from region 2 then flows horizontally in a stable layer, in the top half of region 3, forming a head of buoyant fluid, ultimately flowing out of one or more vents in the surface of the duct. The thickness of the buoyant layer decreasing gradually due to shear stresses.

When there is a vent closer to the release point the situation is more complicated. A ventilation point within the primary *circulation zone allows fluid from the environment to be drawn in* due to the pressure drop associated with the circulating fluid. However, a ventilation point overlapping the primary cell and the excited region adjacent to it (region 2 in figure 1) allows ambient fluid to be drawn into the duct but can also vent buoyant fluid.

Full-scale experimental work

A detailed account of the full-scale experimental study can be found in Cumber et al (1993), a brief statement of the main features of the study are given below. The experimental rig consisted of a full-scale duct, typical of those used to protect gas pipelines. The duct height and width was 0.62m. The gas leaks were simulated using a jet of gas from a nozzle with a diameter of 0.59mm. A number of vent configurations were used in which the frequency and area of vents were varied. Other parameters varied were the pressure (from 7 to 70 bar) and the release orientation. The concentrations were measured using flame ionisation detectors located at a number of stations within the duct. These were arranged in vertical columns in order that the height of the buoyant layer and the bulk concentration could be determined.

SIMPLE MATHEMATICAL MODEL

Full details of the derivation of the original mathematical model for the flow are given in Barnett (1). Cumber et al(2) showed how this model can be extended so as to be applied to high pressure natural gas releases. This was achieved by including the pseudo-source model of Birch et al(3) to deal with the initial expansion of a high pressure gas leak. A general treatment for the inflow of ambient fluid through vents near the source, was also included by incorporating the radial wall jet model described by Cleaver et al(4).

In brief, given the geometry of the duct, vent configuration and the volume flow rate of the leak, the model predicts the bulk concentration and velocity in the stratified region together with the buoyant layer depth and the number of vents required to vent the release.

Comparison of the model with the small-scale data

In this section comparisons of the model with the small-scale data of Barnett are presented. Figure 2 shows the variation of outflow velocity u_2 with the source flow rate Q_0. Figure 3 shows the variation of reduced gravity,

$$g'_2 = ((\rho_a - \rho_2)/\rho_a)\, g, \qquad (1)$$

in the buoyant layer with Q_0. Following Barnett the data is plotted in a way to demonstrate the power law dependencies expected on theoretical grounds. The predicted velocity and reduced gravity are in good agreement with the small-scale data.

Figure 4 is a comparison of the thickness of the buoyant layer after the first vent $h_2(1)$ with vent area. It should be noted that the graph is made dimensionless using the duct height and the area required to totally vent the release. The curve defined by the solution of the model equations is in good agreement with the experimental data. The overall capability of the model in predicting the small-scale data is good.

Comparison of model with field scale data

Cumber et al(2) showed how the model could be applied and compared with the full-scale data obtained by British Gas. Figure 5 shows a comparison of predictions of the mathematical model and experimental bulk concentration data for all of the tests, both vertical and non-vertical gas leaks. In over 80% of simulations the model prediction is within 30% of the observed values.

The error distribution of the predictions for concentration in the buoyant layer can be further analysed to derive confidence levels for the relative difference between the predicted value and the observed value. The error sample had a mean of $x_e = 17\%$ and a standard deviation of $\sigma_e = 11\%$. From these statistical parameters a normalised independent variable for the cumulative frequency of the error distribution is defined by

$$z_e = \frac{\xi_e - x_e}{\sigma_e} \tag{2}$$

Considering the intervals $[z_-, z_+]$ $z_\pm = \pm 0.67, \pm 1.15, \pm 1.96$ of the independent variable z_e, the proportion of the error sample in these intervals are 51%, 76%, and 89% respectively. This compares with 50%, 75% and 95% respectively for a normal distribution for the same intervals, Owen and Jones (5). Therefore the error sample is well approximated by a normal distribution. Assuming that the error sample is normally distributed, then with 95% confidence, the relative error satisfies the inequality,

$$100 \left| \frac{c_{exp} - c_{pred}}{c_{exp}} \right| \leq x_e + 1.96\ \sigma_e \tag{3}$$

Which can be used to derive a 95% confidence interval for the actual gas concentration from the predicted gas concentration.

CFD MODELLING

In the main the small-scale experiments agree with the field-scale experiments; however, in some aspects of the flow they differ. One example is that the field-scale data exhibits a dependency on the leak flow rate and the extent of the mixed recirculation zone, which is not present in the small-scale study. The gas concentration within the zones does, however, agree. It is attractive to consider some other independent method whereby the significance of these differences can be assessed. Modelling of the flow field using a computational fluid dynamics code offers one such alternative.

CFD is a fundamentally based modelling technique requiring a different set of modelling assumptions, such as the use of turbulence models to account for the interaction of the mean and fluctuating components of the flow, compared to more application orientated assumptions used in integral models. The fundamental basis of CFD makes it a highly flexible technique that has been applied successfully to a number of situations where a primary objective is the maintenance of a safe environment, examples being venting and flaring operations, Askari et al(6); Fairweather et al(7) and dense gas dispersion, Riou (8). Another advantage of CFD is the detailed information provided throughout the domain, allowing visualisation of the flow, giving insight in this case, into the mixing processes. The cost of this generality is the large computational resource required to run CFD codes. This prohibits their routine use by safety engineers with todays computer technology, restricting their role to one of support for the development of integral models or the analysis of complex flow regimes, an example being that described by Pericleous et al(9).

Governing Equations

A detailed statement of the mathematical basis of the model can be found in Jones and Whitelaw (10). The high Reynolds number form of the fluid flow equations expressing the conservation of mass, momentum and a conserved scalar (mixture fraction) has been used in this study. The turbulent momentum and scalar fluxes that appear in these equations were approximated using the standard k-ε turbulence model of Jones and Launder (11). Two further transport equations are solved for the turbulent kinetic energy and its dissipation rate. The transport equations describing the fluid motion for a steady flow all take the form,

$$\frac{\partial}{\partial x_i}(\rho U_i \phi) - \frac{\partial}{\partial x_i}\left(\frac{\mu_t}{\sigma_t}\frac{\partial \phi}{\partial x_i}\right) = S_\phi, \qquad (4)$$

where ϕ is a generic variable which represents the three Cartesian mean velocity components (U_i), mixture fraction, turbulence kinetic energy, and the dissipation rate of turbulence kinetic energy. The term S_ϕ is a source or sink term describing, for example, the buoyancy force in the vertical direction.

Computational Procedure and Boundary Conditions

The system of transport equations was integrated by superimposing a computational mesh over the physical domain and applying a second order finite volume method. This transformed the system of differential equations into an algebraic nonlinear system which was solved using a pressure correction algorithm, see for example Patankar and Spalding (12).

One difficulty of applying a CFD code to the scenario of a high pressure leak into a duct is the wide range of physical scales between the shock-containing underexpanded free jet downstream of the leak and the stratified region remote from the leak. As our interest was in predicting the gas concentration remote from the leak, an integral model for jet dispersion, Caulfield et al(13) was used to predict concentration and velocity decay in the underexpanded jet. At 0.1m downstream of the leak where the flow is incompressible (Ma=0.2) the integral model's predictions were used as boundary conditions for the CFD model. This introduced an error in the near field of the leak, but the flow remote from the point of release was unaffected.

As the computational cost of applying CFD techniques to 3 dimensional flows can be large our objective was modest; that was to predict the flow qualitatively, for only two scenarios.
The two scenarios differed in their ventilation configuration; in the first the vents were remote from the mixing region, whereas in the second there were vents close to the source. In each case the duct had dimensions 0.6mx0.6m. The gas leak had a diameter of 0.59mm and a stagnation pressure of 70bar. The leak was located at the base of the duct on the centre-plane. For the second case, the vents were located symmetrically either side of the leak with each having an area of $0.25m^2$. The distance between the vents was 1.3m. Specifying the leak and vent location thus, there were two planes of symmetry, reducing the computational domain to a quarter that of the physical domain, the computational domain being 4.mx 0.3mx 0.6m. At the plane x=4.m a fixed pressure boundary was imposed. At the perimeter of the duct fully turbulent local equilibrium wall law profiles were imposed as boundary conditions. For the second case the computational domain was extended above the duct to z=1.2m and the pressure fixed. By carrying out a sensitivity study, the flow was found to be insensitive to the location of the fixed pressure boundaries.

The grids used consisted of 68x18x30 and 68x18x40 control volumes, for the two cases, without and with vents near the leak respectively. The grids were nonuniform, with a fine grid spacing specified near the leak, and the grid geometrically expanding in all three co-ordinate directions. The geometric expansion rate was approximately 5% within the duct. Figure 6 shows the grid used for the second case. The grid resolution for the first case, where the vents were remote from the leak, was comparable to the grid shown in figure 6. A further simulation with 53x16x24 control volumes for the first case reproduced the same features of the flow as the fine grid simulation, indicating the predicted flow was qualitatively insensitive to further grid refinement. However, quantitatively the flow was not grid-independent.

Analysis of Predictions

Figure 7a and b shows the predicted gas concentration field on the plane y=0 for the two cases simulated. Comparing the two simulations, for the case with vents remote from the leak the flammable zone extends from x=1m to 3m approximately. However, for the vented case, the flammable zone is restricted to a region near the leak, with the gas concentration in the majority of the duct not exceeding 3%.

In the region x=0m to 1.5m for the first case, the flow has a strong recirculation in both the x-z and y-z planes, whereas the recirculation in the second case is restricted to the x-z plane. The recirculation in the y-z plane is inhibited in the second case by the inflow of ambient air through the vent adjacent to the leak. An interesting feature of the predicted flows is a floor jet in the region x=0 to 1.5m with axis y=0m. The floor jet is the product of the leak being located on the centre line y=0m and the flow being attached to the duct perimeter in the recirculation zone. The floor jet is present in both simulations, being strongest in the first case as the inflow through the vent adjacent to the leak in the second case disrupts the jet. The floor jet is responsible for the shape of the 15% contour in figure 7a. The floor jet was unobserved in the sm some evidence for it being present in the field scale experimental study in that significant gas concentrations were observed at the base of the duct for the higher pressure releases.

The predicted flow for the second case is in agreement with the small scale experiments, with the recirculation near the leak inducing ambient fluid to flow into the duct through the vent adjacent to the leak and buoyant fluid to disperse through the vent remote from the leak, (see figure 7b). Comparing the predicted flow with the large-scale experiments, qualitatively they are similar in that the nonstratified region extends to over 4.m from the leak. Quantitatively the CFD model underpredicts the measured gas concentration by 30%. The grid sensitivity studies mentioned above suggest that this discrepancy would be reduced by further grid refinement.

Although the CFD predictions confirm the dependency between the leak flow rate and the extent of the mixed recirculation zone observed in the field scale experiments, the derivation of the simpler model is still valid. The size of the well mixed region does not affect the steady state gas concentration, only the transient phase of gas build up in the duct, Barnett (1).

DISCUSSION

It is of interest to show how the simple model could be used in practice to calculate the frequency and minimum vent area required to maintain a safe environment in a duct, given a maximum 'credible' leak and a safe concentration. Suppose that the maximum 'credible' leak can be taken to have a diameter of 0.59mm and a stagnation pressure of 70bar. Suppose also that it is required that with 95% confidence the concentration remote from the leak does not exceed 5%. Applying equation (3) this requires that the predicted concentration does not exceed 3.1%.

Table 1 shows the predicted gas concentration for a number of vent spacings, vent areas and two square ducts, d=0.6m and d=0.8m.

From Table 1, for the leak specified, the bulk concentration is less than or equal to 3.1%, for a duct height d=0.6m, a vent spacing $\Delta V=d$ and vent area $A_i = 0.3m^2$. If the duct height is increased to d=0.8m, a safe environment is maintained with a vent spacing of $\Delta V=3d$ and $A_i=0.4m^2$.

CONCLUSION

In this paper it has been shown how a combination of small-scale physical modelling, full-scale experiments, simple mathematical models and a computational fluid dynamic model may all be used to investigate the flow produced by a high pressure leak of natural gas in a duct. In particular, it has been shown how the flow fiel that is produced can be predicted by both physical modelling and computational fluid dynamic models. Given this understanding, a satisfactory simple mathematical model can be developed, taking into account the effects of vents both near to the release and remote from it.

The simpler model has been applied to realistic, high pressur releases. The model has been compared to both small-scale and field-scale releases. Though the model has been derived primarily for vertical releases of gas, predictions of bulk concentration fo all leak orientations are satisfactory, (see figure 5).

The error sample of the validation of the model against the field-scale experiments has been analysed statistically to derive confidence levels for the predicted bulk concentration in ducts. The capacity to provide concentrations with associated confidence levels makes this model a useful tool that can be used to support the existing guidelines on the minimum vent area and frequency necessary to maintain a safe environment.

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The CFD calculations reported in this paper were made using a modified version of the Mantis Numerics Ltd. code, COBRA.

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NOTATION

A_i Area of a vent

A_1	Area of a vent in the stratified zone
c_{exp}	Measured bulk concentration
c_{pred}	Predicted bulk concentration
d	Depth of duct
g	Acceleration due to gravity
g'_2	Reduced gravity of buoyant layer
h_2	Thickness of buoyant outflowing layer
$h_2(1)$	Thickness of buoyant layer after first vent
k_1	Constant value 0.5
Ma	Local Mach number
$Q_{0,2}$	Flow rate of source and buoyant layer
S_ϕ	Source term in transport equation
$u_{1,2}$	Horizontal velocity of buoyant and ambient layers
U_i	Velocity components
x	Horizontal co-ordinate
x_e	Mean relative error
x_i	General Cartesian co-ordinate
w	Width of duct
z	Vertical co-ordinate
z_e	Normalised variable in error analysis
Δv	Distance between vents
μ_t	Turbulent viscosity
$\rho_{0,2,a}$	Density of source, buoyant layer and environment
ϕ	Generic fluid variable
σ_e	Standard deviation of relative error distribution
σ_t	Turbulent Prandtl number
ξ_e	Relative error of bulk concentration prediction

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TABLE 1- Simple model predictions of bulk gas concentration (Vol. %)

Vent Spacing (m)	Duct Height (m)	Vent Area (m2)				
		0.	0.1	0.2	0.3	0.4
0.6	0.6	6.5	4.5	3.4	2.7	-
1.8	0.6	6.5	5.6	4.9	4.3	-
2.4	0.8	4.0	3.8	3.5	3.3	3.1

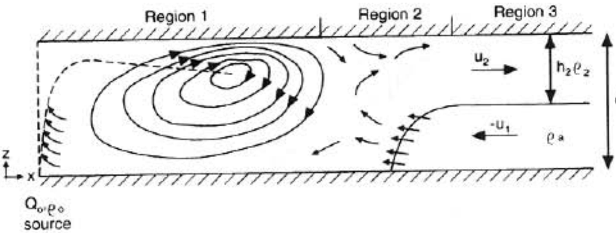


Figure 1- A schematic diagram of the flow produced by a buoyant source with high momentum.

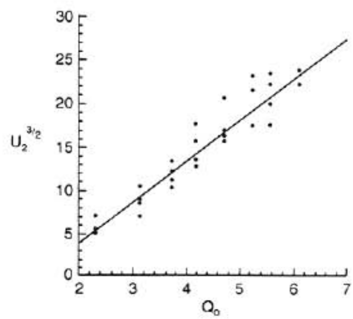


Figure 2- The variation of outflow velocity u_2 with source flow rate Q_0 (—— theory, o expt.)

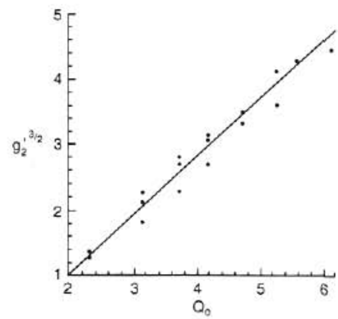


Figure 3- The variation of g'_2 with Q_0 (—— theory, o expt.)

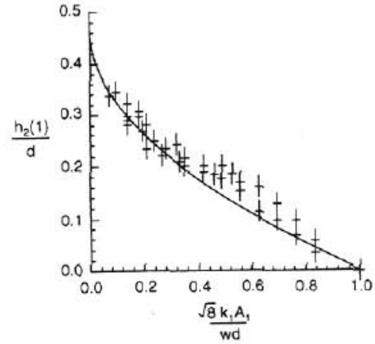


Figure 4- The variation of secondary outflow height with vent area. (—— theory, + expt.)

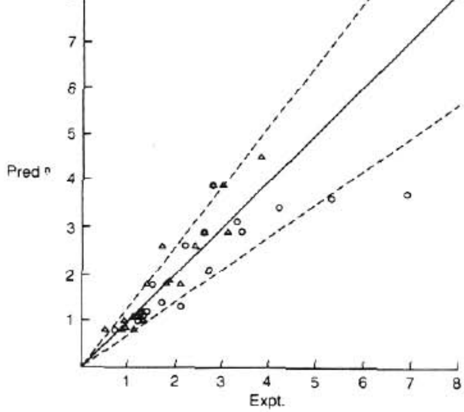
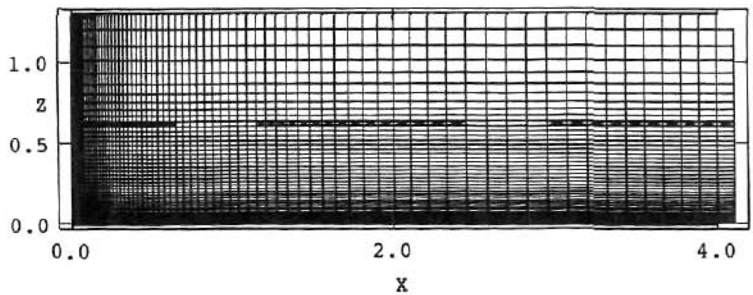


Figure 5- Comparison between model prediction and large scale bulk concentration data (- - - 30% relative difference), (o Vertical releases, Δ Non-vertical releases).

a) x-z grid



b) y-z grid

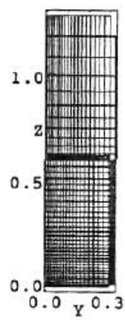
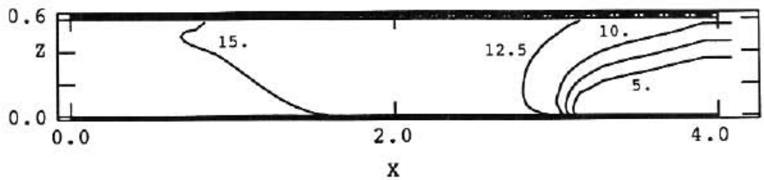


Figure 6- Grid used for simulating gas build up in a duct with vents adjacent to the source.

a) Vents remote from leak



b) Vents adjacent to leak

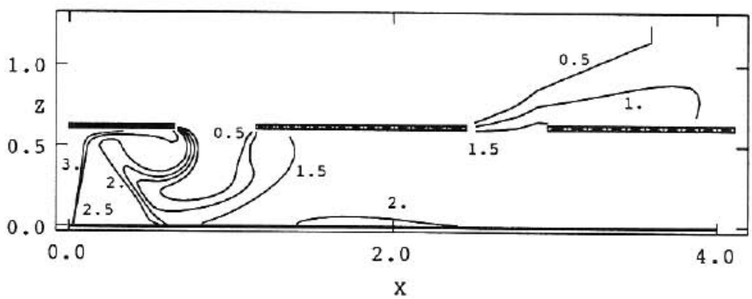


Figure 7- Predicted gas concentration (Vol. %) on the centreplane.