Modelling Releases of Carbon Dioxide from Buried Pipelines

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A large Research and Development programme has been initiated by National Grid to determine the feasibility of transporting carbon dioxide (CO_2) by pipeline. As part of this programme, National Grid commissioned a series of experimental studies to investigate the behaviour of releases of CO_2 mixtures in the gaseous and the liquid (or dense) phase. A programme of theoretical studies has been carried out in parallel with the experiments at University College London (UCL), the Universities of Leeds, Kingston University, the University of Warwick and Newcastle University. These studies have resulted in the further development of 'state of the art', advanced predictive models for various aspects of the flow behaviour. The information from both the experimental and theoretical studies has been analysed in order to help develop a simpler, more pragmatic package of models to predict the risks from possible releases from a high pressure, below ground pipeline transporting CO_2 in the data has been used to help develop the models.

In particular, correlations that predict the velocity and dilution of the flow emerging from a crater following a puncture or rupture of a buried pipeline are presented and it is shown how these initial conditions are important in determining whether the emerging plume of CO_2 stalls and falls back on itself to form a 'blanket' around the crater. Appropriate starting conditions for predicting the dispersion of the plume at greater distances from the crater are discussed and it is shown how these can be used to help predict the subsequent plume behaviour. The effect of concentration fluctuations on the dosage calculated from the experimental data is investigated and a way in which this can be included in the modelling is proposed.

The application of these models to risk assessment is discussed and some of the findings from this work are given.

Keywords: CO₂, CCS, pipelines, source model for pipeline releases, QRA

Introduction

In support of its plans to take a leading role in Carbon Capture and Storage (CCS) projects, National Grid initiated the COOLTRANS research programme to address gaps in knowledge on the safe design and operation of onshore pipelines for transporting anthropogenic, high pressure, gaseous and dense phase carbon dioxide (CO₂) from industrial emitters to storage. This programme was funded by National Grid with financial assistance from the European Union and consisted of a mixture of experimental and theoretical work carried out by a range of university and industrial partners, see Cooper et al (2011).

As part of this programme DNV GL (formerly GL Noble Denton) developed a number of correlations to predict the size of the crater formed following either a puncture or rupture of a below ground pipeline transporting CO₂. The correlations were based on observations of the full scale puncture and scaled rupture experiments, carried out by DNV GL as part of the COOLTRANS research programme (see Allason et al (2012) for an overview of the experiments). Further modelling work was aided by the parallel programme of computational fluid dynamics (CFD) modelling being undertaken as part of COOLTRANS by University College London (UCL), the University of Leeds, Kingston University and the University of Warwick. Examples of this work are available in the publications of Brown et al (2013), Wareing et al (2013) and Wen et al (2013). The more detailed, fundamental modelling studies undertaken by these universities provided insight into the reasons for the observed behaviour and valuable predicted information used in formulating the simpler models.

It was decided that a further model should be developed, using a simplified description of the flow emerging from the crater to define the initial conditions of any plume that is formed at ground level that disperses in the wind. This model was used as part of a risk assessment approach containing a range of the more practical type of models, such as correlations or simpler integral or similarity models.

The purpose of this paper is to provide the details of the above simpler models and to describe how the models could be used to assess a dispersing dense phase CO_2 release produced following a failure of a below ground pipeline.

Overview of the Models

The approach in developing the models was to apply a series of simplifications to break what is a highly complex, transient multi-phase fluid flow problem into a number of tractable, discrete stages. Unlike the CFD modelling approach, no attempt is made to solve the governing set of fluid flow and thermodynamic relationships, but a simplified 'model' of the flow is taken at each of these hypothetical stages, as follows:

- **Outflow.** A method of calculating the outflow from a puncture or rupture in a buried pipeline is provided in this work using the model based on the original work of Morrow et al.(1983), updated to take account of the thermodynamic properties of CO₂ and to consider a wider range of boundary conditions. The way in which the original model was implemented was described in outline by Cleaver et al (2003)]. The updated model has been compared with the predictions provided by UCL, using a state of the art, sophisticated CFD model, Brown et al (2013). As would be expected, the simple model is unable to duplicate all of the flow features predicted by the more sophisticated model, but its predictions for the rate of outflow are not significantly different in the cases examined.
- **Crater formation.** The size and shape of the crater produced by the release is predicted, as it influences the nature of the outflow to the atmosphere. The correlations developed for this purpose were presented by Cleaver et al. (2013) at the Fourth International Forum on the Transportation of CO₂ by Pipeline, held in Newcastle, although details were not published at that time. The equations are given here in Appendix A, for reference.
- Flow within and from the crater. The outflow from the crater, taking into account any entrainment of air, is required to calculate the subsequent behaviour. The model that has been produced predicts an equivalent flow out of the crater at atmospheric pressure, prior to any significant re-entrainment of CO₂ caused by stalling of the cloud above the source (see later). This was developed specifically as part of the COOLTRANS research programme using results of the calculations from UCL on the outflow and the University of Leeds in modelling the flow from the crater prior to any re-entrainment. This model is described in Appendix B.
- **Ground level source.** This model is required to predict the initial conditions of any ground level cloud produced by the release, taking into account the possibility that the flow might stall above the crater. This model is needed to link the crater outflow model to the ground level dispersion model. This is based on an assessment of the experimental results from the COOLTRANS programme.
- **Ground level dispersion.** A method of calculating the dispersion of any ground level cloud in the atmosphere is provided by using an existing dense gas dispersion model see Cleaver et al (1995). There is a requirement to predict the dose that any person would receive at a fixed location from the turbulent fluctuating cloud that is produced. The way in which this has been implemented is described in Appendix C. This model enables the vulnerability of people exposed to the varying concentration of CO₂ to be evaluated and provides a link between the consequence and risk models.

The way in which the various stages are assumed to be linked is shown schematically in Figure 1 below.



Figure 1. Stages in defining an effective source for a ground level cloud: 1. Outlow from the pipe; 2. Flow through the expanded or pseudo source; 3. Flow from out of the crater of a defined size and 4. The ground level dispersion source.

The flow in Stage 1 is defined by the outflow model. The pressure is generally above atmospheric at the pipe exit for a choked, two-phase flow. A conventional pseudo source model, Birch et al (1987), is used to define an equivalent set of conditions for the flow when it expands to atmospheric pressure, ignoring any air entrainment or interaction with the crater sides but including an enthalpy conservation relationship to take account of the formation of solid CO₂ in defining the equivalent conditions at atmospheric pressure. Note that this is a hypothetical set of source conditions that preserve the momentum, mass and enthalpy flux from Stage 1, assuming a uniform flow through the circular source. It would take a detailed CFD model, such as that produced by the University of Leeds, Wareing et al (2013), to solve the equations for the flow and its interaction with the crater walls. This would define the shape, velocity and temperature distribution downstream of the Mach shock region where the flow actually relaxes to atmospheric pressure. The conditions from Stage 2 are used to define an equivalent 'crater exit' flow at Stage 3, where some air has been entrained into the emerging flow and the velocity has reduced due to interaction with the crater sides, bottom or the opposing plume from the opposite pipe end, if a full bore rupture has occurred. This model assumes that the dimensions of the crater that is formed by the release are known and assumes at this stage that there is no significant re-entrainment of CO_2 into the crater as a result of the plume stalling and returning to ground level around the crater formed by the release. Some evidence for the applicability of this approach was provided by Allason et al (2014), who compared the observed and predicted plume heights initially. This gives an indication of the uncertainty attached to the description of the flow at Stage 3. Details of the equations that are used in this model are provided in Appendix B.

Figure 1 above shows a likely case for a double ended rupture in the pipeline, with a fountain like flow above the crater falling back on itself to form a 'blanket' around the crater, with some upwind spread. The model for the source includes a correlation to predict if the blanket forms and defines initial conditions irrespective of whether the plume does form a 'blanket' around the source with some upwind spread of the cloud and is defined for both ruptures and punctures in a below ground pipe. An overview of this was provided in Allason et al (2014), who illustrated the different types of behaviour that were observed in the experiments by two snapshots from the video record of two particular puncture experiments carried out with the same size of release.

Source Type

The correlation that is used to define whether the flow from the crater falls back on itself to form a source blanket or behaves like a free plume (with minimal interaction) is based on the observed behaviour in National Grid's puncture and scaled rupture experiments and the $COSHER^1$ series of rupture experiments. In addition, the observations of the CO_2 venting experiments carried out by DNV GL on behalf of National Grid, see Allason et al (2014), were included to ensure that this correlation is based on as wide a range of initial flow conditions as possible. A judgement was made if the flow stalled above the crater to form a 'source blanket' and dimensionless variables were evaluated for each experiment to represent the forces of gravity and initial momentum in the flow and the momentum of the wind.

In this work, the source Richardson number is used to measure the ratio of the source buoyancy to the source momentum. The source buoyancy acts to cause the flow to return towards the ground, whereas the source momentum acts to direct the flows vertically upwards away from the ground. The source Richardson number gives an indication of which of these forces might dominate. This number, Ri_{Source} , is defined by

$$Ri_{Source} = \frac{D_{Crater} g'_{Crater}}{U_{Crater}^2}$$

where

 D_{Crater} is the bulk diameter of the flow out of the crater

 U_{Crater} is the bulk velocity of the flow out of the crater

and

 g'_{Crater} is the reduced gravity of the flow out of the crater.

The reduced gravity is defined by

$$g'_{Crater} = \frac{g(\rho_{Crater} - \rho_{Air})}{\rho_{Crater}}$$

where

g is the acceleration due to gravity

 ρ_{Crater} is the bulk density of the flow out of the crater

and

 ρ_{Air} is the density of the ambient air.

(1)

(2)

¹ The COSHER programme of scaled rupture experiments were carried out at the Spadeadam Test Site by DNV GL on behalf of a Joint Industry Project (JIP) led by what was formerly KEMA (now part of DNV GL). National Grid was a sponsor of the COSHER programme and so provided access to the data for modelling purposes.

flow away from the crater.

The wind to crater exit velocity ratio is used to measure the tendency of the wind to displace the flow sideways in a

downwind direction. This value is defined by the non-dimensional wind speed W_{ND} as:

where

 $W_{ND} = \frac{W_{10}}{U_{Crater}}$

 W_{10} is the wind speed at an elevation of 10 m.

The larger the velocity ratio, the more likely the plume is to have been displaced away from the crater when it eventually returns to ground. Conversely, the smaller the velocity ratio, the less likely the plume is to have been displaced away from the crater when it returns to ground.

A plot of the source Richardson number against the wind to crater exit velocity was produced and lines were drawn on the graph to separate those points that represent experiments that formed blankets from those that formed free (non-interacting) plumes. To calculate the variables in the above process, it is assumed that the air and the gaseous and condensed phase CO_2 are in equilibrium as the flow emerges from the crater. The equation for the critical value of the non-dimensional wind speed W_{NDCrit} as a function of Ri_{source} that separates the source blankets and free plumes is given by

$$W_{NDCrit} = \begin{cases} 0.08 \frac{Ri_{source}}{0.001} & Ri_{source} < 0.001\\ 0.08 \sqrt{\frac{Ri_{source}}{0.001}} & Ri_{source} \ge 0.001 \end{cases}$$
(4)

This was shown in Allason et al (2014).

The assessment above is used to determine whether releases behave as blankets or as freely dispersing plumes. In general, the concentrations, and hence the risk, predicted by the blanket model are greater than those predicted by the model for freely dispersing plumes. A cautious approach has been used, with all releases lying below the line being modelled as blankets, and only those lying more than half an order of magnitude above the line being modelled as freely dispersing plumes. To avoid discontinuities in the predictions of the model, releases that lie between these two cases are modelled by interpolating between the blanket and freely dispersing plume models. The equations that are used are as follows:

$W_{ND} < W_{NDCrit}$	Blanket	
$W_{NDCrit} \leq W_{ND} \leq \sqrt{10} W_{NDCrit}$	Borderline,	(5)
$\sqrt{10} W_{NDCrit} < W_{ND}$	Freely dispersing plume	

where the function W_{NDCrit} describes the equation of the bounding line defined in equation (4).

In the borderline region, weighting factors for jet and blanket behaviour, F_{let} and F_{Blanket}, are defined by

$$F_{Jet} = 2 \log_{10} \left(\frac{W_{ND}}{W_{NDCrit}} \right) \text{ and}$$

$$F_{Blanket} = 1 - F_{Jet} .$$
(6)

In the case of a freely dispersing plume, it is assumed that the plume returns to ground at some distance downwind of the crater to produce a downwind ground level plume but there is no enveloping blanket formed on the upwind side of the crater.

The slope of the line at the smaller source Richardson numbers is 1, as would be deduced using a simple argument based on the time of flight and horizontal distance travelled by a heavy particle thrown upward and assumed to be displaced sideways at the wind speed. The slope of the line at higher values of the source Richardson number is ¹/₂, expressing a balance between the buoyancy induced gravity spreading upwind once the cloud lands on the ground and the opposing wind speed that is independent of the source velocity. That is, even though the source buoyancy dominates over its initial momentum, the wind is sometimes capable of preventing a blanket from forming around the upwind parts of the crater, in higher wind speed conditions.

Initial Conditions for Ground Level Plume

In order to define the correlations for the dispersing ground source at Stage 4, the experimental results were examined firstly and a set of representative starting conditions were defined by judgement (using the video records from the experiments and the observed concentration records). In order to match these observations with the assumptions of the ground level dense

The larger the source Richardson number, the quicker the flow would be expected to stall and return to ground. Conversely, the smaller the source Richardson number, the more opportunity there is for the source momentum or the wind to carry the

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gas dispersion model, the source was defined in the form of a cross-wind 'box' of a specified aspect ratio of height to width and uniform concentration that moved downwind with the wind speed at a representative height. The dense gas dispersion model was used to predict the resulting decay of concentration downwind and the predicted maxima on each measurement arc, located at different distances downwind in the experiment, were compared with the observed values. As the definitions of the equivalent starting sources were subject to some judgement, the starting parameters were varied either side of the initial estimated values to see the sensitivity of the predictions to the variations. In general, this had a minimal impact over a credible range so a final set of values was selected for each case. These starting conditions were correlated as functions of the values at the crater exit (the Stage 3 source in Figure 1) to provide a general predictive approach.

The correlations depend on the Richardson number and the non-dimensional wind speed defined earlier. For convenience, some of the correlations can be expressed more conveniently in terms of an additional dimensionless number, the wind Richardson number, Ri_{Wind} defined below. This is not independent in that it depends on the original two non-dimensional quantities, the original Richardson number and the non-dimensional wind speed.

$$Ri_{Wind} = \frac{D_{Crater}g'_{Crater}}{W_{10}^2} = \frac{Ri_{Source}}{W_{ND}^2}$$
(7)

Some of the correlations depend on whether the source blanket is assumed to form. However, where a single correlation could be found that fitted all of the experimental observations, this was used.

The correlations that were produced are defined below.

For all releases

The mass concentration of the ground level source, C_{Ground}^{Mass} , is defined as a fraction of the mass concentration of the flow out of the crater by

$$C_{Ground}^{Mass} = Min\left(0.9, Max(0.2, Min(175 Ri_{Source}, 5 Ri_{Wind}))\right) C_{Crater}^{Mass}.$$
(8)

The cloud moves downwind initially at a representative wind speed, taken to be W_{10} , the wind speed at a height of 10 m above the ground.

For all releases forming blankets

The initial aspect ratio (ratio of half width to height) of the dispersion source is taken to be 30.

The dispersion source is placed at the crater centre.

The upwind spread, x_{Upwind} , is given as a multiple of the bulk diameter of the flow out of the crater, d_{Crater} , by

$$x_{Upwind} = 45 \sqrt{Max(0.01, Min(1, Ri_{Source}))} d_{Crater}.$$
(9)

For jet or plume like (non-interacting) flows

The plume is assumed to return to ground at a certain distance downwind (the offset distance) to form a ground level dispersion source. The initial aspect ratio (ratio of half width to height) of the dispersion source is taken to be 10.

The downwind offset of the dispersion source, x_{offset} , is given as a multiple of the bulk diameter of the crater source by

$$x_{Offset} = \frac{2}{\sqrt{Max(0.05,Min(0.75,W_{ND}))}} d_{Crater}$$
(10)

There is assumed to be no upwind spread in this case. (It should be noted that the models used to calculate the risks have separate sub-models to account for billowing and fluctuations in the flow emerging from the crater, and these will predict some risk upwind of the release.)

Borderline flows

In the borderline region where $W_{NDcrit}(Ri_{Source}) \leq W_{ND} \leq \sqrt{10}W_{NDCrit}(Ri_{Source})$ the initial aspect ratio, upwind spread and downwind offset of the ground-level dispersion source are calculated by interpolating between the separate values calculated for a blanket and a freely dispersing plume. The interpolation factors F_{Jet} and $F_{Blanket}$ are as defined in equation (6) above.

Dispersing Plume

The previous sections described a series of models that define the initial conditions of a ground level source. The subsequent dispersion of the ground level plume is modelled with a similarity type of dense gas dispersion model, see Cleaver et al (1995). This model uses a simplified approach to predicting the dispersion for different averaging times. The time scale of interest in assessing the highly toxic effects of CO_2 is taken to be 5 seconds, a timescale for significant exposure within the lungs (typically about 2 breaths). The way in which the averaging time influences the toxic dose calculated from the experimental measurements was referred to in Allason et al (2014), where examples were given that show the effect on the calculated dose. The dispersion model was selected in this work to use a short averaging time. That is, the dispersion model

predicts a 'snapshot' of the dispersing plume, corresponding to a short time average. The way in which these predictions are post-processed to give peak and mean concentration profiles across the width of the plume and to evaluate the toxic dose to take account of the fluctuations are described in Appendix C.

Comparison with Experimental Work

The performance of the above combination of models, when used on the experiments for which they were derived, was illustrated for three of the COOLTRANS rupture experiments in Allason et al (2014). The predictions were made assuming that the dispersion is taking place over flat, horizontal ground. Figure 2 below shows a summary of the comparison of the maximum peak concentration on each arc of sensors for 4 puncture experiments and 5 scaled rupture experiments from the same programme.



Figure 2. Comparison of predicted short-time averaged maximum concentration on each arc with observations for all of the punctures (red symbols) and scaled rupture experiments (blue symbols).

The comparison shows that the model performs satisfactorily in predicting the short-time averaged maximum value of the concentration observed on each arc, but tends to over-predict the observed values at each sensor for concentrations above about 4%. This means that all other things being equal, use of this dense gas dispersion model with the COOLTRANS source models will tend to over-predict the peak value of the concentration - that is, the combination will err on the side of caution.

Discussion

The outflow model used in making the predictions in this report has been compared previously with the predictions provided by UCL, using a state of the art, sophisticated CFD model. The basis of the simple model has been published previously by Cleaver et al (2003). It is unable to duplicate all of the flow features predicted by the more sophisticated model, but its predictions for the rate of outflow are not significantly different in the cases examined.

Models have been developed to predict the source conditions to use when evaluating the dispersion of any ground level cloud formed following an accidental release from a buried pipeline carrying dense phase CO_2 . Separate models are used to predict the size of the crater that forms, the flow out of the crater, and an equivalent ground level dispersion source. The computational results from the University of Leeds have been used directly in formulating some of the correlations for the crater source description and the experimental results have been used directly to help formulate the equivalent ground level dispersion source.

The predictions of the crater source and ground level dispersion source models, using the observed crater size as an input, have been compared to the experiments conducted. The resulting predictions of the short time averaged arc-wise maxima have been found to be in reasonable agreement with the experimental data from the punctures and scaled rupture

experiments. However, this is not a 'blind' test of the model, as the correlations have been based on these experiments. Nevertheless, it does suggest that if the ground level dispersion model can be provided with appropriate initial conditions, by whatever means, it is capable of predicting the observed maxima in a downwind direction.

The predictions of the dense gas dispersion model have been post-processed to predict mean, or longer time averaged concentrations, and to predict the mean and peak concentrations at each sensor location in the experiments. There is significantly more scatter in the prediction of these quantities and it is possible that the agreement could be improved significantly if a more theoretically based model could be produced relating peak to average values and the time variation of the concentration record. One of the significant achievements of the COOLTRANS research programme is that there is sufficient data available to allow this to be attempted at some future date. For the present though, the predictions of the existing model are found to exceed the observations in most cases, with very few predictions where the predicted concentration is less than half the observed concentration anywhere in the dispersing CO_2 cloud. This means that the predictions made with the combination of the new source models and the existing dense gas dispersion model will tend to err on the side of caution.

The results of the calculations from the University of Warwick are available to help assess any specific effects of slopes or obstructions that can be applied to these 'flat terrain' predictions, (see Wen et al (2013) for an example of their predictive methods).

The above model has been demonstrated for a full sized pipeline and the output used in assessing the risks from such a pipeline. This provides a benchmark result using the information provided from the COOLTRANS research programme, with existing outflow and dense gas dispersion modelling. It is possible that as a result of further work some of the model will be refined further. Based on the comparison of the overall package of models with the experimental data for the scaled rupture experiments, this is most likely to lead to a reduction in the over-prediction of the observed concentrations by the package and hence a reduction in the calculated risks.

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APPENDIX A: Crater Size Model

The size of the crater produced by a rupture or a puncture can be estimated using a range of techniques. A simple approach was taken in the COOLTRANS research programme, in that a series of correlations were deduced for the crater dimensions, using the experimental work undertaken on simulated failures of buried CO_2 pipelines. Four programmes of experimental work in the COOLTRANS research programme were used to derive the correlations:

- **Instrumented Burst Tests**. Three tests were undertaken using 914.4 mm outside diameter, L450 grade pipe, with a 25.4 mm wall thickness, at a pressure of 150 barg. All three tests were conducted in clay soil.
- **Puncture Release Experiments.** A series of eight experiments were undertaken on a 914.4 mm outside diameter pipeline, with a puncture diameter of 25 mm (1") or 50 mm (2"). It is noted that as the final test used a pre-formed crater, it was not included in the development of the crater size correlations. The tests covered a range of release orientations and were undertaken in two different soil types: clay and sandy. The first test used gaseous phase CO₂ at 35 barg; the other seven tests used dense phase CO₂ at 150 barg.
- **Fracture Propagation Experiments**. Two full-scale fracture propagation experiments were undertaken using 914.4 mm outside diameter pipe at a pressure of 150 barg. These tests were conducted in clay soil.
- **Rupture Release Experiments.** Three 1/6 scale pipeline rupture experiments, undertaken on 152 mm diameter pipe at pressures of 150 to 151 barg. The pipe was buried 0.3 m below ground level and the soil was clay in one test and sandy in the other two tests.

The equations for the correlations that were deduced are provided below for reference.

Crater Width

A correlation for the total crater width at ground level, W, based on the diameter of the pseudo source, length of the fracture and the depth of the release is as follows:

Clay soil:	$W = 1.1 DoR + Min(2D_{PS}, 3\sqrt{D_{PS}Max(D_{PS}, L_F)} - 2D_{PS})$	
Sandy soil:	$W = 1.6DoR + Min(5D_{PS}, 7.5\sqrt{D_{PS}Max(D_{PS}, L_F)} - 5D_{PS})$	(11)

where

 L_F is the fracture length (m),

 D_{PS} is the diameter of the pseudo source (combining the flows from a two-ended pipe for ruptures) (m) and

DoR is the depth of the centre of the release below ground (m).

The above definitions mean that the depth of release term, *DoR*, is defined as the depth to the centre of the pipe for ruptures and the depth to the centre of the hole for puncture failures. This latter value is dependent on the location of the puncture on the pipeline.

Crater Length

The correlation for the crater length, L, is as follows:

$$L = W + Max(L_F - D_{PS}, 0)$$

For punctures, it can be seen that this expression simply reduces to L = W. The observed craters in the puncture experiments were all relatively circular in shape, although they were offset towards the side of the pipe on which the release took place.

Crater Area

The area of the crater that is formed, A, is given by the following correlation:

$$A = SW^{2} + Max(W(L-W), 0)$$
(13)

where S is a shape factor given by:

$$S = Max \left(\frac{\pi}{4Max(L_F, D_{PS})/D_{PS}}, 0.5 \right)$$
⁽¹⁴⁾

It is noted that the shape factor reduces to $\pi/4$ for punctures, so that the crater area is taken to be the area of a circle with diameter W.

(12)

(16)

Crater Depth

The observations to-date indicate that the maximum crater depth is not overly dependent on the fracture length for ruptures. However, it has been found to depend on the release direction for punctures. As a result, it has been assumed that the maximum crater depth depends on the pseudo diameter of the pipeline outflow and the direction of the release for punctures, but that it is always greater than the depth of release.

Correlation for the maximum crater depth, D, are as follows:

Ruptures

Clay soil:
$$D = DoR + Min(0.3D_{PS}, 2.5D_{Pipe})$$

Sandy soil:
$$D = DoR + Min(0.75D_{PS}, 6.25D_{Pipe}), \qquad (15)$$

where D_{pipe} is the diameter of the pipe.

Punctures

The correlation for punctures is in the same form as that for ruptures, except that it is also dependent on the orientation of the release and is given by:

$$D = DoR + Min(K_1D_{PS}, K_2D_{Pipe})$$

where K_1 and K_2 are coefficients determined according to the location of the release and the soil type and are defined in Table 1.

Table 1. Councients for use in the crater acpuir correlation for punctury	Table 1. C	Coefficients fo	r use in tl	he crater de	oth correlation	for puncture
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Confficient		Location of Release			
Coenicient	Son type	Тор	Middle	Bottom	
K ₁	Sandy	0	3.5	3.75	
	Clay	0	1.4	1.5	
K ₂	Sandy	0	1.5	2.0	
	Clay	0	0.6	0.8	

APPENDIX B: Crater Exit Source Model

The preliminary formulation of this model was taken to follow an equivalent model for natural gas releases, but this was updated following completion of the detailed CFD calculations by the University of Leeds. See Wareing et al (2014), for a typical example of the use of the CFD model. In the majority of cases, the work by the University of Leeds predicted the behaviour of the outflow from the crater in the absence of any re-entrainment of CO_2 into the flow.

Correlation

The crater source model uses a non-dimensional path length parameter, P, in order to calculate the required mass concentration or momentum retained factor for the flow leaving the crater (assumed to be in a vertically upwards direction). This path length depends on the dimensions of the crater, type of release and, for a puncture, the position of release on the pipeline. The associated equations are given below, where D_p denotes the depth to top of pipe; D_c the depth of crater; L_c the length of crater in direction of release; d_p the diameter of pipe and d_{ps} the diameter of the pseudo source of the flow leaving the pipeline (no dilution assumed at this stage).



The path length reflects the distance travelled by the flow from the pipe to the crater exit and is made non-dimensional by a length scale associated with the release. The use of a pseudo-diameter to make length scales non-dimensional as above follows previous work, such as in Birch et al. (1987) on scaling free natural gas jets.

The plot of the predictions obtained from the University of Leeds as part of the COOLTRANS research programme for the mass concentration against a non-dimensional path length is given in Figure 3 along with the proposed, simplified, correlation model, represented by the continuous solid curve.



Figure 3. Percentage mass concentration against non-dimensional path length for University of Leeds data.

(19)

The equation below is used to define the percentage mass concentration at the crater exit, C_{ps}^{Mass} .

$$C_{ps}^{Mass} = Max\left(45, Min\left(100, \frac{1200}{P+10}\right)\right)$$
(18)

The decrease in concentration with the inverse of the scaled distance is in line with previous work describing jet behaviour.

Similarly, the values of the percentage momentum retained, inferred from the predictions of the flow out of the crater produced by the University of Leeds, are plotted against the non-dimensional path length is given in Figure 4 along with the proposed correlation model, shown as the solid line. Again, this follows the same form used for other jetted releases.



Figure 4. Percentage momentum retained against non-dimensional path length for University of Leeds data.

The equation below is used to define the percentage of the momentum at the pseudo-source (Stage 2) that is retained at the crater source, *MomRet*.

$$MomRet = Max\left(15, Min\left(60, \frac{500}{P+5}\right)\right)$$

The data point seen as an outlier in Figure 4 corresponds to the CFD prediction for the vertically upwards puncture on the top of the pipeline. The predictions for the punctures have been examined further by the University of Leeds. They have suggested that deposition of solid CO_2 could have occurred during the experiment. This may have made the crater walls smoother and the crater cross-section narrower than the final observed shape of the crater, which was used by the University of Leeds in their simulations. Sensitivity studies carried out by the University of Leeds suggest that the momentum fluxes in the punctures would have been higher if the observed shaper edged craters were 'rounded'. In particular, the momentum retained would have increased significantly if the crater profile at the predicted location of impaction of solid for the vertically upwards puncture had been smoother and narrower. This would have brought the data point closer to the other points in Figure 4. For this reason the correlation proposed in Equation (19) has been used, leaving the upwards puncture data point as an outlier.

A comparison of this model with observations of the initial plume height, prior to any significant re-entrainment of flow into the crater if a blanket formed, was provided in Allason et al (2014). This showed that the predicted heights were well within 50% of the observed values, suggesting that the combination of using the predicted crater size and the pseudo-source conditions at Stage 2 is providing reasonable predictions for the flow leaving the crater.

(22)

APPENDIX C: Concentration Fluctuations

Dispersion Sub-Model for Peak and Mean Concentration

The differential equations solved by the model outlined in Cleaver et al (1995) predict various parameters including the bulk concentration, bulk width and bulk height of a ground level dispersing dense gas plume. A separate sub-model is used to post-process the predictions to give a concentration profile across the width of the plume, for a short-time 'snapshot' of the plume, as follows:

For a plume at any distance downwind from the source, with a bulk half width of R_{Bulk} and a bulk concentration of C_{Bulk} , the short time averaged crosswind concentration variation, at ground level, is assumed to be given by

$$C(y) = C_{Bulk} \qquad |y| \le R_{inner}$$

$$C(y) = \frac{1}{2}C_{Bulk} \left(1 + \cos\left(\pi \frac{|y| - R_{inner}}{2\delta}\right)\right) \qquad R_{inner} \le |y| \le R_{outer} \qquad (20)$$

$$C(y) = 0 \qquad R_{outer} \le |y|$$

where

 $R_{inner} = Max(R_{bulk} - \sigma_y, 0)$

 $\delta = Min\left(R_{bulk}, \sigma_{y}\right)$

 $R_{outer} = R_{inner} + 2 \,\delta$

C(y) is the ground level concentration,

y is the crosswind distance from the plume centre line and

 σ_{v} is the standard passive dispersion coefficient (5 second averaging).

In order to derive the peak and mean concentrations seen over a longer period of time, the above 'snapshot' of the plume is assumed in the model to fluctuate in position in the cross wind direction. This means that over a longer time period, exposure to any concentration is predicted to occur in a region that is wider than predicted by the 'snapshot' model.

The profile for the short time averaged peak concentration, $C_{Peak}(y)$, that would be experienced during the longer time period is assumed to be a stretched version of the snapshot profile, with the ratio of the widths of the two profiles a constant factor *K*. That is, the inner constant region occurs over a width KR_{inner} and the profile extends to KR_{outer} .

The mean concentration profile, $C_{Mean}(y)$, recorded over the longer time period must have the same maximum width as the above peak concentration profile above, and it is assumed to take the following form:

$$C_{Mean}(y) = \frac{1}{2} C_{Mean}^{Centre} \left(1 + \cos\left(\pi \frac{|y|}{K(R_{outer})}\right) \right) \qquad |y| < K(R_{outer})$$

$$C_{Mean}(y) = 0 \qquad \qquad K(R_{outer}) \le |y| \qquad (21)$$

Conservation of the total mass flow rate of CO_2 can be used to determine the average concentration on the centre line, C_{Mean}^{Centre} .

$$\int_{C_{Mean}}^{C_{entre}} K(R_{outer}) = C_{Bulk} R_{Bulk}$$

An examination of the centreline data from the puncture experiments suggests that the mean concentration, averaged over the period when a steady plume is present, is approximately 75% of the peak of the 5 second average concentration on the closer sensor arcs. Hence, the constant *K* was defined to take the value $\frac{2}{0.75} = 2\frac{2}{3}$

The predictions of a snapshot of the short time averaged plume, and the predicted peak and mean concentrations for one location in puncture Test 5 are shown in Figure 5, using these values.



Figure 5. Predicted peak and mean crosswind concentration profiles for puncture test 5, 50 m downwind of the release.

Calculation of Dose from Transient Concentration

Within a risk assessment, the above dispersion models can be used to predict both peak and mean concentrations, C_{peak} and C_{Mean} respectively. A further simple model can be used to predict a time varying concentration with this peak and mean, from which the dose is calculated, as follows:

• If the peak value exceeds the mean by more than a factor of 2, it is assumed that the concentration is zero for a fraction $1 - 2 \frac{C_{mean}}{C_{peak}}$ of the time, and varies between zero and C_{peak} in a sinusoidal manner for the

remaining time.

• If the peak value exceeds the mean by less than a factor of 2, it is assumed that the concentration varies between $2C_{mean} - C_{peak}$ and the C_{peak} in a sinusoidal manner.

Figure 6 illustrates the time varying concentration that would be assumed for a mean concentration of 5% and a range of peak concentrations.



Figure 6. Assumed time varying concentration for a mean concentration of 5%.

It should be noted that the period of the sinusoidal variations does not affect the calculated dose, provided that these fluctuations are assumed to occur over a shorter time scale than the concentration variations due to a transient release rate.

An analysis of the fluctuations in the observed concentration records obtained in the COOLTRANS puncture experiments was provided in Allason et al (2014). This showed that if the experimentally observed values of the peak and mean are used, the dependence on the dose on the averaging time that is used is correctly reproduced by the above simple approach to representing the time variation of the concentration at each location. Figure 7 shows a comparison for the COOLTRANS

rupture experiments performed in a similar way, comparing the dose evaluated over a certain time period, typically 180 seconds, when calculated from the separate values of observed 5 second average concentrations with the dose calculated using the averaged concentration over that period with the ratio of the peak to mean concentration over that period. The predictions based on the model above, assuming time variation as illustrated in Figure 6, are shown for comparison, assuming the observed values of the peak and mean concentration are used.



Figure 7. Relationship between the dose evaluated using different time averaged values of the observed concentration for the COOLTRANS rupture experiments and the peak to mean ratio of the concentration (analysis as in Allason et al (2014), but including additional data from Rupture Test 4). Predictions with the simple time sinusoidal variation model obtained using the observed peak and mean values shown for comparison.

This figure shows that there is a good agreement between the doses calculated from the assumed sinusoidal concentration variation and the doses calculated from the observed time varying concentrations if the peak and mean values at any location are known. This gives some confidence in the use of this approach to representing the time variation in a general risk assessment in which the peak and mean values are predicted.

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