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Framework for Validation of Pipeline Release and Dispersion Models for the COOLTRANS Research programme

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Abstract

The framework of a Model Evaluation Protocol (MEP) is presented for Carbon Dioxide (CO_2) discharge and dispersion models. Its purpose is to provide a comprehensive evaluation methodology for determining the suitability of models for simulating releases from CO_2 transport infrastructure, i.e. pipelines and associated equipment. The protocol has been developed by the Health and Safety Laboratory (HSL) in support of the National Grid COOLTRANS research programme and it follows a similar structure to that developed previously by HSL for Liquefied Natural Gas (LNG).

The proposed MEP consists of five elements: context definition, scientific assessment, verification, validation and sensitivity analysis. The first of these involves the definition of the set of operating conditions and credible release scenarios that are to be simulated, together with identification of potential models. The second step of scientific assessment involves an examination of the underpinning physics of the models to discern whether they are suitable for the relevant release scenario. In the present work, verification is taken to mean the process of ensuring that the model equations are implemented in the computer software correctly, which includes some consideration of code quality assurance. The validation step is a key component in the MEP and involves the assessment of model performance against experimental data. In the present work, four validation scenarios are considered: above-ground discharges from vents, transient discharges from a shock tube, steady releases from simulated punctures in a buried pipeline, and full-bore ruptures of a buried pipeline. For each of these scenarios, experiments are being conducted at GLND Spadeadam as part of the COOLTRANS research programme. The final element of the MEP involves sensitivity analysis, where model input parameters are varied in order to understand the effect of uncertainties in the physical and model conditions. This final stage of the evaluation procedure also includes simulations of a “realistic” full-scale release scenario that could, for example, be studied as part of a pipeline risk assessment.

The outcome of the MEP will be a review of the capabilities and limitations of various pipeline discharge and dispersion models, and an independent assessment of their performance. This will be of benefit to both pipeline operators seeking to use appropriate consequence modelling tools and regulatory authorities in assessing pipeline quantified risk assessments (QRAs).

Introduction

As part of the Carbon Capture and Storage (CCS) design and risk assessment process, it is necessary to understand the consequences of an intentional or accidental release from the CO_2 transport infrastructure. This infrastructure includes pipelines transporting the CO_2 from the emitter to the reservoir injection site, compressor stations and, in some cases, equipment on offshore platforms.

In many of the proposed CCS projects in the UK, the CO_2 will be transported in pipelines as a dense-phase fluid (i.e. in a liquid or supercritical state). When this material is released into the atmosphere, it changes state into a two-phase mixture of gas and solid CO_2 particles (dry-ice). This presents new challenges for consequence models, in terms of predicting the complex depressurisation behaviour within pipelines, the expansion of CO_2 to atmospheric pressure and the dispersion of the two-phase mixture.

Over the last five years, various calculation methods have been developed to calculate the flow rate and atmospheric dispersion from a dense-phase CO_2 inventory (Dixon and Hasson, 2007; Witlox *et al.*, 2009; Webber, 2011; Mahgerefteh *et al.*, 2011; Hill *et al.*, 2011). These have mainly been based on extending methods previously developed for flashing liquid releases (e.g. liquefied petroleum gas). However, the accuracy of these models for full-scale CO_2 releases remains uncertain and guidance on the best practice use of these models in risk assessments has yet to be produced. A recent study by TNO showed that variations in modelling assumptions and risk criteria could lead to significant variations in the predicted hazard distances. As a consequence, the individual risk contour was found to vary between 0 m and 204 m from the pipeline, depending on assumptions made (Koornneef *et al.*, 2010).

To address this issue, National Grid has commissioned a comprehensive programme of experimental tests and modelling exercises as part of the COOLTRANS research programme. The partners in this project include: Pipeline Integrity Engineers (PIE), Atkins, GL Noble Denton (GLND), Nottingham University, University College London (UCL), University of Leeds, Kingston University, and the Health and Safety Laboratory (HSL). PIE is supporting National Grid in defining the technical strategy and project management of the programme. Atkins are involved principally on the pipeline fracture propagation aspects rather than the release and dispersion modelling analysis. The role of GLND is to conduct field-scale CO_2 release experiments and to provide predictions using consequence models suitable for use in risk assessments. Nottingham University are conducting laboratory experiments to develop an equation of state for CO_2 (with and without impurities) and are also conducting separate field-scale experiments to examine the effect of fugitive CO_2 emissions on vegetation etc. UCL, University of Leeds and Kingston University are tasked with modelling, respectively, the release rate, near-field and far-field dispersion behaviour of CO_2 using sophisticated Computational Fluid Dynamics (CFD) models. Finally, the role of HSL is to develop a Model Evaluation Protocol (MEP) and to conduct some limited tests using the Det Norske Veritas (DNV) consequence modelling package, Phast. The COOLTRANS project started in January 2011 and is due to be completed in December 2013. HSL's involvement in the project is financially supported solely by the UK Health and Safety Executive (HSE).

The aim of the present paper is to describe the MEP that is being developed by HSL for the COOLTRANS research programme. At the present time, the programme of CO_2 release experiments is still ongoing and therefore details of the MEP, such as the choice of quantitative model acceptance criteria, have yet to be finalised. Nevertheless, it is possible to describe the general structure of the proposed MEP at this stage and constructive feedback on the proposals is welcomed.

The MEP proposed here is based on that developed previously by HSL for assessing Liquefied Natural Gas (LNG) dispersion models (Ivings *et al.*, 2008), which is currently used by the U.S. regulatory authorities for selecting models used in siting LNG terminals[1]. This

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[1] NFPA 59A: Standard for the Production, Storage, and Handling of Liquefied Natural Gas (LNG) – see: http://tinyurl.com/crd6525, accessed May 2012

methodology was itself based on the earlier work of the Model Evaluation Group (MEG), which is described in various papers produced by the EU-sponsored REDIPHEM and SMEDIS projects (Nielsen and Ott, 1996; Daish *et al.*, 2000; Carissimo *et al.*, 2001; Duijm and Carissimo, 2002).

The proposed model evaluation protocol consists of the following five elements:

- Context definition
- Scientific assessment
- Verification
- Validation
- Sensitivity analysis

Each of these items are discussed in more detail in the later sections, as applied to the case of CO_2 discharge and release modelling.

Context Definition

A wide range of potential release scenarios needs to be considered as part of the MEP. The transport of CO_2 from capture locations to sequestration reservoirs is likely to involve gaseous-phase CO_2 in the initial collection stage from power stations and other emitters, supercritical CO_2 following compression, and liquid-phase CO_2 once the supercritical fluid has cooled within the pipeline network, either naturally from heat loss to the ground or through forced cooling following compression. The locations of potential CO_2 releases include discharges from both above-ground (e.g. from compressor stations) and below-ground, from the buried pipelines. Since the main focus of pipeline risk assessment is on the impact of hazardous CO_2 clouds on populated areas, there is an interest in considering typical populations and location topography. Finally, the CO_2 may contain various impurities depending upon the emission source and pipeline specification.

To simulate this wide range of potential release scenarios requires three stages of models:

1. Discharge model
2. Near-field dispersion model
3. Far-field dispersion model

The primary role of the discharge model is to predict the mass release rate of CO_2 and the conditions at the release orifice in terms of pressure, temperature and CO_2 quality (i.e. the proportions of gas, liquid, solid and supercritical CO_2). Different discharge models are needed in different circumstances. For instance, a small leak from a large diameter pipeline may be treated similarly to a leak from a vessel, in which case the conditions upstream of the orifice are assumed to remain unchanged over time. Full-bore pipeline ruptures, however, require a model that predicts the time-varying depressurisation of the pipeline and accounts for the changing conditions near the orifice. Various discharge models have been developed for these scenarios that incorporate different assumptions and varying levels of complexity. For the pipeline depressurisation scenario, three models are being tested in the COOLTRANS research programme: the PipeTech model from UCL (Oke *et al.*, 2003), the GLND model (Cleaver *et al.*, 2003) and the Pipebreak model in Phast (Webber *et al.*, 1999).

Immediately downstream from the orifice there is a zone in which the CO_2 expands to atmospheric pressure. The behaviour here is complex and may feature shocks and phase transition from an initial high-pressure gas, supercritical, liquid or two-phase state into the final gas and solid state at atmospheric pressure. Three different approaches to model the expansion behaviour are being tested in the COOLTRANS research programme: a compressible multi-phase CFD model developed by University of Leeds and two simpler integral models used by GLND and DNV (i.e. the Phast software).

For the near-field models, one of the major challenges is to simulate releases from buried pipelines, where the high-speed jet of CO_2 produces a crater around the release location. This has a significant effect on the dispersion behaviour, and hence the hazard range. The entrainment of air into the crater and the impact of the CO_2 onto the crater walls (with the potential for CO_2 solids to deposit) make this a very difficult scenario to model. There are also uncertainties associated with the nature of the surrounding soil and the way in which the pipelines fracture (i.e. for full-bore ruptures, whether the two pipeline ends become misaligned). Furthermore, under low wind speed conditions, the dense CO_2 gas ejected from the crater may fall back and be re-entrained into the crater, coupling the behaviour in the near-field to the far-field dispersion.

In the COOLTRANS research programme, experiments are being conducted to assess the shape and size of craters formed by buried pipeline punctures and full-bore ruptures. CFD simulations of the flow within the crater are being conducted by the University of Leeds, whilst GLND are developing a simple empirically-based crater source model.

In the far-field, dispersion models need to account for the sublimation of any solid CO_2 particles present, the potential for solids to “rain-out” and the effects of ambient humidity, which may lead to water vapour condensing into the cold CO_2 cloud. Previous dense gas dispersion incidents, such as the Lake Nyos disaster (Stager, 1987) and the Buncefield Incident (Gant and Atkinson, 2011), have shown that the far-field dispersion behaviour can be strongly driven by topography and the presence of obstacles, especially under low wind speed conditions. Ideally, far-field dispersion models therefore need to take into account these effects. In the COOLTRANS research programme, experiments are being conducted in which the gas cloud disperses over either flat ground or obstacles and slopes. Simulations of these experiments are being performed by Kingston University using two different CFD codes and by GLND and HSL, using integral far-field dispersion models.

Ultimately, the purpose of the discharge, near-field and far-field dispersion models is to estimate the hazard range. For potential exposures to toxic substances, such as CO_2, the hazard and risk is estimated by HSE on the basis of the “toxic load”. For CO_2, this is calculated from the time-integral of the gas concentration to the power eight[2]. As a consequence of this highly non-linear dependence of the toxic load on the concentration, turbulent concentration fluctuations in the dispersing plume of CO_2 have a significant effect on the calculated hazard range (Gant and Kelsey, 2012). The assessment of far-field CO_2 dispersion models therefore needs to take into account the treatment of concentration fluctuations.

Scientific Assessment

The scientific assessment involves a critical review of the physical, mathematical and numerical basis of the models to ensure that they are fit for the purpose of simulating CO_2 releases. In the proposed MEP, the first stage of this assessment will involve a questionnaire that is completed by the model developers. The objective of this exercise will be to ascertain information from the model developers in a standardised format that will enable model features to be compared. The information recorded in the questionnaire will be examined by one or more independent experts. Additional material may be considered in the assessment

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[2] http://www.hse.gov.uk/hid/haztox.htm, accessed May 2012

process in the form of user-manuals, peer-reviewed publications, reports and the results of validation exercises (including those made independently of the COOLTRANS research programme).

The format of the questionnaire will be similar to that previously developed by Ivings *et al*. (2008). A list of the likely topics is given below for the far-field dispersion models. Suitably modified questionnaires will be developed for the discharge and near-field dispersion models.

1. General Model Description
    a. Model version number and release
    b. Short description
    c. History of model
    d. Availability of model
    e. Level of expertise required to use model
    f. Hardware and software requirements

2. Scientific Basis
    a. Model type (empirical, integral, CFD)
    b. Specification of the source
        i. Type of sources (single/two-phase jet, area source, multiple sources)
        ii. Continuous or time-varying
        iii. Thermodynamic properties of source
    c. Specification of the environment
        i. Reference frame (2D/3D Cartesian, Cylindrical Polar, Spherical)
        ii. Atmosphere (wind profiles, stratification, humidity, zero wind)
        iii. Turbulence parameterisation
        iv. Terrain
        v. Surface roughness characteristics
        vi. Obstacles
    d. Model Physics and Formulation
        i. Transport equations solved
        ii. Turbulence model
        iii. Initial and boundary conditions allowed
        iv. Dispersion treatment (advection, gravity spreading, dilution, concentration fluctuations)
        v. Concentration profiles assumed
        vi. Treatment of aerosols
        vii. Thermodynamics
        viii. Transition to passive dispersion
    e. Solution Technique
        i. Equation types
        ii. Analytical/numerical solution methods
    f. Results output from model
        i. Concentration data output (centreline/centroid values, pointwise etc)
        ii. Further outputs (velocity, turbulence, etc)
    g. Source of model uncertainty
    h. Limits of applicability
    i. Special Features
    j. Planned developments

3. User-Oriented Aspects of Model
    a. Documentation and help
    b. Installation procedures
    c. User interface
    d. Internal databases
    e. Guidance in selecting model options
    f. Assistance in data input
    g. Error/warning messages and checks on use of model beyond its scope
    h. Computational aspects

    i. Programming language
    j. User programming options
    k. Typical execution times
    l. Model output
    m. Facilities for post-processing results
    n. Model suitability to users and usage
    o. Possible Improvements
4. Verification
    a. Verification undertaken
    b. Quality assurance

5. Validation
    a. Previous validation studies

Verification

In the present work, verification is taken to mean the process of ensuring that the model equations are implemented in the computer software correctly. This is distinct from the process of model validation, which consists of ensuring that the model provides an accurate representation of the flow physics. More precise definitions can be found, for example, in the book by Roache (1998).

Information will be sought from the model developers on verification as part of the scientific assessment exercise. This will include consideration of code version control, comparison of model predictions to known analytical solutions, and use of the method of manufactured solutions. It is not proposed to undertake specific demonstrations of model verification as part of the MEP. The extent to which a model has been verified will be assessed qualitatively by an independent expert, based on the information provided by the model developers.

Validation and Model Sensitivity Analysis

The objective of the model validation stage of the MEP is to assess the accuracy of CO_2 discharge and release models by comparing their predictions to experimental measurements for a range of representative scenarios.

Atmospheric dispersion involves inherent randomness due to turbulence and so, for the far-field dispersion modelling at least, the predictions can only be assessed in terms of their statistical performance rather than their ability to predict directly the time-varying concentrations in a particular experiment. Comparisons will therefore be made on the basis of the mean, variance or frequencies of occurrence of the temperatures or concentrations, rather than their instantaneous values at a particular position and point in time.

In the previous LNG MEP (Ivings *et al.*, 2008), a dispersion model was considered to be “acceptable” provided that the following statistical performance criteria were met:

- Mean bias of the predictions within ±50% of the measured mean, corresponding to a Mean Relative Bias (MRB) of between -0.4 and 0.4, and a Mean Geometric Bias (MG) of between 0.67 and 1.5
- A scatter of a factor of three of the mean, corresponding to a Mean Relative Square Error (MRSE) of less than 2.3 and a Geometric Variance (VG) less than 3.3
- The fraction of model predictions within a factor of two of the measurements (FAC2) to be at least 50%

Definitions of the statistical performance measures: MRB, MG, MRSE, VG and FAC2 can be found in the report by Ivings *et al.* (2008). These criteria were applied to maximum arc-wise concentration and plume-width concentration data in the LNG MEP. However, it was considered that there was insufficient experience to apply the same criteria to concentrations at particular point locations or to temperatures.

The purpose in calculating these different measures is to help understand the different facets of a model's performance. For example, one model may be "correct" on average but exhibit a high degree of scatter. This would show up in the values of the MRB and the relatively large value of the MRSE and VG. Another model may nearly always over-predict the experiments by a small percentage. This would show up in the sign and value of the MRSE and the value of the MG. It is useful for a user or assessor to be aware of the values such as these, to help in the interpretation of the predictions of a particular model.

At present, it is unclear whether the same model acceptance criteria will be adopted in the CO_2 MEP as for the LNG MEP. This choice will depend upon the quality of the measurement data from the COOLTRANS experiments. Consideration also needs to be given to the fact that the LNG MEP was devised to assess flammable gas dispersion, whereas in the case of CO_2 it is toxicity that is the concern. The hazardous concentrations of CO_2 and natural gas are in fact reasonably close (in terms of a constant, non-time-varying concentration). The lower explosive limit of methane is 4.4% vol/vol as compared to the Immediately Dangerous to Life and Health (IDLH) concentration for CO_2 of 4.0% vol/vol (NIOSH, 1995). However, the HSE harm criteria in the case of CO_2 is determined from the time integral of concentration to the power eight, which means that peak values of concentration in the plume have a significant effect. This is somewhat different from the criteria used to assess flammable hazards, which is based on the predicted concentration, rather than a time-integrated dose.

In the LNG MEP, data was provided for model validation based on short and long time-averaged concentrations, where in the former case averaging was typically over a period of 1 second (Coldrick *et al.*, 2010). Preference was given to validation using the short time-averaged data in view of the fact that the application was for flammable releases. In the CO_2 MEP, different averaging times will be investigated. If possible, experimental data for model validation will be presented on the basis of the toxic load, which will be calculated by integrating the time-averaged concentration to the power eight over time, where the averaging period is similar to duration of a human breath (i.e. a few seconds).

The dispersion models' performance in the LNG MEP was categorised into two groups, according to whether dispersion took place over flat, open ground or complex terrain. A similar methodology to this will be adopted in the proposed CO_2 MEP.

One approach to model validation is to compare model predictions to the experiments "blind", which would involve the modellers being given only the release geometry, the reservoir state and the weather conditions, without any measurement data. This replicates the way in which models tend to be used in risk assessments, when there is no measurement data available. However, in most of the scenarios simulated in the CO_2 MEP, the discharge, near-field and far-field models are used in sequence, with the outputs from one model being used as inputs to the next model. This introduces difficulties, for example, in independently assessing the performance of the far-field dispersion model, since the input conditions provided to it from the upstream discharge and near-field models could be quite inaccurate. If the far-field model used a mass release rate (from the discharge model) that was much lower than the actual release rate in the experiment, its predictions could not be expected to be the same as the measurements.

The alternative approach of allowing modellers free access to the measurement data prior to the submission of results in order to optimise their choice of model inputs (and obtain the best agreement with the results) is also not entirely acceptable. Different combinations of model inputs could be used in each scenario and the models would then no longer be being used as predictive tools.

To address this issue, it is proposed in the CO_2 MEP to request two sets of predictions from the modellers:

- “Standard” model predictions, using the default input parameters for the particular model, without any tuning
- “Optimised” model predictions using tuned input parameters that achieve the best agreement with the measurement data

For example, in the shock-tube scenario (discussed in more detail below), one of the model input parameters to the pipeline discharge model is the orifice discharge coefficient, C_d. A default value of C_d is used by integral models such as Phast, but it is known that C_d is a function of the particular orifice design and, moreover, the value of C_d has a significant effect on the discharge rate. In the proposed approach, “standard” model predictions would be produced with the default value of C_d. Better agreement with the results may be achieved by changing C_d to some other value. The results from both of these tests would be submitted for the model evaluation exercise. In addition to providing two alternative model inputs to the near-field and far-field models (one “default” and the other more accurate), the two sets of results will help to provide a measure of the sensitivity of the results to uncertainties in the input parameters.

A tree diagram is shown in Figure 1 that describes how it is proposed to combine “standard” and “optimised” variants of the discharge, near-field and far-field dispersion models. The combinations of model inputs and outputs have been selected here in order to assess the accuracy of each model independently (based on accurate input values) and separately to provide model predictions using the “standard” version of all three models, to replicate the type of behaviour that is expected if the models were used as they would be in an industrial risk assessment. In some cases, the default values may in fact be found to provide “optimum” results, or it may be difficult to determine tuned values (due to a lack of validation data in the near-field, for example). If this is the case, then the number of simulations required will be reduced.

Whilst it is feasible to run multiple scenarios and optimise model inputs using integral models such as Phast, the situation is different for the CFD models used by UCL, the University of Leeds and Kingston University. Their simulations are more time-consuming to run and it is less clear what the “default” values would be for these models. Moreover, they are unlikely to be used directly for consequence modelling as part of a pipeline risk assessment. Instead, their role in the COOLTRANS research programme is primarily to provide reference solutions, using state-of-the-art computational methods. Therefore, only one set of model predictions from the university partners will be considered for each of the validation cases, based on the “optimum” input conditions that have been found to produce the best agreement with the measurements.

The following sections consider the modelling scenarios being considered as part of the COOLTRANS research programme.

Scenario 1: Above-Ground Vent Releases

The first validation scenario involves above-ground releases of CO_2 from circular orifices. The results from this case are relevant to leaks from large-diameter above-ground pipelines or vessels, and full-bore ruptures of short lengths of small diameter pipes attached to vessels.

In total 16 release experiments were conducted at Spadeadam that could potentially be used for model validation of this scenario, comprising 11 vertical and 5 horizontal releases, with orifice diameters of between 13 mm (½”) and 51 mm (2”). An example of one of the vertical release tests is shown in Figure 2. Mass release rates of CO_2 were measured in most of the vertical releases but not in the horizontal releases. Both gaseous and liquid-phase CO_2 was released in the vertical cases, with the pressure maintained at an approximately constant value using nitrogen padding gas on the input side to the CO_2 reservoir. For the vertical liquid-phase CO_2 releases, this meant that conditions were maintained in the storage vessel above the saturation conditions, at around 150 barg and ambient temperatures.

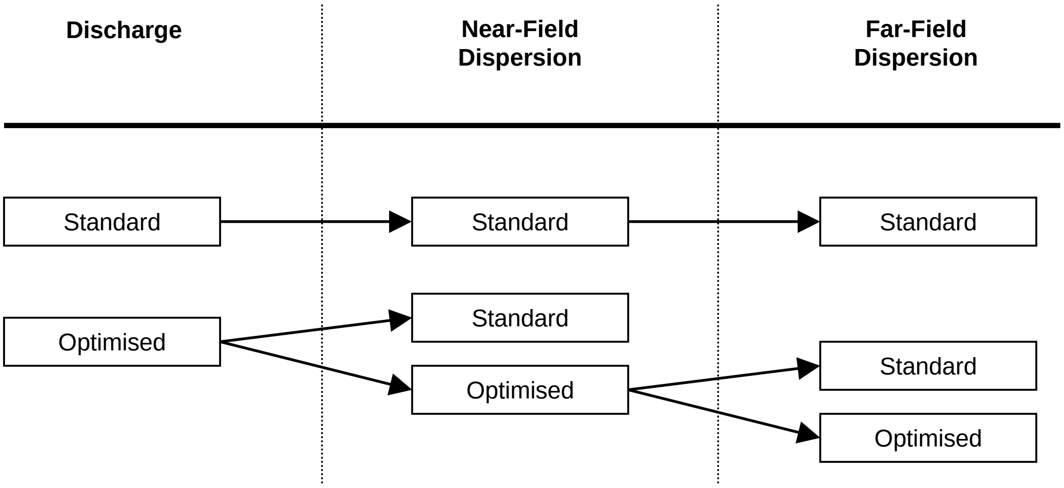

Figure 1 Proposed combinations of model variants for the discharge, near-and far-field dispersion models

Figure 2 Vertical vent release experiment

The horizontal releases were through either 13 mm (½”) or 25 mm (1”) diameter orifices from the end of the 144 m long, 152 mm (6”) diameter, shock tube rig. After an initial very fast transient, the pressure in shock tube fell to the saturation conditions and then slowly decayed to ambient pressure over a few tens of minutes. Tests were conducted with the circular vent located in either the top or the bottom of the shock tube end face, in order to release either the gaseous or liquid-phase CO_2.

It would be very onerous to simulate all 16 releases as part of the validation exercise. Instead, it is proposed to select four cases that cover a range of different conditions:

1a. Vertical gaseous-phase CO_2 release at approximately 34 barg from a 25 mm diameter orifice
1b. Vertical liquid-phase CO_2 release at approximately 150 barg from a 25 mm diameter orifice
1c. Vertical liquid-phase CO_2 release at approximately 150 barg from a 51 mm diameter orifice
1d. Horizontal liquid-phase CO_2 release from the bottom of the shock tube end face through a 25 mm diameter orifice

For the vertical tests (Cases 1a to 1c), a short section of pipe leading to the orifice was instrumented to take pressure and temperature measurements at either end of the pipe. Therefore, it should be possible to validate the discharge models using measured pressure, temperature and mass release rate. Temperatures were also measured on a horizontal array of points at two heights close to the release orifice in these cases, as shown in Figure 2. This data may be used for validating the near-field models, in terms of the plume centreline temperatures and plume-widths. In the far-field, for practical reasons, the measurements were limited to probes close to ground level (rather than in the elevated plume). There is therefore insufficient data to derive the plume centreline concentrations, but the measurements should still provide sufficient information for the purposes of identifying qualitative differences in cloud behaviour (i.e. occurrence of cloud touchdown).

For the horizontal release (Case 1d), a short section of 25 mm vent pipe was attached to the shock tube end face, which was instrumented to record the pressure and temperature. The mass release rate was not measured directly. Only partial validation of the discharge model is therefore possible (since even if P and T were measured, the relative amounts of gaseous and liquid-phase CO_2 are unknown and therefore the mass release rate cannot be determined). However, some indication of whether the mass release rate is predicted accurately can be determined from the time taken for the shock tube to depressurise.

Scenario 2: Transient Shock Tube Releases

The second validation scenario consists of full-bore discharges from the end of a 144 m long, 152 mm diameter, shock-tube test rig (Figure 3). The primary purpose of these experiments was to record the highly transient depressurisation to saturation conditions that occurs within the first second or so of a release, in order to validate predictions of the decompression wave speed. The wave speed is an important parameter in determining the driving force for pipeline fracture propagation models.

For the purposes of pipeline outflow model validation, the only data available from these tests consist of the time-varying pipe wall temperatures along the length of the tube, and the fluid pressure and temperature at a position close to its closed end. No measurements are available for the mass flow rate or the fluid pressure and temperature at the open end of the shock tube, as the primary purpose of the tests were to obtain depressurisation data. The amount of data is less than ideal for the assessment of outflow and dispersion, but useful comparisons to model predictions can still be made. The rate at which the pressure and temperature decays over time provides some indication of the release rate. Comparisons between model predictions and measurements will therefore be made initially by comparing time-varying profiles of pressure and temperature. Other quantitative measures, such as the time taken for the pressure to halve, may be considered later.

In the plume produced by the shock tube releases, measurements were made of the temperature, concentration and flow velocity, in order to study how such a highly transient release behaves, i.e. whether it exhibits behaviour similar to a steady plume or an instantaneous "puff". The effect of localised topographical features on the dispersion behaviour was also studied by performing tests across either open, flat terrain, or across terrain that was sculpted into mounds and/or surface depressions.

Figure 3 Photo of the shock tube test rig

In total, 31 gaseous and liquid-phase CO_2 shock tube tests were conducted which considered a range of initial fluid pressures, temperatures and compositions (including mixtures of CO_2 with various proportions of hydrogen, nitrogen, oxygen and methane), and also various types of terrain. Three of these tests have been selected for the model validation exercise:

2a. Pure liquid-phase CO_2 at an initial pressure of around 150 bar, with flat terrain
2b. Pure liquid-phase CO_2 at an initial pressure of around 150 bar, with complex terrain featuring a slope and a 5 m high mound
2c. A CO_2 rich mixture comprising 92% CO_2 + 4% N_2 + 4% H_2 at and initial pressure of around 140 bar, with complex terrain featuring a slope and a 5 m high mound

If the effect of impurities is found to have a significant effect on the mass release rate and dispersion behaviour, further validation cases may have to be considered.

Validation of the far-field dispersion models will be more challenging for this scenario as compared to the previous above-ground vent release, due to the highly transient nature of the discharge and the uncertainty over the predicted mass release rate.

Scenario 3: Buried Pipeline Punctures

The third model validation scenario consists of steady releases through 25 mm and 51 mm diameter orifices from a buried 914 mm (36”) diameter section of pipeline. The pressure in the pipeline was maintained approximately constant during each release using a long length of pipe filled with CO_2 that formed a charge line, which was connected to a nitrogen padding system. Mass flow rates were measured in the CO_2 supply line using a Coriolis flow meter. A series of eight experiments were conducted with either gaseous or liquid-phase CO_2, using different release orientations from the 914 mm pipeline (horizontal, vertically up and vertically down) and in different atmospheric conditions. In most of the releases, the high-speed discharge from the buried pipe was allowed to form its own crater. Two different types of soil were studied: clay and sand. In a final test, a pre-formed crater manufactured from sheet steel was used instead to allow instrumentation to be placed closer to the release location (Figure 4). The dimensions of this crater were chosen to match the naturally-formed crater from one of the previous tests.

Figure 4 Pre-formed crater prior to burial

In the experiments, the pressure and temperature close to the release location within the pipeline was measured in addition to the mass flow rate into the section of pipeline. For the dispersion aspects, temperatures and concentrations were measured on four arcs in the far-field and at other locations up to 200 m from the release point. For the pre-formed crater test, additional instrumentation was located immediately above the crater to measure the plume temperatures, which may be used to validate the near-field dispersion model.

The experiments for Scenario 3 have only recently been conducted and the data has yet to be processed fully. However, it is currently proposed to use results from four tests for the purposes of model validation:

3a. Horizontal release from a 25 mm orifice into a pre-formed crater in a low wind speed

3b. Vertically down release from a 51 mm orifice into sand in a high wind speed
3c. Horizontal release from a 25 mm orifice into sand in a low wind speed
3d. Horizontal release from a 25 mm orifice into clay in a medium wind speed

Scenario 4: Buried Pipeline Ruptures

The final validation scenario consists of full-bore ruptures of a buried section of 152 mm (6") diameter pipeline. Each end of the ruptured pipeline will be fed from CO_2 reservoirs in order to produce a long duration release. Fluid pressure and temperature will be measured within the pipeline ends, close to the release location, and the installation of Coriolis meters in the two ends of the pipeline is currently being considered. To validate the dispersion models, temperatures and concentrations will be measured on arcs in the far-field and at other locations up to 200 m from the release point. Some velocity measurements will also be made. Releases will take place into soil, forming natural craters, and at least one test is planned to take place using a pre-formed crater. For the pre-formed crater test, additional instrumentation will be located close to the release point.

Details of the cases to be considered for model validation will be decided upon when the experimental programme is finalised, but they will probably consist of the following:

4a. Gaseous-phase CO_2 release forming a natural crater
4b. Liquid-phase CO_2 release forming a natural crater
4c. Liquid-phase CO_2 release with a pre-formed crater

Scenario 5: "Realistic" full-scale pipeline release scenario

The final scenario considered for the model evaluation exercise consists of a "realistic" full-scale pipeline release that may be considered as part of a pipeline risk assessment. The conditions modelled are currently planned to consist of a full-bore rupture of a 914 mm (36") diameter, 70 km pipeline with a mid-point break. Although no measurement data will be available for this case, useful information will be obtained by comparing results from the different models.

Conclusions

A framework methodology has been proposed for evaluating CO_2 discharge and dispersion models as part of National Grid's COOLTRANS research programme. The aim of the MEP is to produce an independent assessment of models, in terms of their scientific basis, verification and validation.

One of the difficulties faced in validating CO_2 discharge, near-field dispersion and far-field dispersion models is the interdependence of models, where errors in the output from one model may propagate into the inputs of the next model. In the present work, it has been proposed to address this issue by performing multiple integral model simulations using both default and optimised model input parameters. Additionally, "reference" simulations will be obtained using state-of-the-art CFD models.

An initial selection of validation case studies has been made, based on four release scenarios, including: above-ground discharges from vents, transient discharges from a shock tube, steady releases from simulated punctures in a buried pipeline, and full-bore ruptures of a buried pipeline. For each of these scenarios, experiments are being conducted at GLND

Spadeadam as part of the COOLTRANS research programme. A final stage of the evaluation procedure includes simulations of a “realistic” full-scale release scenario that could, for example, be studied as part of a pipeline risk assessment.

The range of scenarios will be used to validate each of the models (discharge, near-field and far-field dispersion) at a range of scales, from 25 mm diameter steady vent releases to 152 mm diameter full-bore pipeline ruptures. Most of the validation cases will involve releases of liquid phase CO_2 at an initial pressure of around 150 barg, but some tests will consider gaseous-phase CO_2 releases and, in one case, a 140 barg CO_2 rich mixture with small amounts of nitrogen and hydrogen. For the far-field dispersion modelling, most of the validation cases will involve flat open terrain but in some of the shock tube tests the CO_2 disperses across complex terrain featuring a slope and a mound.

One area where it could be argued that uncertainties will remain following the proposed validation exercise is in predicting the outflow from pipeline ruptures. It is important to have confidence in the predicted mass release rate from the pipeline outflow model, since it has a strong effect on the subsequent dispersion behaviour. Validation of the outflow models is limited to comparing the time-varying pressure and temperature at the closed end of the shock tube. No mass release rate data or information from measurements of temperature and pressure near the open end of the tube are currently available. This limitation is to a large extent understandable, given the severe technical challenges to be overcome in measuring experimentally the mass release rate from full-bore pipeline ruptures. To partially address this issue, it is proposed to compare in detail the predictions of different pipeline depressurisation models and study model sensitivities. If in the future, mass release rate data becomes available, it would be useful to incorporate this into the validation exercise.

A second area where uncertainties remain is in scaling the results from the 152 mm diameter rupture tests to full-scale CO_2 pipelines. In part, this issue should be addressed in the review of the scientific basis of models, which will examine whether the models account for scaling issues appropriately. Model predictions will also be compared and sensitivity tests undertaken for full-scale releases as part of the final evaluation test case involving a simulated “realistic” pipeline rupture. As part of the COOLTRANS research programme, experiments are currently being conducted at GLND Spadeadam to investigate crack propagation using lengths of 914 mm diameter pipeline. These should help to identify any significant qualitative changes in the release and dispersion behaviour at full scale.

The outcome of the MEP will be a review of the capabilities and limitations of various pipeline discharge and dispersion models, and an independent assessment of their performance. This will be of benefit to both pipeline operators seeking to use appropriate consequence modelling tools and regulatory authorities in assessing pipeline QRAs.

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