Evaluating vapor dispersion models for safety analysis of LNG facilities

FINAL REPORT BY:

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FOREWORD

This report describes a Model Evaluation Protocol (MEP) that can be used for assessing the suitability of Liquefied Natural Gas (LNG) dispersion models for estimating the size of exclusion zones around LNG facilities. The development of this MEP was funded by the Fire Protection Research Foundation (FPRF) of the National Fire Protection Association (NFPA) and the work was carried out by the UK Health and Safety Laboratory. This led to the publication of the first edition of this report in 2007 by Ivings et al. (2007).

Following the publication of this report in 2007, further work was carried out in the period 2008 to 2010 to develop and revise a database of experimental data that could be used to validate models as part of the MEP process (Coldrick et al., 2010). In addition, a review of LNG source models was produced (Webber et al., 2009) and PHMSA published an Advisory Bulletin clarifying the process for model validation (PHMSA, 2010).

More recently, substantial changes to the validation database have been made and further advice has been produced to describe how the MEP should be applied in practice (Stewart et al., 2016). This has led to a requirement to update the MEP and hence the publication of this second edition of the MEP report. This revision was carried out by the UK Health and Safety Laboratory, funded by Oak Ridge National Laboratory.

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FOREWORD

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EXECUTIVE SUMMARY

Background

The US Code of Federal Regulations governing Liquefied Natural Gas (LNG) facilities (49 CFR 193), which incorporates by reference the 2001 edition of the NFPA 59A Standard, requires dispersion exclusion zones to be defined around each LNG container and LNG transfer system as part of the siting requirements for LNG facilities. The size of these exclusion zones must be calculated using a vapor dispersion model. Prior to 2010, two vapor dispersion models were accepted for this purpose: DEGADIS and FEM3A. The Regulations permitted the use of alternative models, subject to the Administrator’s approval, provided that they incorporated the correct physics and had been validated against experimental test data.

To assist in this approval process, an LNG dispersion model evaluation procedure was developed in 2007, which is now widely known as the LNG Model Evaluation Protocol or LNG MEP. The development of the LNG MEP was undertaken by the UK Health and Safety Laboratory, under contract to the Fire Protection Research Foundation of the NFPA.

Following the initial development of the MEP, an LNG dispersion model validation database was also constructed, which has been updated a number of times over the following years. The most recent update of the database (Version 12) includes several significant changes from the previous version. To address both these changes and incorporate other guidelines on model validation published by PHMSA in 2010, it was decided to produce this second edition of the MEP report.

Objectives

The objectives of the MEP are:

- To develop a methodology for the evaluation of predictive models for vapor dispersion from LNG spills on land, to assist with the approval process for selecting alternate models under 49 CFR 193
- To include recommendations to the NFPA regarding qualitative and quantitative criteria for model evaluation and provide these in a form suitable for use for model selection
- To provide an initial review of appropriate versions of the DEGADIS, FEM3A and FLUENT models for LNG dispersion
- To provide guidance on the application of models to large LNG spills

Main Outcome

This work has led to the development of an MEP that can be used to assess the suitability of dispersion models for predicting hazard ranges associated with large spills of LNG. The protocol is based on that developed by the EU SMEDIS project for dense gas dispersion, with modifications to make it specifically applicable to the dispersion of LNG on land.

The MEP is based on three distinct phases: scientific assessment, model verification and model validation. The scientific assessment is carried out by obtaining detailed information on a model from its current developer using a specifically designed questionnaire and with the aid of other papers, reports and user guides. The scientific assessment examines the various aspects of a model including its physical, mathematical and numerical basis, as well as user-oriented aspects. This assessment allows the model to be evaluated against 11 proposed qualitative assessment criteria. The outcome of the scientific assessment is recorded in a Model Evaluation Report (MER), along with the outcomes of the verification and validation stages. The template for the MER has been designed to aid the reviewer to extract all of the necessary information to complete the scientific assessment.
The verification stage of the protocol is treated passively as in the original application of the SMEDIS protocol. This means that instead of carrying out a specific exercise to verify that the model has been implemented correctly and accurately, evidence of model verification is sought from the model developer and this is then assessed and reported in the MER.

The validation stage of the MEP involves applying the model to a database of 33 experimental test cases, including both wind-tunnel experiments and large-scale field trials. The aim of the validation stage is to quantify the performance of a model by comparing its predictions to measurements. The specific datasets and validation cases included in Version 12 of the validation database have been outlined; comprehensive details of each trial are included in a separate Model Validation Database Guide. A number of physical comparison parameters and statistical performance measures have been defined that allow the model to be assessed via a number of proposed quantitative assessment criteria.

The MEP has been applied, excluding the full validation stage, to “DEGADIS Version 2.1”, “FEM3A February 2007 version” and “DOE-NETL LNG Dispersion Module for FLUENT 6.2/6.3”. This exercise was primarily undertaken to assess the suitability of the MEP itself, rather than to serve as a validation exercise for models. This is the reason for only partially applying the MEP here. A full scientific assessment of the three models has been undertaken and the MER’s have been included in full in the Appendices of this report. All three models met all of the qualitative assessment criteria. For each model a general description of the model has been given along with the scientific basis of the model. The limits of applicability of each model are described and an assessment of previous validation of the model is given.

The way in which a model is used is at least as important as the choice of model itself. Therefore, some brief guidance is given on the application of dispersion models for assessing the hazards from LNG spills. The importance of the source model is discussed and concerns are raised for situations where the ‘source’ model includes a model for the initial dispersion of the vapor. In cases such as these, it is recommended that the LNG dispersion MEP is applied to the ‘dispersion’ part of the source model.

The full application of the MEP will help the NFPA to make decisions on the appropriateness of dispersion models for predicting hazard ranges for large LNG spills. However, like the models themselves, the MEP is subject to uncertainty and, although the best possible use of previous work on model evaluation has been made, the MEP would benefit from continued refinement following further research and use of the MEP. This could include, for example, extending the database to include test cases for flashing jets of pressure-liquefied gases that are relevant to releases from the refrigerant systems at LNG export facilities. Another possible extension of the LNG MEP would be to include scenarios involving active mitigation systems.
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1 INTRODUCTION

1.1 BACKGROUND

The US Code of Federal Regulations governing Liquefied Natural Gas (LNG) facilities (49 CFR 193), which incorporates by reference the 2001 edition of the NFPA 59A Standard, requires dispersion exclusion zones to be defined around each LNG container and LNG transfer system as part of the siting requirements for LNG facilities. The exclusion zone must not extend beyond the area controlled by the operator or government agency, where the limit of the exclusion zone is defined as the maximum distance from the release point to where the predicted mean vapor concentration falls to half the Lower Flammability Limit (LFL).

The NFPA 59A standard prescribes the LNG releases which must be considered in this analysis, so-called “design spills”, and it provides guidance on the approach which should be used to predict the resulting hazard zones. Prior to 2010, two vapor dispersion models were accepted for calculating the extent of the vapor exclusion zones: DEGADIS (Havens and Spicer, 1985, 1988, 1990) and FEM3A (Spicer and Havens, 1997). However, the Regulations permitted the use of alternative models, subject to the Administrator’s approval, provided that they incorporated the correct physics and had been validated against experimental test data. To assist in this approval process, an LNG dispersion model evaluation procedure was developed in 2007, which is now widely known as the LNG Model Evaluation Protocol or LNG MEP. The development of the LNG MEP was undertaken by the UK Health and Safety Laboratory, under contract to the Fire Protection Research Foundation of the NFPA.

Following the initial development of the MEP, an LNG dispersion model validation database was also constructed, which has been updated a number of times over the following years. The database (up to Version 11) was described in the Model Validation Database Guide by Coldrick et al. (2010). More extensive updates to the Database and the associated guide have recently been made to bring it up to Version 12, as described by Stewart et al. (2016).

Following the publication of the 2007 version of the current report, much experience has been gained in the application of the MEP. This has required some minor changes and clarification of the recommended approaches for the use of the MEP. This report has therefore been revised to take into account the development of the MEP.

The Model Validation Database Guide Version 12 (Stewart et al., 2016) provides the factual information needed to validate a model following the MEP procedures. The current report provides a higher-level overview of the MEP in general, and justification for the approach.

A critical aspect of the application of an LNG dispersion model is the use of an appropriate source term model. This issue is addressed in the report by Webber et al. (2009).

1.2 OUTLINE OF REPORT

The remainder of the Introduction provides some background information on LNG hazards and an introduction to model evaluation. Further background information can be found in the reviews by Luketa-Hanlin (2006) and Cleaver et al. (2007) and the references cited therein. Volume 140 (2007) of the Journal of Hazardous Materials also provides much information on the hazards associated with LNG.
Section 2 of this report introduces the MEP for LNG dispersion models and describes in detail how the information is gathered and then evaluated using a number of qualitative and quantitative assessment criteria. Sections 3 to 5 then describe the three main aspects of the MEP individually, namely, the scientific assessment, verification and validation of a model.

A review of the different classes of dispersion models is presented in Section 6. Application of the protocol, excluding active validation of the model, is presented in Section 7 as applied to three models: DEGADIS Version 2.1, FEM3A February 2007 version and DOE-NETL LNG Dispersion Module for FLUENT 6.2/6.3. These reviews were undertaken at the time the original version of the LNG MEP was published in 2007 and so may be outdated.

Section 8 of the report provides guidance on the application of models to large LNG spills and the conclusions from this project are presented in Section 9. References are provided in Section 10.

A Glossary of key terms used within this report is provided in Section 11.

1.3 LIQUEFIED NATURAL GAS (LNG)

1.3.1 LNG as methane

Liquefied Natural Gas (LNG) is mainly methane (CH\textsubscript{4}) with a small admixture of higher, less volatile hydrocarbons. For the purposes of hazard assessment, LNG is usually considered effectively to be methane to a very good first approximation and this will be adopted throughout this report.

1.3.2 Properties of methane

Table 1.1 below provides the properties of methane (Reid et al., 1987). We use SI units, except for the adoption of kmol instead of mol to make molecular weights look more familiar, and bar instead of Pascals to make pressures more manageable (1 bar = 10\textsuperscript{5} Pa). The vapor pressure curve up to the critical point is shown in Figure 1.1 and the section focusing on a range around the normal boiling point is presented in Figure 1.2.

<table>
<thead>
<tr>
<th>Physical property</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>16.04</td>
<td>kg/kmol</td>
</tr>
<tr>
<td>Freezing point</td>
<td>90.7</td>
<td>K</td>
</tr>
<tr>
<td>Boiling point</td>
<td>111.7</td>
<td>K</td>
</tr>
<tr>
<td>Liquid density at B.P.</td>
<td>425</td>
<td>kg/m\textsuperscript{3}</td>
</tr>
<tr>
<td>Critical temperature</td>
<td>190.4</td>
<td>K</td>
</tr>
<tr>
<td>Critical pressure</td>
<td>46.0</td>
<td>bar</td>
</tr>
</tbody>
</table>

Table 1.1 Physical properties of methane
The critical temperature of 190.4 K means that methane cannot be liquefied by pressure at ambient temperature. Therefore to liquefy methane at ambient pressure it needs to be cooled to the boiling point at 111.7 K. (In practice, LNG liquefaction is carried out at pressures above atmospheric and therefore temperatures above the atmospheric pressure boiling point). This is quite different from LPG (liquefied petroleum gas, which is largely propane and butane) that is liquefied under a pressure of several bar at ambient temperature.

The liquid density means that a large tank of LNG – say 30 m high – would have a liquid head of around 1.3 bar. This gives a measure of the sort of pressures one has to pump against. They are significantly lower than those involved in LPG storage.
An increase of temperature by only a few degrees corresponds with an increase of saturated vapor pressure comparable with the head of liquid.

The low molecular weight of methane (16.04 kg/kmol, as compared to air with a molecular weight of around 29 kg/kmol) means that methane is lighter than air at ambient temperature. However, methane at its boiling point is significantly denser than ambient temperature air (typically by about a factor of 1.5), and LNG spills are therefore likely to result in heavy gas clouds.

1.3.3 The source of the hazard

Liquid spills

If LNG escapes from its containment, a cold flammable gas cloud will result. A breach in pipework or the side of a tank may result in a boiling liquid pool.

The source term for a heavy gas cloud dispersion calculation is crucially dependent on the area of the pool and its rate of vaporization. There are broadly two modes of vaporization:

Boiling: the liquid temperature is the boiling point, and the rate of vaporization is controlled by the rate at which heat is transferred from the surroundings (primarily the substrate in most cases) to supply the heat of vaporization. The methane gas concentration immediately above the pool surface is 100%.

Evaporation: the liquid is well below the boiling point and the rate of vaporization is controlled by the rate at which air flow above the pool can carry the vapor away. The methane gas concentration immediately above the pool surface is governed by its partial pressure and is significantly less than 100%.

In reality, vaporization is a combination of both modes. The heat balance is governed by an equation schematically of the form:

\[ \frac{dT}{dt} = \frac{Q_{in}}{Q_{vap}} \]

where \( Q_{in} \) is proportional to the heat transfer rate to the pool, and \( Q_{vap} \) is proportional to the heat of vaporization multiplied by the vaporization rate. In the boiling scenario the temperature \( T \) is constant at the boiling point and \( Q_{vap} = Q_{in} \) determines the vaporization rate. As heat is extracted from the surroundings and the ground cools, \( Q_{in} \) may drop to the point where the air stream can remove material faster than the incoming heat can vaporize it. At this point \( Q_{vap} > Q_{in} \) and the pool will start to cool. In this case, there will thus be a gradual transition to the “evaporation mode” described above. Whether or not this happens may depend on the detailed spill scenario: for example a spreading pool can continually reach warm ground and the boiling regime may be prolonged.

Rollover

Another hazard potentially posed by LNG storage sites is the escape of gas through the roof of the tank. This can happen following “rollover”. If one considers the liquid at the top of a high tank to be at a pressure of 1 bar, then the liquid at the bottom also experiences the head of the liquid above it and may be at approximately 2 bar. A glance at the vapor pressure reveals that it can exist there as a liquid at a higher temperature (by quite a few degrees K). If this is allowed to happen, then the equilibrium in the tank can become unstable, and a sudden rollover can send liquid from the bottom
of the tank to the top. Its higher temperature means that its higher vapor pressure is applied to the roof of the tank, which may then fail, leading to the escape of a significant gas cloud. The quantity of gas created will depend on the temperature and heat capacity of the liquid. It is not clear whether hazard analyses routinely consider this scenario, though it is known to have happened. Rollover was considered by Cleaver et al. (2007).

Rapid phase transition (RPT)

Also of interest is the possibility of Rapid Phase Transitions (RPTs), where a rapid vaporization occurs causing a shock wave. RPT’s typically occur during LNG spills onto water. If heat transfer to the liquid LNG is rapid enough then an RPT may occur. Predicting when they occur is difficult, and they are not generally considered in hazard analysis. However, RPT’s were shown to be of importance in several experimental trials included in the LNG Model Validation Database and the majority of the field scale experiments included in the Database involved spills of LNG onto water, giving the potential for RPT’s.

Cleaver et al. (2007) included a summary of possible effects of RPT’s and Luketa-Hanlin (2006) also reviewed RPTs and noted that the enhanced vaporization rate, should an RPT occur, can lead to significantly longer hazard ranges.

1.3.4 LNG Dispersion and modeling

General considerations

LNG hazards are usually analyzed in three phases: source term (usually covering the development and vaporization of a pool), dispersion (the transport of the gas) and effect (radiation from fire or pressure wave from explosion).

Initially an LNG pool will boil very rapidly, and the vaporization rate is controlled mainly by the heat flux into the pool from the ground. If the pool is bunded, the ground beneath it will cool and the heat flux will diminish with time, leaving a still very hazardous pool which vaporizes more slowly. If the pool is not bunded then it will be able to spread on to new warm ground and rapid boiling may continue. The rate of production of gas also increases with increasing surface area of the pool. An LNG cloud formed in this way is cold, concentrated and flammable, and requires a dispersion calculation to estimate the hazard range.

As noted above, the result of vaporization will typically be a heavy cloud – the heaviness being caused by the coldness. It will initially both slump and disperse, and a heavy gas model is required in order to make predictions. As the cloud mixes and dilutes with ambient air, the behavior of the cloud may transition into a passive and/or buoyant regime.

Thermodynamic considerations

A key consideration for LNG dispersion is the rate of heat transfer to/from the LNG pool. The rate of vaporization from the pool is greatly affected by the rate at which the pool is heated, consequently affecting the cloud temperature and concentration, and therefore the extent of the flammable cloud.

Temperature variations in the LNG vapor cloud influence its density. The initially very cold cloud will be very dense. As the cloud is heated the cloud density will reduce and the dispersion of the LNG cloud could switch from density-driven spreading to the passive dispersion regime. With sufficient heat input the LNG vapor cloud may even become buoyant (methane at room temperature is lighter
than air). It is therefore important that models used to simulate LNG dispersion incorporate both temperature and density effects and such models should be capable of modeling dense, passive and buoyant dispersion.

The main mechanism responsible for the warming of an LNG vapor cloud is through mixing and dilution with the surrounding ambient air. As the LNG vapor warms it also dilutes and the rate at which these two processes occur is the same. This leads to a scenario in which the vapor cloud asymptotically approaches neutral buoyancy.

However, the initial temperature of the LNG vapor can have a significant impact on the density of the vapor cloud as it disperses. For cryogenic spills it is possible for the vapor evolving from a liquid pool to have an initial temperature significantly higher than the gas boiling temperature. Ruff et al. (1988) observed this for a spill of liquid nitrogen onto water where the cloud temperature was measured as nearly 50 K above the boiling temperature. The increased cloud temperature, and corresponding reduction in vapor density, results in a cloud with reduced potential for gravity-driven spreading. Taking the vapor source temperature to be the boiling point of methane represents a conservative modeling approach for determining hazard distances.

A further consequence of having a vapor temperature much greater than the gas boiling temperature is that the vapor cloud will approach neutral buoyancy more quickly and is more likely to transition to the buoyant regime. This emphasizes the need to use models capable of accounting for dense, passive and buoyant dispersion when predicting hazard distances for LNG releases.

Humidity

Another important factor to consider in the context of modeling LNG dispersion is the effect of humidity on the characteristics of the vapor cloud. Atmospheric water vapor can affect an LNG cloud, as air is entrained into the cloud, the water vapor will condense (and even freeze). In doing so, the droplets will tend to increase the density of the cloud, but the heat released by condensation will tend to warm it up and make it less dense. Later as the cloud dilutes and warms up, the water will evaporate again, and the two opposing effects on the density will each be reversed. Temperature effects dominate, and the early effect of water vapor condensation is to warm up the cloud faster than would otherwise be the case, making it less dense. Although entrainment rates are affected by density, this makes very little difference to the concentration of methane. However, the dispersion behavior of an LNG vapor cloud may be influenced by atmospheric humidity effects. Ruff et al. (1988) found that the primary causes of heating of the vapor cloud above a cryogenic liquid pool are due to heat transfer from atmospheric moisture and due to the heat released through condensation of the water picked up by the vapor cloud from the atmosphere. This effect can cause the vapor cloud to gain sufficient heat at the source such that it is possible for the vapor to disperse in the buoyant, rather than dense-gas, regime. It is therefore important that humidity effects are accounted for when modeling LNG vapor dispersion.

Geometric considerations: obstacles

Another point of interest is whether dispersion models should include obstacles, or whether it is sufficient to ignore them. Some, though perhaps relatively few, integral models consider obstacles. CFD models can usually cope with obstacles.

Far from the source where the cloud is high, obstacles may often make little difference to the dispersion (an exception occurs at very low wind speed, where the cloud remains heavy and low). Duijm and Webber (1994) and Jones et al. (1992) show how a fence across the flow may be incorporated into any integral model. The model, which gives a good overall fit to field data, indicated that the fence only makes a difference if the cloud is actually lower than the fence when it encounters it; otherwise the turbulent wake of the fence just mixes the already well mixed cloud.
Thus it would appear that individual obstacles only affect cloud dispersion when they are bigger than the cloud.

It is possible that concentrations at some locations, close to an obstacle situated near the source, may be larger owing to its presence. (In addition, the presence of obstacles increases congestion within the dense gas cloud which can lead to an increase in the potential for explosion hazards, though very substantial congestion is typically needed for LNG to pose any explosion risk in unconfined areas.) However, far down-stream of an obstacle (where public safety is affected) the net effect is usually one of extra dilution in the turbulent wake of the obstacle and a reduction in concentration as a consequence.

One does not only have to consider obstacles in the path of a cloud downstream of the source. If a pool of LNG forms just downwind of a large obstacle, then turbulence in the wind field may enhance the vaporization rate, usually not initially while it is controlled by the heat flux into the pool, but later when the surfaces in contact with the pool have cooled.

In summary: ignoring obstacles will usually, but not always, result in higher concentration predictions in the far-field with increased hazard distances and exclusion zones as a result. Overall therefore the presence of obstacles is considered important with regard to hazards modeling and obstacles should be included in a model where possible.

However, when modeling obstacles their effects may be over-estimated, resulting in excessively reduced downwind concentration predictions. Thus any safety case which relies on the existence of obstacles to dilute the cloud, should also present results in the absence of obstacles, and also present a credible case that the difference has not been over-estimated. Simple checks are available: for example Duijm and Webber (1994) indicate that the distance to any given concentration is reduced effectively by the distance which the cloud would have to travel, in the absence of the obstacle, to increase in height from its height at the obstacle, to the height of the obstacle. If a model produces an effect greater than that, then further explanation should be sought.

**Geometric considerations: terrain**

Sloping and complex terrain can also usually be handled by 3D CFD models. Integral models of gas dispersion have also considered it, but few have used it in hazard analysis. Interestingly, theoretical analysis (e.g. Webber et al. 1992) indicates that the process may be better described by slumping followed by down-slope flow, rather than both simultaneously. For flammable gases, it may not often be important, as sites are usually fairly level out to the sort of distances expected to (say) half the LFL. However, in low wind speeds it can be a factor, and the gas may be channeled under gravity by obstacles and terrain in quite complicated ways, which might be difficult to consider in a hazard analysis. Sloping terrain within an impoundment may be very important for liquid flow, possibly by design as a “run-off”.

**Concentration**

Models must be clear on what they mean by concentration. In the literature on heavy gas dispersion, concentrations have been averaged over 0.6 s, over 6 s and assorted other time intervals, and in the literature on passive dispersion 10 minute averages are common. These are very different things, although correlations have been produced which attempt to relate them. Models must be clear about what they are predicting. Webber (2002) has reviewed this subject in some detail, in particular noting various reasons why ½ LFL may be a more valid safety criterion than LFL (with an appropriate choice of concentration). Further attention is given to averaging time in Section 5.4.7.
1.4 MODEL EVALUATION

1.4.1 General considerations

Mathematical modeling

Mathematical modeling of a physical process involves schematically the steps summarized in Figure 1.3.

This is a very general summary of what lies at the heart of the scientific method. It is a recipe for gaining an improved understanding of the physical processes in question.

Some things are usually considered so obvious (to academic theorists among others) that they do not need to be said. These include:

(i) Implicit in step 1 is the idea that the model should be consistent with what one knows about related phenomena: the model must have a sound scientific basis. Without that the procedure is worthless.

(ii) Implicit in step 2 is the idea that the solution procedure is accurate, and does indeed provide a solution of the equations.

(iii) Implicit in all of it is the concept of a fitness for purpose. There is some purpose for which we are studying the process; the model must satisfy that purpose and the solutions must be accurate enough for that purpose.

Figure 1.3 Schematic outline of mathematical modeling of a physical process
Application to consequence analysis for industrial safety

This process underlies consequence modeling in industrial hazard analysis, where an understanding of what might happen in an accident is required. Predictions are required for the consequences of an accident which may never happen, and it may be so severe that an experimental simulation at full scale is impossible to perform. Therefore, the process would reach as far as step 4 in the flow diagram, with predictions for the accident, but with no means to test against experimental data.

For this reason, we require confidence in everything that has been done up to this point. With this uppermost in mind, the “Model Evaluation Group” (MEG) was set up by the Commission of the European Communities and tasked with providing a very general summary of how the scientific method should be applied to consequence assessments.

They emphasized (MEG, 1994a, b) three important aspects of the procedure as:

- The scientific basis: the model must be credible and fit for purpose, (see (i) above)
- Verification: it must be shown that the solution procedure (usually a computer program) produces solutions of the model equations to satisfactory accuracy, (see (ii) above)
- Validation: the model must be shown to agree with relevant experimental observations to satisfactory accuracy, (see (iii) above)

The concept of “validation” requires some consideration: Comparison with an experiment can never show that a model is “valid”. The best it can do is to fail to show that the model is “invalid”. A validated model is therefore one where tests have been performed which could have shown it to be invalid, but which failed to do so.

Therefore, it is often a useful exercise to compare the predictions of different models. If they are found to disagree significantly then further examination of one or both should be made to identify the reasons for the discrepancies. Such model comparisons can be done with envisaged accident scenarios where experimental data may be hard to come by.

Validation is an open ended process (corresponding with the non-closure of the scientific method outlined above) but in practice it ends when one has sufficient confidence in the model.

However, the MEG was aware that the model evaluation procedure would need further particularization and refinement (in different directions) so that it could be applied to different specific areas of consequence analysis, and different authors have derived protocols for model comparison and validation in different areas. The objective in this report is to derive a protocol appropriate for models used in analyzing the safety of the handling of LNG.

1.4.2 SMEDIS

The EU-sponsored SMEDIS project (Carissimo et al., 2001; Daish et al., 2000) took as its starting point the MEG’s reports (MEG, 1994a, b) and produced a more detailed protocol for evaluating heavy gas dispersion models.

In order to develop a specific protocol for LNG dispersion models, the SMEDIS protocol is used as a starting point with the following objectives:

- To particularize to the physical phenomena expected in LNG dispersion, omitting irrelevant aspects which may be present in other heavy gases
- To give due consideration to the relevant source terms
1.4.3 The work of Hanna et al.

In the USA, the prime example of heavy gas dispersion model evaluation was work undertaken by Hanna et al. (1991, 1993). They compared a number of models with a number of data sets and presented overall measures of the average fit of each model to the data, and of the variability of the fit for continuous passive releases, continuous dense gas releases, and instantaneous dense gas releases.

It is important to note that Hanna et al. were not involved in developing any of the models, but rather used them as independent assessors. Hanna et al. did not review the scientific basis of any of the chosen models or their verification, and so this should be regarded as a (major) validation exercise rather than a full model evaluation in the sense of the MEG, although they did give some reasons for certain aspects of the results.

In order to compare the models and data on the same basis, Hanna et al. created an archive with data from all the experiments included in a common format. They also wrote pre-processing software to read the data archive and generate the input conditions for each model, and post-processing routines to produce the defined physical comparison parameters and statistical performance measures used to determine ‘goodness of fit’. This was a major, four year long, exercise.

Hanna et al. also observed that model documentation seldom contained anything concerning the models’ limitations, but the developers of the models tended to claim a very wide applicability for their models. The MEG make a point of mentioning the desirability of documenting the design limitations.

Hanna et al. also observed that allowing models, where possible, to predict the emission rate resulted in much greater discrepancies than would have been the case had they input the best approximation to the observed emission rates. This emphasizes the need to evaluate source models along with dispersion models.

1.4.4 Recent work

Since this report was first published in 2007, further work has been carried out in developing approaches for evaluating models used in safety assessments. In particular, a project called SAPHEDRA was jointly undertaken by a number of European organizations, on “Building a European platform for evaluation of consequence models dedicated to emerging risks”. The project members were: INERIS (France), BAM (Germany), Demokritos (Greece), the Health and Safety Laboratory, HSE (UK), RIVM (The Netherlands), TNO (The Netherlands) and Università di Bologna (Italy). The project is currently nearing completion and a number of publications are currently available¹:

- WP1: Identification of existing tools for the modeling of hazardous phenomena
- WP2: Gap Analysis for Emerging Risk Issues
- WP3: Review and analysis of previous model evaluation protocols

¹ [http://projects.safera.eu/project/14](http://projects.safera.eu/project/14) (accessed 30th June 2016)
• WP4: List of experimental campaigns and information available to be used to evaluate existing tools or new tools

A further European project on model evaluation, SUSANA, has been carried out specifically looking at the use of CFD models for hydrogen safety applications (Coldrick et al., 2015; Baraldi et al., 2016). The project included the development of a validation database including experiments on gas dispersion, fires and deflagrations.

1.4.5 LNG Dispersion Model Validation

Before concluding this section, it is important to note that any model validation exercise focused on LNG dispersion should not limit itself to datasets involving only LNG. Any appropriate model will also cover isothermal gas dispersion and possibly other, more complex situations. Any validation should cover all of these: the validity of a model which fits LNG dispersion data, but fails to fit simpler cases, would clearly be in some doubt.
2 LNG DISPERSION MODEL EVALUATION PROTOCOL

2.1 OVERVIEW

This Section describes the LNG Model Evaluation Protocol (MEP). It is based on the SMEDIS protocol for dense gas dispersion models, which itself was in a form consistent with the EC Model Evaluation Group (MEG) generic protocol (MEG, 1994a, b) and the Heavy Gas Dispersion Expert Group (HGDEG) protocol (Mercer et al., 1998). However, the SMEDIS protocol contained much content that is not relevant to LNG vapor dispersion and so a specific version of the protocol has been developed.

The objectives and guiding principles of the LNG MEP are as follows.

The purpose of the MEP is to provide a comprehensive evaluation methodology for determining the suitability of models to accurately simulate the dispersion of vapors emanating from accidental spills of LNG on land.

The protocol is applicable to a wide range of dispersion models, primarily CFD and integral models, but also empirical models and shallow layer models. Some of these models will be designed specifically for modeling the dispersion of LNG vapors, others, particularly the CFD models, will not.

The key steps in the application of the MEP are a scientific assessment, verification and validation of the model. These three key stages of the MEP are described in detail in the following three Sections.

The information required to undertake the scientific assessment is obtained via a questionnaire that is completed by the ‘model developer’ or a ‘proponent for the model’. This person does not necessarily have to be the original model developer, but it does need to be someone who has an intimate knowledge of the model.

The MEP is specific to one and only one version of a model. This will be recorded clearly in the model evaluation report. After the MEP has been applied to a particular model it is the responsibility of the user to ensure that the model is the same as that which has undergone the evaluation using the MEP.

A key principle in the application of the MEP is that model evaluation is either carried out, or reviewed in detail, by a suitably qualified independent third party. Ideally the scientific assessment should be carried out by the independent expert. However, in practice the MER may be written by the model developer and then reviewed by the independent expert. In general, due to the effort involved, the validation exercise may be carried out by the model developer. The validation exercise is not expected to be a ‘blind test’, although any changes made to the model during the validation exercise should be documented.

Parts of the procedure involving the active use of the model must be documented to make them auditable and the results reproducible. This would apply even if an independent third party were performing the evaluation. For the validation of the model against the LNG MEP Database, the model should be used in the manner in which it would be used in practice for an LNG siting application.

The MEP should not be biased to any one model or type of model. Two examples illustrate the point. The MEP consists of a number of qualitative acceptance criteria (see Section 3.1) which include a number of physical factors that the model should take into account. These have been designed such that they do not exclude models which can be appropriately used where neglecting these physical parameters leads to conservative results or has negligible effects on the result. Secondly, the validation database consists of two sets of data, one for flat terrain the other for cases with
obstacles or complex terrain, such that even if a model were to perform poorly for the latter cases, it
could still be accepted as suitable for the former.

The performance of the models is quantified using a range of data sets and performance measures,
including quantitative statistical comparison techniques. However, ranking of models according to
their performance is not carried out.

This MEP is only applicable to dispersion models, although it is recognized that accompanying
models and in particular the associated source model play a very important role in determining the
hazard associated with a spill of LNG.

Ideally, the information produced by the evaluation should be available to the public. However, it is
recognized that for proprietary models this may not be possible, although some form of openly-
available results would be desirable, and it is hoped the Model Evaluation Report (MER), see below,
would be treated in the same way as other documentation on a model.

The development of the MEP includes some uncertainty. It would be appropriate to review the
updated MEP after it has been applied to a number of models, particularly the quantitative
evaluation criteria with respect to point-wise concentrations. Application of the MEP will reveal
what a model does and highlight whether it is obviously poorly designed but, in the case of a
generally acceptable model, the MEP may fall short of conveying/acquiring a full understanding of
the system. Therefore, the application of the MEP should be undertaken very much in the spirit of
“validation”, which never makes a model valid: if successful, it merely fails to invalidate it.

2.2 HOW TO USE THE MEP

The MEP is split into three main phases: Scientific Assessment, Verification and Validation. Further
details are provided in Sections 3, 4 and 5, respectively. The three phases can be carried out in
parallel with each other. The validation exercise requires the model to be run against the LNG Model
Validation Database (Stewart et al., 2016), as described in Section 5, and will therefore be the most
time consuming of these phases (considerably so for CFD models).

2.3 QUESTIONNAIRE

The purpose of the questionnaire is to request the information which is needed for the scientific
assessment of an LNG dispersion model from the model developer or proponent. The model
developer or proponent should have an intimate knowledge of the model and this may therefore
exclude developers who merely package an existing model. The questionnaire is included as an
appendix to this report (see Section 13.1).

The completed questionnaire should be returned with a set of documentation covering all aspects of
the model and, preferably, cross-referenced to the topics in the questionnaire. The accompanying
documentation should include user manuals, published papers, reports etc. Confidential documents
should be clearly indicated. Of particular interest are peer-reviewed applications of the model in the
technical literature, validation exercises and also any other validation exercises that may not have
been made publicly available (note that confidential information will not be included in the model
evaluation report).
The questionnaire includes a set of guidelines following the questions to help the model developer/proponent to provide the required information. It is essential that these guidelines are used to complete the questionnaire.

The information supplied should refer to a single well-defined version of the model, which should be unambiguously identified.

The questionnaire is based on the form derived by the European Commission’s SMEDIS project but has been particularized (with emphasis on guidelines to support interpretation of the questions) to models dealing with the dispersion of LNG.

The questionnaire is aimed at all types of model such that they can be compared on an equal basis, and therefore answers to some questions may be almost trivial in some cases.

The questionnaire is split into the following sections:

1. General information
2. Information for scientific assessment
3. Information for user-oriented assessment
4. Information on verification
5. Information on validation
6. Administrative details
   - Guidance on completing the questionnaire

### 2.4 MODEL EVALUATION REPORT (MER)

The MER is the key output of the application of the MEP. It contains the full details of the scientific assessment, which is based on information provided in the questionnaire and associated documentation. The model evaluation report is presented in the appendices of this report as applied to DEGADIS (Section 10.2), FEM3A (10.3) and FLUENT (10.4).

The MER provides conclusions on the scientific basis of the model, limitations of the model, user-orientated aspects of the model, the model verification and validation performed as well as the evaluation against the MEP qualitative and quantitative assessment criteria.

Additionally, the PHMSA Advisory Bulletin ADB-10-07 (PHMSA, 2010) provides specific further information to be included in the MER. This additional information should be included in the MER where approval is sought for an alternative vapor-gas dispersion model to be used for performing LNG dispersion calculations for LNG siting applications under 49 CFR 193.2059. The MER also makes provision for comments from the model developer, which in practice will prove to be essential in ensuring that all of the details of the model are captured accurately.

The MER is structured as follows:

0. Evaluation information
1. General model description
2. Scientific basis of model

3. User-orientated basis of model

4. Verification performed

5. Evaluation against MEP qualitative assessment criteria

6. Validation performed and evaluation against MEP quantitative assessment criteria

7. Conclusions

A1 Actively-generated information

A2 Comments from model supplier / proponent

The main headings above (1-6) are subdivided into the assessment categories which are structured in a consistent way as follows:

- General remarks on the category

- Topics of interest describing the subjects relevant to the category. This means that there should be information available covering each subject and the evaluator should check that this is the case. If none is available this can be noted together with the reason for its absence and recorded later in the MER (this may prove useful in the revision of the protocol)

- Assessment and comment gives aspects of the topics of interest that should be considered by the evaluator, i.e. this section suggests ways that the information on the topics of interest can be assessed

- Contribution to the evaluation record describes the part to be added to the evaluation record, i.e. the MER, for this category. It gives the relevant headings from the MER, followed by the general form of the content under each heading. The contribution typically involves a combination of some reporting of the information describing the topics of interest, e.g. summarizing that aspect of the model, followed by assessment of/comment on the information.

The evaluator must provide a description or an assessment of the model under each category in turn. Note that each category should be addressed to a level of detail that:

- Concentrates on the most relevant features, and does not reproduce the information to an excessive degree

- Does not demand an unreasonable amount of analysis, e.g. assessing the limits of applicability of a model

It is recognized that further advisory bulletins may be issued in the future; where this is the case, the MER should incorporate all requirements of such.
3 SCIENTIFIC ASSESSMENT

The scientific assessment is carried out by critically reviewing the physical, mathematical and numerical basis of the model. The information on which this review is based is taken from literature made available for this purpose, which may include published material, and a completed questionnaire that has been specifically designed to extract the necessary information. When this information has been obtained the scientific assessment is carried out and the findings are recorded in the MER.

To carry out the scientific assessment, the reviewer should have an in-depth understanding of the behavior of dense gas clouds and the application of dispersion models. To carry out a review of a CFD model then the reviewer should have additional understanding of this modeling approach. Clearly the reviewer should also be independent of the model developer and should have no vested interest in the outcome of the model evaluation. However, it is accepted that it may be appropriate for the model developer to be involved in, or carry out some or all of the validation exercise.

3.1 SCIENTIFIC ASSESSMENT/ QUALITATIVE CRITERIA

The qualitative assessment criteria are presented below. The following further description of the criteria (Section 3.2) should be read in conjunction with this summary.

Scientific criteria

1. Key details of the model available for scientific assessment
2. Model based on accepted/published science
3. Model accepts a credible source term
4. Model accounts for the effects of wind speed
5. Model accounts for the effects of surface roughness on dispersion
6. Model accounts for the effects of atmospheric stability on dispersion
7. Model accounts for passive dispersion
8. Model accounts for gravity-driven spreading
9. Model accounts for the effects of buoyancy on dilution
10. Numerical methods are based on accepted / published good practice

Output criteria

11. Model produces output suitable for assessment against MEP statistical performance measures

3.2 JUSTIFICATION FOR QUALITATIVE CRITERIA

In this Section, the reasons for choosing the qualitative assessment criteria are justified. In some cases, the reasons are obvious and therefore little reasoning is included. In general, the predictions
of distance to ½ LFL correlate strongly with the physical parameters that make up the qualitative criteria. We additionally describe why some other possible criteria have not been included.

1. **Key details of the model available for scientific assessment:** To carry out a scientific assessment of a model requires that detailed information on the physical and numerical basis of the model is available.

At a more fundamental level, the model’s results must be entirely reproducible. If two methods of analysis obtain different results, then both must be open to scrutiny in order to resolve why. In this case, two parties with opposing ideas on the safety of an installation, or a proposed installation, based on the results of different models (or indeed different applications of the same model) must be able to resolve the situation scientifically, by examination of the differences in their procedures. Use of models whose details are not available for scrutiny prevents this.

2. **Model based on accepted/published science:** The model should be based on sound physical principles building on, or using, modeling techniques that have gained acceptance through publication in peer reviewed journals etc.

Importantly, it is not sufficient that a model has been published in a peer-reviewed journal, for a number of reasons, not least because published papers may reflect the state of knowledge at the time of publication but contain ideas which are found to be erroneous by subsequent research. Moreover, industrial employers (rather than academia) may prefer publication in internal reports, or reports to clients. These reports also have the advantage that they can go into more detail of a model than would be considered appropriate for some peer review journals. Furthermore a new model, which is based on science now thoroughly accepted, may not be thought worthy of publication in a journal which is looking for innovative ideas.

However, it is important that the model is based on accepted ideas, which have been subjected to scientific scrutiny in journals and conference papers.

Any innovative modeling aspects should be specifically highlighted and their use justified by scientific argument, verification, and validation.

Furthermore the effect of any “innovative aspect” on the results of a hazard analysis should be made clear. For example, if it is argued that model A is “better” than model B because it includes such and such an effect, then model A should also be run with the effect switched off, and arguments presented to show that

- The results are then comparable with those of model B
- The differences in model A when the effect is included/excluded are scientifically reasonable

If either of these is not demonstrable, then the need for further work is signaled. In the case of clouds from LNG releases, these considerations may include the effect of obstacles to the flow, or the effect of atmospheric humidity.

3. **Model accepts a credible source term:** The specification of the source is probably at least as important as the dispersion model itself and therefore it is important that an appropriate source model is used. Guidance on LNG source term models is provided by Webber et al. (2009). Any uncertainty in the model’s predictions should ideally lead to conservative results.

In the case of LNG, the usual scenario will be a liquid spill resulting in a boiling pool. This may also be spreading (on the ground or on water). A pool restrained by a dike may cool the ground under it, reducing and the heat transfer rate and hence also the boiling rate. The boiling rate may decrease to
the extent that the air removes material faster than it is vaporizing, in which case the pool will cool. However, a spreading pool (on land) will continue to encounter new warm ground and may boil vigorously for longer. A pool floating on deep water can continue to acquire heat by convective transfer in the water.

The interface between the source and dispersion in this case is clear: the liquid flow is part of the source whereas the gas flow is dispersion. If it is necessary to use an input model to the dispersion model which takes into account the initial dispersion of the gas, e.g. due to a limitation of the dispersion model to take into account the presence of obstacles, then this input model should also be subject to the model evaluation protocol. If this does not happen then the ‘dispersion model’ has only been partially evaluated.

The cloud above the pool may spread across the wind direction and upwind from the source, and dispersion models should allow for this. The cloud may also encounter walls near the source but will be less affected than is the liquid. Any such considerations will be part of the dispersion model.

4. Model accounts for the effects of wind speed: Higher wind speeds will advect the cloud more rapidly but also, other things being equal, higher atmospheric turbulence will dilute the cloud more rapidly. The relative importance of these effects on concentration as a function of downwind distance is not always the same, as the wind speed varies with height and there is also gravity driven turbulence production even in the absence of wind. Allowing for all of this is crucial.

5. Model accounts for the effects of surface roughness on dispersion: The aerodynamic roughness length is a property of the air flow, which relates wind speed at a given height to turbulent transport. Its value is determined in a complicated way by the nature of the ground surface. It is one of the factors affecting the relative rates of advection and dilution mentioned in the previous paragraph.

6. Model accounts for the effects of atmospheric stability on dispersion: Turbulent transport in the atmosphere is affected by more than just the wind speed and the surface roughness. The third important determinant is atmospheric stability. If air near the ground is colder than air above (stable atmosphere), mixing is suppressed as the vertical density gradient acts to damp out vertical movement and mixing of air. Conversely warmer, less dense, air near the ground (unstable atmosphere) will result in enhanced vertical mixing. Thus for any given wind speed and roughness length, both the vertical wind-speed profile and the turbulence intensity, will depend on atmospheric stability.

It should be noted that a heavy gas cloud can easily introduce a stronger vertical density gradient than anything inherently in the atmosphere. However, gravity spreading also generates turbulence and this is increased by the same factors suppressing vertical mixing. For a period, gravity driven mixing (edge entrainment) will dominate and atmospheric stability makes little difference. However, a more stable atmosphere will delay the onset of atmosphere-driven mixing (top entrainment) and atmospheric stability is therefore important.

7. Model accounts for passive dispersion: the most important quantity which distinguishes heavy gas dispersion from passive dispersion is typically the Richardson number $g'h/(u^*)^2$. Here $g'$ is the acceleration due to gravity multiplied by the relative density difference and so for a cloud of great enough height $h$, in an atmosphere of small enough friction velocity $u^*$, the cloud can still be ‘heavy’ when it dilutes to LFL and below. Conversely, a smaller cloud of the same gas in a more turbulent atmosphere can disperse effectively passively even while it is relatively concentrated. It is therefore important that models can cope with this.

8. Model accounts for gravity-driven spreading: Heavy gas clouds spread under their own weight forming a gravity current. Thus, heavy plumes tend to be lower and wider than passive plumes.
9. **Model accounts for the effects of buoyancy on dilution:** A heavy cloud suppresses any vertical mixing due to atmospheric turbulence because of the strong stable density gradient. Models must encompass this. However, in the early stages, much of the turbulence powering the mixing can be generated by the gravity driven spreading motion; the stronger the gravity current, the stronger the turbulence generation. In contrast with atmospheric turbulence, mixing powered by gravity does not suffer the same suppression as that powered by atmospheric turbulence. In this way, the spreading significantly affects the dilution near the source, a feature which must be included in any model. These features are all expected to be controlled by a Richardson number.

10. **Numerical methods are based on accepted/published good practice:** Current best practice should be employed by the numerical model. This is not just to ensure that the results are of the highest accuracy possible, but more importantly to make sure that erroneous solutions are avoided that could be due to the use of inappropriate numerical methods.

Extensive guidelines exist for CFD in particular (e.g. Casey and Wintergate, 2000) and they cover topics such as numerical discretization and mesh dependence.

In the case of integral models, which typically employ ordinary differential equations, the importance of applying best practice in the numerical model is equally true. Despite the ready availability of a number of well-tested commercial solvers, which employ sophisticated methods that control errors, many model authors prefer to recode their own, using relatively simple methods with no real error control in the modern sense. Examples of such include the 4th-order Runge-Kutta method, or, even worse, Euler’s method. Runge-Kutta may be satisfactory in some cases, but it is better to simply by-pass any uncertainties with the method (and its implementation in the model) by using a more sophisticated approach generated by specialists in numerical mathematics.

A further advantage in using a commercial library is that it forces a separation in the code of the calculation of terms in the equations from their use in the solver. If one does not do this, it is all too easy to introduce “corrections” which are only first-order accurate, leading to an erroneous impression that one is using a 4th-order accurate method just because some “Runge-Kutta equations” are also present.

11. **Model produces output suitable for assessment against MEP statistical performance measures:** In general, suitable output consists of a (well defined) measure of the concentration expected at different points and or times. However, output of a wider variety of information makes the task easier and more reliable. This includes temperature, density, and aerosol content, Richardson number, cloud center position, and cloud dimensions.

**Final comments:** There are some features that have not been included in the qualitative criteria allowed for by some models and not by others.

As a general principle, if a model does not take into account physical factors, e.g. the existence of a fence, then it should be demonstrated that this will lead to conservative results, i.e. longer hazard ranges, or that the effect on the results is negligible. Indeed, this will influence the choice of model from the outset, for example in cases where there are significant variations in terrain then a model that cannot take this into account is unlikely to be appropriate. Additionally, where a model has taken into account physical factors that a model indicates will lead to a shortening of hazard ranges, then this should be shown to be appropriate.

Note that the following physical factors have not been included as qualitative acceptance criteria but are in the current version of NFPA 59A: heat transfer, humidity and wind direction. Although heat transfer is clearly of vital importance in modeling the source, its effect on the LNG vapor dispersion is likely to be small. The wind direction is irrelevant in many cases for integral models that do not take into account topography or other physical obstruction in the vicinity of the vapor source.
Similarly the humidity of the air is unlikely to have a dominant effect on the vapor dispersion (although it is important for the dispersion of hydrogen fluoride and ammonia, which will undergo an exothermic chemical reaction with the water) and even if it were significant its influence will generally tend to result in shorter hazard ranges, see Section 1.3.4. Therefore a model that does not take these factors into account should not necessarily be excluded.
4 VERIFICATION

4.1 INTRODUCTION

Verification of a model is the process of comparing the implementation of a model with its mathematical basis. Most commonly this refers to checking that a computer implementation of a model (computer software) accurately represents its mathematical description.

Verification is essential, and should be demonstrable. A good start is provided if a numerical solver with a good track record (and published verification) is adopted. But even so, it should be demonstrated that the solutions presented are indeed solutions of the programmed equations. Models sometimes admit analytic solutions in special cases, and comparison with these is always useful. In other cases, asymptotes can be found analytically and a comparison can provide a useful test. In yet other cases, things are known about the solution, which emerge non-trivially from the numerical procedure, such as conservation of buoyancy, and this can be checked.

The European SUSANA\(^2\) project (Coldrick et al., 2015; Baraldi et al., 2016) has developed a database\(^3\) of verification tests for hydrogen CFD models that illustrates the type of tests that could be used in a verification exercise for LNG dispersion models. In the specific case of CFD models, the method of manufactured solutions (Roache, 1998) can also be used as a verification tool.

Verification does require a certain amount of mathematical skill, which is quite different from many of the engineering skills needed to model hazards.

4.2 MEP VERIFICATION

The verification of a model within the MEP follows the same approach as SMEDIS. This means that verification is treated passively as part of the scientific assessment instead of an exercise in its own right. Evidence for verification is therefore sought from the model developer and this is assessed and recorded in the MER.

Note that verification of the model is not a qualitative assessment criterion, although it is reported in the MER. The reason for this is that the absence of information or evidence of verification would not be a sufficient reason to reject a model. Also, the judgment that needs to be made on whether a model has been verified is subjective as well as being reliant on claims made by the model developer/proponent, which are impractical to substantiate. For example, two different reviewers could easily reach different conclusions depending on how rigorous they choose to be in demanding evidence of verification.


5 VALIDATION

5.1 INTRODUCTION

Validation is the process of comparing model results to measured data for scenarios that test the physics that the model is intended to predict. A validation database containing these measurements provides the means to assess the performance of a model. The end objective of validation is to establish whether a model replicates reality to an acceptable degree.

Although we use the term ‘validation’, and this is the accepted terminology, what we actually mean is ‘evaluation’. Over a prescribed range of applications sufficient confidence in a model may be gained by comparison with measurements such that the model has been evaluated and found to perform acceptably well across this range of applications.

In this Section we set out the basis of the validation procedure based on the approach adopted and developed during the SMEDIS project (Daish et al., 2000; Carissimo et al., 2001) and further explained in Duijm & Carissimo (2002).

The validation procedure involves a number of differing aspects, addressed in the following steps:

a) Specification of the objective: this being the quantification and assessment of model performance for dispersion of LNG vapor from spills on land

b) Identification of the key physics and variables involved in the dispersion of LNG vapor from spills on land

c) Identification of target scenarios that cover the key physical processes involved in the dispersion of LNG vapor from spills on land. Ideally, these scenarios are sufficiently wide-ranging that the performance of a model can be tested over the full range of key physical variables (source terms, atmospheric conditions, terrain, etc.)

d) Identification of suitable validation datasets

e) Selection of specific cases from these datasets so as to cover the range of target scenarios

f) Definition of physical comparison parameters (PCP) that are measured or derived from measurements and which form the basis of comparisons with model predictions

g) Selection of statistical performance measures (SPM) that allow a quantitative comparison of predictions against measurements

h) Review and definition of quantitative assessment criteria that define the acceptable numerical range of the SPM which result from applying this validation procedure

Steps b) and c) are addressed in Section 5.2.

Steps d) and e) are addressed in Section 5.3.

Steps f) and g) are covered in Section 5.4 and 5.5.

Step h) is covered in Section 5.7.
5.2 KEY PHYSICS AND TARGET SCENARIOS

The key physical processes involved in the dispersion of LNG vapor over land have been discussed in Section 1.3.

More comprehensive descriptions of the phenomenology can be found in a series of reports and papers from the Lawrence Livermore National Laboratory (Koopman et al., 1982a; Morgan et al., 1984; Koopman & Ermak, 2007). These stem primarily from large-scale, unobstructed, field trial spills of LNG at China Lake, California, in which dispersion occurred over land. Phenomenology in the presence of obstructions comprising a vapor fence and barrier is provided by Brown et al. (1990) and also addressed briefly by Koopman & Ermak (2007).

Additional phenomenology, gained from LNG spills at Maplin Sands in the UK and in which dispersion occurred over the sea, is provided by Puttock et al. (1982) and Colenbrander & Puttock (1983).

Other recent reviews (Luketa-Hanlin 2006; Cleaver et al., 2007) also provide further insight into the key physical processes involved in the dispersion of LNG vapor.

In summary form, the key physical processes involved in the dispersion of LNG vapor over land are as follows:

- Formation of a dense cloud due to the low boiling point of LNG
- Gravity-driven spreading
- Advection by the ambient wind field
- Reduction in turbulent mixing due to the resulting stable density stratification
- Dispersion influenced by atmospheric stability

Other physical processes can also be important, with their significance dependent on the particular circumstances of a release. These could include:

- Enhanced mixing and dilution due to obstacle-generated turbulence
- Influence of terrain on gravity spreading
- Vapor hold-up due to fences or dikes
- Heat addition and removal due to condensation and evaporation of water vapor
- Heat transfer from the ground

Ideally, scenarios which are used to define the specific test cases in the validation database should encompass the key physical processes. This is most comprehensively achieved by consideration of field trial spills of LNG.

It is also preferable to test a model over as wide a range of conditions as possible, i.e. for a broad range of scenarios. As outlined in Section 5.1, these scenarios should ideally be sufficiently wide-ranging that the performance of a model can be tested over the full range of key physical variables (variation in source terms, atmospheric conditions, terrain, etc.).
The key physical variables affecting dispersion of LNG vapor over land are as follows:

- Source configuration: release rate, duration and pool geometry
- Atmospheric conditions: stability, wind speed, humidity
- Terrain: surface roughness, flat/sloping/complex terrain
- Obstacles: tank, dike, fence, etc.

In principle, a matrix of target scenarios based on the above physical variables, which encompass the key physical processes, could be constructed. Test cases would then be defined which meet entries in this matrix. This was the approach adopted in SMEDIS, which led to a matrix of 45 scenarios for which test cases were found. As will become more apparent in Section 5.3, such an approach is not practicable for dispersion of LNG vapor over land because:

- Data do not exist to allow all target scenarios (i.e. all combinations of factors which may be relevant for LNG dispersion in different circumstances) to be met
- Even if data were available, the matrix could become impractically large (note that the SMEDIS project extended from 1996 to 1999 and in that time only about one third of the entire set of test cases were computed and analyzed, approximately 300 in total)

This being the case, a modified approach is required such that the main physical processes are tested for a set of scenarios covering a more focused range of key physical variables. In practice, the scenarios and test cases are governed by the availability of appropriate data.

5.3 DATASET SELECTION

5.3.1 Data requirements

To be useful for model validation, data must fulfill several requirements. These include:

- The quality of the data must be fit for purpose, i.e. model evaluation. Nielsen & Ott (1996) discuss the meaning of data quality in this context and describe methods of screening and checking the quality of data for model evaluation
- The test conditions must be known, including source configuration, atmospheric conditions, surface roughness etc. Duijm & Carissimo (2002) stress the importance of reliable information on the source term and release rate
- The time-averaging applied to the data must be specified. For flammables, as here, data should be available for short time-averages
- If wind tunnel data are to be used then scaling effects are crucial and must have been considered in the design and reporting of experiments. Scale factors should be within acceptable ranges. Meroney & Neff (1982) discusses appropriate scaling rules and scale factors for wind tunnel simulations of LNG releases
- The data must be available and in suitable formats
Although the above requirements are quite stringent, they can be met for a range of test cases that do address the main physical processes involved in dispersion of LNG vapor over land.

Ideally, multiple realizations of an experiment will also have been undertaken so that ensemble-mean values are available. Note that the vast majority of models produce an output which is essentially an ensemble-mean. Davies (1987) showed, by analysis of wind-tunnel trials, that multiple repeats of an instantaneous release of a dense gas under nominally identical conditions can produce concentrations at downstream locations that vary by roughly a factor of two. Unfortunately, ensemble-mean data are rarely available, especially for field trials.

5.3.2 Dataset Overview

Further details of the following experimental datasets, which are included in the validation database, are provided in the Model Validation Database Guide Version 12 (Stewart et al., 2016). The remainder of this section provides a brief overview.

The most significant and useful datasets resulting from field-trial spills of LNG without obstructions are from Maplin Sands performed by Shell Research in 1980 (Puttock et al., 1982; Colenbrander & Puttock, 1983), and the Burro and Coyote trials performed by Lawrence Livermore National Laboratory in 1980 and 1981 (Morgan et al., 1984). A comprehensive overview of these trials is provided by Ermak et al. (1988).

The only significant field-trial spills of LNG in the presence of obstructions are the Falcon trials undertaken in 1987, by Lawrence Livermore National Laboratory (Brown et al., 1990).

These four trials have recently been reviewed by Luketa-Hanlin (2006) and Koopman & Ermak (2007) and so only a brief summary is provided here.

The Maplin Sands trials undertaken by Shell Research in 1980 comprised spills of either LNG or LPG onto water with dispersion occurring over tidal sands (most experiments were performed at high tide). Some releases were ignited. Both continuous and instantaneous releases of LNG were undertaken. Of the thirteen continuous LNG releases, eight were deemed to provide useful data. These continuous releases were directed vertically downwards onto the sea surface from a range of heights, and in some trials the release impinged on a cone and plate device designed to restrict initial spreading of the liquid to the horizontal direction. The release rates ranged from 1 to 4.5 m$^3$/min, in wind speeds of between 2 and 10 m/s, all in neutral atmospheric conditions. A large number of sensors were arranged in downstream arcs floating on 71 pontoons. Data was obtained at a minimum averaging time of 3 s. The trials and their analysis are described by Puttock et al. (1982) and Colenbrander & Puttock (1983) and a useful summary of the test conditions is given by Ermak et al. (1988).

The Burro trials were undertaken at China Lake, California in 1980. Dispersion occurred over land, although the spill was onto a 58 m diameter water pool. The releases were initially directed vertically downwards but impinged on a splash plate to limit LNG penetration into the water. A series of nine tests were undertaken. Spill rates ranged from 11.3 to 18.4 m$^3$/min, in wind speeds from 1.8 to 9.1 m/s. With one notable exception, all of the releases were undertaken in either neutral or slightly unstable atmospheric conditions. The exception was the Burro 8 trial, which took place in stable conditions (Pasquill-Gifford stability class E) at a relatively low wind speed of 1.8 m/s. The Burro 8 test is the only well-instrumented unobstructed field trial release of LNG in stable atmospheric conditions. Gas concentration sensors were arranged in four arcs at 57, 140, 400 and 800 m downstream from the release point. Data were obtained at a minimum averaging time of 1 s. The test site terrain was not flat, in general tending to slope upwards downwind from the release,
but in a non-uniform manner. The trials are presented, described and analyzed in Koopman et al. (1982a, 1982b) and Morgan et al. (1984), and are also summarized in Ermak et al. (1988).

The Coyote trials were a follow-up to the Burro trials and were primarily designed to investigate RPTs and the consequences of ignition. Nevertheless, significant dispersion data were also obtained. Releases took place using the same release configuration as the Burro trials. Spill rates ranged from 6 to 19 m³/min, although the trials that are useful for dispersion model evaluation involved spill rates in the range 13.5 to 17 m³/min. The wind speeds for these useful dispersion trials ranged from 4.6 to 9.7 m/s. The atmospheric stability was either neutral or slightly unstable. The gas concentration sensors were clustered in four arcs between 140 and 400 m downstream from the point of release. The trials are presented, described and analyzed in Goldwire et al. (1983) and Morgan et al. (1984), and are also summarized by Ermak et al. (1988).

The Falcon trials were undertaken to examine the effectiveness of fences to mitigate the effects of accidental releases of LNG. The trials were carried out at Frenchman Flat, Nevada in 1987. Five trials were undertaken in which LNG was released onto a 40 × 60 m water pond via 4 spill pipes. A splash plate was fitted underneath each pipe so that LNG was directed across the surface of the pond. A fence of height 8.7 m surrounded the water pond. Upwind of the pond, but inside the fence, a ‘billboard’ structure was located to generate turbulence in a similar manner to that which could be expected from a storage tank. This billboard was 17.7 m long by 13.3 m high. Spill rates from 8.7 to 30.3 m³/min were obtained in these trials. The wind speed ranged from 1.7 to 5.2 m/s. Significantly, the atmospheric stability was either neutral or stable during these trials. In particular, the Falcon 1 trial was undertaken in very stable conditions (Pasquill-Gifford stability class G). Gas concentration sensors were clustered along three lines at 50, 150 and 250 m from the downwind edge of the fence. The data report (Brown et al., 1990) provides a comprehensive description of the tests and presents the data in graphical form.

Table 5.1 summarizes the main features of these four sets of LNG trials.

<table>
<thead>
<tr>
<th>Trial</th>
<th>Spill type</th>
<th>Release rates (m³/min)</th>
<th>Wind speeds (m/s)</th>
<th>Atmospheric stability</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maplin Sands, 1980</td>
<td>Water pool</td>
<td>1 - 4.5</td>
<td>2 - 10</td>
<td>D</td>
</tr>
<tr>
<td>Burro, 1980</td>
<td>Water pool</td>
<td>11 - 18</td>
<td>1.8 - 9.1</td>
<td>C - E</td>
</tr>
<tr>
<td>Coyote, 1981</td>
<td>Water pool</td>
<td>13.5 - 17</td>
<td>4.6 - 9.7</td>
<td>C - D</td>
</tr>
<tr>
<td>Falcon, 1987</td>
<td>Water pool</td>
<td>9 - 30</td>
<td>1.7 - 5.2</td>
<td>D - G</td>
</tr>
</tbody>
</table>

Several observations can usefully be made at this point:

- Almost all field trial spills of LNG are under neutral conditions and mostly at moderate to high wind speed
- With the exception of the Falcon trials, most field trial spills of LNG are in unobstructed conditions
- The source configuration for field trial spills of LNG is limited to pools, rather than line sources characteristic of spills in a trench

In addition, although the LNG release rate is essentially steady for a period of typically a few minutes in these trials – leading to quasi-continuous releases - almost no information exists on the time-varying dimension of the resulting LNG pool (although, where practicable, mass balance calculations indicated that the release rate was approximately matched by the overall vaporization rate). This introduces uncertainty in the specification of the vapor source term. As an illustration of how the
pool dimension may vary, HSL has applied a sophisticated liquid spill model, GASP (Webber, 1990), to the Burro 8 trial. Figures 5.1 and 5.2 indicate that the pool radius never reaches a steady-state and is likely to grow to a maximum radius of about 16 m.

![Figure 5.1 GASP prediction of LNG pool radius for Burro 8 trial](image)

![Figure 5.2 GASP prediction of mass of LNG vaporized for Burro 8 trial](image)

Ermak et al. (1982) modeled the Burro trials assuming that the LNG covers the entire surface of the 58 m diameter water pond, but the LNG spill model results in Figure 5.1 indicate that this is unlikely to be the case; Ermak et al. recognized this uncertainty in the source term.

The uncertainty in the pool radius, which is common to all four sets of field trials, can be reduced if an appropriate liquid spill model is used to predict the characteristics of the LNG spill. However, since there is some uncertainty in the LNG vapor source term for these trials, and also because the range of conditions in which experiments have been conducted is mostly limited to near-neutral conditions, it is also very useful to consider other field trial releases of dense gas.
Pre-eminent amongst these other field trials are those at Thorney Island, carried out from 1982 to 1984 in the UK, in which instantaneous or continuous releases of Freon/nitrogen mixtures were undertaken over flat terrain. For the continuous cases a release rate of approximately 4.3 m³/s of gas was obtained at an initial density ratio of about 2.0. The wind speed ranged from 1.5 to 3.2 m/s and the atmospheric stability from neutral to stable. Gas concentration sensors were located in a rectangular grid with distances up to about 800 m from the release point. Data was originally taken at high frequency. The trials are presented and analyzed in two special editions of the Journal of Hazardous Materials (Volumes 11 and 16, 1985 and 1987, respectively). The continuous releases are presented and analyzed in McQuaid (1987), Mercer & Nussey (1987) and Mercer & Davies (1987). Tabulated data for the continuous releases is also presented in Ermak et al. (1988) and is available from the HSL archives.

Wind-tunnel data is also included in the validation database. Indeed, any exclusion of wind tunnel tests would be unduly restrictive to the range of scenarios considered. Wind-tunnel tests, if carried out appropriately (Meroney & Neff, 1982), are also widely recognized and accepted as a valuable addition to field-trials data for model evaluation. They allow for more control and repeatability of tests. However, the effects of heat transfer and atmospheric stability are difficult to replicate in a wind tunnel, so most wind-tunnel data are for dense, isothermal, releases in neutral stability.

Wind-tunnel modeling has been completed by the Chemical Hazards Research Center, University of Arkansas, specifically to provide data for the evaluation of LNG dispersion models. Three sets of experiments have been undertaken, all with release of CO₂ as the dense gas simulant. Case A is a release without obstacles; Case B is in the presence of a storage tank and ‘high’ dike; Case C is in the presence of the dike only. A description of the experiments, as well as the tabulated data, is given in Havens & Spicer (2006a). The scaling relations and scale factor employed (150:1) are discussed in Havens & Spicer (2005, 2007) together with the implications of the results. This work repeats earlier work undertaken at the Chemical Hazards Research Center in the mid 1990’s. However, the earlier work used a smooth floor, whilst this later work used roughness elements on the floor of the tunnel to create turbulence properties similar to those which might be encountered in full-scale releases. The scaled spill is equivalent to a full-scale LNG release rate of 36 m³/min.

Extensive wind-tunnel modeling of LNG releases has also been carried out at Colorado State University from about the mid 1970’s to mid 1980’s, including examination of the effects of tanks and dikes. This body of work is reported in several publications, for example Meroney & Neff (1979, 1980 and 1982), Kothari & Meroney (1984). It established the validity and range of applicability of wind-tunnel experiments for simulating releases of LNG, provided analysis and guidelines on scaling rules and scale factors, and reported on the phenomenology of LNG releases, including the effects of tanks in enhancing mixing and dilution of LNG vapor.

The SMEDIS project also made extensive use of two wind-tunnel datasets generated as part of a project funded by the European Commission and undertaken by the University of Hamburg (Germany) and TNO (Netherlands), as well as other European organizations. These datasets are commonly referred to as BA-Hamburg and BA-TNO. In each case, sulfur hexafluoride (SF₆) was used as the dense gas simulant.

A very wide range of configurations was examined in the BA-Hamburg trials including a semi-circular fence placed upwind or downwind from a release, a fence completely surrounding a release, crosswind canyons, and sloping terrain. Most configurations were modeled with both instantaneous and continuous releases. Multiple repeats of many cases were also undertaken.

The BA-TNO trials consisted primarily of continuous releases over flat terrain with or without the presence of a fence of variable height. The fence was located downwind from the release and was perpendicular to the wind direction.
The BA-Hamburg and BA-TNO trials provide data on dense gas dispersion in the presence of a wider, more generic, range of obstacle configurations than that of the recent work at the Chemical Hazards Research Center, including sloping terrain.

Detailed electronic records are available for the Burro, Coyote, BA-Hamburg and BA-TNO trials via the REDIPHEM database (Nielsen & Ott, 1996). This database was constructed during the REDIPHEM project (1992 – 1995), funded by the European Commission. It comprises measurements from a significant number of field trials and wind-tunnel experiments. The database details the experimental configurations including release and atmospheric conditions, sensor positions, and time-series of measured parameters. The time-series are typically at 1 s intervals for the field trials. These time-series can be visualized, processed and exported using the REDIPHEM data browser. It is an extremely valuable resource for the evaluation of dense gas dispersion models. HSL was in direct contact with the original developers and custodians of the REDIPHEM database, at the Riso National Laboratory, Denmark, to obtain the database – which was freely available at the time of writing.

Detailed data reports for the Burro and Coyote trials are also available in the reports by Koopman et al. (1982b) and Goldwire et al. (1983).

Electronic records for the key Maplin Sands and Thorney Island field trials are available via the Modelers Data Archive (MDA) created by Hanna and co-workers during their extensive dense gas model validation exercise (Hanna et al., 1991, 1993). The MDA also contains data for the Burro and Coyote trials, as well as other dense gas field trials. The MDA consists of a summary of the experimental configurations, including release and atmospheric conditions, together with processed concentration measurements at arc-wise locations, maximum arc-wise concentrations and cloud widths. HSL has been in direct contact with the original developers and current custodians of the MDA to obtain the database and supporting documentation, which is available upon request (Hanna et al., 1991).

Tabulated data for the key Maplin Sands and Thorney Island trials are also available in the paper by Ermak et al. (1988). Data reports for the Maplin Sands trials are also available (Colenbrander et al., 1984a, b, c), which contain figures showing the measured time-varying concentration signals. Electronic data for the Thorney Island continuous release trials is available in the REDIPHEM database.

An extensive data report for the Falcon trials is available (Brown et al., 1990), from which long time-averages of gas concentration can be obtained.

The wind tunnel work undertaken at the Chemical Hazards Research Center, University of Arkansas, is available in tabulated form in Havens & Spicer (2006a).

It should also be noted that the quality of the data in the REDIPHEM and MDA database can usually be regarded as being the best which is available. In both cases, it has undergone in-depth scrutiny by the original developers before acceptance. Some errors in the REDIPHEM database that have recently been identified are discussed in the Model Validation Database Guide by Stewart et al. (2016).

5.3.3 Specific datasets and test cases

Specific test cases included in the validation database (Stewart et al., 2016) have been selected from the Maplin Sands, Burro, Coyote, Falcon and Thorney Island field trials, and the Chemical Hazards Research Center (CHRC), BA-Hamburg and BA-TNO wind tunnel experiments, and are presented in Table 5.2.
Table 5.2 Specific test cases for the validation database

<table>
<thead>
<tr>
<th>Trial</th>
<th>Field (F) or Wind tunnel (WT)</th>
<th>Trial/Case number and/or description</th>
<th>Atmospheric stability</th>
<th>Data source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maplin Sands, 1980</td>
<td>F</td>
<td>27 dispersion over sea</td>
<td>C-D</td>
<td>MDA. Also Ermak et al. (1988) and Colenbrander (1984a, b, c)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>34 dispersion over sea</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>35 dispersion over sea</td>
<td>D</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Burro, 1980</td>
<td>F</td>
<td>3</td>
<td>B</td>
<td>REDIPHEM. Also MDA, Burro data report, and Ermak et al. (1988).</td>
</tr>
<tr>
<td></td>
<td></td>
<td>7</td>
<td>D</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>8</td>
<td>E</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>9</td>
<td>D</td>
<td></td>
</tr>
<tr>
<td>Coyote, 1981</td>
<td>F</td>
<td>3</td>
<td>B-C</td>
<td>REDIPHEM. Also MDA, Coyote data report, and Ermak et al. (1988).</td>
</tr>
<tr>
<td></td>
<td></td>
<td>5</td>
<td>C-D</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>6</td>
<td>D</td>
<td></td>
</tr>
<tr>
<td>Falcon, 1987</td>
<td>F</td>
<td>1</td>
<td>G</td>
<td>Data report (Brown et al., 1990)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3</td>
<td>D</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>4</td>
<td>D-E</td>
<td></td>
</tr>
<tr>
<td>Thorney Island 1982-4</td>
<td>F</td>
<td>45 – continuous release</td>
<td>E-F</td>
<td>MDA. Also Ermak et al. (1988). HSE Data Archive</td>
</tr>
<tr>
<td></td>
<td></td>
<td>47 – continuous release</td>
<td>F</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>B – with storage tank &amp; dike</td>
<td>D</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>C – with dike</td>
<td>D</td>
<td></td>
</tr>
<tr>
<td>BA-Hamburg</td>
<td>WT</td>
<td>Unobstructed DA0120/DAT223</td>
<td>D</td>
<td>REDIPHEM.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Upwind fence 039051/039072</td>
<td>D</td>
<td>Also see Schatzmann et al. (1991), Nielsen &amp; Ott (1996), Marotzke (1993)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Downwind fence DA0501/DA0532</td>
<td>D</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Circular fence 039094/...097</td>
<td>D</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Slope DAT647/...631/...632/...637</td>
<td>D</td>
<td></td>
</tr>
<tr>
<td>BA-TNO</td>
<td>WT</td>
<td>TUV01 - unobstructed</td>
<td>D</td>
<td>REDIPHEM.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TUV02 – downwind fence</td>
<td>D</td>
<td>Also see Nielsen &amp; Ott (1996)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FLS – 3-D mapping</td>
<td>D</td>
<td></td>
</tr>
</tbody>
</table>

The selected Maplin Sands test cases are three of the four releases in the MDA of Hanna et al. (1991, 1993). Case 29 is omitted, since Ermak et al. (1988) stated that for this case sub-surface vaporization was considerable, leading to gas jetting as high as 10 m in the source area, such that specification of a vapor source term could prove problematic.

The four selected Burro test cases are those which have been most extensively analyzed and cover the widest range of meteorological and spill conditions (Koopman et al., 1982a; Morgan et al., 1984; Koopman & Ermak 2007). They include the Burro 8 case, which was undertaken in stable atmospheric conditions.

The three selected Coyote test cases are again those cases which have been most extensively analyzed (Morgan et al., 1984) and are regarded as benchmarks for dispersion model validation (Koopman & Ermak, 2007).

The three Falcon test cases are again those which are regarded as benchmarks (Koopman & Ermak, 2007) from the total of five tests carried out in these trials. They include the Falcon 1 case, which was undertaken in very stable atmospheric conditions.
The two Thorney Island test cases are taken from the three continuous release experiments. One of these experiments is not included (case 46), since the plume missed many of the gas sensors.

All three of the CHRC test cases are selected.

The selected test cases from the very extensive BA-Hamburg trials are those covering the most pertinent range of obstacle and terrain configurations. For each of the selected configurations, there are multiple test cases covering parameter variations, such as a slope angle and fence size. The configurations selected include: unobstructed; sloping terrain; upwind and downwind semi-circular fence obstructions and circular fence obstructions. The TUV01 and TUV02 test cases from the BA-TNO trials are similar in outline to some of those from the BA-Hamburg trials, but for differing release rates and wind speeds. The FLS case is a very comprehensive 3-D mapping of the concentration field. All three of these trials are included in the validation database.

Table 5.2 shows that the validation database consists of a total of 33 test cases. Many of these test cases have been used in previous model validation exercises.

All of the selected wind-tunnel trials are for continuous releases. The field-trial test cases are also continuous in the case of the Thorney Island data.

For the remaining four field trial spills of LNG, releases were typically carried out over a period of a few minutes at most. In some cases, the release ceased before the cloud reached sensors at the furthest downstream location. Strictly, these are not continuous releases (Hanna et al., 1996), but from the point of view of LNG dispersion (at least for spills on a water pool) they are probably closer in character to continuous than instantaneous releases.

Modeling of the wind tunnel test cases must be carried out at wind-tunnel scale to avoid uncertainties introduced as a result of scaling effects. For comparison purposes, the wind tunnel data is also provided in the validation database at a scale representative of an equivalent field-scale experiment, using well-established scaling rules (Meroney & Neff, 1982). Section 5.6 provides more information on the scaling rules. In the first edition of the LNG MEP, an allowance was given for models to be compared to the wind-tunnel data at equivalent field scale if this was the only practicable option. However, integral and CFD models that are used for LNG vapor dispersion can simulate these experiments at wind-tunnel scale. This topic was discussed amongst an international panel of experts at the UKELG meeting in 2012\(^4\), and it was concluded that the experiments should be simulated at the wind-tunnel scale. Therefore, to enable models to be compared on a like-for-like basis, without uncertainties associated with scaling effects, this second edition of the LNG MEP stipulates that the experiments must be simulated at wind-tunnel scale.

### 5.4 PHYSICAL COMPARISON PARAMETERS

The physical comparison parameters are the physical quantities against which the performance of a model is evaluated. They can be directly measured or derived from measurements.

Physical comparison parameters can be separated into those which are based on point-wise and arc-wise data. The former involves comparison between model predictions and measurements paired at specific points. The latter involves comparison between model predictions and measurements at specific distances downstream from a release, typically along circular arcs. The advantage of arc-wise comparisons is that uncertainties in wind direction, or those introduced as a result of lateral meandering of a plume, are circumvented. Arc-wise comparisons are most appropriate for situations

\(^4\) [http://ukelg.ps.ic.ac.uk/UKELG49.htm](http://ukelg.ps.ic.ac.uk/UKELG49.htm), accessed 13 July 2016.
in which plume direction is dominated by the wind direction. However, for other situations, for example in which the model performance depends on the correct prediction of the path of the plume as a consequence of the effects of obstacles or terrain, then point-wise comparisons should also be made (Duijm & Carissimo, 2002). SMEDIS included both point-wise and arc-wise based physical comparison parameters (Carissimo et al., 2001). Hanna et al. (1993) based their study on arc-wise comparisons. Further discussion of the advantages and disadvantages of point-wise and arc-wise comparisons can be found in Duijm et al. (1996).

Model predictions are compared to experimental data in Version 12 of the Validation Database (Stewart et al., 2016) using the following six physical comparison parameters:

i. Point-wise concentrations
ii. Maximum arc-wise concentrations
iii. Cloud widths
iv. Predicted distances to the measured maximum arc-wise concentrations
v. Distances to the LFL concentration
vi. Predicted concentration at the measured distance to the LFL

The following Sections describe these physical comparison parameters in turn, followed by a discussion on averaging times and the use of low concentration measurements in calculating the physical comparison parameters.

5.4.1 Point-wise Concentrations

Measured point-wise concentrations are the concentrations recorded at sensor locations in a given experiment, which have been processed using a specified averaging time. In some experiments, two sets of measured point-wise concentrations may be produced, based on a short and a long time-average. The short time-average is typically one second and the long time-average is usually the duration of the steady period of the release. To determine the short time-averaged point-wise value, the concentration data from the sensor is first filtered using a running average (as noted, typically a one second running average). The maximum value of this time-series is then taken as the point-wise value. To determine predicted point-wise concentrations from dispersion models, different approaches may be used depending upon the type of model. Integral models typically predict concentrations with a defined averaging period, whilst CFD models usually predict time-varying concentrations. The CFD data can be processed in the same way as the experimental data to arrive at the predicted point-wise concentrations for short and long averaging times.

Point-wise time-average concentrations at specific locations were included in SMEDIS as a physical comparison parameter for continuous releases. The use of point-wise concentrations allows credit to be given to models which provide spatial information on the concentration field (e.g. in situations where the cloud is affected by the presence of obstacles and/or terrain). It also provides additional information on the spatial performance of a model for trials in which an arc contains insufficient sensors to allow determination of cloud width. Point-wise data are the primary means for inputting data into the validation database, upon which all of the other physical performance parameters are automatically calculated.

However, there is unfortunately rather little information available in the literature on quantitative values of statistical performance measures for this parameter. Point-wise comparisons provide a more stringent test of model performance than arc-wise comparisons (Carissimo et al., 2001).
Point-wise concentrations are included as a physical comparison parameter to allow a more detailed comparison between measurements and predictions to be made if required. Their inclusion also means that, over time, knowledge of model performance can be built-up which may ultimately lead to quantitative acceptance criteria being proposed for this comparison parameter.

5.4.2 Maximum Arc-wise Concentrations

The most commonly-used physical comparison parameter for arc-wise data for the continuous and quasi-continuous releases in Table 5.2 is the maximum concentration across an arc at a specific distance downwind from a release. This ‘maximum arc-wise concentration’ has been interpreted differently in various validation studies, and it is therefore carefully defined here to avoid any confusion. For each given arc distance, the maximum arc-wise concentration is taken as the maximum of the point-wise concentrations on that arc, i.e. the maximum of the concentrations at the sensors positions (at both their circumferential position and height). The approach is applied consistently to both measured and predicted data. Figure 5.3 shows schematically the method used for determining both the measured and predicted maximum arc-wise concentrations.

It is important to note that when predicting the maximum arc-wise concentration, the model should use the mean wind direction that was measured in the experiments (rather than assume the wind is directed along the centerline of the array of sensors). Due to wind meandering effects and turbulent fluctuations in the dispersing cloud, the location of the measured and predicted maximum arc-wise concentrations may differ. Some models may be able to account for wind-meandering effects whilst others may just use the fixed mean wind direction.

![Figure 5.3 Schematic illustration of methods used for determining the measured (left) and predicted (right) maximum arc-wise concentration](image)

Other dense-gas model evaluation exercises (e.g. Hanna *et al*., 1993; Duijm *et al*., 1996; Witlox *et al*., 2013) have used a different method to determine the predicted maximum arc-wise concentrations from that described above. They have commonly used the predicted maximum concentration at any circumferential position along the measurement arc, irrespective of the location of the sensors in the experiment. The advantages of using the method shown in Figure 5.3 for the LNG Model Evaluation Protocol are as follows:

a. There are limitations to the quality of the experimental data for maximum arc-wise concentrations. There were only a certain number of sensors used in each of the experiments and the field-scale experiments were not repeated to obtain ensemble-averaged maximum arc-wise concentrations. It is therefore unclear whether the
experiments measured the “true” maximum arc-wise concentration. Faced with this uncertainty in the representativeness of the measured value, the recommended approach takes a cautious approach. There are different methods that could be used to calculate the predicted maximum arc-wise concentration and the present method is more likely to make the model appear to under-predict concentrations.

b. The recommended method favors models that more accurately simulate plume meandering. Models that predict an overly narrow plume with no meandering are more likely to miss the sensor positions and they will therefore perform poorly. The recommended approach therefore encourages the development of more accurate models.

c. In the Thorney Island and Falcon experiments, the sensors were not arranged in arcs around the source but were instead arranged in an array of straight lines. The method used for calculating maximum arc-wise concentrations takes into account this fact, whereas other approaches assume implicitly that the sensors were arranged in arcs.

d. The method illustrated in Figure 5.3 was used previously by PHMSA to evaluate the following models: DEGADIS v2.1 (FERC, 2010), PHAST v6.6 and v6.7 and FLACS v9.1r2. It is important to ensure continuity and consistency in the evaluation procedure, where possible.

There could be adverse consequences of comparing the measured maximum arc-wise concentration to the predicted maximum concentration at any circumferential location along the measurement arc (e.g. Hanna et al., 1993b; Duijm et al., 1996; Witlox et al., 2013). Using that method, a model could falsely be considered to over-predict the measurements.

To illustrate this point, an example is shown in Figure 5.4. In this example, the plume in the experiments is relatively narrow so that it passes between sensors. The measured concentrations at the two middle sensors on the arc, \( C_{m2} \) and \( C_{m3} \), are both below the LFL, but the LFL cloud in the experiments extends beyond the arc to a distance of around \( 2R \).

The model results shown in Figure 5.4 predict a maximum concentration at any circumferential location on the arc that is above the LFL (at the position marked “x”). If the predicted concentration at this location is taken to be the maximum arc-wise concentration, it appears that the model over-predicts the measured concentrations and it would therefore be considered to provide a conservative result, yet the opposite is true (the model under-predicts the distance to the LFL).

In contrast, if the LNG MEP method of determining predicted maximum arc-wise concentrations is applied to Figure 5.4 (using the predicted concentrations \( C_{p2} \) and \( C_{p3} \)), it correctly identifies that the model is under-predictive.

Further information on the different methods for evaluating maximum arc-wise concentrations can be found in the papers by Duijm et al. (1996), Chang & Hanna (2004) and Gant et al. (2016).

---

The maximum arc-wise concentration is useful in assessing the ability of a model to predict the correct decay of concentration with downwind distance. It has the practical advantage of having been used as a physical comparison parameter in other dense gas dispersion model evaluation exercises (Hanna et al., 1993; Carissimo et al., 2001; Chang & Hanna, 2004; Hanna et al., 2004) which means that there is information available in the literature on the quantitative values of statistical performance measures for this parameter (see Section 5.5.3). Hanna et al. (1993), Duijm et al. (1996) and Duijm & Carissimo (2002) point out that comparison of maximum arc-wise concentrations should be combined with comparison of the plume width at an arc to provide a more comprehensive evaluation of the performance of a model for predicting concentration in both the downwind and lateral directions.

All of the recommended test cases in Table 5.2 allow for extraction of maximum concentration across a number of arcs downwind from the release, with the exception of the BA-TNO and BA-Hamburg trials. In these two trials, measurements were typically made downwind of the release in the wind direction only (i.e. on the nominal plume centerline). However, uncertainty in the wind direction is negligible in these wind tunnel trials, so the measured concentration can reasonably be assumed to be equal to the maximum concentration at the particular downwind distance. Cloud width cannot be obtained for these two wind tunnel trials (with the exception of test case ‘FLS’ for BA-TNO).

**Figure 5.4** Illustration of a possible pitfall that would occur in calculating maximum arc-wise concentrations from the predicted concentration at any circumferential location along an arc.
5.4.3 Cloud Width

The cloud width is typically calculated using moments of the concentration distribution across the arc (Hanna et al., 1991; Carissimo et al., 2001). Unfortunately, there is significantly less information available in the literature on quantitative values of statistical performance measures for cloud width. It should also be noted that cloud width appears to be a less discriminating test of a model than maximum concentration at downwind distances (Hanna et al., 1991).

For both the measured and predicted data, the cloud width is determined in the model validation database using the following formula, which is derived from standard deviation of a frequency distribution (Pasquill, 1977):

\[
\sigma_y = \frac{\sum C y^2}{\sum C} - \left(\frac{\sum C y}{\sum C}\right)^2
\]

(5.1)

where \(\sigma_y\) is the cloud width, \(C\) is the long time-averaged concentration, \(y\) is the crosswind displacement of each sensor and the summation (indicated by \(\Sigma\)) is performed over the point-wise values from the lowest sensor height on each measurement arc.

For some of the experimental trials, it is not appropriate to try to calculate a cloud width. Following a similar approach to that taken by Hanna et al. (1991), three conditions must be met before a measured cloud width is determined:

a. There must be at least four sensors on an arc that register long time-averaged concentrations greater than 0.1% v/v

b. The sensor that registers the maximum long time-averaged concentration must not be located at either end of an arc

c. The lateral concentration distribution must not exhibit a bi-modal pattern with two peaks

The example concentration profiles shown in Figure 5.5 illustrate a cloud that is bifurcated and one that is not bifurcated.

![Figure 5.5 Examples of bifurcated and non-bifurcated clouds (left and right, respectively)](image)

The calculation method used to determine the predicted cloud width should give the same cloud width as that measured if the predicted point-wise concentrations exactly match those measured in the experiments. Therefore predicted plume widths should not be calculated where the measured concentrations are less than or equal to 0.1% v/v.
This approach was chosen based on an evaluation of the alternative methods. For example, one alternative would be to exclude all of the predicted point-wise concentrations below 0.1% v/v in the plume-width calculation. However, the lower limit of 0.1% v/v is introduced to account for the uncertainty in the measurement accuracy of very low concentrations (see Section 5.4.8). The model predictions of low concentrations are not uncertain and they should be used wherever possible. If low predicted concentrations were ignored, it could bias the plume-width calculation.

Another alternative approach would be to ignore predicted point-wise concentrations at those locations where both the measured and predicted concentration were below 0.1% v/v. This approach is not recommended though because it could lead to plume widths being calculated inconsistently; using a different number of points depending upon whether the measured or the predicted plume width was being calculated.

A final alternative approach is possible with integral-type dispersion models that calculate an integral plume width. An option would be to use the integral plume width in comparison with data rather than calculate it independently from the point-wise concentrations. This is not recommended because the definition of the integral plume width may differ from that used to measure the plume width in the experiments. By using point-wise concentrations, the measured and predicted plume widths are calculated on a common basis.

5.4.4 Predicted Distance to the Measured Maximum Arc-Wise Concentration

The concept of the predicted distance to the measured maximum arc-wise concentration is illustrated in Figure 5.6. The idea behind making this comparison is to assess the ability of the model to calculate the distance to a certain concentration, as opposed to its ability to predict the concentration at a certain distance. The maximum concentration measured along each arc is chosen as the most appropriate concentration on which to base the comparison. It is highly unlikely that the specified concentration will be predicted at one of the arc locations. Therefore interpolation between the predicted maximum arc-wise concentrations is required. This is carried out using a power-law:

$$C = Ax^{-B}$$

(5.2)

where $C$ is the predicted maximum arc-wise concentration, $x$ is the distance downstream from the source and $A$ and $B$ are constants whose values are determined by fitting the curve between the maximum arc-wise concentrations at two neighboring arcs. The slope of the curve may not necessarily be continuous with distance downwind, since it is based on a piecewise fit between concentrations at neighboring arcs.

In theory, instead of using interpolation between predicted point-wise concentrations, the model itself could be used to predict the distance to the specified concentration. The main reason why the interpolation approach is used instead is that for some models it is difficult to output the distance at a specified concentration. The use of interpolation allows for a consistent approach to be applied across all model types evaluated against the LNG MEP.

Further details on how this interpolation is carried out can be found in the Model Validation Database report (Stewart et al., 2016).
5.4.5 Distance to the LFL Concentration

An obvious choice for a physical performance parameter is the distance to the LFL or ½ LFL, since the predicted distance to the ½ LFL is the one of the key outputs of a dispersion model that is used in LNG siting applications (49 CFR 193). However, whilst such a physical comparison parameter initially appears attractive, it is not without its potential problems.

One of the key issues is whether reliable data on the distance to the LFL are available, since this parameter is not directly measured. Morgan et al. (1984) have examined the variation of concentration with distance for the Burro and Coyote trials at some length and the possibility of extracting a distance to the LFL would appear promising. Data on the variation of concentration with distance are available from the MDA for two of the Maplin Sands and both of the Thorney Island trials. Nevertheless, for all of these trials the distance to the LFL will inevitably rely on the appropriateness of interpolation or extrapolation functions fitted to data obtained at relatively few distances downwind from a release.

A further issue with using the distance to the LFL as a physical comparison parameter is that there appears to be no information available in the literature on which to base quantitative assessment criteria for this quantity.

Although the distance to the LFL (or ½ LFL) is the key output from a dispersion model, it is important that this performance comparison parameter is not given undue prominence in the evaluation of the model, for the reasons outlined above. However, its inclusion in the model evaluation process can provide insight into the predictive ability of a model.

The measured and predicted distances to the LFL are calculated using a similar method to that described above in Section 5.4.4, except that the LFL concentration of 5% v/v (for LNG) is used instead of the measured maximum arc-wise concentration. The approach is illustrated in Figure 5.7.
To maintain consistency between the way in which the model predictions and the measurement data is handled, interpolation is used on both sets of data to calculate the distance to the LFL. This approach means that if the point-wise data are the same for both the predictions and the measurements then this method will give identical distances to the LFL. This would not necessarily be the case if the interpolation was used solely for the measurement data.

If the LFL falls outside of the range of measured or predicted concentrations then extrapolating the data to find the appropriate distance would introduce significant uncertainty into the value of the parameter. Therefore, comparisons are only made when distance to the LFL can be interpolated between arcs, not extrapolated beyond the furthest arc.

![Figure 5.7 Illustration of the interpolation used to calculate measured and predicted distance to LFL. Symbols are: ■ measurements ▲ model predictions](image)

**5.4.6 Predicted Concentration at the Measured Distance to the LFL**

This physical performance parameter is similar to the distance to the LFL physical performance parameter, but in this case the comparison is made in terms of concentration rather than distance. To interpolate the measured distance to the LFL, the measured maximum arc-wise concentration is assumed to decay as a power-law. Then the predictions of maximum arc-wise concentration are interpolated to find the concentration at that distance. Figure 5.8 provides an illustration of the method used to determine the predicted concentration at the measured distance to the LFL.

For the same reasons given above, it is not considered appropriate to use extrapolation to extend the curve of predicted maximum arc-wise concentrations beyond the arcs.
5.4.7 Averaging Times

Long time-averaged concentrations should be used to calculate the cloud width parameter, whereas the other physical comparison parameters (e.g. distance to LFL) should be based on the shortest averaging period available from the data. This is consistent with the fact that for flammable vapors, concentrations may only need to briefly rise above the LFL for the vapor to ignite at an ignition source. Further details on averaging times can be found in the works of Hanna et al. (1993, 1996). The short averaging time is typically around one second and the long averaging time is usually comparable to the steady period of the release.

The averaging times used for each set of experimental data and how the data are processed using these averaging times is provided in the Model Validation Database report (Stewart et al., 2016). Where possible, models should use the same averaging time as the experimental data.

5.4.8 Lower Limit (Threshold) Concentration

Due to the uncertainty in the measurement accuracy of low gas concentrations, physical comparison parameters should only be calculated using concentrations above a certain threshold concentration. If SPMs are calculated based on the ratio of two small numbers then small measurement errors (in absolute terms) could lead to large errors in the SPMs.

However, it is useful to include the low concentration data in the model validation database, since it provides useful information for model evaluation. The precise value of the concentration may be uncertain, but if a model predicts a much higher value then this indicates (qualitatively) that there is poor agreement between the model prediction and the measurement.

For these reasons, in Version 12 of the model validation database, measured point-wise concentrations less than 0.1% v/v are included in the database, but they are not used in the calculation of the SPMs.
5.5 STATISTICAL PERFORMANCE MEASURES

Quantitative evaluation of the performance of atmospheric dispersion models requires the definition of appropriate statistical performance measures (SPMs) which compare model predictions with measurements. There is a wide range of SPMs which have been devised for this purpose and all have their advantages and disadvantages (Duijm et al., 1996; Carissimo et al., 2001; Chang & Hanna, 2004). The main requirements of SPMs are as follows (Duijm & Carissimo, 2002):

- They should provide a measure of the bias in the predictions, i.e. the tendency of a model to over/under-predict
- They should provide a measure of the spread in the predictions, i.e. the level of scatter from the average over/under-prediction

In addition, it is very helpful if the SPMs that are selected have been used in previous dense gas model evaluation studies, since this provides a source of information on the typical range of quantitative values of SPMs, which can be used as a basis of recommendations for quantitative assessment criteria (see Section 5.7).

The PHMSA Advisory Bulletin (PHMSA, 2010) requires additional SPMs to be calculated to those specified in the previous version of the LNG MEP (Ivings et al., 2007). The full set of SPMs, including both those in the previous version of the LNG MEP and the PHMSA Advisory Bulletin, are shown in Table 5.3.

### Table 5.3 Chosen Statistical Performance Measures (SPM)

<table>
<thead>
<tr>
<th>SPM</th>
<th>Definition</th>
<th>Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean Relative Bias</td>
<td>$MRB = \frac{C_m - C_p}{\frac{1}{2}(C_p + C_m)}$</td>
<td>Accepts zero values. Less sensitive than other measures. Symmetric for under/over-prediction.</td>
<td>Allows differences between models with $C_m/C_p$ up to $\sim 10$ to become apparent, but not so outside this range.</td>
</tr>
<tr>
<td>Mean Relative Square Error</td>
<td>$MRSE = \frac{(C_p - C_m)^2}{\frac{1}{4}(C_p + C_m)^2}$</td>
<td>More transparent than VG in allowing standard deviation of predictions to be obtained.</td>
<td></td>
</tr>
<tr>
<td>FAC2: the fraction of predictions within a factor of two of the measurements</td>
<td>$0.5 \leq \left( \frac{C_p}{C_m} \right) \leq 2.0$</td>
<td>Robust, consistent, easy to understand.</td>
<td></td>
</tr>
<tr>
<td>Geometric Mean Bias</td>
<td>$MG = \exp \left( \ln \left( \frac{C_m}{C_p} \right) \right)$</td>
<td>Mitigates the dominating effects of a few extreme values in measured/predicted concentrations. Loge(MG) symmetric about zero in under/over-prediction.</td>
<td>Less transparent than MRB. Cannot accept zero values and so requires a threshold to be set.</td>
</tr>
</tbody>
</table>

7 CSF, CSF$_{LFL}$ and DSF$_{LFL}$ are the SPM additionally required following the PHMSA Advisory Bulletin ADB-10-07 (PHMSA, 2010).
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Formula</th>
<th>Description</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Geometric Variance</td>
<td>$VG = \exp\left(\left[\ln\left(\frac{C_m}{C_p}\right)\right]^2\right)$</td>
<td>Mitigates the dominating effects of a few extreme values in measured/predicted concentrations. Variance measure related to MG.</td>
<td>Less transparent than MRSE. Cannot accept zero values and so requires a threshold to be set.</td>
</tr>
<tr>
<td>Concentration Safety Factor</td>
<td>$CSF = \left{ \frac{C_p}{C_m} \right}$</td>
<td>Straightforward metric comparing the predicted and measured concentrations.</td>
<td></td>
</tr>
<tr>
<td>Concentration Safety Factor to the Lower Flammability Limit (LFL)</td>
<td>$CSF_{LFL} = \left{ \frac{C_p}{LFL} \right}$</td>
<td>Straightforward metric comparing the predicted and LFL concentrations at the measured/interpolated distance to the LFL.</td>
<td>Cannot be calculated from predictions that do not span the LFL concentration.</td>
</tr>
<tr>
<td>Distance Safety Factor</td>
<td>$DSF = \left{ \frac{x_p}{x_m} \right}$</td>
<td>Straightforward metric comparing the distance to the measured maximum arc-wise concentration to the interpolated predicted distance to those concentrations.</td>
<td>Cannot be calculated where measured concentration is not within the range of model predicted concentrations.</td>
</tr>
<tr>
<td>Distance Safety Factor to the Lower Flammability Limit (LFL)</td>
<td>$DSF_{LFL} = \left{ \frac{x_{p,LFL}}{x_{m,LFL}} \right}$</td>
<td>Straightforward metric comparing the predicted to the measured/interpolated distance to the LFL.</td>
<td>Cannot be calculated from predictions that do not span the LFL concentration.</td>
</tr>
</tbody>
</table>

In Table 5.3 the angle brackets $<...>$ denote an average over all measured/predicted pairs of concentration. The most easily understood parameters are the Mean Relative Bias (MRB) and the Mean Relative Square Error (MRSE), together with the Factor of 2 (FAC2) and the Concentration Safety Factor (CSF). The Geometric Mean and Geometric Variance, MG and VG, respectively, are less easily understood but have been included partly because they have been used in several previous model evaluation studies (Hanna et al., 1993; Duijm et al., 1996; Carissimo et al., 2001; Chang & Hanna, 2004; Hanna et al., 2004) and partly because they help ensure that a few very large or very small values of predicted/measured concentrations do not dominate the SPM. The set of SPMs in Table 5.3 are the same as those used in SMEDIS (other than those added following the PHMSA Advisory Bulletin ADB-10-07).

The SPMs listed in Table 5.3 should be computed for each of the 33 trials included in the validation database individually. In addition, the SPMs should be calculated for the following groups of trials:

- **Group 1**: Maplin Sands; Burro; Coyote; Thorney Island; CHRC A; BA-Hamburg DA0120 and DAT223; BA-TNO TUV01 and FLS
  - Group 1a: Maplin Sands; Burro; Coyote; Thorney Island
  - Group 1b: BA-Hamburg DA0120 and DAT223; BA-TNO TUV01 and FLS
- **Group 2**: Falcon; CHRC B and C; BA-Hamburg 039094, 039097, DA0501, DA0532, 039051, 039072; BA-TNO TUV02
  - Group 2a: Falcon
Group 2b: CHRC B and C; BA-Hamburg 039094, 039097, DA0501, DA0532, 039051, 039072; BA-TNO TUV02

The grouped-trial SPMs should be computed for both short and long time-averaged results, where appropriate, for the six groups of trials listed above.

The validation database automatically computes and tabulates the individual and grouped-trial SPMs needed as part of the quantitative evaluation of a model. For further information see Stewart et al. (2016) and Section 5.7 of this report.

5.6 DATABASE

The LNG Model Validation Database v12 (Stewart et al., 2016) contains configuration details and measured concentration data for the 33 trials listed in Table 5.2. The details for each trial are listed in individual worksheets that contain the following headings and associated entries to summaries the trial conditions:

a) **Trial name** – The recognized name of the experimental series, i.e. Burro, Coyote etc.

b) **Test identifier** – A simplified identifier of the test within the experimental series

c) **Date of test** – The date of the experiment

d) **Origin of the data and date of inclusion** – The data sources used, and the date of entry into the validation database

e) **Test description** – A brief note describing the nature of the experiment

f) **Substance released** – Information relating to the physical and chemical properties of the substance released

g) **Release conditions** – Information relating to the storage and release conditions

h) **Atmospheric conditions** – Information relating to the atmospheric conditions (e.g. wind speed, atmospheric stability) and details of their measurement

i) **Terrain and obstacles** – Details of the terrain and obstacles, where this is straightforward. In complex cases (e.g. the terrain elevations for the Burro and Coyote experiments), references are provided for the original data reports, where this information can be found.

j) **Physical comparison parameters** – These entries contain the point-wise and arc-wise data describing the cloud and the locations of measurements, as well as the associated averaging times

k) **Units** – SI units are provided for all physical quantities

For the wind-tunnel trials in the database, the data is provided at both wind-tunnel scale and equivalent field scale data, together with the scaling relations. As noted in Section 5.3.3, the wind-tunnel trials must be modelled at wind-tunnel scale for the LNG MEP. The data is provided at equivalent field-scale experiment for comparison purposes only.
As an example of the scaling of wind-tunnel data to equivalent field scale, the Chemical Hazards Research Center wind tunnel trials (Havens & Spicer, 2005, 2006, 2007) were based on a 1:150 scale model (i.e. L is 150), giving the following relations between model and full-scale:

\[
L_m = L_f / 150 \\
U_m = U_f / 150^{1/2} \\
Q_m = Q_f / 150^{5/2}
\]

where \(L\) refers to length, \(U\) to velocity and \(Q\) to volumetric flow rate. Subscripts \(m\) and \(f\) are model and field scales, respectively.

Application of the above scaling rules preserves the measured concentration data so allowing it to be re-interpreted unchanged at full-scale, but obviously with all length scales changed by a factor \(L\) (i.e. the measured concentrations remain unchanged at equivalent field scale but the distance to the sensors increases). Strictly this is only true if the specific gravity is unchanged at full-scale.

Users of the validation database should enter their model predicted point-wise concentration data for each trial into the appropriate worksheet. The validation database will then compute the maximum arc-wise gas concentrations from the point-wise model predictions, the predicted cloud widths (where appropriate) and all of the individual and grouped-trial SPMs.

Comprehensive details of the validation database contents is provided by Stewart et al. (2016). Section 5.8 of this report discusses the presentation of model validation outputs for the LNG MEP.

### 5.7 VALIDATION / QUANTITATIVE CRITERIA

An absolute definition of what constitutes a ‘good’ or ‘acceptable’ model is not straightforward. The decision criteria comprise a combination of elements drawn from the scientific assessment (in particular whether the qualitative assessment criteria are met – Section 3.1), the verification process, and the extent to which quantitative values of the SPM output from the validation exercise are also met. Some guidance on the choice of these values can be obtained from previous model evaluation exercises, but it needs to be recognized that there is only limited experience in conducting model evaluations of this type and therefore there is some uncertainty in values of ‘good’ or ‘acceptable’ quantitative ranges for SPM. This uncertainty can be reduced as models are evaluated against the protocol and it is refined in the light of this experience.

Hanna et al. (1993) carried out the first extensive validation exercise on a range of dense gas dispersion models. They compared measured arc-wise maximum concentrations and plume widths with predicted values for continuous, instantaneous dense releases and some neutral density experiments and computed two SPMs: the geometric mean bias (MG) to measure the bias of the predictions; the geometric variance (VG) to indicate the degree of scatter. See Section 5.5 for a definition of these SPMs. Overall they found that the better-performing models gave relative mean biases of about ±30-50% and relative scatters about equal to the mean. For the continuous dense gas releases they found that the better performing models lay within the following range: 0.7 < MG < 1.5 and 1.4 < VG < 2.6. The plume widths were better predicted.

Touma et al. (1995) carried out a similar exercise for evaluation of dense gas dispersion models but used a different measure of bias – the Fractional Bias – finding overall that the models predicted arc-wise maximum concentrations with a fractional bias of <70%. They also noted that the models performed better when plume width was examined.
Hanna et al. (2004) and Chang and Hanna (2004) have carried out further examinations of how a validation exercise should be performed. They conclude that a range of SPMs should be computed and model performance assessed using this full range of SPMs since each individual SPM has advantages and disadvantages (as outlined in Section 5.5) and measure a different aspect of model performance. They suggested that two SPMs be used for each of the bias and scatter, namely:

- the Fractional Bias (FB) and Geometric Mean (MG), for the bias in the mean
- the Normalized Mean Square Error (NMSE) and Geometric Variance (VG), for scatter about the mean

alongside the simple measure Factor of Two (FAC2). FB is similar to the MRB measure in Table 5.3 and NMSE is similar to the MRSE (also in Table 5.3).

Hanna et al. (2004) and Chang and Hanna (2004) conclude that a ‘good’ model would be expected to have a fractional bias within ±30%, a relative scatter of about a factor of two or three, and about 50% of the predictions within a factor of two of observations. These recommendations were qualified by the statement that these criteria apply to comparisons against research-grade field experiments. It should also be noted that the experiments upon which these criteria were based tend to be those relevant to air quality modeling, rather than being exclusively limited to dense gas dispersion. Chang and Hanna (2004) also commented that these criteria can be expected to be revised as more evidence appears from new model evaluation exercises.

Hanna et al. (2004) used this range of SPMs to examine the performance of the CFD code FLACS over a range of dispersion trials with releases over a range of densities. For maximum concentrations they described the model performance as ‘fairly good’ and ‘well within the criteria of acceptance for dispersion models’. This statement was made on the basis of 20% under-prediction of the mean, a relative scatter of 50% and a factor of two of 86%. For a separate dataset for a complex situation of dispersion around buildings the model produced a FAC2 of 72%.

SMEDIS (Carissimo et al., 2001) adopted a slightly different approach. The majority of validation datasets involved a complicating effect with potential influence on the dispersion process such as obstacles, complex terrain or presence of aerosols. SMEDIS also sought to compare predicted and measured concentrations paired in space and time, as well as arc-wise maximum concentrations and plume widths, for a range of models from the simple workbook methods through to CFD codes. They computed SPMs which are very similar to those suggested by Chang and Hanna (2004) and are based on the recommendations of Duijm et al. (1996). In fact these are the SPMs as recommended in Section 5.4.4.2. The results were divided according to model type and complex effect rather than individual model. SMEDIS showed that the better performing models were the integral and CFD-based types. For these class of models, maximum arc-wise concentrations showed biases within ±30% of the mean and scatters about the mean within a factor of two. Also, the values of FAC2 were well in excess of 50%. The only exception was for releases into complex terrain for which integral models produced biases and scatter well in excess of these figures, while the CFD codes coped better by producing results only slightly worse than these figures.

As expected, SMEDIS showed that the SPMs for concentrations paired in space and time were significantly worse, since this is more severe test for models, due to the complicating effect of fluctuations in the wind direction. The integral models produced surprisingly small biases within ±60% for all cases except complex terrain, but the scatter about the mean was high, suggesting that the bias results were fortuitous. The results for CFD codes were poor for bias and similar for scatter, except for the complex terrain case where the bias to the mean was <60% and the scatter about the mean less than a factor of two.
Sklavounos and Rigas (2006) have also used a range of SPM to evaluate dense gas dispersion models but it is difficult to draw useful general conclusions from their study because only one set of field trials was used as the basis for model validation and in addition only a small number of models (three) were evaluated.

In conclusion it is difficult to disagree strongly with the criteria for a ‘good’ or ‘acceptable’ model outlined by Chang and Hanna (2004). To recap, they suggest that two measures of bias should be used – FB (or MRB) and MG, and that the bias in the mean should be < ±30%. Measures for scatter about the mean should include NMSE (or equivalently MRSE) and VG, and take values corresponding to a relative scatter of between two to three. These should be used alongside a FAC2 with a value in excess of 50%.

However, since there is some uncertainty in the absolute relevance of Chang and Hanna’s criteria to the dispersion of LNG vapor and guided by the study of Hanna et al. (1993) which did concentrate on dense gas dispersion datasets we propose the following modified quantitative assessment criteria to be met by a model:

- A mean bias within ±50% of the mean, corresponding to: -0.4<MRB<0.4 and 0.67<MG<1.5
- A scatter of a factor of three of the mean, corresponding to: MRSE<2.3 and VG<3.3
- The fraction of model observations within a factor of two of observations to be at least 50%

Such criteria apply to maximum arc-wise concentration and plume width data. Unfortunately, there appears as yet insufficient experience to set criteria for point-wise concentration comparisons. Nevertheless, SPMs for point-wise concentration comparisons should be computed so as to build experience in the expected range of values and which could be used at a later date to set additional criteria. A summary of the SPM and their quantitative acceptance criteria is given in Appendix A.

For the additional SPMs given in the PHMSA Advisory Bulletin (PHMSA, 2010), namely CSF, CSF<sub>LFL</sub>, DSF and DSF<sub>LFL</sub>, predictions within a factor of two of the measurements are deemed to be quantitatively acceptable, i.e. 0.5 < CSF < 2.0 etc.

The full set of SPMs (MRB, MG, MRSE, VG, FAC2, CSF, CSF<sub>LFL</sub>, DSF and DSF<sub>LFL</sub>) should be computed for each of the validation trials individually. In addition, grouped-trial SPMs should be computed as averages over all of the trials in each of the six SPM groupings given in Section 5.5. The SPM groups are repeated below, for reference:

- **Group 1:** Maplin Sands; Burro; Coyote; Thorney Island; CHRC A; BA-Hamburg DA0120 and DAT223; BA-TNO TUV01 and FLS
  - Group 1a: Maplin Sands; Burro; Coyote; Thorney Island
  - Group 1b: BA-Hamburg DA0120 and DAT223; BA-TNO TUV01 and FLS
- **Group 2:** Falcon; CHRC B and C; BA-Hamburg 039094, 039097, DA0501, DA0532, 039051, 039072; BA-TNO TUV02
  - Group 2a: Falcon
  - Group 2b: CHRC B and C; BA-Hamburg 039094, 039097, DA0501, DA0532, 039051, 039072; BA-TNO TUV02
All models should be run against the Group 1 trials. This will allow evaluation of models suitable in principle for dispersion of LNG vapor over flat, unobstructed, terrain. Both integral and CFD models are capable of modeling these trials, which will enable easy model comparisons.

Optionally, models can also be run against the Group 2 trials. This will allow the wider evaluation of models that are in principle suitable for dispersion of LNG vapor in the presence of obstacles or non-flat terrain. Many CFD models are expected to be suitable for such scenarios.

5.7.1 Averaging

In order for the above SPM to be computed correctly it is important that models are set-up to run for the averaging-time stated in the validation database. In some cases data will be available for two averaging-times: a short and long time-average. If a model is capable of being run and providing output relevant to the short time-average then preference should be given to simulation of and comparison with that data. In some cases this is not possible: most CFD models produce outputs which are mean values that are not usually characteristic of a short time-average. In such circumstances a correction to the model predictions might be used to convert from a long averaging-time to a short averaging-time (Hanna et al., 1996; Webber, 2002). In any case, the person who applies the model and carries out the comparison against data to compute the SPM should state the averaging-time set-up/employed by the model, whether any correction has been made, and the averaging-time of the data used as a basis of comparisons. The model reviewer should then comment on the validity of the model for concentration predictions relevant to short and/or long averaging-times.

Model evaluation is complicated by the fact that the maximum concentration at a particular sensor in a trial depends on the averaging time used to process the raw concentration data. The use of a short time-average is more appropriate as the basis of evaluation of models for the dispersion of flammables (Hanna et al., 1996), but not all models may be able to provide such output directly. For instance, most CFD models will produce output which more closely represents a long time-average than a very short time-average when applied to the dispersion of a continuous release. In the LNG MEP, models should use the same averaging time as the measurements. Various options are available to account for short averaging times with CFD models, such as empirically-based peak-to-mean models or adoption of safety factors (Hanna et al., 1996; Webber, 2002).

5.8 PRESENTATION OF VALIDATION OUTPUTS

Evaluation of a model against the LNG MEP culminates in the production of a Model Evaluation Report (MER), which describes the outcomes of the scientific assessment of the model, the model verification and the results of the validation exercise. The MER should contain a number of validation outputs, which are used to help determine the suitability of a model for performing LNG vapor dispersion calculations as required under 49 CFR 193.2059 for LNG siting applications.

In the validation section of the MER, model performance should be discussed for each trial individually. Comparison of measured and model predicted maximum arc-wise concentrations should be provided graphically and, in accordance with the PHMSA Advisory Bulletin ADB-10-07 (PHMSA, 2010), vertical error bars should be included to represent the extent of model sensitivity to experimental and model input uncertainties. An example is shown in Figure 5.9. In addition,
predicted and measured maximum arc-wise concentrations should be tabulated. It is suggested that individual SPM values are also provided for each trial.

Figure 5.9 Example of graphical comparison of measured and predicted maximum arc-wise concentrations with model sensitivity represented with vertical error bars

Tables containing SPM values for maximum arc-wise gas concentration, maximum point-wise gas concentration, cloud width and predicted distance to measured concentrations for all of the validation trials should also be provided. SPM values that fall outside the quantitative acceptability limits should be highlighted. Version 12 of the model validation database automatically generates these tables (see Appendix A of Stewart et al., 2016), and an example is given in Table 5.4.

Similarly, tables of SPMs for the groups of trials described in Section 5.7 should be provided in the Model Evaluation Report. Such tables of SPMs are automatically generated in Version 12 of the model validation database (see Appendix B of Stewart et al., 2016).

In addition to the comparison of measured and predicted maximum arc-wise gas concentrations on an individual trial basis, scatter plots showing comparisons of measurements and predictions across the entire set of completed validation trials should also be provided. The final worksheet of the validation database automatically generates several of these plots, including ones for: all trials, all field trials, all wind-tunnel trials, all unobstructed trials and all obstructed trials. An example is shown in Figure 5.10.

The reason for standardizing the presentation of the validation outputs is so that the performance of different models can be compared more easily. Furthermore, using the same validation outputs to inform decisions about model suitability should ensure more consistent model evaluations.

Table 5.4 Partial table from Database v12 of individual trial SPMs

8 In Table 5.4, and the tables in Appendix A and Appendix B of Stewart et al. (2016), (short) and (long) relate to the averaging time of the concentration data used to generate the SPMs, e.g. Burro 3 (short) and Burro 3
5.9 SENSITIVITY AND UNCERTAINTY ANALYSIS

(long) indicate SPM values for the short time-averaged and long time-averaged concentration predictions for the Burro 3 trial, respectively.

Figure 5.10 Partial measured vs predicted maximum arc-wise gas concentration scatter plot from the Model Validation Database v12 (Stewart et al., 2016)
The PHMSA Advisory Bulletin ADB-10-07 (PHMSA, 2010) requires that models evaluated against the LNG MEP should be subject to a parametric analysis to assess model sensitivity to a range of uncertain model inputs.

An uncertainty analysis should be provided in the MER that presents the uncertainty of user input parameters and the associated sensitivity of the model. The following key model inputs should be addressed:

- Source term
- Boundary conditions, e.g. wall conditions, surface roughness
- Wind profile
- Sub-models
- Spatial discretization
- Temporal discretization
- Geometrical representation, e.g. sloping/complex terrain, obstacles

It is likely that the above model inputs will have different parameters, limitations and uncertainties depending on the model type. It is therefore recommended that the listed model inputs are addressed as appropriate on a model-by-model basis. For example, FERC presented a sensitivity analysis in the evaluation of DEGADIS (FERC, 2010) which could be used as a starting point for other models evaluated against the LNG MEP.

Experimental uncertainties should also be considered and should be used to inform the choice of sensitivity analysis parameters. The Model Validation Database Guide (Stewart et al., 2016) provides a discussion of the experimental uncertainties for each series of trials included in the validation database. Finally, uncertainties in model output should also be discussed. Particular focus should be given to the following:

- Spatial output: i.e. are there uncertainties associated with the model outputting concentrations at the required spatial locations, e.g. due to the grid resolution or use of assumed Gaussian concentration profiles in the crosswind direction?
- Temporal output: does the model provide output that is appropriate for comparison to the averaging times specified in the validation database?

Further details of these requirements can be found in the Advisory Bulletin (PHMSA, 2010).
6 CLASSIFICATION OF MODELS

6.1 INTRODUCTION

There is a wide choice of models available for simulating the dispersion of vapors from a spill of LNG. As discussed in the introduction, there have been a number of extensive model evaluation exercises undertaken including in-depth validation studies, see Hanna et al. (1993), Carissimo et al. (2001), and Luketa-Hanlin (2006) for an overview.

Models for LNG dispersion can be categorized into four classes: Workbooks/Correlations, Integral models, Shallow-layer models and Computational Fluid Dynamics (CFD) models. Many models are available commercially, whilst others are available for free.

It is impractical to carry out a review of all available models for LNG vapor dispersion at least in a short time-scale. A selection of well-known models is listed in Table 6.1 to provide an indication of their extent and diversity. Rather than provide a review of individual models, a review of the main classes of dense gas dispersion models is therefore presented here using a format similar to that in the MEP. Integral models and CFD models are covered in detail as they cover the majority of models available and brief reviews are provided of the other model types.

<table>
<thead>
<tr>
<th>Model's Name</th>
<th>Model Type</th>
<th>Supported by</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALOHA</td>
<td>Integral</td>
<td>Publicly available (CAMEO, EPA)</td>
</tr>
<tr>
<td>CANARY</td>
<td>Integral</td>
<td>Quest Consultants Inc.</td>
</tr>
<tr>
<td>CFX</td>
<td>3D-CFD</td>
<td>ANSYS</td>
</tr>
<tr>
<td>DEGADIS</td>
<td>Integral</td>
<td>Publicly available (e.g. Trinity consultants, Lakes Environmental)</td>
</tr>
<tr>
<td>DRIFT</td>
<td>Integral</td>
<td>ESR Technology , UK</td>
</tr>
<tr>
<td>FDS</td>
<td>3D-CFD</td>
<td>Publicly available, NIST</td>
</tr>
<tr>
<td>FEM3A</td>
<td>3D-CFD</td>
<td>University of Arkansas</td>
</tr>
<tr>
<td>FLACS</td>
<td>3D-CFD</td>
<td>Gexcon AS, Norway</td>
</tr>
<tr>
<td>FLUENT</td>
<td>3D-CFD</td>
<td>ANSYS</td>
</tr>
<tr>
<td>GASTAR</td>
<td>Integral</td>
<td>CERC, UK</td>
</tr>
<tr>
<td>HGSystem (HEGADAS)</td>
<td>Integral</td>
<td>Shell, UK</td>
</tr>
<tr>
<td>SLAB</td>
<td>Integral</td>
<td>Publicly available (e.g. EPA, Trinity consultants, Lakes Environmental )</td>
</tr>
<tr>
<td>SLAM</td>
<td>Shallow Layer</td>
<td>Risø, Denmark</td>
</tr>
<tr>
<td>SCIPUFF</td>
<td>Lagrangian</td>
<td>L3 Communications Titan Group, Trinity consultants</td>
</tr>
<tr>
<td>STAR-CD</td>
<td>3D-CFD</td>
<td>CD-Adapco</td>
</tr>
<tr>
<td>SUPERCHEMS EXPERT</td>
<td>Integral</td>
<td>IoMosaic</td>
</tr>
<tr>
<td>TSSCREEN (Britter-McQuaid model)</td>
<td>Box</td>
<td>Publicly available (e.g. EPA, Lakes Environmental)</td>
</tr>
<tr>
<td>PHAST (UDM)</td>
<td>Integral</td>
<td>Det Norske Veritas (DNV), Norway</td>
</tr>
<tr>
<td>BREEZE (DEGADIS, SLAB)</td>
<td>Integral</td>
<td>Trinity consultants</td>
</tr>
</tbody>
</table>
6.2 WORKBOOKS / CORRELATION

6.2.1 General model description

Also known as an engineering correlation, this type of model seeks to relate two quantities by an empirical relation. The model is based on the assumption that this relationships which may hold under one set of conditions, will also hold under other conditions.

Dense gas dispersion is sufficiently complicated that there is essentially no place for the use of simple correlations for predicting, say, concentration simply as a function of distance.

Correlations can be, and are, however used as sub-models within all the other kinds of models. A notable example is that of the terms used to describe the spreading rate in Gaussian passive dispersion models (which are expressed as correlations with downstream distance and atmospheric stability). Moreover, the simpler turbulence closure sub-models in CFD models may also be thought of as correlations.

6.2.2 Advantages and disadvantages of model

Advantages: Where appropriate, it is very quick and simple to apply the model.

Disadvantages: It can only be applied where things are simple. If applied to a situation which is not very closely related to that of the original observations which gave rise to the correlation, then it can be very misleading.

6.3 INTEGRAL MODELS

6.3.1 General model description

Integral models attempt to derive a few, partly phenomenological, equations to describe the overall properties (integral properties) of a flow. For example in the case of a plume the radius of the plume, height of its centerline, velocity, and centerline temperature and concentration may be solved. Simple differential equations are used for these, justifying the equations on the basis of sound scientific derivation and assumptions.

Integral models of instantaneously released heavy gas clouds tend to model the cloud as a cylindrical box and use the radius and volume of the box as two of the appropriate integral properties which vary with time. For this reason, integral models are sometimes known as "box" models, a name applied by some of the earliest heavy gas dispersion models, though this kind of fluid dynamic modeling has a history which long predates its application to heavy gas dispersion.

6.3.2 Scientific basis of model

Integral models of gas dispersion typically model dispersion from a point just downstream of the source to a point where the cloud no longer poses a hazard.

Physical processes modeled

Sometimes the source model may be included, but more typically it will be done by a separate model, possibly in the same suite of models. In the case of LNG dispersion, the source will most often be a pool. The dispersion model may be able only to cope with a circular pool of fixed size at
constant temperature, constant surface gas concentration, and constant vaporization rate, or it may be able to handle a more general situation.

Many integral models technically handle only an instantaneous release of a fixed mass of gas and/or a steady continuous release.

As LNG problems often involve non-circular pools whose size, shape, temperature, surface concentration, and (especially) vaporization rate vary with time, it is important how the model is applied to cope with this. Often the authors of the model will give recommendations.

Integral models idealize the state of the atmosphere, but usually allow for different wind speeds, surface roughness, and atmospheric stability. Mixing is usually incorporated in the form of entrainment velocities, with lower entrainment at high Richardson number.

Some research has been done on understanding the behavior of heavy clouds on sloping terrain, in such a way that it could be incorporated into an integral model, but most models will probably only simulate flat terrain.

Some integral models consider certain types of obstacles including a fence across the wind, one or more cuboidal buildings (with releases upstream or downstream in a wake) and/or a statistically-uniform distribution of obstacles.

There is probably no “standard” way of incorporating some of the more complex effects above, and if complex effects are included in the model, the reviewer should expect to see evidence from validation tests indicating that these have been modeled adequately.

**Mathematical formulation of the problem:** Integral models are characteristically formulated in terms of a few, or several, ordinary differential equations for bulk properties of the cloud. For example, for an instantaneously released, cylindrically symmetric, isothermally dispersing cloud, equations will be derived for the rate of change of (for example) the cloud radius, cloud volume and cloud centroid position. Similarly, for a steady continuous release, equations for time derivatives of the plume width and cross-sectional area can be derived.

In more sophisticated models, extra differential equations are added for other quantities (varying with time or downstream distance) such as temperature and aerosol content.

**Profiles:** The governing equations often appear to relate to a cylinder of gas at uniform concentration with none outside and to a plume of rectangular cross-section with uniform concentration. This is a useful, simple way of thinking about the models, and they have been called “box models” when viewed in this light. But the dimensions are better thought of as coming from some self-similar profile. In this perspective, the radius, $R$, becomes a measure of the horizontal extent of the concentration profile, the height, $H$, a measure of the vertical extent of the concentration profile, and $V=\pi R^2H$ is a measure of the cloud volume, rather than exactly the volume.

In practice, in the heavy gas dispersion regime clouds often have sharp edges, and the language applied to these quantities tends to be rather loose with no particular disadvantage. However, it is important to note that the same concepts (possibly with the extra feature of an evolving profile) can be applied even into the passive dispersion regime. Usually, such profiles are less well validated than the bulk parameters and care must be taken if results are likely to be sensitive to their precise form.

**Dimensional analysis and entrainment:** The success of integral models depends to a large extent on the fact that there are rather few significant groupings of dimensionless parameters on which the overall properties of the cloud can depend. Another way of looking at this is to observe that the
governing equations can only be constructed in a limited number of ways, which are dimensionally correct, and so dimensional analysis is a powerful tool in constructing models.

The importance of the model equations being dimensionally correct cannot be overemphasized. Any model which is not dimensionally correct should be rejected, as it can introduce uncontrolled errors. The broadly accepted concepts of “edge” and “top” entrainment rely entirely on dimensional analysis and are worthless if one bypasses it for other purposes.

One important theoretical result is that top entrainment must vanish in the limit of zero wind. If such a model is adopted, then the cloud’s potential energy increases indefinitely with no wind to power the increase, and conservation of energy is violated at a very fundamental level.

**Transition to passive dispersion:** Early models simply stopped solving the equations somewhere where the cloud had “gone passive” and replaced them with a new set appropriate for passive dispersion. However, the criterion should be based on the value of the Richardson number, or a similar quantity (certainly not just the density or relative density), but this was not always realized in early models. Predictions from early models were often discontinuous at this transition but more modern models formulate their equations smoothly so that the same equations apply to heavy gas dispersion and passive dispersion.

**Thermodynamics:** Although the source of LNG vapor is at or below 112 K, integral models do not necessarily have an explicit temperature equation. The reasons why this is actually a reasonable approach are discussed in Section 1, along with the role and possible effect of atmospheric humidity.

**Solution method:** There are numerous commercially available software packages for solving ordinary differential equations. Their accuracy is known, they have been verified, and use of one of them is generally to be expected for integral models of gas dispersion.

### 6.3.3 Limits of applicability

Integral models have proved remarkably successful and have wide limits of applicability. They have been shown to be useful for doing a hazard analysis in advance of a possible accident, rather than a detailed analysis after a specific accident. Research suggests that integral models can be expected to cope well with heavy gas dispersion, passive dispersion, temperature effects, aerosol effects, humidity, at least some simple chemical reactions, and the effects of certain simple obstacles. In principle, simple terrain features (such as a uniform slope) could be introduced.

### 6.3.4 User-oriented aspects of model

One of the advantages of integral models is that the equations present a simple intuitive description of the cloud dynamics. A model which allows the output of many different variables can enhance understanding of the underlying processes.

Integral models tend to run on desktop computers and will usually take a few seconds to provide a solution for a given problem.

Sometimes, important properties such as the liquid density and vapor specific heat will come from an internal database.

Very little knowledge may be needed to run the program, whereas more knowledge may be needed to configure the appropriate input.
6.3.5 Advantages and disadvantages of model

**Advantages:** Integral models predict the specific data required for hazard analysis and they are usually very quick to run.

**Disadvantages:** Extra features (such as obstacles or non-flat terrain, or anything other than a highly idealized situation) require additional effort to include, and the assumptions employed require further testing against experimental data.

Integral models, because of their advantages, are the most frequently encountered models in hazard assessments.

6.4 SHALLOW LAYER MODELS

6.4.1 General model description

These have some of the features of 3D CFD and some of the features of integral models. In the case of a heavy cloud the properties, concentration, temperature etc., are modeled as depending on horizontal co-ordinates but in a depth-integral sense, in which the cloud height becomes another local property.

6.4.2 Advantages and disadvantages of model

Such models have a combination of the advantages and disadvantages of CFD and Integral models. They would be ideally suited to dispersion over complex sloping terrain, where they would be less empirical than integral models but easier to use (and faster) than CFD models.

However, we are not aware of any model of this kind which has moved from the status of a research tool to the point where it is routinely usable as a hazard analysis code.

6.5 CFD MODELS

6.5.1 General model description

CFD involves the numerical solution of the three-dimensional time-dependent fluid flow equations. Assumptions have to be made in the form of a "turbulence closure" model, which determines the local rate of mixing. Such closure models have been used extensively in modeling a diverse range of flows. An obvious feature of heavy gas dispersion is the suppression of turbulent mixing due to strong, stable, vertical density gradients. A turbulence closure scheme needs to take this into account, and the model should be used in such a way that these density gradients are adequately resolved.

The main advantage of a CFD modeling approach is that it allows for the representation of complex geometry and its effects on flow and dispersion. This can be particularly significant in the case of LNG vapor dispersion if complex terrain and obstacles such as storage tanks and dikes are thought to be of importance. The main disadvantage of CFD approaches for LNG vapor dispersion is that they are generally costly and time-consuming.

CFD modeling is particularly useful for post-accident analysis. However, if the exact source is unknown or assumed (as in the case of hazard analysis) then the ability of CFD to specify precise...
sources is largely irrelevant, whereas for analyzing the event post disaster, where the source is relatively well known, then CFD can be advantageous.

6.5.2 Scientific basis of model

CFD is based on the numerical solution of the Navier-Stokes equations that describe fluid flow. In practice, the Reynolds-averaged form of the equations is commonly used, and therefore equations are solved for the mean (time or ensemble-averaged) values rather than the instantaneous values of velocity, pressure, temperature and concentration. Reynolds-averaged models require a turbulence model to describe the effects of the fluctuating components on the mean fluid properties.

Having derived a set of appropriate equations that describe the fluid flow, these are then discretized and solved on a grid of cells or control volumes. Typically, a finer mesh will give a more accurate solution, but at the expense of increased computational cost. One of the main advantages of CFD is that modern meshing algorithms, typically using unstructured grids, can allow complex topographies and an arbitrary arrangement of obstacles to be modeled relatively easily.

The vapor source term for the dispersion calculation in many CFD models can be specified over an arbitrary area (which may vary in size over time), or by specifying a volumetric source within the computational domain. Additionally, in theory, arbitrary wind conditions can be applied by specifying appropriate boundary conditions, although it is important to ensure that a converged solution to the wind field problem is obtained first, in the absence of any spill.

6.5.3 Limits of applicability

CFD models are applicable to the widest set of circumstances of all the models reviewed here, although they are often not best suited to hazard analyses where a large number of different configurations need to be modeled, due to the time and effort required to configure, compute and post-process the results of a simulation. However, it is likely that in many cases using CFD will be the only practical option if the local topography is very complex or the situation to be modeled is far from the experiments on which the simpler models were derived (although of course the CFD will not be validated for that case either).

In theory, CFD models should be able to model an arbitrarily-shaped source and any wind conditions, including zero wind speed. In practice, obtaining a converged solution for unstable atmospheric conditions can be very difficult, although fortunately this is not important in hazard analysis as this case tends to lead to the shortest hazard ranges.

Most CFD models are based on the Reynolds-averaged Navier-Stokes equations and so no information is provided on short time-averaged concentration fluctuations. Large Eddy Simulations (LES), which would provide such concentration information, are less frequently used for routine hazard analysis, due to increased computational expense.

6.5.4 User-oriented aspects of model

CFD models have traditionally been difficult and time consuming to set up and run. However, the modern general purpose CFD codes, such as ANSYS CFX, STAR-CCM+ and ANSYS FLUENT, are becoming easier to use and they employ sophisticated user-interfaces. Although this means that they are now useable by a wider range of people, they still require considerably more time to set up even the simplest cases compared to the other model types reviewed here. Modern CFD codes use a Computer-Aided Design (CAD) front end to generate the geometry followed by the mesh. The
interface guides the user through a series of forms where the appropriate physical parameters, sub-models and boundary conditions can be specified.

Once the model is running, various output data will be provided to allow the user to monitor how the simulation is progressing. Importantly, information on model convergence will be provided, and it is essential that appropriate convergence criteria are specified and met for each simulation. CFD simulations can take from a few hours to many days or weeks to run, depending on the complexity of the scenario and the number of cells used within the computational mesh.

CFD models provide a very detailed description of the flow field. The output from a CFD model is typically many megabytes of 3-D data. This can make it very time consuming to assess whether or not the solution is credible. However, it does have the advantage that a very wide range of derived parameters can be calculated from the numerical solution.

Despite the ease of use of modern CFD models, it is vital to stress the importance of the expertise of the CFD model user in addition to that required for other types of dispersion model. Studies have shown that different CFD users can produce different results for the same test case, even using the same CFD software.

6.5.5 Advantages and disadvantages of model

**Advantages:** Complex features such obstacles and terrain can be relatively straightforward to model.

**Disadvantages:** The models are labor intensive to use as well as requiring significant computer resources; setting up the problem requires skill and experience and the results can be sensitive to how it is set up; the validation exercise is also very labor and computer intensive.
7 Model Reviews

A partial application of the earlier version of the LNG MEP (Ivings et al., 2007) was made to three models: DEGADIS Version 2.1, FEM3A February 2007 version and DOE-NETL LNG Dispersion Module for FLUENT 6.2/6.3. This exercise was primarily undertaken to assess the suitability of the MEP itself, rather than to serve as a validation exercise for models. A full scientific assessment of the three models was undertaken and the corresponding model evaluation reports are attached as appendices. Although active validation of the model was not undertaken, previous published validation was reviewed. The conclusions from each of these reviews are provided in Sections 7.1 to 7.3 below. Given that these evaluations were undertaken in 2007, it is possible that the reviews provided below are now outdated.

A more recent evaluation of DEGADIS Version 2.1 was undertaken by FERC (2010). The earlier version of the LNG MEP (Ivings et al., 2007) was also applied to evaluate PHAST Versions 6.6/6.7 and FLACS Version 9.1 release 2. Details of these studies can be found on the PHMSA website9. The Fire Dynamics Simulator (FDS) was also evaluated by Kohout (2011). All of these studies mentioned above were evaluated based on the earlier version of the LNG MEP (Ivings et al., 2007).

7.1 DEGADIS

These are the conclusions drawn from Version 3 of the MER for DEGADIS Version 2.1. See Section 12.2 for the report in full. The review was carried out by Dr. D. Webber in 2007.

7.1.1 General model description

The model describes a steady plume, advecting downwind, spreading (with a constant Froude number condition determining the width) and entraining via a fairly standard top entrainment mechanism with entrainment suppression at high Richardson number. Continuity into the passive regime is assured by a relationship derived between turbulent diffusivity and entrainment velocity.

An interesting feature is a secondary source model (present, as far as we know, only in this model and that of Colenbrander (1980) from which DEGADIS was adapted) consisting of a vapor blanket spreading above the source, but not advecting with the wind.

In Colenbrander’s model the vapor blanket does not entrain, whereas in DEGADIS a fairly standard edge entrainment model is used. In both cases the vapor blanket feeds the plume above.

The numerical method used to solve the equations is a variant of a 4th order Runge-Kutta method.

The model includes transient releases, modeled by using a series of virtual observers moving downwind with the plume, each observing a slightly different plume according to the time at which it sets off. The results are combined to give an unsteady plume model. This approach would appear to use an ad hoc solution of partial differential dispersion equations (in time \( t \) and downstream distance \( x \)), but the equations have never been written down and the solution method never shown to converge to the actual solution. However, this may not be a problem if things change slowly enough with time, although whether a boiling LNG pool satisfies this criterion is uncertain.

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It would appear that instantaneous releases are modeled as a special case of transient releases. In this case the non-advecting vapor blanket detraining into a plume above, does not resemble a gas cloud spreading axisymmetrically while advecting downwind (as shown in the Thorney Island trials). An exception is the case of zero wind, where the model must reduce essentially to that of the vapor blanket, and neither top entrainment nor advection would be expected. For the current application to LNG pools, perhaps this is of less concern, unless the gas release looks to be essentially of short duration.

The temperature of the cloud is modeled and there is some discussion of heat transfer from the ground. Atmospheric humidity is one of the inputs. However, this review has not discovered an explicit equation of state of the cloud, or the way in which humidity is considered to affect the dynamics.

### 7.1.2 Scientific basis of model

The assorted sub-models all have a firm scientific basis. The steady plume model puts these together in a well-established way to form an overall model of a structure which few would argue with. In this case the vapor blanket secondary source provides a useful and attractive model of cross-wind and upwind spreading near the source.

The transient release model is built on this but moves a little further from the scientific basis, particularly for releases which are not quasi-steady. LNG vaporization is likely to be a transient continuous release with a large “spike” in the release rate followed by a long tail. Modeling the spike may stretch the scientific basis of the model.

The instantaneous release model has an equally firm scientific basis in the limit of zero wind, but there are some questions regarding the basis when the wind is incorporated. It is worth noting that the Colenbrander model was not only oriented towards continuous releases but also predated the Thorney Island trials, which are by far the best data source for instantaneous releases, with clear side and aerial cinematography in addition to the concentration measurements. It would appear that DEGADIS requires a little coercion to fit instantaneous releases in a wind, although this may not be completely relevant for LNG pool vaporization, if that can successfully be treated as a transient continuous release.

### 7.1.3 Limits of applicability

The model is well suited to gas vaporizing from LNG pools with the caveats expressed above (which may not be large in the general context of integral models, most of which do not even attempt to model transient releases).

It does not handle non-flat terrain or obstacles. But these issues should not be considered as obstacles to its use.

### 7.1.4 User-oriented aspects of model

The user interface is not particularly sophisticated and predates popular use of graphical user interfaces. The output is presented in ASCII files and any results wanted in other formats require some manual post-processing.
7.1.5 Verification performed

The verification reported is very much commensurate with what has generally been done for models like this.

7.1.6 Evaluation against MEP qualitative assessment criteria

It conforms.

7.1.7 Validation performed and evaluation against MEP quantitative assessment criteria

A significant amount of validation has been done. It is possible that, because it is mentioned in the US regulations and easily available free of charge as an internet download, more comparisons with data have been done using this model than any other.

Therefore it should be noted that other analysts have not always found such good agreement with data as the model developers, we have to note also that few models have had the same exposure. But these analyses also indicate areas which may benefit from further analysis or development, including:

- Instantaneous releases: in particular are different independent users of the code liable to use it slightly differently and get different results?
- Performance of the model at low wind speed/stable atmosphere

7.1.8 Advantages and disadvantages of model

Advantages

- Quick to use, especially for steady releases, but probably for all on a modern PC
- A well-considered model which has undergone significant validation
- The vapor blanket estimates upwind and crosswind spreading at the source, a feature missing from many integral models

Disadvantages

- Some doubts arise from some validation exercises
- Obstacles and terrain are not modeled

7.1.9 Suitability of protocol for assessment of model

The protocol has achieved its objectives.

7.2 FEM3A

These are the conclusions drawn from Version 2.0 of the MER for FEM3A, February 2007 version. See Section 12.3 for the report in full. The review was carried out by Dr. C. Lea in 2007.

7.2.1 General model description
FEM3A February 2007 is a finite element based 3-D unsteady Reynolds-averaged CFD code. It was originally developed at Lawrence Livermore National Laboratory by Chan and Ermak (1987), during the 1980’s and 1990’s, specifically for the modeling of dense gas dispersion in the atmospheric boundary layer. It appears to be most closely related to the FEM3C model from Lawrence Livermore National Laboratory (Chan, 1994a). It has undergone further, more minor development and application, specifically for the modeling of LNG vapor dispersion, at the Chemical Hazards Research Center, University of Arkansas.

FEM3A February 2007 is based on a single-block structured mesh composed of general hexahedrons. Turbulence closure models and other sub-models are specifically developed to model the important features of dispersion of LNG vapor clouds in the atmosphere.

The model requires text-based, formatted input files and produces output as text files. There is a conversion program available which operates on this output file to produce a format suitable for input to TECPLOT, a commercial post-processing software package.

The source and executables of FEM3A February 2007, the pre-processing tools for setting-up a flat terrain simulation with or without a tank/dike and the post-processing program for converting FEM3A February 2007 text output to a form suitable for input to TECPLOT can all be licensed from the Gas Technology Institute.

### 7.2.2 Scientific basis of model

The numerical basis of FEM3A February 2007 is inherited from the original FEM3 model (Chan, 1983). FEM3A February 2007 uses a modified form of the Galerkin finite-element method for integration in space along with an Euler explicit finite-difference method for integration in time to solve the conservation equations for total mass, momentum and energy. The temporal and spatial schemes are stated as being second-order-accurate.

There are two turbulence models in FEM3A February 2007: an anisotropic algebraic planetary boundary layer (PBL) model; a $k$-$\varepsilon$ model in which the effects of buoyancy are included as a variation of the model proposed by Betts and Haroutunian (1988) and a simple means of allowing for anisotropy in the turbulent diffusivity is also included (Chan, 1994a, 1994b). The algebraic model is similar to that of ‘model C’ from Ermak & Chan (1986) for the FEM3 model and in particular is very similar to that of FEM3C as reported in Chan (1994a). The $k$-$\varepsilon$ turbulence model was originally implemented by Lawrence Livermore National Laboratory, but with some more recent relatively minor modifications. Both of these turbulence models include mechanisms which lead to a local damping of turbulent mixing in the presence of stable density gradients, a phenomenon important for LNG spills or stable atmospheric conditions.

A water vapor transport, evaporation and condensation model is available in FEM3A February 2007 as originally implemented by Lawrence Livermore National Laboratory (Chan, 1988). A model to account for cooling of the ground has recently been implemented and tested in FEM3A February 2007 (Havens & Spicer, 2005).

The model does not include an LNG spill and vaporization sub-model and therefore a credible vapor source term has to be defined by the user.

### 7.2.3 Limits of applicability

Source: FEM3A February 2007 is most easily used by applying pre-processing tools to create the required text input files. These pre-processing tools are available, although they are limited to the
specification of a constant-area rectangular source at ground level, with constant flux of vapor. Time-variation in the extent of the rectangular source and/or its emission rate can only be approximated by conducting multiple runs of FEM3A February 2007 with differing input conditions.

In principle, non-rectangular sources at ground level can be handled by FEM3A February 2007, although this requires the user to become involved in setting-up or modifying text input files. This will not be a trivial task.

It is unclear as to whether FEM3A February 2007 can handle an arbitrary location and orientation of an area source. If this is possible, the user would again be required to set-up or modify text input files, which would be a very involved task and may be impractical.

**Environment:** It is not clear that zero wind speed could be modeled or would give a numerically-stable solution.

Non-flat terrain can be modeled using FEM3A February 2007. However, pre-processing tools are only available for flat terrain and simulations of non-flat terrain would require the user to specify or modify text input files, which would be an involved process.

Obstacles can be modeled using FEM3A February 2007. However, pre-processing tools are only available for setting-up a single tank in a rectangular dike. Simulation of differing or multiple obstacles, such as multiple storage tanks, would require the user to specify or modify text input files and this would be a very involved process and may not be practical.

**Targets/output:** In common with other Reynolds-averaged CFD approaches, no information on short time-averaged concentration fluctuations is available from the model. Only mean (time or ensemble averaged) values are output, but these can be time-varying provided that the time variation is long compared to turbulent time-scales.

All simulations must be run in transient mode.

It is possible that the cumulative execution time could be lengthy for a time-varying source.

### 7.2.4 User-oriented aspects of model

Model input and output is via formatted text files: there is no user interface.

However, pre-processing tools are available for creating text input files for the case of a rectangular constant-area source, with or without a storage tank/rectangular dike. In addition, a post-processing program for converting FEM3A February 2007 text output to a form suitable for input to TECPLOT, a commercial graphical post-processing software package, is available.

A new user manual is being written, but the key basis and use of FEM3A February 2007 is already documented in Spicer & Havens (1997) and earlier reports by the Lawrence Livermore National Laboratory.

Limited user support and training is available subject to the limitations of resources at the Chemical Hazards Research Center, University of Arkansas.

The source of FEM3A February 2007 is available. The code is written in FORTRAN 77. Model run-times could be lengthy (24 hours or more).
7.2.5 Verification performed

The vast majority of the development of FEM3A February 2007 was undertaken by the Lawrence Livermore National Laboratory during the 1980’s and early 1990’s. The coding modifications and additions by the University of Arkansas since that time have been relatively minor, for example: modification of the clipping procedures to ensure numerical stability for a range of atmospheric conditions; additional code to allow for ground cooling. The additional coding introduced by University of Arkansas to allow for ground cooling has been verified.

The coding of FEM3A February 2007 and its predecessors FEM3, FEM3A, FEM3B and FEM3C, by the Lawrence Livermore National Laboratory during the 1980’s and early 1990’s, does not appear to have been formally and rigorously verified. However, there have been numerous broadly successful evaluations published by Lawrence Livermore National Laboratory in which comparisons have been made against both wind tunnel and field trials data. Whilst this does not formally constitute rigorous verification of FEM3A February 2007, it does nevertheless provide some confidence in the coding of FEM3A February 2007.

7.2.6 Evaluation against MEP qualitative assessment criteria

Model meets the qualitative assessment criteria.

7.2.7 Validation performed and evaluation against MEP quantitative assessment criteria

From the existing validation studies it appears that:

- Overall, the algebraic PBL turbulence model provides broadly acceptable predictions when compared to continuous, unobstructed, field trial releases of LNG.
- For an instantaneous field trial release of Freon, the algebraic PBL turbulence model leads to a significant under-prediction in the maximum downwind distance to concentrations comparable to that of ½ LFL for LNG.
- For wind tunnel continuous releases of carbon dioxide in the presence of a tank and dike, and when using the $k$-$\varepsilon$ turbulence model with buoyancy modifications and anisotropy effects, FEM3A February 2007 provides accurate prediction of the downwind distance to concentrations equivalent to the upper flammability limit of methane, but under-predicts the distance to LFL and ½ LFL by 22% and 26%, respectively.
- For continuous, unobstructed, field trial releases of LNG, FEM3C (using the same form of $k$-$\varepsilon$ turbulence model as implemented in FEM3A February 2007) was broadly successful in capturing both the qualitative and quantitative features of the measured concentration field.

7.2.8 Advantages and disadvantages of model

Advantages

- FEM3A February 2007 is based on previously tested and published numerical and physical sub-models.
- The physical sub-models are specifically tailored to the modeling of LNG vapor dispersion.
• For the specific case of a rectangular constant-area source with or without a storage tank/rectangular dike, pre-processing tools are provided which permit relatively rapid set-up of the model (the model developer indicates about 8 hours)

• A user manual is available (Spicer & Haveins, 1997) which will soon be updated.

• Validation against field trials and wind tunnel data has been reported which indicates that the model is capable of providing credible and broadly acceptable predictions when compared against this data

**Disadvantages**

• There is no user interface. All input and output is via formatted text files

• Model set-up for configurations comprising non-flat terrain/multiple obstacles/non-rectangular area source, could be very involved and may be impractical

• There is very limited error handling of model input and limited information is output whilst the model is running

• Quality of the results will depend strongly on the way in which the model has been applied

• Model use will require user experience in CFD and some knowledge of atmospheric dispersion

• Run-times are lengthy (24 hours or more)

7.2.9 **Suitability of protocol for assessment of model**

The protocol is suitable for assessment of the model.

7.3 **FLUENT**

These are the conclusions drawn from Version 3.0 of the MER on the DOE-NETL LNG Dispersion Module for FLUENT 6.2/6.3. See Section 12.4 for the report in full. The review was carried out by Dr. C. Lea in 2007.

7.3.1 **General model description**

The model is a 3-D CFD code, whose underlying basis is the FLUENT package. FLUENT is a general-purpose commercially-available CFD package, which is under continual development and with regular releases. The current release is 6.3. FLUENT allows users to extend the capabilities of the package by User Defined Functions (UDF).

A set of UDFs are being developed to improve the capability of the FLUENT package to predict the dispersion of dense gas, specifically LNG vapor in the atmosphere. These UDFs are collectively referred to as the LNG dispersion module.

The development of the model is being guided by the outcome of evaluations against wind tunnel data from the Chemical Hazards Research Center, University of Arkansas, and field trial spills of LNG, i.e. 1980 Burro trials at China Lake, California.

The development version of the model is compatible with FLUENT Versions 6.2 and 6.3.

David Huckaby at DOE-NETL, and a team of NETL site support contractors are developing and validating these UDFs. David Huckaby is the main developer of the UDFs. The main FLUENT package is developed by ANSYS Inc. (www.ansys.com).
The model is still under active development and has not yet been released. Distribution of the UDFs has not yet been determined.

### 7.3.2 Scientific basis of the model

The model is based on the 3-D Reynolds-averaged Navier Stokes equations, closed by one of two turbulence models developed specifically for dispersion of LNG in the atmosphere and implemented in the FLUENT package via UDFs; referred to as the LNG module.

The primary components of the LNG module are: (1) an anisotropic algebraic turbulence model based on dense gas Planetary Boundary Layer theory, (2) a two-equation turbulence model built on the standard $k$-$\varepsilon$ model in which the effects of buoyancy on turbulent diffusivity are included and a simple means of allowing for anisotropy in the turbulent diffusivity is also incorporated (3) a water vaporization/condensation model. These physical sub-models were developed and have been published by the Lawrence Livermore National Laboratory.

Other turbulence models are also available, of which the two most significant are an isotropic buoyancy-modified $k$-$\varepsilon$ model and a Reynolds stress transport model.

The model does not yet include a fully tested LNG spill and vaporization sub-model, but this is under development. Therefore a credible vapor source term has to be defined by the user. The model allows for a wide range of source characteristics to be input as boundary conditions.

The atmospheric flow is predicted by the model, subject to user-specified boundary conditions applied at the boundaries of the computational domain.

Single, multiple or arbitrary arrangements of obstacles varying in size and shape can be handled.

Complex terrain can be handled.

The model is implemented within a finite-volume framework.

The module has been developed around FLUENT’s segregated, implicit solver, which implements several pressure-correction algorithms. A range of flux discretization schemes are available, including bounded higher-order schemes. First or second-order temporal discretization schemes are available. The user has to define acceptable convergence criteria.

### 7.3.3 Limits of applicability

**Source:** A separate model is required to provide the specification of a vapor source term. This is under development.

**Environment:** No obvious limitations, other than spatial mesh resolution. Complex geometries may require a large number of mesh cells for adequate resolution of the flow, with correspondingly-large execution times (days). In addition, simulation of a long transient release may also require significant execution time.

**Targets/output:** In common with other Reynolds-averaged CFD approaches no information on short time-averaged concentration fluctuations is available from the model. Only relatively long time-mean values are output but these can be time-varying provided that the time variation is long compared to turbulent time-scales.
### 7.3.4 User-oriented aspects of model

Model set-up, run and post-processing of output is mostly via a Graphical User Interface (GUI). No comments can be made on the user-friendliness of the GUI.

At present formal documentation of the model theory, advice on model set-up, examples of model applications for LNG spills are not available, although these are planned as a future development.

The output can be post-processed to produce a very wide range of data suitable for model evaluation and the needs of hazard assessment.

The results will depend strongly on the way in which the model is set-up and applied by the user. Significant experience in CFD and knowledge of atmospheric dispersion will be required of a user.

Model run-times could be lengthy (24 hours or more), on single processor hardware.

### 7.3.5 Verification performed

Only a limited amount of verification has been performed to date. The model developer states that formal verification is something they intend to address.

### 7.3.6 Evaluation against MEP qualitative assessment criteria

Model meets the qualitative assessment criteria.

### 7.3.7 Validation performed and evaluation against MEP quantitative assessment criteria

Validation thus far has primarily been against wind tunnel data from the Chemical Hazards Research Center at the University of Arkansas. Test cases include release of carbon dioxide in unobstructed conditions and release of carbon dioxide from within an impoundment surrounding a tank, under neutral stability, for both low and high dike walls. The test data stem from work undertaken for the GRI in the mid 1990’s by Havens et al. (1996) and much more recent work undertaken for the GTI also by Havens & Spicer (2006a, b). Some validation has also been carried out against the Burro LNG field trials, test 3 (Koopman et al., 1982a, b).

The outcome of this validation work has been presented at two conferences in the latter half of 2006. There are no peer-reviewed publications associated with application of this model.

The model is still under development. Validation is continuing against a wider set of wind tunnel and field trials data and the outcome of the on-going validation is being fed back into model development.

### 7.3.8 Advantages and disadvantages of model

Note that this model is still under active development and has not been released yet.

**Advantages**

- Model is flexible and can be applied to a very wide range of scenarios
- Model can handle complex geometries and terrain
- LNG module is based on previously published physical sub-models
• Base model – FLUENT – is widely accepted as a ‘state-of-the-art’ commercial CFD package
• Solution methods are up-to-date and can take advantage of current hardware
• Wide variety of output can be obtained
• Support could potentially be available for the model for the foreseeable future

Disadvantages

• Limited range of validation cases examined thus far
• Only a limited amount of verification of the model implementation has been undertaken to date
• Quality of the results will depend strongly on the way in which the model has been applied
• Model use will require user experience in CFD and some knowledge of atmospheric dispersion
• Run-times are lengthy (24 hours or more)
• Base model – FLUENT – is proprietary and must be licensed

7.3.9 Suitability of protocol for assessment of model

The DOE-NETL LNG dispersion module for FLUENT 6.2/6.3 is still under development. However this protocol is designed for evaluation of the full release of a model whose status is fixed and identified by a specific version number. It is therefore strongly recommended that the assessment be repeated upon issue of a full release of this model.
8 GUIDANCE ON MODEL APPLICATION

The general guidance on model application for LNG vapor dispersion given in the Section 8.1 was included in the original version of the LNG MEP Report (Ivings et al., 2007). Since that time, further guidance has been produced on the use of LNG vapor dispersion models, which can be found in the PHMSA website “LNG Plant Requirements: Frequently Asked Questions”\(^\text{10}\), in the paper by Kohout (2012), in the 49 CFR 193 regulations and in the NFPA 59A standard.

Specific guidance on the use of models that have been approved for simulating LNG vapor dispersion can be found in the relevant PHMSA Final Decision Letters\(^\text{11}\) and the review of DEGADIS by FERC (2010). This includes a description of appropriate safety factors and any model limitations. Developers of each of the approved models also publish user guides, which should be followed.

For CFD models, there is generic good practice guidance published by ERCOFTAC (Casey and Wintergate, 2000). More specific guidance on CFD modeling of atmospheric boundary layers has been published by the European COST Action 732 (Franke et al., 2007) and INERIS\(^\text{12}\). For LNG vapor dispersion in particular, there is further guidance published by Luketa-Hanlin et al. (2007).

8.1 GENERAL GUIDANCE

One of the areas sometimes neglected is the difficulty of applying a model or models consistently. Different users may arrive at different conclusions about the same hazard because they used different models or they applied the models (even the same model) differently. The latter possibility is of some concern.

Model developers should be encouraged to supply guidance, possibly in the form of worked examples, on how their models were intended to be applied to the hazards it is designed for. Moreover, inputs need to be specified, including whether they were based on a different choice of source model or a different usage of the same source model. It is therefore recommended that source models should be reviewed on the same basis as dispersion models.

In the case of an LNG pool, not all source models may predict the gradual change from boiling to evaporation and thus may underestimate the release rate in the latter period. It may be productive to compare the effects of using different source term models.

Not all dispersion models may explicitly handle transient releases, in which case (and possibly even if they do) it should be specified how the varying source of gas from the vaporizing pool should be handled. In the past, Webber et al. (1994) found it productive to model the release both as steady continuous and as instantaneous and to compare the maximum concentration against distance predicted in each case. In fact, for the Goldfish HF trials (Blewitt et al., 1987a, b) the difference was not too great and a reasonably coherent picture emerged, despite the fact that the dispersion model being used did not explicitly handle transient releases. Such an approach was also recommended by Hanna et al. (1996).

A range of atmospheric conditions should always be considered. Models which agree in medium wind speed and neutral stability, where there is sufficient data for validation, may not show the same level of predictive performance in stable low wind speed conditions, where data are more sparse. If so, that should be noted as an uncertainty. Atmospheric stability and wind-speed


combinations of Pasquill-Gifford Class D and 5m/s (D5) and Pasquill-Gifford Class F and 2m/s (F2) are often chosen as representative of typical neutral and stable conditions, respectively, but other combinations should be considered in case they result in longer predicted hazard ranges.

The sensitivity of the model output to other factors should also be considered. For example, the best choice ground roughness length is never absolutely certain and it should also be varied to assess its effect. For example, a very large ground roughness length, for any given wind speed, can generate arbitrarily high levels of turbulence causing very short hazard ranges to be predicted. The aerodynamic roughness length is always much less than the height of the roughness elements from which it comes; if it is large, it may be appropriate for the wind flow over the tops of the buildings (which are then considered as “roughness”) but for the flow at ground level the buildings should be considered as obstacles or not at all.

In any event, presenting a single run of a model or even a very limited number of runs as the definitive answer, is unsatisfactory, and as wide a view of the hazard as possible should be presented by testing various hypotheses.

Some expertise on the part of the model user is always going to be required. A black box where one can press the button to predict a hazard range does not exist, and will almost certainly never exist. For example, if a model asks the user for a roughness length, or the atmospheric stability, then the user must know what is being asked for, and not just choose values according to convenience. Generally, the user will be expected to know something of the atmosphere and the factors affecting vaporization and dispersion.

Effects of obstacles near the source should not be overestimated and this is another area where some general fluid dynamics expertise is required of the user. While an LNG pool is boiling, its vaporization rate is controlled by heat transfer, irrespective of the air flow. If the surroundings have cooled to the extent where it is vaporizing more slowly, then obstacles, such as a storage tank, will create turbulence in their wake, and turbulence over the pool will assist vaporization rather than hinder it. A high dike wall may mean that a heavy cloud within it may have to dilute in the turbulent flow caused by the wind over the top before it escapes but, for example, we know of no reason to assume that it does not escape, or that there would be any very significant delay in its escape. For the Falcon series of LNG field trials (Brown et al., 1990) and in the first test undertaken, LNG vapor was observed to escape over an 8.7 m high fence surrounding a spill on water, even under low wind speed and very stable atmospheric conditions: Pasquill-Gifford Class G.

This is an area where application of CFD models to some idealized examples may be very productive, not only to provide hazard estimates, but also specifically with a view to drawing conclusions for the application of integral models with the optimal assumptions about the source.
9 CONCLUSIONS

A Model Evaluation Protocol (MEP) has been presented here that can be used to assess the suitability of dispersion models for predicting hazard ranges associated with large spills of LNG. The MEP is based on one that was previously developed by the EU SMEDIS project for dense gas dispersion (Carissimo et al., 2001; Daish et al., 2000), with modifications to make it specifically applicable to the dispersion of LNG vapor on land.

The MEP is based on three distinct phases: scientific assessment, model verification and model validation. The scientific assessment is carried out by first obtaining detailed information on a model from its current developer using a specifically designed questionnaire, with the aid of other papers, reports and user guides. The scientific assessment then examines the various aspects of a model including its physical, mathematical and numerical basis, as well as user-oriented aspects. This assessment allows the model to be evaluated against eleven qualitative assessment criteria. The outcome of the scientific assessment is recorded in a Model Evaluation Report (MER), along with the outcomes of the verification and validation stages. The template for the MER has been designed to aid the reviewer to extract all of the necessary information to complete the scientific assessment.

The verification stage of the protocol is treated passively, as in the original application of the SMEDIS protocol. This means that instead of carrying out a specific exercise to verify that the model has been implemented correctly and accurately, evidence of model verification is sought from the model developer and this is then assessed and reported in the MER.

The validation stage of the MEP involves applying the model against a database of 33 experimental test cases, including both wind-tunnel experiments and large field-scale trials. The aim of the validation stage is to quantify the performance of a model by comparing its predictions to measurements. The specific datasets and validation cases included in Version 12 of the LNG Model Validation Database have been outlined here, and further details of each trial can be found in the Model Validation Database Guide (Stewart et al., 2016). A number of physical comparison parameters and statistical performance measures have been defined which allow the model to be assessed via a number of quantitative assessment criteria.

In early 2007 (at the time of the first version of this MEP was published), the MEP was applied to three models: “DEGADIS Version 2.1”, “FEM3A February 2007 version” and “DOE-NETL LNG Dispersion Module for FLUENT 6.2/6.3”. A full scientific assessment of these models was undertaken and the resulting MER’s are included as Appendices to this report. For each model, a general description of the model is given along with its scientific basis. The limits of applicability of each model are then described and the previous validation of the model is assessed. All three models met all of the qualitative assessment criteria, based on their scientific assessment. The performance of the three models was not assessed against the LNG Model Validation Database since, at the time of the review, the database had not been created.

However, since then, the full MEP (including the validation stage) has been applied to evaluate PHAST Version 6.6/6.7 and FLACS Version 9.1 release 2. Details of these studies can be found on the PHMSA website\(^\text{13}\). In addition, DEGADIS Version 2.1 has been assessed by FERC (2010) and the Fire Dynamics Simulator (FDS) has been evaluated by Kohout (2011) using the MEP.

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In the past year, changes have been made to the validation database to correct various errors that have recently been found, and further clarification has been provided on the use of the database (Stewart et al., 2016). This has led to a requirement to update the MEP and publish this second edition of the MEP report.

The continued application of the MEP will help the NFPA and PHMSA to make decisions on the appropriateness of dispersion models for predicting hazard ranges for large LNG spills. However, like the models themselves, the MEP is subject to uncertainty and it may be beneficial to review and refine the MEP once it has been applied in full to other models.

A final point worth reiterating is that model predictions are often sensitive to user effects. Studies have shown that different users can produce different results for the same test case, even using the same model. To address this issue, this report provides guidance on the application of dispersion models for assessing the hazards from LNG spills and provides references for other relevant guidance documents.

9.1 RECOMMENDATIONS

Based on the work that has been carried out, the following recommendations are made:

- A number of models should be subjected to the full MEP, including the validation exercise. The MEP should then be refined in the light of this new information, in particular with regards to the choice of quantitative assessment criteria for point-wise concentration and distance SPMs.
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11 GLOSSARY

**DGD models** Dense gas dispersion models, i.e. models that are able to simulate the spreading and dilution of clouds of gas whose initial density is greater than that of the ambient air.

**evaluation procedure** The list of activities in a model evaluation, including gathering information on a model, performing the scientific assessment, scrutinizing model verification, assessing model performance against validation data, recording the outcome of the evaluation and agreeing this outcome with the model developer.

**MEP** – see model evaluation protocol

**MER** – see model evaluation report

**model** A theoretical representation of a physical scenario. In the present circumstances, models are broadly speaking either mathematical or physical. Mathematical models lead to mathematical problems to solve, whilst physical models are predominantly based on experimental representations of the problem, typically at reduced scale.

**model evaluation protocol** The evaluation of a model according to a set of well-defined procedures. Although the scientific assessment and validation of the model are the central activities, “evaluation” is used to mean the entire range of activities before, during and after the scientific assessment and validation.

**model evaluation report** The Model Evaluation Report (MER) is the key output following application of the MEP. It contains the scientific assessment and the outcomes of model application against test cases in a validation database. It provides conclusions and an assessment of the model against qualitative and quantitative assessment criteria.

**model developer** A person who has an intimate knowledge of the model and is usually the person responsible for developing the current version of the model.

Richardson number A measure of the relative importance of buoyancy forces and kinetic energy of a flow. A low Richardson number indicates a flow where buoyancy is negligible.

**scientific assessment** The assessment of the scientific basis of a model based on information provided via the questionnaire.

**source** The origin of the material that eventually forms a cloud of dense gas. Two meaning are commonly attributed to ‘the source’: Firstly the source can be defined as the initial conditions to a dispersion calculation, i.e. the vaporization of a liquid pool; alternatively it can be defined as the input to a dispersion model. In this report it refers to the latter unless otherwise stated. Also see source model.

**source model** A model that provides the initial conditions for a dispersion model. Note that this may include a model for the initial dispersion of the gas (e.g. within an impoundment), in which case this part of the ‘source model’ should also be subject to the model evaluation protocol. The source model may or may not be a separate piece of software from the dispersion model.

**user-oriented aspects** Those aspects of a model connected with the practical usage of the model to solve a given problem, including setting-up a problem and handling the output produced, experience requirements of a user, etc.

**validation** The process of comparing the predictions of a model which has been run to simulate a given event, with the observations made in connection with the same event. It is a test of the extent
to which the model reproduces reality. In the case of the MEP, validation is the only part of the evaluation procedure that requires running the model.

**validation database** A structured source of information on a set of test cases against which a model should be validated. A validation database contains sufficient information on each test configuration, release conditions and meteorological data to permit model set-up and simulation. The database also contains tabulated test results against which model output is compared.

**verification** The process of comparing the implementation of a model with its mathematical basis. Most commonly this refers to checking that a computer implementation of a model (computer software) accurately represents its mathematical description. In the case of the MEP this is treated passively as part of the scientific assessment, i.e. it is based on information provided by the model developer.
## 12 APPENDIX A

**Table 12.1** Summary of the Statistical Performance Measures (SPM) and their quantitative acceptance criteria

<table>
<thead>
<tr>
<th>SPM</th>
<th>Definition</th>
<th>Quantitative Acceptance Criteria</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean Relative Bias</td>
<td>[ MRB = \left( \frac{C_m - C_p}{\frac{1}{2}(C_p + C_m)} \right) ]</td>
<td>(-0.4 &lt; MRB &lt; 0.4)</td>
</tr>
<tr>
<td>Mean Relative Square Error</td>
<td>[ MRSE = \left( \frac{(C_p - C_m)^2}{\frac{1}{4}(C_p + C_m)^2} \right) ]</td>
<td>(MRSE &lt; 2.3)</td>
</tr>
<tr>
<td>FAC2: the fraction of predictions within a factor of two of the measurements</td>
<td>(0.5 \leq \frac{C_p}{C_m} \leq 2.0)</td>
<td>(0.5 \leq FAC2)</td>
</tr>
<tr>
<td>Geometric Mean Bias</td>
<td>[ MG = \exp \left( \ln \left( \frac{C_m}{C_p} \right) \right) ]</td>
<td>(0.67 &lt; MG &lt; 1.5)</td>
</tr>
<tr>
<td>Geometric Variance</td>
<td>[ VG = \exp \left( \left[ \ln \left( \frac{C_m}{C_p} \right)^2 \right] \right) ]</td>
<td>(VG &lt; 3.3)</td>
</tr>
<tr>
<td>Concentration Safety Factor</td>
<td>[ CSF = \left( \frac{C_p}{C_m} \right) ]</td>
<td>(0.5 &lt; CSF &lt; 2.0)</td>
</tr>
<tr>
<td>Concentration Safety Factor to the Lower Flammability Limit (LFL)</td>
<td>[ CSF_{LFL} = \left( \frac{C_p}{LFL} \right) ]</td>
<td>(0.5 &lt; CSF_{LFL} &lt; 2.0)</td>
</tr>
<tr>
<td>Distance Safety Factor</td>
<td>[ DSF = \left( \frac{x_p}{x_m} \right) ]</td>
<td>(0.5 &lt; DSF &lt; 2.0)</td>
</tr>
<tr>
<td>Distance Safety Factor to the Lower Flammability Limit (LFL)</td>
<td>[ DSF_{LFL} = \left( \frac{x_{p,LFL}}{x_{m,LFL}} \right) ]</td>
<td>(0.5 &lt; DSF_{LFL} &lt; 2.0)</td>
</tr>
</tbody>
</table>
13 APPENDIX B

The following are attached as appendices. Note that they all have their own page numbering, independent of this report.

13.1 QUESTIONNAIRE

13.2 DEGADIS MER

13.3 FEM3A MER

13.4 FLUENT MER
HSL: HSE’s Health and Safety Laboratory is one of the world's leading providers of health and safety solutions to industry, government and professional bodies.

The main focus of our work is on understanding and reducing health and safety risks. We provide health and safety expert advice and consultancy, research, specialist training and products.

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