Model Validation Database for Toxic Dispersion

Blue Engineering and Consulting Company

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EXECUTIVE SUMMARY

The safe siting of LNG facilities requires the quantification of the consequences to people and property from a loss of containment and release of hazardous materials (e.g., flammable and/or toxic). Calculating the distance to which hazardous conditions may extend for each type of scenario requires the use of computational models.

The quality of models, especially those used to evaluate the consequences of hazardous scenarios on the public or public property, has always been a concern to regulatory bodies. Therefore, the U.S. Department of Transportation, Pipeline and Hazardous Materials Safety Administration (PHMSA) funded a research project to develop means to evaluate computational models for the calculations of the different types of hazards associated with the operation of LNG facilities. This research project is being conducted by Blue Engineering and Consulting Company (BLUE), in collaboration with the Gas Technology Institute (GTI).

A general methodology for the evaluation of models was developed and described in an earlier report as part of this project [1]. From the general methodology, a set of hazard-specific model evaluation protocols (MEPs) are developed.

The scope of the MVD presented in this document is to evaluate toxic streams from liquid spills or pressurized releases, dispersing over different types of terrain (unobstructed, obstructed or including complex geometries). Given the focus on toxic exposure, this database includes test data with measured concentrations on the order of 10-1,000 ppm. Some of the data sets included in the flammable dispersion database are also included in the current document, as their characteristics match both scopes. However, this report provides only a brief summary of those test series; the reader is redirected to the flammable MVD report [2] for additional information.

The database for toxic dispersion model validation presented in this report includes experimental data from the following test series:

- BA-Hamburg;
- FLADIS;
- Goldfish;
- Jack Rabbit II;

- Kit Fox;
- Lathen;
- MUST;
- Prairie Grass; and
- Thorney Island.

1 Structure of the Model Validation Database

Validation is the process of comparing model results to measured data for scenarios that test the physics that the model is intended to predict [3]. In the context of a model evaluation protocol for regulatory purposes, the term "validation" is not intended in absolute terms but, rather, it implies "relative to the scenarios against which it was compared".

Therefore, the purpose of a model validation database is to identify a set of scenarios to be simulated with a computational model, in such a manner that qualitative and/or quantitative comparisons may be made between model predictions and actual observations. In general, the scenarios in the database will consist of experimental data sets; however, real-world scenarios (e.g., accidents) can also be included, provided that there is sufficient information to set up a simulation and evaluate the modeling results.

In addition to specifying data sets for model validation, the MVD needs to include the information necessary to set up and perform the simulations, as well as to define the criteria for comparison of the model predictions with the observations. The following sections describe the different components of the model validation database for toxic dispersion.

1.1 Requirements for Suitable Data Sets

In order to be suitable for the validation of a toxic dispersion model, a dataset should meet the following requirements [4]–[6]:

- The test configuration should be representative of realistic scenarios. The scale of the experiment should also be comparable to actual scenarios; in particular, focus will be placed on test series that tracked gas concentrations below 1,000 ppm (0.1%), as toxic hazard thresholds are typically associated with much lower concentrations than flammable hazards.
- The tests should be described in sufficient detail for modelers to set up their simulations in an accurate and consistent manner, with as few assumptions as possible.
- Meteorological data (i.e., ambient temperature, humidity, wind speed and atmospheric stability, etc.) should be available from sensors in/near the area of interest. Location and height of sensors should be provided. The resolution should be sufficient to define the atmospheric boundary layer profiles, or those values should be provided in the test series report.
- The test series should include a wide range of meteorological regimes.
- Sensor data should include measurement of the key variables: in the case of atmospheric dispersion experiments, gas concentration measurements must be

available; temperature measurements are less likely to be useful for toxic dispersion scenarios due to the high dilution of the cloud.
- Measurements should be of a sufficient quantity to be statistically representative.
- Uncertainty of all measured and derived quantities should be provided, together with a description of the method used to define such uncertainty.
- If the raw data is not provided, the time-averaging applied to the data must be specified. Since toxic hazards are typically associated with prolonged exposure, long time-averages tend to be more relevant in this case.
- The data must be freely available.
- Concentrations should be available at more than one distance downwind, with sufficient lateral resolution to document the spatial structure of the cloud. Vertical resolution should also be included, to define the cloud stratification.

1.2 Dataset grouping

Every experimental data set generally has a well-defined scope which determines the details of the test series, including the material being released, type of release, the scale, type and quantity of instrumentation, etc. In order to optimize the database, the selected data should span a broad range of conditions and should strike a balance between the number of trials included for each type of scenario. Therefore, it is useful to combine different test series into groups with similar characteristics. Grouping the test series will clearly identify which sets of conditions have sufficient data for model validation and which ones will require additional research and a suitable near-term alternative.

The following sets of parameters have been selected for the purpose of grouping the toxic dispersion test series:

- Material:[1]
    A. Heavier-than-air
    B. Lighter-than-air
- Release Type:
    A. Liquid spill or low-momentum gas source
    B. Jet (flashing liquid or gas)
    C. Tracer
- Dispersion Area:
    A. Unobstructed (e.g., “rural”)
    B. Obstructed (e.g., barriers)

[1] A distinction between toxic and non-toxic materials would appear more logical; however, such distinction is less meaningful in terms of cloud dispersion behavior than the buoyancy of the gas.

C. Complex Geometry (e.g., “urban” setting, or topography effects)

1.3 Dataset rating

Given the complexities associated with performing atmospheric dispersion experiments, particularly at scales typical of industrial facilities, it is unlikely that many experimental test series would meet each of the requirements listed in 1.1. Therefore, each experimental dataset reviewed for potential inclusion in this MVD is “rated” according to several categories, following an approach first introduced by Skjold et al. [7]. The different ratings are then combined into an average score, which informs the selection of data sets for the validation database.

The following categories are used to rate experimental datasets for the toxic dispersion MVD:

- Relevance to actual scenarios: this category evaluates whether the experimental set up replicates toxic dispersion scenarios that are likely to be modeled in an actual hazard analysis. In particular, given the focus on toxic exposure modeling, relevant trials should have two or more measurement arcs with peak concentrations below 1%.
- Material: this category evaluates the relevance of the fluid released during the experiments to those typically evaluated in an actual hazard analysis.
- Scale: this category compares the scale of the experimental set up to typical hazard analysis scenarios. “Scale” should consider the physical dimensions of the test area (i.e., the distance from the source to the measurement stations), the strength of the source term (i.e., release flowrate), and the range of gas concentrations measured during each trial. As discussed in the flammable dispersion MVD report, the purpose of this project is to evaluate models for industrial-scale applications, therefore, “full” scale trials will be rated higher than reduced scale or wind tunnel tests.
- Repeatability: this category addresses the inherent uncertainty associated with atmospheric dispersion. For example, if a field scale experiment is run just once, the measurements will be affected by stochastic conditions specific to that run, which cannot easily be quantified; if the same experiment were to be repeated multiple times, an ensemble average of the data could be calculated as well as a measure of the stochastic uncertainty. Typically, field experiments are rarely repeated due to the complexity of ambient conditions; smaller scale experiments (e.g., wind tunnel or laboratory scale) can be repeated more easily and are subject to more controlled ambient conditions.
- Data quality/availability: this category evaluates whether the data publicly available is adequate to evaluate a model’s predictions. Data quality considers the type of measurement performed, the instruments used and the sampling rate. Data availability considers the number and placement of sensors, and whether time traces are available or just peak values.

For each category, ratings will range between 0 and 5, as follows:

- 0 = Not Acceptable
- 1 = Poor
- 3 = Acceptable
- 5 = Excellent

A rating of "0" in any one category will eliminate the data set from consideration for the MVD. An average rating of 3 is considered as the acceptability threshold for a test series. However, the average rating is intended as guidance and not as a strict pass/fail criterion. Other considerations, such as the number of trials addressing a given type of scenario, will also factor into the decision of including a given test series in the database.

Each data set reviewed in Section 2 was rated as described above; the rating for each test series is reported on the summary page.

1.4 Datasets and Trials Selected for the Toxic Dispersion MVD

A review of available literature and discussions with various LNG safety and atmospheric dispersion experts led to the identification of over 20 experimental test series focused on the dispersion of gas or vapor clouds. A summary description of each test series is provided in Section 2, including ratings and classification, and the information necessary to set up and run model simulations. The test series included in the toxic dispersion database are shown in Table 1.4-1, grouped by type of release and dispersion area. Test series involving toxic streams are in red text; non–toxic streams are shown in green text. The number in parentheses following each test series name represents the number of trials included in the MVD.

Table 1.4-1. Experimental test series included in the Toxic Dispersion MVD.

	Unobstructed	Obstructed	Complex Geometry
Spill / Low-Momentum	BA-Hamburg (1) Thorney Island (2)	BA-Hamburg (2)	Kit Fox (8)
Jet	FLADIS (3) Goldfish (3)	Lathen (4)	Jack Rabbit II (6)
Tracer	Prairie Grass (5)		MUST (6)

The toxic dispersion MVD includes a total of 40 trials, of which 13 (33%) are spills or low-momentum releases, 16 (40%) are jet releases and 11 (28%) are tracer gas releases. Cloud dispersion occurred over flat terrain in 14 trials (35%), whereas 6 trials (15%) included obstructions (e.g., barriers) and 20 trials (50%) included an urban style "complex" geometry.

Table 1.4-2 lists each of the 40 trials included in the toxic dispersion model validation database. It should be noted that 19 of the 40 trials (48%) are the same as in the flammable dispersion MVD, which significantly reduces the total modeling effort required for models to be evaluated against both the flammable and toxic dispersion databases.

Data from each trial is included in a spreadsheet ("Toxic Dispersion MVD – rev #.xlsx")[2] that accompanies this report; the data includes ambient conditions, source term characteristics, and measured gas concentrations at individual sensors.

[2] The "#" indicates the revision number for the spreadsheet, which may be updated more frequently than this report.

Table 1.4-2. Experimental trials included in the Toxic Dispersion MVD.

Series	Test No.	Release Type	Fluid	Notes
BA-Hamburg	BAH DA0120	Low-momentum	SF_6	-
	BAH 039051	Low-momentum	SF_6	Upwind fence, 19.15 cm radius
	BAH 039072	Low-momentum	SF_6	Upwind fence, 30.64 cm radius
FLADIS	FL 16	Flashing jet	Ammonia	-
	FL 25	Flashing jet	Ammonia	-
	FL 27	Flashing jet	Ammonia	-
Goldfish	GF 1	Flashing jet	Hydrogen Fluoride	-
	GF 2	Flashing jet	Hydrogen Fluoride	-
	GF 3	Flashing jet	Hydrogen Fluoride	-
Jack Rabbit II	JRII 2	Flashing jet	Chlorine	Downward release; Urban array
	JRII 3	Flashing jet	Chlorine	Downward release; Urban array
	JRII 4	Flashing jet	Chlorine	Downward release; Urban array
	JRII 5	Flashing jet	Chlorine	Downward release; Urban array
	JRII 7	Flashing jet	Chlorine	45-deg. down; Reduced array
	JRII 8	Flashing jet	Chlorine	Vertical release; Reduced array
Kit Fox	KF 5-3	Low-momentum	CO_2	Urban array
	KF 5-4	Low-momentum	CO_2	Urban array
	KF 6-4	Low-momentum	CO_2	Urban array
	KF 6-5	Low-momentum	CO_2	Urban array
	KF 6-6	Low-momentum	CO_2	Urban array
	KF 6-9	Low-momentum	CO_2	Urban array
	KF 7-3	Low-momentum	CO_2	Urban array
	KF 8-8	Low-momentum	CO_2	Urban array
Lathen (EEC)	EEC 07	Flashing jet	Propane	Curved barrier
	EEC 08	Flashing jet	Propane	Curved barrier, 50% porous
	EEC 17	Flashing jet	Propane	Curved barrier
	EEC 18	Flashing jet	Propane	Curved barrier, 50% porous
MUST	MUST 4	Gas Jet	Propylene	Urban array

Series	Test No.	Release Type	Fluid	Notes
	MUST 5	Gas Jet	Propylene	Urban array
	MUST 15	Gas Jet	Propylene	Urban array
	MUST 19	Gas Jet	Propylene	Urban array
	MUST 20	Gas Jet	Propylene	Urban array
	MUST 21	Gas Jet	Propylene	Urban array
Prairie Grass	PG 17	Tracer	SO_2	-
	PG 32	Tracer	SO_2	-
	PG 36	Tracer	SO_2	-
	PG 53	Tracer	SO_2	-
	PG 66	Tracer	SO_2	-
Thorney Island	TI 45	Low-momentum	Freon-12 / Nitrogen	-
	TI 47	Low-momentum	Freon-12 / Nitrogen	-

1.5 Key Physics of Toxic Dispersion Scenarios

Describing the physics of toxic dispersion within the scope of this database is quite complex; in fact, the behavior of the toxic cloud can vary significantly depending on the characteristics of the scenario, including the type of release, the released fluid, and the area over which the toxic cloud disperses. It can also vary with the distance from the source, as the cloud entrains ambient air and (potentially) exchanges heat with the environment; both of these effects tend to modify the density of the cloud relative to the ambient air, thereby affecting its buoyancy. The toxic dispersion database includes different types of releases, which are typically encountered in LNG facility siting scenarios. Even though the evaluation of the source term is part of a separate model evaluation protocol, a brief description of the release types considered in this MVD is provided below.

1.5.1 Liquid spills

Liquid spills represent scenarios in which a loss of containment results in the formation of a liquid pool on a surface. This can occur, for example, if a low-pressure liquid storage tank is breached, resulting in a liquid outflow that collects on the ground; or it can occur if a pressurized pipe or vessel is breached, resulting in a flashing liquid spray, part of which may deposit on the ground or collect onto a surface.

The liquid pool is driven by gravity to spread thinner and to follow any slopes towards lower elevations; this behavior is used to direct liquid spills into a liquid conveyance system (a.k.a., a set of trenches) that terminates at an impoundment area, where the liquid can collect.

Vapors are formed above the surface of the liquid pool; the amount of vapor being generated depends on the properties of the spilled material (e.g., the boiling temperature) and the ambient conditions (e.g., the temperature of the substrate beneath the pool). If the boiling temperature is below the substrate temperature, boiling heat transfer generates intense vaporization of the liquid, resulting in large amounts of vapor which is heavier than the surrounding ambient air and therefore forms a dense vapor cloud above the pool. Over time, the substrate cools down thus reducing the rate of heat transfer to the pool and the vapor generation rate. If the boiling temperature of the liquid is above the temperature of the substrate, vapors are still formed but at a lower rate: vapor generation is now driven by diffusion (and non-boiling heat transfer, if the liquid is colder than the substrate) and the resulting cloud tends to be smaller and have a lower gas concentration.

As more vapor is generated, the vapor cloud tends to spread horizontally but remains low to the ground due to its higher density. In the presence of terrain gradients, the cloud may move away from the pool, driven by gravity; more commonly, however, wind is the mechanism that drives the vapor cloud away from the source. The dispersion of the lowlying, slow-moving cloud is easily affected by obstacles and obstructions, including barriers intended to stop or redirect it away from areas of concern. As the dense cloud is advected, it mixes with ambient air and absorbs heat from the warmer ground. Eventually, the gas concentration within the vapor cloud falls below the toxic hazard concentration threshold for the spilled material and the toxic dispersion hazard ceases to exist.

1.5.2 Jet releases

Jet releases occur when a pipe or vessel containing a fluid under pressure is breached. If the fluid is liquefied under pressure, the release scenario results in a flashing jet, where a portion of the stream immediately flashes to vapor upon discharge while the rest is atomized into liquid droplets; the liquid droplets tend to evaporate as the jet moves away from the source and entrains air, however, a portion of the liquid droplets may impinge onto a surface (or the ground) before fully evaporating and result in rainout and the formation of a liquid spill.

The air entrainment results in a less dense and generally “taller” cloud than in the case of a liquid spill; additionally, the cloud can carry momentum from the initial jet for some distance. Therefore, while obstacles and obstruction can affect the dispersion of a vapor cloud from a flashing jet release, controlling this type of cloud using barriers is generally more challenging.

If the fluid is in the gas phase before the breach, the release scenario is likely a choked gas flow, since most gas streams in an LNG facility operate above the critical pressure ratio. If the released gas is lighter than air, the cloud tends to rise shortly after the release, as the jet slows down and buoyancy becomes dominant; if the gas is heavier than air, the cloud tends to fall to the ground and spread as described above for a flashing jet release. As for the spill scenario, eventually the gas concentration within the cloud falls below the toxic hazard concentration threshold for the released material and the toxic dispersion hazard ceases to exist.

1.5.3 Tracer releases

Tracer releases include scenarios in which the material of interest is released at rates small enough that it is rapidly diluted to low concentrations (e.g., less than 1,000 ppm). Examples may include a small release rate of toxic gas into a highly ventilated area, a large release of a mixture with only a small fraction being toxic, the spill of a toxic liquid, etc. Tracer release scenarios are not common in LNG facility siting. Furthermore, the behavior of tracer releases can therefore be related to one of the other release types discussed above. However, since several experimental test series have been conducted with this type of release and the focus of the measurements is much more on the far field, tracer releases are considered separately to specifically evaluate the model performance against these scenarios.

1.5.4 Parameters affecting Toxic Cloud Dispersion

The brief descriptions provided above suggest that, while the characteristics of the cloud formation and dispersion can vary significantly from scenario to scenario, the toxic dispersion scenarios are generally affected by the same parameters, such as:

- Thermodynamic properties of the released material (boiling point, molecular weight, etc.)
- Release characteristics (release rate, temperature, momentum, liquid fraction, etc.)
- Terrain or substrate characteristics (temperature, heat transfer properties)
- Ambient conditions (wind, temperature, humidity)
- Topography and other geometric considerations (barriers, obstructions)

Models applied to toxic dispersion scenarios should therefore include as many of these parameters as possible; however, it is not necessary for all parameters to be included in a model – for example, several widely used models do not include the effects of topography or obstacles, yet their results can frequently be considered conservative and therefore they are still applicable to many scenarios.

1.6 Variables and Physical Comparison Parameters

The quantity most frequently measured during dispersion experiments is the gas concentration in air, which also represents the variable of concern in siting scenarios. Other quantities, such as oxygen concentration or gas temperature, are sometimes measured in addition, or in alternative, to gas concentration; while measurements based on these quantities may allow to quantify the gas concentration in the flammable range (approximately 1-5%), they are likely to result in large uncertainty at the concentrations typical of toxic hazard thresholds (10-1,000 ppm).

The selection of physical comparison parameters is critical to ensure that model performance is properly evaluated. The physical comparison parameters (PCPs) for toxic dispersion were selected according to prior evaluation protocols for atmospheric dispersion models and to the flammable dispersion MVD, as follows:

1. Maximum point-wise concentration;
2. Maximum arc-wise concentration;
3. Predicted distance to a measured maximum arc-wise concentration.

Note that the cloud width, which was included as PCP in the flammable dispersion MVD, is not included in the toxic dispersion PCP. The main reason for the omission is that the concept of cloud width loses meaning when cloud dispersion is affected by obstacles or complex geometries, which together represent nearly half of the trials in this database and significantly limit the applicability of this PCP to toxic dispersion scenarios. Additionally, even when cloud width can be calculated, it represents a less discriminating test than the peak concentration.

1.6.1 Maximum point-wise concentration

Point-wise concentrations are the gas concentrations in air measured at individual sensor locations, processed using a specified averaging time. Frequently, gas concentrations are reported for both short and long time-averages: the short time-average is typically 1 second, while the long time-average is typically equal to the duration of the steady period of the release. The peak value measured at each sensor and for each averaging time is recorded for comparison with the model's prediction at the same location and under the same averaging time.

The use of point-wise concentrations challenges the model's ability to predict the cloud distribution away from the centerline; therefore, it is a more difficult test than the use of arc-wise maximum concentrations (discussed in the next subsection). The use of point-wise concentrations is also more easily affected by experimental uncertainties, such as wind speed or direction. However, point-wise concentrations provide critical information on the model's performance in obstructed or complex dispersion scenarios, where arc-wise data may lose significance. Point-wise data are also the primary means for inputting data into the validation database, upon which all of the other physical performance parameters are automatically calculated.

Therefore, point-wise concentrations are included as a physical comparison parameter to allow a more detailed comparison between measurements and predictions, where appropriate.

1.6.2 Maximum arc-wise concentration

The maximum arc-wise concentration is the maximum concentration (measured or predicted) across an arc, at a given distance from a release. This definition has been interpreted differently in various validation studies, which has caused confusion when evaluating model performances. Throughout this database and model evaluation protocol, maximum arc-wise concentrations will be compared as specified in the flammable dispersion MVD (and previously by Ivings et al. [3]): at each arc distance, the maximum arc-wise concentration will be taken as the maximum at the sensors positions (including elevation); it is critical for this approach to be applied consistently to both experimental data and model predictions, or the model performance will be determined incorrectly. This is particularly important for non-CFD models, that calculate the peak concentration at each distance along the cloud centerline and then apply a distribution profile to calculate the concentration off-axis: if the experiment does not include a sensor along the cloud centerline at a given distance, the maximum measured arc-wise concentration should not be compared with the model's centerline prediction at that same distance; instead, the maximum measured concentration should be compared with the maximum of the predicted concentrations at the same off-axis locations as the sensors.

This approach has the following advantages:

- It tends to result in lower predicted concentrations, which is important given the experimental uncertainty in the measured data. Conversely, using the centerline value as the maximum arc-wise prediction could lead to overprediction of the experimental results and nonconservative statistical performance measures (SPMs).
- It allows the comparison to be made in cases where sensors are aligned in rows perpendicular to the array centerline rather than in concentric arcs.
- It is consistent with the approach followed in previous model evaluations by PHMSA ([8], [9]) and in earlier dense gas dispersion model evaluation exercises ([4], [10]–[12]).

The use of maximum arc-wise concentrations for model evaluation is generally a simpler test than the use of maximum point-wise concentrations; it is also less dependent on the experimental boundary conditions. Its simplicity makes it useful in assessing the ability of a model to predict the correct decay of concentration with downwind distance.

The maximum arc-wise concentrations are automatically calculated in the spreadsheet based on the maximum point-wise concentrations predicted by the model. It should be noted that, in several cases, sensors were placed along a straight line perpendicular to the release direction or to the expected wind direction, instead of along an arc centered on the release location; for consistency with previous validation efforts, sensors along these lines are treated as if being along the same arc. It should also be noted that, in some trials, the placement of sensors and obstacles or obstructions did not lend itself to a representation by arcs; in such cases, only point-wise comparisons were performed.

1.6.3 Predicted distance to a measured concentration

The predicted distance to a measured concentration evaluates the ability of the model to accurately predict the distance to a given concentration, as opposed to its ability to accurately predict the concentration at a given distance, as evaluated by the point-wise and arc-wise PCPs.

Given a target concentration, it is unlikely that the predicted value will fall exactly on one of the measurement arc locations. Therefore, data interpolation is required between the maximum arc-wise concentrations predicted at the available arcs. The interpolation is based on a power-law concentration profile:

$$C(x) = Ax^{-B}$$

Where:

- x = downwind distance from the release
- C(x) = predicted maximum arc-wise concentration at distance x
- A, B = power-law constants

The values of A and B are obtained by fitting the power-law profile between the maximum arc-wise concentrations at two consecutive arcs, as shown in Figure 1.6-1. It is important to note that the power law is fitted between the two arcs that bracket the target concentration, not across the entire cloud concentration profile; therefore, the slope of the curve may not necessarily be continuous across the entire range. It is also important to observe that this approach cannot be applied to extrapolate the curve outside the range of measurement arcs; therefore this PCP can only be calculated for concentrations falling between the measurements along the first and last arc.

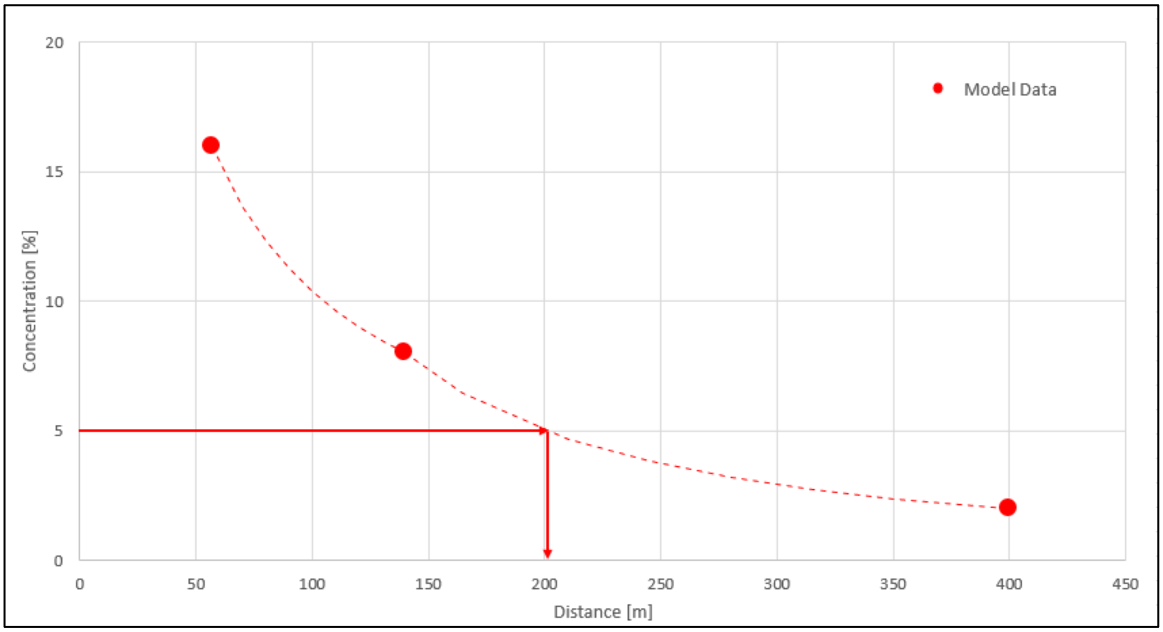

Figure 1.6-1 Example of power-law interpolation to predicted data.

As discussed for the cloud width PCP, the same interpolation method must be applied for any model type, including those that can directly calculate the distance to a given concentration, in order to have a consistent evaluation approach across all model types.

The predicted distance to a measured concentration is automatically calculated in the spreadsheet based on the maximum point-wise concentrations predicted by the model.

1.7 Statistical performance measures

Model performance relative to experimental observation can be evaluated on a qualitative and/or quantitative basis.

Qualitative model evaluation consists of comparing predicted and experimental plots of the relevant variables. A qualitative evaluation can be a useful first step in model evaluation as it can provide a general indication of the ability of a model to predict a particular scenario. This procedure can also provide insight on whether a model's behavior is consistent with expectations based on physical understanding of the phenomena involved. Qualitative evaluation should be performed by the model evaluator, and the results should be discussed in the model evaluation report.

The quantitative evaluation consists of defining a set of statistical performance measures (SPMs) that compare predicted and observed physical comparison parameters. The SPMs should be calculated for each available trial as well as for groups of trials with similar characteristics; the calculated SPMs should then be compared to predefined acceptability criteria. Duijm et al. [13] suggested that a suitable set of SPMs should:

- Provide an indication of the model's bias (i.e., whether on average it under- or over-predicts the measurements)
- Provide an indication of the level of scatter (i.e., deviation from the average)
- Give equal weight to all measurements/predictions, regardless of their absolute values

Chang and Hanna [11] suggested that multiple performance measures should be applied as each measure has its advantages and disadvantages. The SPMs should also be consistent with previous work in order to build on prior experience and increase confidence on the specified acceptability criteria (or revise their values). The statistical performance measures selected to evaluate toxic dispersion models are listed in Table 1.7-1; note that they match the SPMs selected for the flammable dispersion MVD, with the exception of those tied to the lower flammable limit (LFL), which do not apply to toxic dispersion scenarios. The SPMs are automatically calculated in the accompanying spreadsheet, for each trial as well as for groups of trials that fit similar categories as defined in Section 1.2.

Table 1.7-1. Statistical Performance Measures for Toxic Dispersion Models

SPM	Definition
Mean Relative Bias	$MRB = \langle \frac{c_m - c_p}{\frac{1}{2}(c_m + c_p)} \rangle$
Mean Relative Square Error	$MRSE = \langle \frac{(c_m - c_p)^2}{\frac{1}{4}(c_m + c_p)^2} \rangle$
Fraction of Predictions Within a Factor of 2	$0.5 \leq \left(\frac{c_p}{c_m}\right) \leq 2.0$
Geometric Mean Bias	$GMB = e^{\langle \ln\left(\frac{c_m}{c_p}\right) \rangle}$
Geometric Variance	$GV = e^{\langle \left(\ln\left(\frac{c_m}{c_p}\right)\right)^2 \rangle}$
Concentration Safety Factor	$CSF = \langle \frac{c_p}{c_m} \rangle$
Distance Safety Factor	$DSF = \langle \frac{x_p}{x_m} \rangle$

1.8 Acceptability criteria

Once the SPMs for a model have been calculated, the quantitative evaluation needs to compare the calculated values to a set of reference values or ranges that define an "acceptable" model.

Acceptability criteria for atmospheric dispersion over unobstructed terrain were first defined by Chang and Hanna [11] and later adopted by Ivings et al. [5]. Only a few models have since been tested against these criteria; therefore, the same acceptability ranges are specified in this MVD. Hanna and Chang [14] later defined a separate set of acceptability criteria for dispersion through an urban environment, recognizing the increased challenge in modeling such scenarios due to the interaction of the cloud with multiple obstacles and obstructions. No models have since been tested against these criteria; therefore, the same acceptability ranges were specified in this MVD.

There is currently no information available to define acceptable values for the more recent SPMs (distance and concentration safety factors). Ivings et al. [3] deemed model predictions to be acceptable if within a factor of two of their respective measurements; therefore, they specified the acceptability range for the distance and concentration safety factors to be the same as for the "fraction of predictions within a factor of 2". For consistency with the earlier protocol, the same acceptability range was specified in the flammable dispersion MVD and is maintained in the toxic dispersion MVD.

It is important to note that all the acceptability criteria previously defined apply to SPMs based on maximum arc-wise concentrations. As discussed in Section 1.6.1, point-wise predictions are generally more challenging; therefore, the acceptability criteria for maximum arc-wise concentrations would be too strict if applied to point-wise predictions. However, given the limited information available on point-wise model comparisons, any relaxation of the acceptability range at this stage would be arbitrary. Therefore, the same stability criteria are applied to point-wise SPMs as to arc-wise SPMs. As more models are evaluated according to this protocol, the acceptability criteria are expected to be reviewed and updated to "not be so stringent that they are not met by most widely used models, and […] not be so easy that they are met by all models" [11].

The acceptability criteria for the SPMs used in this model evaluation protocol are listed in Table 1.8-1. Note that "simple" geometry includes unobstructed dispersion as well as dispersion obstructed by a single barrier, whereas "complex" geometry represents dispersion through urban or industrial environments.

It is important to note that the quantitative assessment is just one of several tasks in the model evaluation. Therefore, it is not necessary for a model to meet all SPM acceptability criteria in order to be approved for use. A model falling outside the acceptability range for one or more SPMs should warrant a closer review in order to understand the cause of such outcome and possibly identify areas for improvement of the model.

Table 1.8-1. Acceptability Criteria for Toxic Dispersion Model Validation.

Statistical Performance Measure	Arc-Wise, Simple Geometry	Arc-Wise, Complex Geometry	Point-Wise, Simple Geometry	Point-Wise, Complex Geometry
Mean Relative Bias	$\|MRB\| < 0.4$	$\|MRB\| < 0.67$	$\|MRB\| < 0.4$	$\|MRB\| < 0.67$
Mean Relative Square Error	$MRSE < 2.3$	$MRSE < 6.0$	$MRSE < 2.3$	$MRSE < 6.0$
Fraction of Predictions Within a Factor of 2	$0.5 \leq FAC2$	$0.3 \leq FAC2$	$0.5 \leq FAC2$	$0.3 \leq FAC2$
Geometric Mean Bias	$0.67 < MG < 1.5$	$0.5 < MG < 2.0$	$0.67 < MG < 1.5$	$0.5 < MG < 2.0$
Geometric Variance	$VG < 3.3$	$VG < 7.5$	$VG < 3.3$	$VG < 7.5$
Concentration Safety Factor	$0.5 < CSF < 2$	$0.5 < CSF < 2$	$0.5 < CSF < 2$	$0.5 < CSF < 2$
Distance Safety Factor	$0.5 < DSF < 2$	$0.5 < DSF < 2$	$0.5 < DSF < 2$	$0.5 < DSF < 2$

1.9 Data processing

Processing the data from an experiment can be quite complicated. Available experimental datasets vary widely in terms of available instrumentation, measurement frequency, data format (electronic data exists for more recent experiments, but for older experiments only printed traces may be available), etc. Therefore, significant effort may be required in order to convert the data into a format suitable for model evaluation. The procedure used to analyze and process the data should be properly documented so that the process may be replicated. Because of the importance of data processing, guidance was provided in many of the existing protocols; additionally, in some cases, the experimental data may have already been analyzed and reduced during earlier database development efforts (e.g., MDA [15], REDIPHEM [16], LNG spills [17]). The current model validation database relies upon these earlier efforts wherever appropriate, in order to avoid unnecessary work and potentially inconsistent outcomes.

1.9.1 Threshold Concentrations for Data Analysis

A common issue in the analysis of experimental data is the treatment of “zero” values. When considering SPMs based on the ratio of predicted to measured values (for example, the concentration safety factor c_p/c_m), as the measured value tends to zero that result becomes very sensitive to measurement uncertainties. However, toxic hazards frequently occur at gas concentrations below 1,000 ppm, therefore, it is important for the validation data to be accurate to very low concentrations. Several of the test series reviewed for this study utilized instruments calibrated for gas concentrations as low as 0.5 ppm; therefore, the minimum threshold for measured data to be included in the SPM calculations is set to 1 ppm. In order to focus on model performance at concentrations of interest for toxic hazards, a maximum threshold of 1% concentration is also set for data to be included in the SPM calculations. It should however be noted that all measured point-wise maximum concentrations (even those below the threshold) are included in the spreadsheet as reported.

1.9.2 Averaging Times

LNG facility siting studies focus on hazards to the public outside the facility boundaries and seek to minimize such hazards. Therefore, the toxic thresholds considered in siting studies are based on criteria such as the Acute Exposure Guideline Levels (AEGL) or the Emergency Response Planning Guidelines (ERPG) levels, which assume exposure to a given toxic gas concentration for periods of time between 10 minutes and 8 hours. This is different from flammable hazards (i.e., flash fires) which can occur if a flammable concentration is present even for a very short period of time. Therefore, data based on long time averaging is considered more relevant than short time averaged data, for the purpose of this MVD.

The long averaging time is set for each trial to the duration of the steady portion of the release. In this database, the maximum measured point-wise concentrations are obtained from rolling averages of the available data (typically at 1 Hz frequencies) using the long averaging times.

Whenever possible, model results should be provided for both short and long averaging times, and those averaging times should match the respective experimental values. Where available, experimental results for each trial in this database are provided based on both short and long time averaging, to allow a closer comparison for models that may have limitations in the choice of averaging times. The accompanying spreadsheet allows the modeling averaging times to be specified for each trial. If the averaging times used in the modeling do not match the experimental values, a discussion should be provided.

The SPMs for the PCPs described in Section 1.6 are calculated for both short and long averaging times as available, with the exception of cloud width which is only calculated for long averaging times. When model predictions are provided for both short and long averaging times, the SPMs based on long averaging times should be given more weight in the evaluation.

1.10 Sensitivity Analysis

Several methods are available to evaluate uncertainty and sensitivity of models, as discussed by Hanna [18] for atmospheric dispersion models. Some of these methods can require significant effort in order to provide detailed evaluations of a model's performance. For the purpose of this MVD, the sensitivity of model predictions to uncertainty in the input parameters is evaluated according to the requirements in PHMSA Advisory Bulletin ADB-10-07 [19], which specifies that model uncertainty analysis should address:

1. Source term
2. Boundary conditions
3. Wind profile
4. Sub-models
5. Temporal discretization/averaging
6. Spatial discretization and grid resolution
7. Geometry representation

1.10.1.1 Source Term

Even though most scenarios required for facility siting involve releases of liquids under pressure, most atmospheric dispersion models require the source term to be specified as a gas at ambient pressure, whose temperature, composition, flow rate and momentum depend on the characteristics of the release (e.g., liquid pool on the ground, flashing jet, etc.). Therefore, many current models include source term packages that can calculate the flashing, rainout, air entrainment and evaporation of a jet, the spreading and evaporation of a liquid spill, etc. Models that include such packages should apply them in the "base" simulation, since it is expected that the same packages will be used in facility siting studies. Some of the trials included in this database may also specify sensitivity cases to be run using alternative source term models (e.g., fixed radius pool with given evaporation rate) in order to evaluate the sensitivity of the model to the source term characteristics. Similarly, the nominal release rate reported for each experiment will define the base case; sensitivity cases to the release rate may be added to address uncertainties in the flow rate measurements.

Source term uncertainties may also be due to the properties of the released stream, for example, whether a mixture is specified in the model or approximated as a single component. For models which require a vapor source term to be specified, the effect of composition can be evaluated by changing the molecular weight of the vapors; models which calculate the pool vaporization internally should modify all relevant material properties to match the given composition.

1.10.1.2 Boundary Conditions

Boundary conditions for atmospheric dispersion modeling include wall properties (e.g., no-slip), and initial conditions (e.g., temperature, pressure, relative humidity), surface roughness, and the placement of computational domain boundaries (for CFD models). Nominal values for the boundary conditions are specified in the base case for each trial; sensitivity cases are specified for some trials, where uncertainty in the values of some parameters is considered likely to affect the model predictions appreciably. The boundary condition parameter most likely to warrant a sensitivity study is the surface roughness, which is often affected by significant uncertainty and whose variations tend to significantly affect gas dispersion.

Ambient temperature tends to have a minor effect on the dispersion of gas clouds, especially when compared to other parameters such as wind speed or atmospheric stability. Therefore, evaluating sensitivity to ambient temperature is not warranted unless significant fluctuations are observed during a trial.

Ambient pressure fluctuations tend to have a minor effect on the dispersion of gas clouds, especially when compared to other parameters such as wind speed or atmospheric stability. However, since siting studies typically assume standard atmospheric pressure, FERC included in their review of DEGADIS [20] sensitivity cases to ambient pressure for trials in which the reported pressure was not 1 atmosphere, in order to determine the sensitivity of the model to this assumption.

Relative humidity may affect the dispersion of vapor clouds, especially from cryogenic releases, as the cold vapor temperatures cause the condensation of water vapor into droplets (“fog”), which later re-evaporate as the cloud is diluted and warmed up. Most dispersion models currently available, however, cannot account for the water condensation/evaporation; rather, models are limited to adjusting the density of moist air according to the specified ambient relative humidity. Similar to temperature and pressure, relative humidity has a minor effect on cloud dispersion, particularly at long distances from the source. Therefore, evaluating sensitivity to relative humidity is not warranted unless significant differences are found in the reported data.

The placement and definition of computational domain boundaries for CFD models can also have a significant effect on the modeling results. Given the multitude of possible approaches, the proper definition of domain boundaries for each trial is left to the modelers; however, this does not preclude the model evaluator from requesting sensitivity cases to be performed during the review.

1.10.1.3 Wind Profile

In most cases of interest for LNG facility siting, the cloud developing from an accidental release starts off heavier than air and close to the ground. Therefore, once the momentum from the release (e.g., in the case of pressurized jet) has dissipated, the behavior of the cloud is determined by the wind profile near the ground and the topography.

The wind profile near the ground is characterized by gradients of velocity and turbulence, which are functions of several parameters including the roughness of the terrain, the wind speed at elevation, cloud cover, etc.

1.10.1.4 Sub-Models

Models used for atmospheric dispersion studies may include several sub-models, such as the source term packages described above, turbulence closure models, or other solvers designed to increase accuracy or performance in specific scenarios. Given the large number of existing sub-models and their respective parameters, this MVD does not include specific sensitivity cases to evaluate their effect on model predictions. The base case for each model should include the most appropriate sub-models, as they are expected to be used in actual facility siting studies; the choice of sub-models and specific parameters used should be described and explained in the model evaluation report. Sensitivity cases may be included for additional information or may be requested by the model evaluator.

1.10.1.5 Temporal discretization/averaging

As discussed in Section1.9.2, each trial in this MVD includes experimental data based on specified averaging times. Models should be run using averaging times equal to or longer than the experimental values listed in this database, since toxic hazards are typically associated with prolonged exposure; the averaging times used in the modeling should be specified in the spreadsheet. If a model cannot be run with averaging times as specified above, sensitivity cases to different averaging times should be included.

1.10.1.6 Spatial discretization and grid resolution

Certain types of models perform their calculations onto a grid of discrete points, whose spacing can be specified by the user. Given the different types of models available for toxic dispersion, a grid sensitivity study is not explicitly required in this MVD. Instead, modelers are considered responsible for selecting a “grid independent” spacing for their model, for each trial, and running the “base” case and any other sensitivity case using the same spacing. Additional information, including grid sensitivity cases or evidence of grid convergence, may be requested by the model evaluator.

1.10.1.7 Geometry representation

Most of the trials in this MVD include flat or nearly flat terrain; the placement and dimensions of all obstacles (barriers, containers) is clearly defined in this report, the accompanying spreadsheet, or test specific references. Therefore, the main cause of uncertainty with regards to geometry representation is the terrain profile, which may affect the dispersion of dense gas clouds particularly at low wind speeds.

For this reason, and to provide consistent boundary conditions for all types of models, the base case for all trials included in this MVD assumes flat terrain. Sensitivity cases may be run to evaluate the effects of topography in models with such capabilities.

1.11 Use of the Database

The model validation database for toxic dispersion consists of the present report and of a spreadsheet (in Microsoft Excel format). The report provides background information on the model validation activities, as well as a description of each data set included in the database. The model developer (or anyone interested in comparing a model to experimental data) should review these documents, and possibly some of the cited references, prior to commencing any simulations.

The spreadsheet includes a sheet for each individual trial, which summarizes the relevant information necessary to set up simulations, such as:

- Overall description, including barriers and other obstacles
- Source term (material properties, flowrate, release location, etc.)
- Sensor location and maximum measured concentration for short and long averaging times
- Boundary conditions (wind speed and direction, temperature, surface roughness, etc.)
- Material properties for the released species, for use with models that do not include that species (or mixture) in their database. The material properties were calculated using the REFPROP database[3]

Each sheet is locked for editing, with the exception of cells highlighted in orange, which are intended for user input: the user should enter model information, scenario characteristics (e.g., for user-selected sensitivity cases) and the modeling results for the base case and the sensitivity cases. The spreadsheet will automatically generate plots to visually compare the model predictions to the measurements; it will also automatically calculate the model uncertainty and the statistical performance measures for each trial. Each sheet is laid out to print in an organized and consistent pattern on “Letter” size pages (however, printing the spreadsheet results is not required).

[3] https://www.nist.gov/srd/refprop

A set of summary sheets is also included in the spreadsheet. These present the SPM calculations for the entire database, as well as for groups of trials with similar characteristics (e.g., jet releases over unobstructed terrain), to aid in the model evaluation.

2 Model Validation Datasets

The scope of the present database includes a wide variety of scenarios, as described by the groupings in Section 1.2. In order to identify suitable data sets for each of the groupings, the project team reviewed several resources and reached out to various entities including:

- Modeler's Data Archive [11], [21];
- REDIPHEM database [22], [23];
- SMEDIS database [10], [24];
- LNG spills database [17], [25];
- Jack Rabbit I and Jack Rabbit II test series [26]–[29];
- Various research and testing organizations.

Each of the test series reviewed for this MVD is listed in the following subsections:

1. A brief description of the test series
2. The grouping and rating of the experiments according to the criteria in Sections 1.2 and 1.3, respectively.

For the test series that are included in the MVD, additional information is provided, such as:

3. Test series observations and comments: includes any particular observations or comments on specific trials that may be of interest for modeling purposes. It also provides a list of the trials included in the MVD, with a summary of the main parameters (e.g., source term, wind, obstacles, etc.).
4. Ambient conditions: describes the type and placement of instruments to measure temperature, wind speed and direction, atmospheric stability, etc. Information regarding the sampling rate and accuracy of the instruments is also included, when available.
5. Discharge system: describes the fluid storage and release system, and associated instrumentation.
6. Dispersion area: describes the characteristics of the terrain over which the released cloud dispersed, including slopes, obstacles and obstructions that may affect the behavior of the cloud.
7. Gas measurement instrumentation: describes the type and placement of instruments to measure gas concentration and other variables that may be used to compare against model "outputs". Information regarding the sampling rate and accuracy of the instruments is also included, when available.
8. Time averaging: sets the averaging times for short- and long-time averaging for each trial, to be used by the modelers for a proper comparison with the experimental data.

9. Experimental uncertainty: describes the sampling rate and accuracy of the instruments, when available. When this information is not available, estimates are provided and identified as such. These values will be used in the model validation spreadsheet to define experimental uncertainty bands in the model comparison plots.
10. Sensitivity cases: specifies a minimum set of sensitivity cases to be modeled, in addition to the "base" case, to evaluate the effect on results from uncertainty in the source term or boundary conditions.

The purpose of the following subsections, coupled with the accompanying spreadsheet, is to provide modelers with sufficient information to set up the simulations. Several references are provided for each test series, where additional information may be obtained by interested readers.

Several of the test series included in this MVD (i.e., Burro, Coyote, Falcon, Maplin Sands, BA-Hamburg and CHRC) were previously included in the "LNG spills" database by Stewart et al. [25], who provided a review and description of each series for model evaluation as well as in the flammable dispersion MVD by Gavelli et al. [2]. Therefore, only a brief description of those series is included in this MVD; the readers are directed to the cited report (or other test-specific references) for additional information.

2.1 BA-Hamburg and BA-TNO Wind Tunnels

Experimental campaign	BA-Hamburg (BAH) and BA-TNO (TNO)
Test dates:	N/A
Number of trials:	146 (BAH); 13 (TNO)
Test location:	University of Hamburg and TNO wind tunnels
Tests performed by:	University of Hamburg and TNO
Brief description:	Sulfur hexafluoride gas release in a wind tunnel. Dispersion over different sets of obstacles.
References:	Stewart et al., 2016 [25] Nielsen and Ott, 1996 [23]
Data confidentiality:	Open (based on publicly available data)
Model validation category **Material:** **Release Type:** **Dispersion Area:**	 Toxic Low-momentum Unobstructed; Obstructed
Test series rating **Overall:** **Relevance:** **Material:** **Scale:** **Repeatability:** **Data Quality/Availability:**	 **2.8** 3 2 1 4 4
Included in MVD:	**Yes**

2.1.1 Description

The BA-Hamburg and BA-TNO test series consisted of sulfur hexafluoride (SF_6) gas releases in wind tunnels; they were conducted at the Meteorological Institute at the University of Hamburg in Germany and at the TNO 'Pollution Industrial Aerodynamics' wind tunnel facility. The source term consisted of a ground-level release through a circular opening, resulting in a low-velocity vertical flow through the wind tunnel floor. Both instantaneous and continuous releases were performed. Different downwind configurations were tested, including unobstructed (flat and sloped floor) and obstructed cases. Figure 2.1-1 shows a schematic of the BA-Hamburg tests.

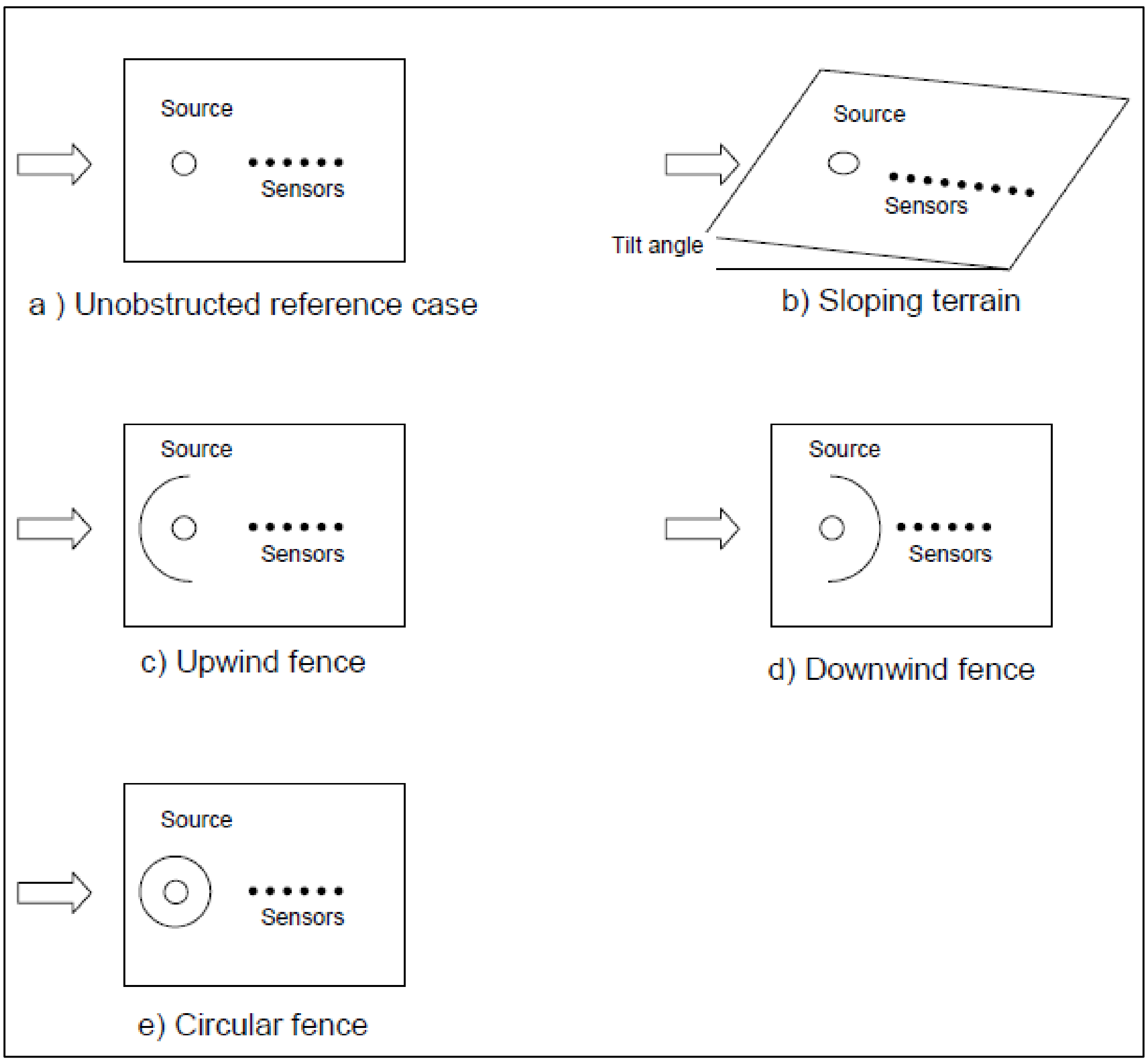

Figure 2.1-1. BA-Hamburg test configurations [25].

The University of Hamburg wind tunnel consisted of a 7.5 m long flow establishment section and a 4 m long test section; air flow was pulled through the test section by a centrifugal fan near the exhaust. The test section was 1.5 m wide and 1 m high. The experiments were set up for a scale of 1:164. SF_6 was introduced through a 7 cm diameter perforated disk, flush with the tunnel floor. The obstructions consisted of 3.01 cm tall barriers, with radius of 19.15 cm or 30.64 cm depending on the trial.

The TNO wind tunnel was 16 m long and consisted of a 10 m long flow establishment section and a 6.8 m long test section; flow was pulled through the test section by a centrifugal fan near the exhaust. The test section was 2.65 m wide and 1.2 m high. The experiments were set up for a scale of 1:78. SF_6 was introduced through a 10.7 cm diameter perforated disk, flush with the tunnel floor. Trial TUV02 included a fence 61.5 cm downwind from the release, 25.6 cm tall and 64 cm long.

2.1.2 Test Series Grouping and Rating

The BA trials consisted of low-momentum, continuous releases of SF_6 through the floor of a wind tunnel. The resulting clouds were advected through the wind tunnel and dispersed over different configurations – both unobstructed (flat or sloped) and obstructed (straight or circular barriers). The test series therefore fit in the following categories:

- Material: Toxic
- Release Type: Low-momentum
- Dispersion Area: Unobstructed; Obstructed

The ground-level source term is representative of vapor generation from an evaporating liquid pool, and the presence of obstacles upwind or downwind of the release is quite common in LNG facilities; however, only a few trials measured gas concentrations in the range of interest for toxic dispersion modeling. Therefore, the scenarios modeled in the BA trials are relevant siting studies (“Relevance” rating = 3). Sulphur hexafluoride is not a material used in LNG facilities or present in feed gas; however, the use of SF_6 as a gas to produce dense clouds in wind tunnel trials is well-established (“Material” rating = 2).

Wind tunnel tests are performed at a scale much smaller than actual plants. While this has benefits in terms of costs and controllability of boundary conditions, the reduced scale tends to increase the effect of near-wall phenomena on the overall behavior of the cloud, which in turn may affect the model’s performance for reasons not relevant to its intended applications. Therefore, the scale of wind tunnel trials is considered a poor fit for this MVD (“Scale” rating = 1).

Wind tunnel trials allow the source term and boundary conditions to be finely controlled, allowing for steady state conditions to be achieved and sustained for long periods of time. Therefore, the repeatability of the experiments is good (“Repeatability” rating = 4).

The overall quality and availability of data is considered more than acceptable for the purpose of this MVD ("Data quality/availability" rating = 4).

Overall, the BA-Hamburg and BA-TNO series are rated at 2.8, which is below the "acceptable" threshold; nonetheless, the inclusion of some wind tunnel trials in this database is considered useful to evaluate a model across different scales. Therefore, the BA-Hamburg test series is included in the toxic dispersion MVD.[4] Note that the BA-Hamburg series is also included in the flammable dispersion MVD [2].

2.1.3 Test Series Observations and Comments

Several trials from the BA-Hamburg test series were included in the flammable dispersion MVD [2] as well as in the earlier LNG spills database [25]. Since the focus of the toxic dispersion model evaluation is to assess a model's ability to accurately predict very small gas concentrations, only trials with more than one measurement row below 1% were included in the toxic dispersion MVD.

Table 2.1-1 lists the main characteristics for the trials included in the toxic dispersion MVD. The values provided in the table are at wind tunnel scale. Some models may be unable to perform simulations at these scales; therefore, for each wind tunnel trial, the accompanying spreadsheet also includes data at full scale. The wind tunnel scale remains the preferred option for models capable of simulating small scales.

Table 2.1-1. BA-Hamburg test characteristics

Test No.	Release Rate [kg/s]	Wind Speed [m/s]	Obstruction
BAH-DA0120	1.74E-4	0.54 @ 7.2 mm	-
BAH-039072	8.72E-4	0.74 @ 7.2 mm	Upwind fence, 30.64 cm radius
BAH-DA0501	8.72E-4	0.74 @ 7.2 mm	Downwind fence, 30.64 cm radius

The thermodynamic properties of SF_6 needed for dispersion modeling are included in the MVD spreadsheet for each trial. These values should be used in models which do not have a species database, or do not include the released material.

[4] The measured concentrations for the BA-TNO trials are above the range of interest for toxic dispersion (1% or below), therefore, those trials are not included in this MVD.

2.1.4 Time Averaging

The BA-Hamburg wind tunnel trials were run to steady state; therefore, the concept of averaging time is not as critical as in a transient scenario and, with the possible exception of the initial and final transients, short- and long-time averaging should provide the same results. Therefore, only long-time averages are considered for the wind tunnel trials. The averaging times, as provided by Stewart et al., are listed in Table 2.1-2.

Table 2.1-2. Averaging times for the BA-Hamburg trials in the toxic dispersion MVD.

Trial	Long time avg.
BAH-DA0120	225 s
BAH-039072	225 s
BAH-DA0501	160 s

2.1.5 Test Series Sensitivity Cases

The BA-Hamburg trials were conducted under well controlled and steady atmospheric conditions, and with well-defined source terms, as is typical of wind tunnel experiments. Sensitivity analyses relative to atmospheric conditions or source term are generally not warranted for wind tunnel trials; however, Stewart et al. [25] suggested that models may require different surface roughness values in order to produce velocity and turbulence profiles consistent with the wind tunnel measurements.

2.1.5.1 Roughness Length

Stewart et al. reported a nominal value of 0.033 mm for the roughness length of the wind tunnel floor; additionally, they specified an uncertainty range of ±0.027 mm within which models should be evaluated to find an adequate match to the experimental velocity and turbulence profiles. The same uncertainty range is used to specify sensitivity cases for the BA-Hamburg wind tunnel trials in this MVD.

2.1.5.2 Summary of Sensitivity Cases

Based on the discussion above, the model validation efforts should include the sensitivity cases listed in Table 2.1-3. If one or more sensitivity cases cannot be run, for example, due to hard-coding of certain parameters in a model, an explanation should be provided in the model questionnaire.

Table 2.1-3. Base and sensitivity cases for the BA-Hamburg trials in the MVD.

Parameter	Case	BAH-DA0120	BAH-039072	BAH-DA0501
Source term	Base	Low-momentum ground level injection	Low-momentum ground level injection	Low-momentum ground level injection
Release Rate	Base	1.74E-4 kg/s	8.72E-4 kg/s	8.72E-4 kg/s
Release Duration	Base	Continuous	Continuous	Continuous
Wind Speed (at 7.18E-3 m height)	Base	0.54 m/s	0.74 m/s	0.74 m/s
Surface Roughness Length	Base	3.3E-5 m	3.3E-5 m	3.3E-5 m
	R1	6.0E-5 m	6.0E-5 m	6.0E-5 m
	R2	6.0E-6 m	6.0E-6 m	6.0E-6 m
Atmospheric Stability	Base	D	D	D
Ambient Temperature	Base	14.0 °C	14.0 °C	14.0 °C
Ambient Pressure	Base	1 atm	1 atm	1 atm
Relative Humidity	Base	N/A	N/A	N/A
Stream Composition	Base	SF_6 = 100%	SF_6 = 100%	SF_6 = 100%

2.2 Burro

Experimental campaign	Burro (BU)
Test dates:	1980
Test location:	China Lake, California
Number of tests:	8
Tests performed by:	Naval Weapons Center and Lawrence Livermore National Laboratory
Brief description:	LNG spills onto water; unobstructed vapor cloud dispersion over land.
References:	Stewart et al., 2016 [25] Koopman et al., 1982 [30], [31] Ermak et al., 1983 [32] Ermak et al., 1989 [33]
Data confidentiality:	Open (based on publicly available data)
Model validation category **Material:** **Release Type:** **Dispersion Area:**	 Non-Toxic Spill Unobstructed
Test series rating **Overall:** **Relevance:** **Material:** **Scale:** **Repeatability:** **Data Quality/Availability:**	 **0** 0
Included in MVD:	**No**

2.2.1 Description

The Burro test series consisted of 8 spills of LNG onto water; they were conducted at the Naval Weapons Center at China Lake. The vapor clouds produced by the evaporation of the liquid spills dispersed over mostly flat terrain.

2.2.2 Test Series Grouping and Rating

The Burro trials included in this MVD consisted of spills of LNG. The spill point is located in the center of a water test basin of approximately 58 m in diameter. The resulting clouds dispersed over open water and then over the terrain immediately downwind of the water test basin, with no obstructions. The test series therefore fits in the following categories:

- Material: Non-Toxic
- Release Type: Spill
- Dispersion Area: Unobstructed

LNG is not toxic, and the peak concentrations measured are above 1% at all measurement arcs. Therefore, the Burro trials included in the MVD are not relevant to the purpose of this database (“Relevance” rating = 0). The Burro test series is not included in the toxic dispersion MVD.

2.3 Chemical Hazards Research Center (CHRC) Wind Tunnel

Experimental campaign	Chemical Hazards Research Center (CHRC)
Test dates:	N/A
Number of trials:	N/A
Test location:	Chemical Hazards Research Center (CHRC) at the University of Arkansas
Tests performed by:	CHRC
Brief description:	Carbon dioxide gas release in a wind tunnel. Dispersion includes cases with a dike and tank.
References:	Stewart et al., 2016 [25] Havens et al., 2007 [34]
Data confidentiality:	Open (based on publicly available data)
<u>Model validation category</u> **Material:** **Release Type:** **Dispersion Area:**	 Non-Toxic Low-momentum Unobstructed; Complex geometry
<u>Test series rating</u> **Overall:** **Relevance:** **Material:** **Scale:** **Repeatability:** **Data Quality/Availability:**	 **0** 0
<u>Included in MVD:</u>	**No**

2.3.1 Description

The CHRC test series consisted of carbon dioxide (CO_2) gas releases in wind tunnels; they were conducted at the University of Arkansas' Chemical Hazards Research Center (CHRC) wind tunnel facility. The source term consisted of a ground-level release, resulting in a low-velocity vertical flow through the wind tunnel floor. Different configurations were tested, including unobstructed, with a dike around the release area, and with a tank in the middle of the release area. Figure 2.3-1 shows a picture of the CHRC wind tunnel configuration for a trial with tank and dike.

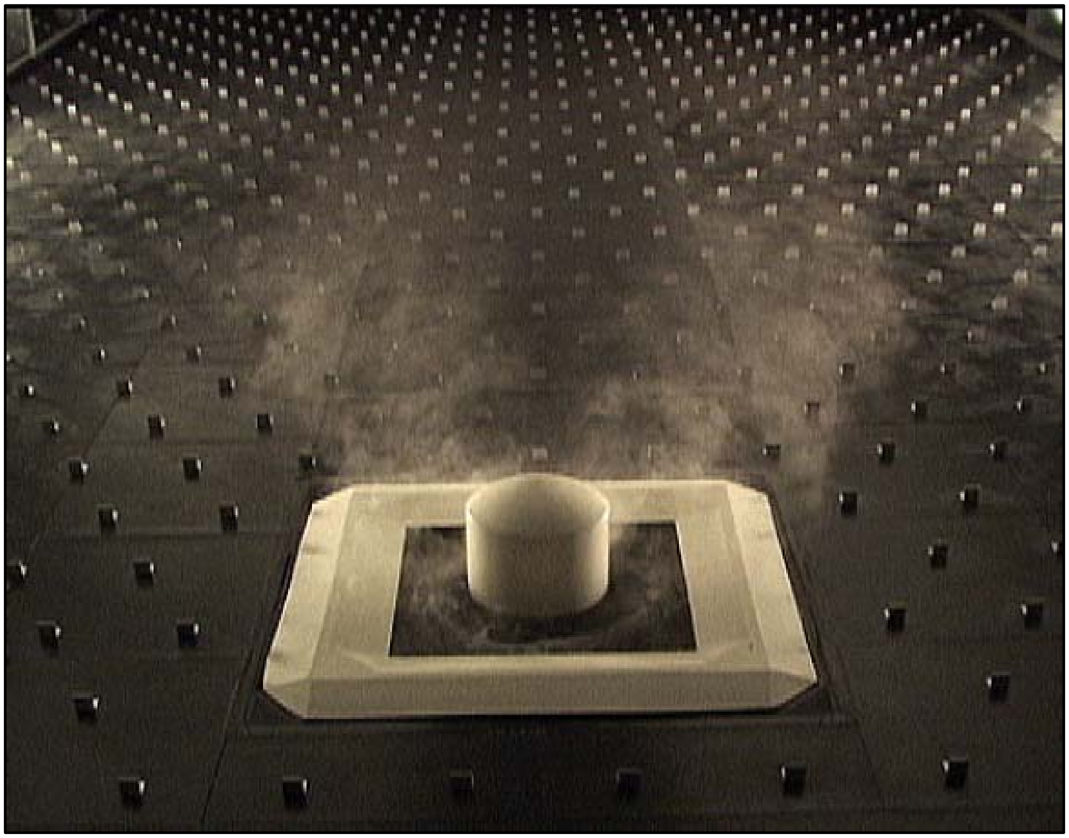

Figure 2.3-1. CHRC configuration for a trial with tank and dike [34].

The CHRC wind tunnel consisted of a working area measuring 24.4 m (80 ft) long, 6.1 m (20 ft) wide, and 2.2 m (7.5 ft) tall; flow was pushed through the test section by upwind fans. The experiments were set up for a scale of 1:150. CO_2 was introduced through a meshed screen over a square area (63 cm length and width) flush with the tunnel floor, with a central disk (31 cm diameter) blocked off; the total flow area measured 0.334 m^2. Some of the trials included a dike (3.7 cm tall) around the square source area, and a tank (28.3 cm tall) over the central blocked area.

2.3.2 Test Series Grouping and Rating

The CHRC trials considered for this MVD consisted of low-momentum, continuous releases of CO_2 (with 1.5% propane as a tracer) through the floor of a wind tunnel. The resulting clouds were advected through the wind tunnel and dispersed over different configurations – both unobstructed and in a layout intended to scale the spill containment system for a single-containment LNG storage tank. The test series therefore fits in the following categories:

- Material: Non-Toxic
- Release Type: Low-momentum
- Dispersion Area: Unobstructed; Complex geometry

The peak concentrations measured are above 1% at all measurement rows. Therefore, the CHRC trials are not relevant to the purpose of this database (“Relevance” rating = 0). The CHRC test series is not included in the toxic dispersion MVD.

2.4 Copenhagen

Experimental campaign	Copenhagen (CP)
Test dates:	September 1978 – July 1979
Test location:	Copenhagen, Denmark
Number of tests:	10
Tests performed by:	Risø National Laboratory
Brief description:	Neutrally buoyant emissions from 115 m tall stack, containing Sulphur hexafluoride (SF_6) at tracer concentrations. Concentration measurements were made at 2-3 m above ground along arcs up to 6 km from the release.
References:	Gryning and Lyck, 2002 [35] Olesen, 2005 [36]
Data confidentiality:	Open (based on publicly available data)
Model validation category	
Material:	Toxic
Release Type:	Tracer
Dispersion Area:	Unobstructed (flat terrain)
Test series rating	
Overall:	**0**
Relevance:	0
Material:	
Scale:	
Repeatability:	
Measurement Quality:	
Data Availability:	
Included in MVD:	**No**

2.4.1 Description

The Model Validation Kit (MVK) [36] includes experimental data from four test series in which a tracer gas was released from an elevated source and concentration was measured at ground level, up to several kilometers downwind. The four test series were conducted, respectively, near Copenhagen (Denmark), Indianapolis (Indiana, United States), Kincaid (Illinois, United States), and Lillestrøm (Norway). While the specific test configurations (released material, source height, terrain) differ for each series, all four present similar characteristics and are therefore discussed together.

2.4.2 Test Series Grouping and Rating

Each of the MVK test series involved the release of a tracer gas from a high elevation. The tracer dispersed over mostly flat terrain in a residential area, and was collected near ground level, up to several kilometers downwind. The test series therefore fit in the following categories:

- Material: Toxic
- Release Type: Tracer
- Dispersion Area: Unobstructed

Neutrally buoyant tracer releases from very high elevations do not represent scenarios of interest for toxic dispersion in a siting study. Therefore, the Copenhagen, Indianapolis, Kincaid and Lillestrøm series are considered not relevant to the purpose of this MVD (“Relevance” rating = 0). As such, none of these four series is considered suitable for inclusion in this toxic dispersion MVD.

2.5 Coyote

Experimental campaign	Coyote (CO)
Test dates:	1981
Test location:	China Lake, California
Number of tests:	9
Tests performed by:	Naval Weapons Center and Lawrence Livermore National Laboratory
Brief description:	LNG spills onto water; unobstructed vapor cloud dispersion over land.
References:	Stewart et al., 2016 [25] Ermak et al., 1989 [33] Goldwire et al., 1983 [37]
Data confidentiality:	Open (based on publicly available data)
Model validation category **Material:** **Release Type:** **Dispersion Area:**	 Non-Toxic Spill Unobstructed
Test series rating **Overall:** **Relevance:** **Material:** **Scale:** **Repeatability:** **Data Quality/Availability:**	 **0** 0
Included in MVD:	**No**

2.5.1 Description

The Coyote test series was conducted at China Lake and included seven spills of LNG and two spills of liquid methane, both on water. The vapor clouds produced by the evaporation of the liquid spills dispersed over mostly flat terrain.

2.5.2 Test Series Grouping and Rating

The Coyote trials included in this MVD consisted of spills of LNG onto water. The spill point was located in the center of a water test basin of approximately 58 m in diameter. The resulting clouds dispersed over open water and then over the terrain immediately downwind of the water test basin, with no obstructions. The test series therefore fits in the following categories:

- Material: Non-Toxic
- Release Type: Spill
- Dispersion Area: Unobstructed

LNG is not toxic, and the peak concentrations measured are above 1% at all measurement arcs. Therefore, the Coyote trials included in the MVD are not relevant to the purpose of this database (“Relevance” rating = 0). The Coyote test series is not included in the toxic dispersion MVD.

2.6 Desert Tortoise

Experimental campaign	Desert Tortoise (DT)
Test dates:	August-September 1983
Test location:	Frenchman Flat, DOE Nevada Test Site
Number of tests:	4
Tests performed by:	Lawrence Livermore National Laboratory
Brief description:	Pressurized and liquefied anhydrous ammonia was released from a tank as a jet directed horizontally downwind. The release was located 0.79 m above ground and the dense vapor cloud dispersed over unobstructed, flat terrain.
References:	Goldwire et al., 1985 [38] Ott, 1995 [22] Ermak et al., 1989 [33]
Data confidentiality:	Open (based on publicly available data)
Model validation category **Material:** **Release Type:** **Dispersion Area:**	 Toxic Flashing Jet Unobstructed
Test series rating **Overall:** **Relevance:** **Material:** **Scale:** **Repeatability:** **Data Quality/Availability:**	 **0** 0
Included in MVD:	**No**

2.6.1 Description

The Desert Tortoise (DT) test series consisted of four large-scale pressurized ammonia releases dispersing over flat, unobstructed terrain. Pressurized liquid ammonia was released at flow rates between approximately 81 and 133 kg/s from a nozzle pointed horizontally downwind at a height of 0.79 m above ground. The release duration varied between approximately 2 and 6 minutes. All trials occurred under fairly strong winds (wind speeds of 5-7 m/s, measured at 2 m above ground), warm and dry air (29-34°C temperature and 10-21% relative humidity). Ammonia concentration was measured at several locations and elevations along two arcs, respectively 100 m and 800 m downwind of the release.

2.6.2 Test Series Grouping and Rating

The Desert Tortoise test series involved the release of anhydrous ammonia, liquefied under pressure and discharged downwind through an orifice of approximately 3–4 in. diameter. The resulting cloud dispersed over flat and unobstructed terrain. The test series therefore fits in the following categories:

- Material: Toxic
- Release Type: Flashing Jet
- Dispersion Area: Unobstructed

Even though anhydrous ammonia is a toxic material, the peak concentrations measured in the Desert Tortoise trials are above 1% at all measurement arcs. Therefore, the trials are not relevant to the purpose of this database (“Relevance” rating = 0). The Desert Tortoise test series is not included in the toxic dispersion MVD.

2.7 Eagle

Experimental campaign	Eagle (EA)
Test dates:	September 17 – October 30, 1983
Test location:	US Department of Energy (DOE) Nevada Test Site (NTS)
Number of tests:	6
Tests performed by:	Lawrence Livermore National Laboratory (LLNL)
Brief description:	Spills of liquid nitrogen tetroxide (N_2O_4) dispersing over flat, unobstructed terrain.
References:	McRae et al., 1984 [39] Ermak et al., 1989 [33]
Data confidentiality:	Open (based on publicly available data)
Model validation category **Material:** **Release Type:** **Dispersion Area:**	 Toxic Spill Unobstructed
Test series rating **Overall:** **Relevance:** **Material:** **Scale:** **Repeatability:** **Data Quality/Availability:**	 **2.4** 2 3 3 2 1
Included in MVD:	**No**

2.7.1 Description

The Eagle test series consisted of six spills of the oxidizer nitrogen tetroxide (N_2O_4): four trials were conducted to evaluate vaporization and dispersion, and two trials evaluated the performance of a Portable Foam Vapor Suppression System. The vapor cloud emanating from the liquid pool dispersed over a mostly flat, unobstructed area. Vapor concentration measurements were performed at downwind locations of 25 m and 785 m.

2.7.2 Test Series Grouping and Rating

The Eagle test series involved spills of liquid nitrogen tetroxide with cloud dispersion over flat and unobstructed terrain. The test series therefore fits in the following categories:

- Material: Toxic
- Release Type: Spill
- Dispersion Area: Unobstructed

Toxic dispersion hazards from liquid spills must be evaluated in LNG facility siting studies; the concentrations measured during the Eagle trials are within the range of interest for toxic dispersion modeling but only at the farthest arc (“Relevance” rating = 2). N_2O_4 is typically not present in LNG facilities but it is a toxic fluid (“Material” rating = 3). The release flow rates are downscaled from typical siting scenarios and are considered medium-scale (“Scale” rating = 3).

In every field scale test series, replicating the same test conditions (including the weather) is extremely difficult, therefore, the repeatability of field scale experiments is inherently limited (“Repeatability” rating = 2).

The experimental data from the Eagle trials is available from the REDIPHEM database; however, concentration measurements were performed only at two downwind distances over 750 m apart and with large gaps (100 m) between the sensors in the farther array. Therefore, the overall quality and availability of the data for the purpose of this MVD is considered poor (“Data quality/availability” rating = 1).

Overall, the Eagle test series is rated at 2.4, which is below the “acceptable” threshold for inclusion in the MVD. The Eagle series is therefore not considered suitable for inclusion in the toxic dispersion MVD.

2.8 Falcon

Experimental campaign	Falcon (FAL)
Test dates:	1981
Test location:	Frenchman Flat, Nevada Test Site
Number of tests:	5
Tests performed by:	Lawrence Livermore National Laboratory
Brief description:	LNG spills onto water; obstructed vapor cloud dispersion.
References:	Stewart et al., 2016 [25] Brown et al., 1983 [40]
Data confidentiality:	Open (based on publicly available data)
Model validation category	
Material:	Non-Toxic
Release Type:	Spill
Dispersion Area:	Obstructed
Test series rating	
Overall:	**0**
Relevance:	0
Material:	
Scale:	
Repeatability:	
Data Quality/Availability:	
Included in MVD:	**No**

2.8.1 Description

The Falcon test series included five trials performed at Frenchman Flat on the Nevada Test Site, which consisted of LNG spills on a water pond inside a fenced area. LNG was spilled at four locations onto a rectangular water basin measuring 40 m by 60 m. The goal of the Falcon tests was to evaluate the effectiveness of vapor barriers as a vapor dispersion mitigation technique; therefore, the spill pond was surrounded by vapor barriers.

2.8.2 Test Series Grouping and Rating

The Falcon trials consisted of LNG spills onto a water surface. The resulting vapor clouds were obstructed by a vapor containment barrier, after which they could disperse over flat terrain. The test series therefore fits in the following categories:

- Material: Non-Toxic
- Release Type: Spill
- Dispersion Area: Obstructed

LNG is not toxic, and the peak concentrations measured are above 1% at all measurement arcs. Therefore, the Falcon trials included in the MVD are not relevant to the purpose of this database (“Relevance” rating = 0). The Falcon test series is not included in the toxic dispersion MVD.

2.9 FLADIS

Experimental campaign	FLADIS Field Experiments
Test dates:	April and August 1993, August 1994
Test location:	Hydro-Care training facilities in Landskrona, Sweden
Number of tests:	27
Tests performed by:	Risø National Laboratory
Brief description:	Dispersion of liquefied ammonia from small-scale releases (diameter 4-6 mm) to study the near-source aerosol jet, the heavy gas dispersion phase, and the transition to passive dispersion.
References:	Nielsen and Ott, 1996 [23] Nielsen, 1998 [41]
Data confidentiality:	Open (based on publicly available data)
Model validation category	
Material:	Toxic
Release Type:	Flashing Jet
Dispersion Area:	Unobstructed
Test series rating	
Overall:	**3.8**
Relevance:	5
Material:	4
Scale:	4
Repeatability:	2
Data Quality/Availability:	4
Included in MVD:	**Yes**

2.9.1 Description

The FLADIS field experiments consisted of 27 small-scale pressurized ammonia releases dispersing over flat, unobstructed grassy terrain. Of these releases, six trials were highlighted for model comparison based on having long release durations and favorable wind conditions.

Pressurized liquid ammonia was released at flow rates between approximately 0.2 and 0.6 kg/s and durations up to 40 minutes, from a nozzle pointed horizontally downwind. The nozzle diameter varied between 4 and 6.3 mm. Measurements of ammonia concentration were taken along three arcs at downwind distances of 20 m, 70 m, and 238 m.

2.9.2 Test Series Grouping and Rating

The FLADIS test series involved the release of liquid ammonia under pressure and discharged downwind through a nozzle with exit diameter 4-6.3 mm. The resulting cloud dispersed over flat and unobstructed terrain. The test series therefore fits in the following categories:

- Material: Toxic
- Release Type: Flashing Jet
- Dispersion Area: Unobstructed

The pressurized release of toxic materials, with unobstructed dispersion of the resulting vapor cloud, is a common scenario for LNG facility siting studies ("Relevance" rating = 5). Ammonia is frequently included in toxic hazard scenarios, although in most cases as an aqueous solution rather than in anhydrous form ("Material" rating = 4). The orifice sizes in the FLADIS trials are small compared with typical siting scenarios, however, the measured concentrations are in the range of interest for toxic hazard modeling ("Scale" rating = 4).

In every field scale test series, replicating the same test conditions (including the weather) is extremely difficult, therefore, the repeatability of field scale experiments is inherently limited ("Repeatability" rating = 2).

Several FLADIS trials were found to have useful data for dispersion model evaluation; the data is available from the REDIPHEM database. The overall quality and availability of the data is therefore considered more than acceptable ("Data availability" rating = 4).

Overall, the FLADIS test series is rated at 3.8, which exceeds the "acceptable" threshold for inclusion in this MVD. Therefore, the FLADIS test series is considered suitable for inclusion in the toxic dispersion MVD.

2.9.3 Ambient Conditions

Meteorological data was acquired from the reference mast located 10 m upwind of the release point. Additional wind and ambient measurements were made at 20, 70 and 238 m downwind of the release. This included a sonic anemometer at a height of 4 meters, to determine the friction velocity and Monin-Obukhov length, and ambient temperature and relative humidity sensors at a height of 1.5 m. Wind speed and direction were averaged across the four measurement locations.

2.9.4 Discharge System

The release system for the FLADIS field trials is shown in Figure 2.9-1. The ammonia tank was pressurized with nitrogen and included both pressure and temperature sensors. Liquid ammonia from the tank flowed through a hose to custom nozzles where the flow rate was calculated by measuring the pressure drop. The ammonia tank was mounted on a load cell to verify the calculated flow rate; the agreement was found to be within 5%. The discharge nozzle was mounted at 1.5 m height and directed horizontally along the test array centerline [41].

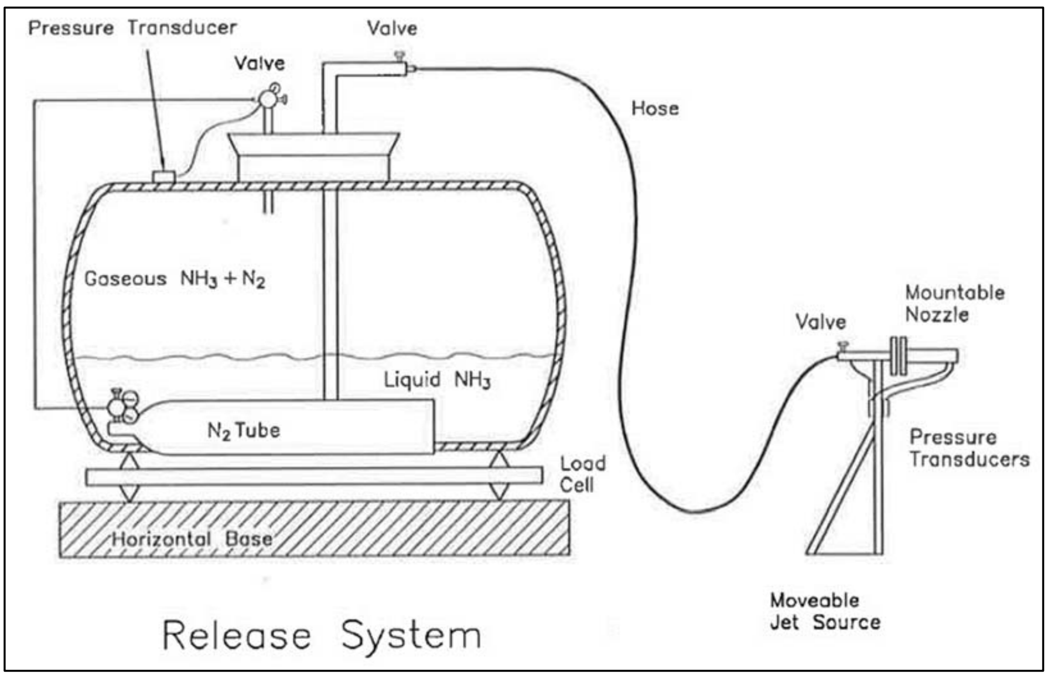

Figure 2.9-1. Schematic of the FLADIS discharge system [23].

2.9.5 Dispersion Area

The dispersion area for the ammonia vapor cloud was relatively flat and unobstructed.

2.9.6 Instrumentation

The ammonia concentration was measured by an array of catalytic and electrochemical sensors, distributed along three arcs respectively at 20, 70 and 238 m from the source as shown in Figure 2.9-2.

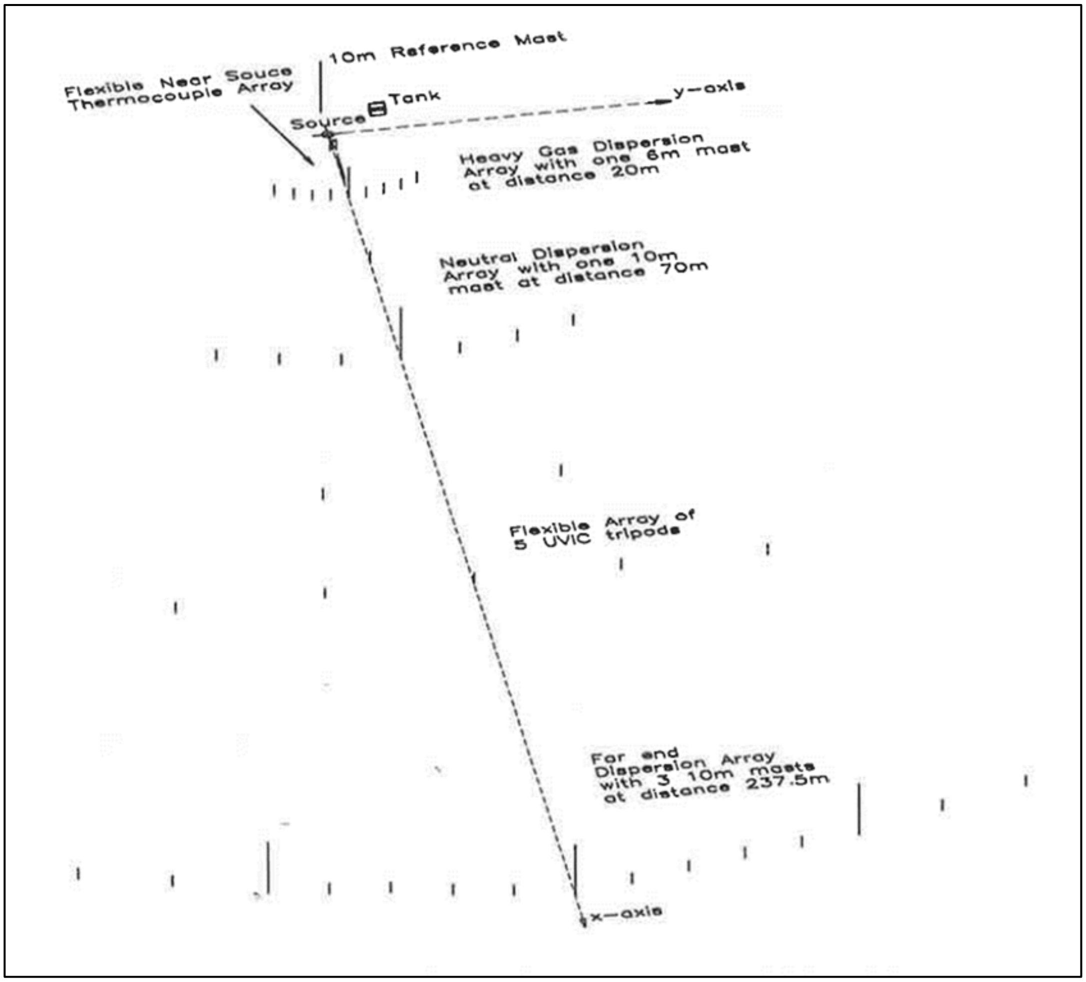

Figure 2.9-2. Sensor array for the FLADIS trials [23].

The first arc, located 20 m downwind, had 9 sensor posts spaced 3 m apart, each with sensors at elevations of 0.5 and 1.5 m; two additional sensors (at 0.7 and 4 m height) were installed on the centerline mast (Figure 2.9-3).

The 70 m arc had 7 sensor sensors posts spaced 10 m apart, each with a sensor at 0.5 m above grade. The centerline mast carried sensors at 0.1, 2, 4 and 9 m but not at 0.5 m (Figure 2.9-4).

The last arc, located 238 m downwind, consisted of 11 sensor posts spaced 10 m apart, each with a sensor at 1.5 m above grade. The centerline and +/-50 m masts also included sensors at 4 and 9 m (Figure 2.9-5). Additionally, moveable tripods with sensors at 2 m height were available and placed at different locations in each trial.

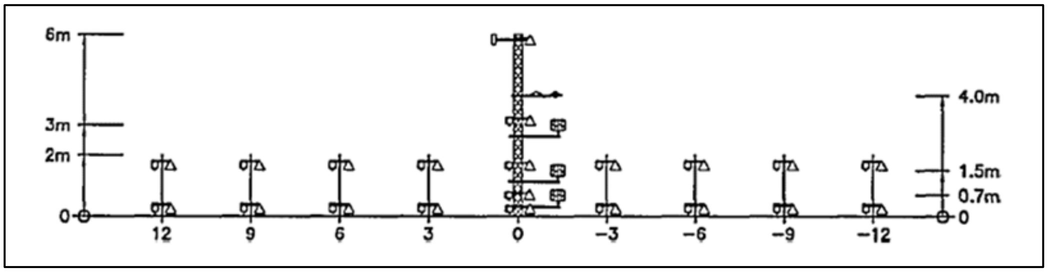

Figure 2.9-3. Sensor array at 20 m [41].

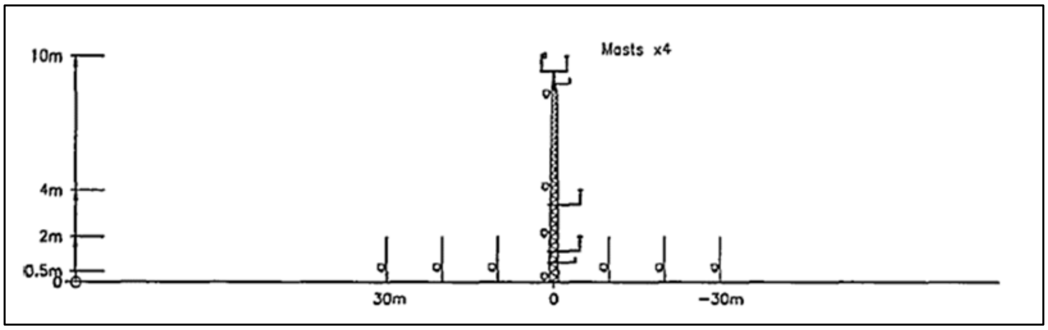

Figure 2.9-4. Sensor array at 70 m [41].

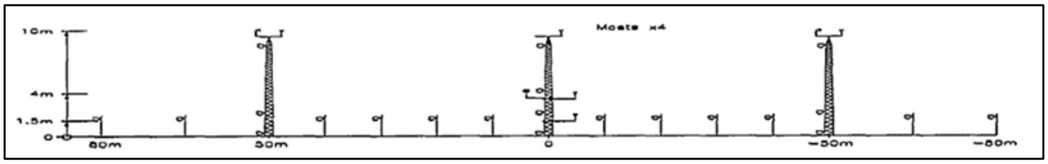

Figure 2.9-5. Sensor array at 238 m [41].

2.9.7 Time Averaging

The response times of the catalytic and electrochemical sensors were 5 and 15 seconds, respectively [41]. Therefore, the short-time averaging for each trial is set to 15 s. Given the long duration of the releases (approximately 20 minutes), which were aimed at achieving near steady gas concentrations, the long time average is set to 600 seconds. Table 2.9-2 summarized the averaging times for the selected trials.

Table 2.9-1. Averaging times for the FLADIS trials.

Test No.	Short Time Avg.	Long Time Avg.
16	15 s	600 s
25	15 s	600 s
27	15 s	600 s

2.9.8 Experimental Uncertainty

The test series final report provides the manufacturer of equipment but does not include information on the accuracy of the various instrumentation [23]. Therefore, for the purpose of estimating uncertainty bands in the MVD, all gas concentration measurements in the FLADIS test series are assumed to have 20% uncertainty.

2.9.9 Test Series Observations and Comments

Nielsen and Ott [23] identified six of the 27 FLADIS trials as most suitable for gas dispersion model comparison: trials number 16, 20, 23, 24, 25, and 27. Data from these trials (and several others) is available in the REDIPHEM database. A review of the experimental data showed that most of these trials were conducted under moderate to high wind speeds and neutral or unstable atmospheric conditions. Therefore, only a subset of these trials were selected for the toxic dispersion MVD: Table 2.9-2 lists the main test parameters for the selected trials. A more complete set of data for each test is included in the model validation spreadsheet; the data included in the spreadsheet was obtained from the REDIPHEM database. Additional information on these trials can be found in the references listed in the summary table.

Table 2.9-2. FLADIS test parameters[5]

Test No.	Spill Rate [kg/s]	Spill Duration [min]	Wind Speed @ 10m [m/s]	Atmospheric Stability Class	Ambient Temperature [C]
16	0.27	20	4.4	E	16
25	0.46	22	4.5	D	17
27	0.22	21	2.4	C	19

[5] These values were obtained from the test series report and may differ slightly from the values in the sensitivity tables and accompanying spreadsheet, which are taken from the REDIPHEM database.

2.9.10 Test Series Sensitivities

The FLADIS trials do not appear to have been widely used for dispersion model validation purposes (Witlox et al. [42] used the FLADIS data to evaluate the atmospheric expansion sub-model in Phast). Therefore, the sensitivity cases specified below are based on a review of the test series data.

2.9.10.1 Source Term

The source term for the FLADIS trials consisted of a flashing liquid jet of anhydrous ammonia; the release rate reported in the REDIPHEM database represents the time-averaged rate based on the total amount released and the duration of the release. Flow variations at the beginning of the release and after the main valve shutoff (i.e., to empty the inventory in the discharge pipe) were reported but no measurement data is available. Given the long release duration, such fluctuations are not expected to significantly affect the results. No rainout was reported. Therefore, no sensitivity cases are specified for the source term.

2.9.10.2 Wind Speed

Wind speed was reportedly steady in most trials, with an unquantified declining tendency toward the end of the release in trial 16. Therefore, no sensitivity cases are specified for wind speed.

2.9.10.3 Atmospheric Stability

Sensitivity cases for atmospheric stability are specified, where the ambient conditions (wind speed, cloud cover, etc.) produced uncertainty in the representative Pasquill-Gifford class.

2.9.10.4 Roughness Length

The FLADIS test series report did not provide information regarding the surface roughness; in a later study, Nielsen [41] indicated a surface roughness value of 0.004 m. Given the uncertainty associated with this value and the effect of surface roughness on atmospheric dispersion, sensitivity cases are specified that span one order of magnitude around the base value.

2.9.10.5 Temperature, Pressure and Humidity

No sensitivity cases to ambient temperature, pressure or relative humidity are specified for the FLADIS trials, given the small fluctuations and uncertainties in the data.

2.9.10.6 Material Properties

The FLADIS series consisted of releases of anhydrous ammonia. Models that include ammonia in their species database should use the built-in properties in their simulations; models that do not include ammonia should use the thermophysical properties listed in the accompanying spreadsheet. No sensitivity cases are specified.

2.9.10.7 Summary of Sensitivity Cases

Based on the discussion above, the model validation efforts should include the sensitivity cases listed in Table 2.9-3. If one or more sensitivity cases cannot be run, for example, due to hard-coding of certain parameters in a model, an explanation should be provided in the model questionnaire.

Table 2.9-3. Base case and sensitivity cases for the FLADIS test series.

Parameter	Case	FLA-16	FLA-25	FLA-27
Source term	Base	Flashing jet	Flashing jet	Flashing jet
Release Rate	Base	0.27 kg/s	0.46 kg/s	0.22 kg/s
Release Duration	Base	19 m 0 s	23 m 0 s	20 m 35 s
Wind Speed (at 10 m height)	Base	4.4 m/s	4.7 m/s	2.5 m/s
Surface Roughness Length	Base	0.004 m	0.004 m	0.004 m
	R1	0.001 m	0.001 m	0.001 m
	R2	0.01 m	0.01 m	0.01 m
Atmospheric Stability	Base	E	D	C
	A1	D	C	D
Ambient Temperature	Base	16.0 C	17.3 C	19.0 C
Ambient Pressure	Base	1.01 atm	1 atm	1.01 atm
Relative Humidity	Base	60%	54%	50%
Stream Composition	Base	Ammonia = 100%	Ammonia = 100%	Ammonia = 100%

2.10 Flashing Liquids in Industrial Environment (FLIE)

Experimental campaign	Flashing Liquids in Industrial Environment (FLIE)
Test dates:	2004
Test location:	INERIS test site
Number of tests:	94
Tests performed by:	INERIS and von Karman Institute
Brief description:	Pressurized releases of propane or butane from a horizontal nozzle between 0.4 in and 2 in diameter. The main purpose of this project was to get a better understanding of the behavior of a two-phase discharge in the presence or in the absence of an obstacle.
References:	Bonnet and Lacome, 2014 [43] Lacome et al., 2020 [44] Bonnet, 2005 [45]
Data confidentiality:	Open (based on publicly available data)
Model validation category **Material:** **Release Type:** **Dispersion Area:**	 Toxic Flashing Jet Unobstructed; Obstructed
Test series rating **Overall:** **Relevance:** **Material:** **Scale:** **Repeatability:** **Measurement Quality:** **Data Availability:**	 **0** 0
Included in MVD:	**No**

2.10.1 Description

The Flashing Liquids in Industrial Environment (FLIE) test series consists of 94 pressurized releases of propane or butane from a horizontal nozzle between 0.4 in and 2 in diameter. The main purpose of this project was to develop models for calculating the interaction between a two-phase jet and an obstacle and to get a better understanding of the mechanisms steering the dispersion of a two-phase discharge in the presence or in the absence of an obstacle [45]. Therefore, while some of the trials allowed the flashing jet to travel unimpeded, most of the trials included a barrier at a distance between 0.8 and 2.6 m downwind, for the purpose of collecting liquid droplets and measuring liquid rainout. All measurements were performed with less than 10 m from the discharge location, as the focus of the trials was to characterize the two-phase region of the jet.

2.10.2 Test Series Grouping and Rating

The FLIE test series involved the release of propane or butane from a horizontal nozzle between 0.4 in and 2 in diameter. Some of the trials allowed the flashing jet to travel unimpeded, while other trials placed a barrier at a distance between 0.8 and 2.6 m downwind. The test series therefore fits in the following categories:

- Material: Toxic
- Release Type: Flashing Jet
- Dispersion Area: Unobstructed; Obstructed

The purpose of the FLIE trials was to examine the flashing jet behavior in proximity of the release (within approximately 10 m downwind), including quantifying the amount of rainout on the ground. While flashing jets represent a large number of facility siting scenarios, the purpose of the toxic dispersion MVD is to evaluate the far-field dispersion capabilities of a model. Therefore, the FLIE series is considered not relevant to the purpose of this MVD (“Relevance” rating = 0).

The FLIE series is thus not suitable for inclusion in the toxic dispersion MVD. The FLIE series will be re-evaluated for possible inclusion in the source term MVD.

2.11 Goldfish

Experimental campaign	**Goldfish (GF)**
Test dates:	Summer 1986
Test location:	Frenchman Flat
Number of tests:	6
Tests performed by:	Lawrence Livermore National Laboratory
Brief description:	Pressurized jet releases of liquefied hydrofluoric acid through an orifice directed horizontally downwind. The release was located 1 m above ground and the dense vapor cloud dispersed over unobstructed, flat terrain. Gas concentrations were measured along arcs at distances 300, 1000 and 3000 m downwind.
References:	Blewitt et al., 1987 [46] Hanna et al., 1991 [15] Zapert et al., 1991 [47]
Data confidentiality:	Open (based on publicly available data)
Model validation category **Material:** **Release Type:** **Dispersion Area:**	 Toxic Flashing Jet Unobstructed
Test series rating **Overall:** **Relevance:** **Material:** **Scale:** **Repeatability:** **Data Quality/Availability:**	 **3.0** 5 2 4 2 2
Included in MVD:	**Yes**

2.11.1 Description

The Goldfish (GF) test series consisted of six large-scale pressurized hydrofluoric acid (HF) releases dispersing over flat, unobstructed terrain. Pressurized liquid HF was released from a 2-4 cm diameter nozzle pointed horizontally downwind at a height of 1 m above ground. All trials occurred under fairly strong winds (wind speeds of 4-7 m/s, measured at 2 m above ground), warm and dry air (21-37°C temperature and less than 20% relative humidity). The tests included a meteorological array and measurements of HF concentration at several locations along three arcs, respectively 300, 1000 and 3000 m downwind of the release. At each location, HF concentrations were measured at 1, 3 and 8 m above ground. The last three trials included water sprays, to evaluate their effectiveness for HF cloud volume control.

2.11.2 Test Series Grouping and Rating

The Goldfish test series involved the release of hydrogen fluoride, liquefied under pressure and discharged downwind through an orifice of 4-inch diameter. The resulting cloud dispersed over flat and unobstructed terrain. The test series therefore fits in the following categories:

- Material: Toxic
- Release Type: Flashing Jet
- Dispersion Area: Unobstructed

The release of pressurized liquid through orifices of approximately 2 inch diameter is a very frequent scenario for facility siting (“Relevance” rating = 5). However, HF is not a material found in LNG facilities; additionally, HF presents peculiar thermodynamic properties that are not representative of other fluids found in LNG facilities (“Material” rating = 2). The measured concentrations were within the range of interest for toxic dispersion modeling (“Scale” rating = 4).

In every field scale test series, replicating the same test conditions (including the weather) is extremely difficult, therefore, the repeatability of field scale experiments is inherently limited (“Repeatability” rating = 2). Limited information is available on the instrumentation and quality of the data recorded during the GF trials. The MDA database includes data for each measurement sensor, but only at discrete times and for long time averages (66.6 s). The overall quality and availability of the data, for the purpose of this MVD is considered less than acceptable (“Data quality/availability” rating = 2).

Overall, the GF series is rated at 3.0, which meets the “acceptable” threshold; therefore, the Goldfish trials that did not involve the use of water sprays are included in this MVD. Note that the same trials were also included in earlier model evaluation databases and protocols [15], [47].

2.11.3 Ambient Conditions

The meteorological array for the GF trials included numerous stations to measure wind and temperature, distributed throughout the sampling array for distances up to 5 km. A total of 18 stations were used to measure wind speed and direction at a reference height of 2 m above ground. The wind speed and direction reported for each test were averaged over all 18 stations for a 15-minute period before the start of each trial.

The flatness of the terrain led to an estimated roughness length of 0.003 m, consistent with other test series performed at the same site (e.g., Desert Tortoise).

2.11.4 Discharge System

Hydrogen fluoride was stored in a pressurized tank at approximately 40°C, which corresponds to approximately 14% flash fraction upon discharge. The pressurized HF was discharged horizontally from a pipe terminating with a 2-4 cm diameter orifice, approximately 1 m above ground.

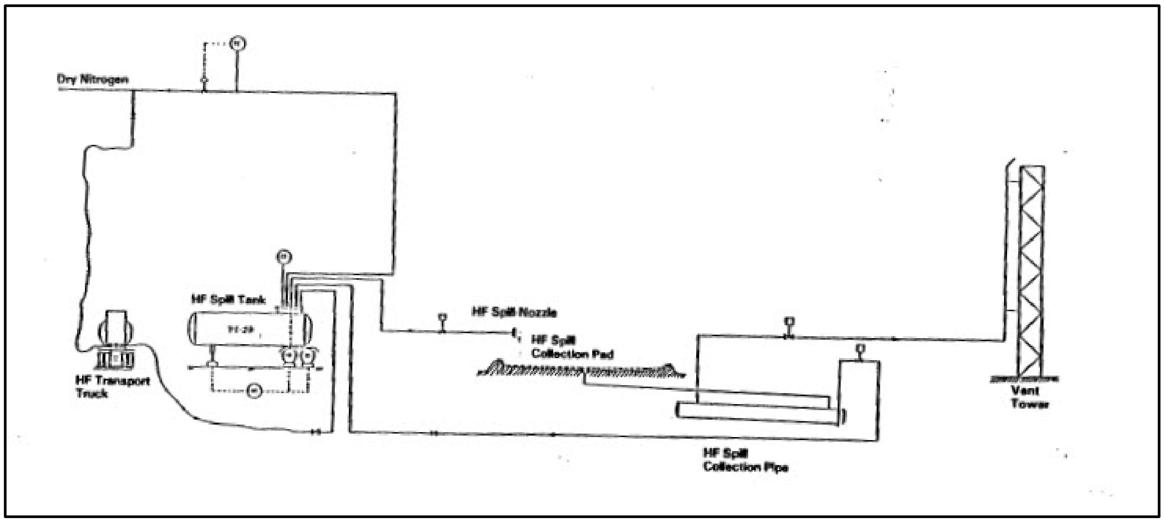

Figure 2.11-1. Schematic of the Goldfish hydrogen fluoride discharge system [46].

A load cell was used to measure the weight of the trailer throughout the release; this measurement was used to calculate the release rate. Pressure and temperature at the orifice were also measured. A liquid collection pad (9 x 61 m) was placed at the end of the discharge pipe, to collect any HF rainout.

2.11.5 Instrumentation

The instrumentation array for the measurement of the dispersing cloud consisted of three rows with instrument stations distributed across the plume, respectively at 300, 1000 and 3000 m distance from the source. The array centerline was aligned 225° with respect to North. The location of the HF measurement stations is shown graphically in Figure 2.11-2. Each station included instruments at three elevations (1, 3 and 8 m above ground) in order to gather information on both the lateral spread of the cloud and its stratification.

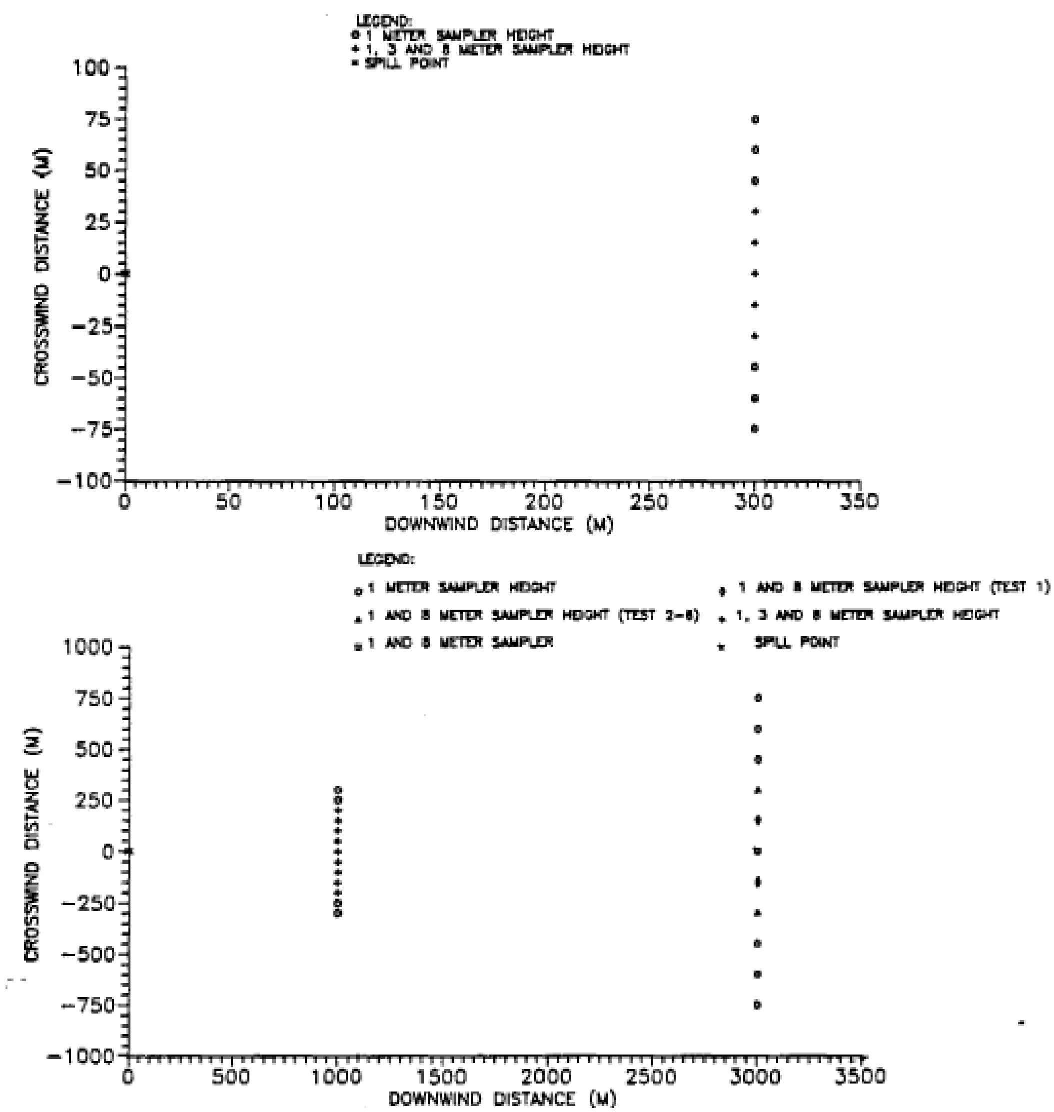

Figure 2.11-2. Location of the gas concentration measurement stations for the Goldfish trials(top: 300 m; bottom: 1,000 and 3,00 m) [46].

Sensors at the 300 m row were spaced 15 m apart, up to ±60 m crosswind of the array centerline. Sensors at the 1,000 m row were spaced 50 m apart, up to ±250 crosswind. Finally, sensors at the 3,000 m row were spaced 150 m apart up to ±750 crosswind. The coordinates of each sensor are provided in the accompanying spreadsheet, for each trial.

The HF concentration measurements used Integrated Filter (IF) samplers with sampling times of 66.6, 83.3 or 100 seconds depending on the location of the sampler and the test conditions. The collected concentration was determined in a laboratory, after the test.

2.11.6 Averaging Times

No comprehensive report was developed for the Goldfish trials; therefore, the availability of data is limited. The source of data for inclusion in the MVD is the Modeler's Data Archive (MDA) [21], which provides the HF concentration at each sampling station at discrete times, based on the sampling duration for each instrument. Given the concentration measurement method, short-time averaging is not possible; the long averaging times are listed in Table 2.11-1.

Table 2.11-1. Time averaging for the Goldfish trials.

Trial	Short time avg.	Long time avg.
GF 1	N/A	66.6 s
GF 2	N/A	66.6 s
GF 3	N/A	66.6 s

2.11.7 Experimental Uncertainty

No information was provided by Blewitt et al. [46] regarding the uncertainty of the gas concentration measurement. Therefore, an overall uncertainty of 20% is assigned to the experimental data.

2.11.8 Test Series Observations and Comments

Goldfish trials 1-3 were intended to observe the unmitigated downwind dispersion of HF releases; a summary of the test parameters is provided in Table 2.11-2. A more complete set of data for each test is included in the model validation spreadsheet.

Table 2.11-2. Goldfish test parameters

Test No.	Spill Rate [kg/s]	Spill Duration [s]	Wind Speed [m/s]	Atmospheric Stability Class
GF 1	29.1	125	5.6	D
GF 2	10.9	360	4.2	D
GF 3	10.6	360	5.4	D

The thermodynamic properties of hydrogen fluoride most frequently needed for dispersion modeling are included in the MVD spreadsheet for each trial, for use in models which may not already include it in their species database.

2.11.9 Test Series Sensitivities

The GF trials were included in previous model evaluation efforts. However, no sensitivity studies were performed to evaluate the effects of uncertainties in the model input parameters. The following sensitivity cases are based on a review of available data.

2.11.9.1 Source Term

The GF source term consisted of a flashing liquid jet, with approximately 14% flash fraction upon discharge. No rainout was reported after any trial. The release rate was not measured directly, but calculated from the tanker load cell measurements. These calculations were reported to be within 10% of the orifice flow calculation based on the measured pressure and temperature at the orifice [46]. Therefore, no source term sensitivity cases are specified for the GF trials.

2.11.9.2 Wind Speed

A review of the wind speed data indicated limited wind speed fluctuations (within approximately ±15% of the average value for each trial). Therefore, no wind speed sensitivity is specified.

2.11.9.3 Atmospheric Stability

Sensitivity cases for atmospheric stability are specified, for trials where the ambient conditions (wind speed, cloud cover, etc.) produced uncertainty in the representative Pasquill-Gifford class.

2.11.9.4 Roughness Length

The roughness length was not reported by Blewitt et al.; Hanna et al. [15] specified a value of 0.003 m to be used for model evaluation purposes based on the flatness of the terrain. Given the uncertainty associated with this estimate, sensitivity cases are specified to span one order of magnitude around the proposed value.

2.11.9.5 Temperature, Pressure and Humidity

No sensitivity cases to ambient temperature, pressure or relative humidity are specified for the Goldfish trials, given the small fluctuations and uncertainties in the data.

2.11.9.6 Material Properties

The GF trials released pure hydrofluoric acid. Models that include HF in their species database should use the built-in properties in their simulations; models that do not include HF should use the thermophysical properties listed in the accompanying spreadsheet. No sensitivity cases are specified.

2.11.9.7 Summary of Sensitivity Cases

Based on the discussion above, the model validation efforts should include the sensitivity cases listed in Table 2.11-3. If one or more sensitivity cases cannot be run, for example, due to hard-coding of certain parameters in a model, an explanation should be provided in the model questionnaire.

Table 2.11-3. Base case and sensitivity cases for the Goldfish test series.

Parameter	Case	GF 1	GF 2	GF 3
Source term	Base	Flashing jet, no rainout	Flashing jet, no rainout	Flashing jet, no rainout
Release Rate	Base	27.7 kg/s	10.5 kg/s	10.3 kg/s
Release Duration	Base	125 s	360 s	360 s
Wind Speed (at 2 m height)	Base	5.6 m/s	4.2 m/s	5.4 m/s
Surface Roughness Length	Base	0.003 m	0.003 m	0.003 m
	R1	0.001 m	0.001 m	0.001 m
	R2	0.01 m	0.01 m	0.01 m
Atmospheric Stability	Base	D	D	D
	A1	-	E	-
Ambient Temperature	Base	37.0°C	36.0°C	24.0°C
Ambient Pressure	Base	0.89 atm	0.88 atm	0.89 atm
	P1	1 atm	1 atm	1 atm
Relative Humidity	Base	5%	11%	18%
Stream Composition	Base	HF = 100%	HF = 100%	HF = 100%

2.12 Hanford-67

Experimental campaign	Hanford-67 (HAN)
Test dates:	1967-1973
Test location:	Hanford Dispersion Grid - Hanford, Washington
Number of tests:	103
Tests performed by:	General Electric Co.
Brief description:	Tracer releases of radioactive isotopes from various release heights (from ground level up to 111 m). Dispersion over flat terrain, with measurements at distances up to 12.8 km.
References:	Droppo, 1986 [48]; Horst et al., 1979 [49]
Data confidentiality:	Open (based on publicly available data)
Model validation category	
Material:	Non-Toxic
Release Type:	Tracer
Dispersion Area:	Unobstructed
Test series rating	
Overall:	**2.4**
Relevance:	2
Material:	1
Scale:	3
Repeatability:	2
Data Quality/Availability:	4
Included in MVD:	**No**

2.12.1 Description

The Hanford-67 (HAN) test series consisted of 104 tracer release experiments during 54 trial dates, distributed over a period of 7 years. The releases occurred from different elevations, from ground level up to 111 m. The tracer dispersed over relatively, unobstructed terrain. The instrumentation included a meteorological array and measurements of tracer concentration along up to 10 arcs at distances up to 12.8 km downwind of the release. Concentration measurements were near ground level (1.5 m height), but vertical concentration profiles were measured in several trials.

2.12.2 Test Series Grouping and Rating

The Hanford-67 test series involved the release of toxic or radioactive isotopes (zinc sulfide, fluorescein, rhodamine-B, and krypton-85) as tracer gas. The releases occurred from different heights and the cloud dispersed over relatively flat and unobstructed terrain. The test series therefore fits in the following categories:

- Material: Toxic
- Release Type: Tracer
- Dispersion Area: Unobstructed

Tracer releases are not frequently included in LNG facility siting studies (“Relevance” rating = 2). None of the tracer materials releases in these trials are present in LNG facilities (“Material” rating = 1). The dimensions of the test area are quite larger than typical dispersion studies (“Scale” rating = 3).

In every field scale test series, replicating the same test conditions (including the weather) is extremely difficult, therefore, the repeatability of field scale experiments is inherently limited (“Repeatability” rating = 2).

Measurements were performed at four different downwind locations, and each location included several sensors distributed crosswind and at different elevations. Data from each sensor is available from the MDA database; the overall quality and availability of data is considered more than acceptable (“Data availability” rating = 4).

Overall, the Hanford-67 series is rated at 2.4, which is below the “acceptable” threshold; therefore, the Hanford-67 series not included in the toxic dispersion MVD.

2.13 HSL-LPG

Experimental campaign	HSL-LPG
Test dates:	N/A
Test location:	Buxton, United Kingdom
Number of tests:	10
Tests performed by:	Health and Safety Laboratory
Brief description:	Horizontal pressurized jet releases of LPG through a 2-inch orifice, dispersing over flat terrain; 6 trials were unobstructed, while 4 included a barrier normal to the jet flow. Gas concentration and temperature measurements were recorded, prior to the vapor cloud being ignited.
References:	Butler and Royle, 2001 [50]
Data confidentiality:	Open (based on publicly available data)
Model validation category	
Material:	Toxic
Release Type:	Flashing Jet
Dispersion Area:	Unobstructed; Obstructed
Test series rating	
Overall:	**0**
Relevance:	
Material:	
Scale:	
Repeatability:	
Data Quality/Availability:	0
Included in MVD:	**No**

2.13.1 Description

The Health and Safety Laboratory (HSL) conducted a series of experiments involving the horizontal release of liquefied petroleum gas (LPG) as part of a joint industry project. A total of 10 trials, with release rates up to 4.9 kg/s through a 2-inch (50 mm) orifice, were performed to investigate the ignition of vapor clouds formed by these releases; however, gas concentration and temperature measurements were performed prior to the ignition, which could be used to test dispersion models. Six of the trials comprised unobstructed release, while the other four included a solid barrier perpendicular to the jet flow.

A report by Butler and Royle [50] represents the only available reference for these trials; the HSL was contacted for additional information or data but none was received beyond what is included in the report.

2.13.2 Test Series Grouping and Rating

The HSL-LPG test series involved the release of propane, liquefied under pressure and discharged downwind through an orifice of approximately 2-inch diameter. The resulting cloud dispersed over slightly sloped terrain; in some trials, a 1-m tall barrier was placed approximately 15 m from the release to obstruct the cloud dispersion. The test series therefore fits in the following categories:

- Material: Toxic
- Release Type: Flashing Jet
- Dispersion Area: Unobstructed; Obstructed

As discussed in the flammable dispersion MVD [2], limited information is available on the instrumentation and quality of the data recorded during the HSL-LPG trials. Additionally, the only available data on the propane cloud dispersion is represented by plots included in the report, which are limited to sample time traces for one trial, and concentration vs. distance plots based on long time averaged measurements at one instance per trial. The data quality and availability is therefore considered not suitable for the purposes of the MVD (“Data quality/availability” rating = 0). The HSL-LPG trials are considered not suitable for inclusion in the toxic dispersion MVD.

2.14 INERIS Ammonia Releases

Experimental campaign	INERIS (IN)
Test dates:	December 1996 – April 1997
Test location:	Centre of Scientific and Technical Studies of Aquitaine Outdoor Testing Site, near Bordeaux, France
Number of tests:	15
Tests performed by:	INERIS
Brief description:	Pressurized ammonia releases at flow rates of 2-4 kg/s, under different configurations: unobstructed; obstructed by impingement on a wall placed in proximity of the discharge; obstructed by impingement on the ground. Cloud dispersion occurred over flat terrain.
References:	Bouet, 2005 [51] Bouet et al., 2005 [52]
Data confidentiality:	Open (based on publicly available data)
Model validation category	
Material:	Toxic
Release Type:	Flashing Jet
Dispersion Area:	Unobstructed; Obstructed
Test series rating	
Overall:	**3.0**
Relevance:	5
Material:	4
Scale:	3
Repeatability:	2
Data Quality/Availability:	1
Included in MVD:	**No**

2.14.1 Description

The INERIS ammonia dispersion test series (IN) consisted of 15 releases of pressurized liquid ammonia. The test series aimed at characterizing the source term, including the potential for rainout; therefore, three different configurations were tested [51]:

1. Unobstructed jet;
2. Jet impinging on a wall close to the source (less than 3 m downwind);
3. Jet impinging on the ground.

The flashing jet of ammonia was released from a storage vessel through a 2-in pipe and 2-in diameter orifice; for some of the trials, other orifice sizes and shapes (e.g., flange gap) were used. The release flow rates were set to 2-4 kg/s in order to fall between the Desert Tortoise (approximately 100 kg/s) and the FLADIS (approximately 0.5 kg/s) test series. The terrain on the test site was flat and free of obstacles, with the exception of the wall placed near the release location in some of the trials.

2.14.2 Test Series Grouping and Rating

The INERIS (IN) test series involved the pressurized release of liquefied anhydrous ammonia through a 2-inch diameter orifice. Different configurations were used, including horizontal and downward releases, free and impinging jets, and water curtains. The cloud then dispersed over flat and unobstructed terrain for up to 2 km. The test series therefore fits in the following categories:

- Material: Toxic
- Release Type: Flashing Jet
- Dispersion Area: Unobstructed; Obstructed

Even though anhydrous ammonia is not a common fluid to be considered in LNG facility siting, the release of pressurized liquids through 2-in diameter orifices is a scenario that frequently needs to be modeled in siting studies ("Relevance" rating = 5). Ammonia is commonly used for toxic analyses at LNG facilities ("Material" rating = 4). The release flow rates are smaller than typically encountered in facility siting scenarios ("Scale" rating = 3).

In every field scale test series, replicating the same test conditions (including the weather) is extremely difficult, therefore, the repeatability of field scale experiments is inherently limited ("Repeatability" rating = 2). The major negative of the INERIS test series is the availability of data. In fact, no information is presented by Bouet on the discharge system besides the total released mass and release duration, even though pressure and temperature were measured at several locations within the storage vessel and all the way to the orifice. Therefore, the source term for these trials is highly uncertain. Similarly, none of the time traces from the numerous sensors are available; instead, only long time averaged peak values are provided. Therefore, the overall quality and availability of the data, for the purpose of this MVD is considered poor ("Data quality/availability" rating = 1).

Overall, the INERIS series is rated at 3.0, which meets the "acceptable" threshold. However, given the availability of higher-rated test series that fit the same categories, the INERIS series is not included in the toxic dispersion MVD.

2.15 Jack Rabbit Phase I

Experimental campaign	Jack Rabbit 1 (JRI)
Test dates:	April-May 2010
Test location:	Dugway Proving Ground, Utah
Number of tests:	10
Tests performed by:	West Desert Test Center
Brief description:	Pressurized and liquefied ammonia or chlorine releases through a 3 or 4-inch orifice directed downward from a 2 m elevation. The dense vapor cloud dispersed over unobstructed, flat terrain. Gas concentrations were measured along arcs at distances up to 2,500 m downwind.
References:	Fox and Storwold, 2011 [26] Storwold et al., 2011 [27] Hanna et al., 2012 [53]
Data confidentiality:	Open (based on publicly available data)
Model validation category	
Material:	Toxic
Release Type:	Flashing Jet
Dispersion Area:	Unobstructed
Test series rating	
Overall:	**3.4**
Relevance:	2
Material:	4
Scale:	5
Repeatability:	2
Data Quality/Availability:	4
Included in MVD:	**No**

2.15.1 Description

The Jack Rabbit I (JRI) test series consisted of 10 large-scale releases of pressurized liquids (either anhydrous ammonia or chlorine) from the bottom of a storage tank, directed down to impinge on the ground at the center of a man-made depression (2 m deep and 50 m diameter); the resulting vapor cloud was then allowed to be dispersed by the wind over flat, unobstructed terrain. The Jack Rabbit test program was conducted by West Desert Test Center (WDTC) at Dugway Proving Ground (DPG), Utah in April/May 2010.

The pressurized liquids were released through nozzles of 3 to 4 in diameter, with flow rates on the order of 50-70 kg/s. All trials were performed under low winds (wind speeds of 1-3 m/s). Measurements of gas concentration were performed at several locations and elevations along eight arcs, ranging from 50 m to 2,500 m downwind of the release.

2.15.2 Test Series Grouping and Rating

The Jack Rabbit I test series involved the release of anhydrous ammonia or chlorine, liquefied under pressure and discharged vertically towards the ground through an orifice of approximately 3–4 in diameter, at an elevation of 2 m. The resulting cloud dispersed over flat and unobstructed terrain, outside of a man-made depression centered around the release location. The test series therefore fits in the following categories:

- Material: Toxic
- Release Type: Flashing Jet
- Dispersion Area: Unobstructed

The release of pressurized liquids through orifices up to 4 inches in diameter is frequently encountered in siting studies; however, downward releases are rarely required as they are frequently bounded by horizontal releases. The man-made depression surrounding the release further separates the JRI layout from scenarios of interest ("Relevance" rating = 2). Anhydrous ammonia and chlorine are not commonly found in LNG facilities; however, they are both toxic ("Material" rating = 4). The release flow rates and measured concentrations are consistent with typical toxic dispersion scenarios ("Scale" rating = 5).

In every field scale test series, replicating the same test conditions (including the weather) is extremely difficult, therefore, the repeatability of field scale experiments is inherently limited ("Repeatability" rating = 2). The measurement data is of high quality and was subjected to rigorous quality control and analysis. However, data access is only possible via request to the Department of Homeland Security ("Data quality/availability" rating = 4).

Overall, the JRI series is rated at 3.4, which exceeds the "acceptable" threshold; given the availability of other flashing jet releases with more relevant configuration, though, the JRI series is not included in the toxic dispersion MVD.

2.16 Jack Rabbit Phase II

Experimental campaign	**Jack Rabbit Phase 2 (JRII)**
Test dates:	August 2015 – September 2016
Test location:	Dugway Proving Ground, Utah
Number of tests:	9
Tests performed by:	West Desert Test Center
Brief description:	Pressurized chlorine jet releases, between 5 and 20 tons per trial, from a 6-inch diameter hole. Tested different release directions (vertical up, vertical down and 45-degrees down) and dispersion through simulated urban area.
References:	Nicholson et al., 2015 [54] Byrnes and Mathew, 2016 [29] Nicholson et al., 2017 [28] Signature Science, 2015 [55]
Data confidentiality:	Open (based on publicly available data)
Model validation category **Material:** **Release Type:** **Dispersion Area:**	 Toxic Flashing Jet Complex terrain
Test series rating **Overall:** **Relevance:** **Material:** **Scale:** **Repeatability:** **Data Quality/Availability:**	 **3.6** 4 3 5 2 4
Included in MVD:	**Yes**

2.16.1 Description

The scope of the Jack Rabbit Phase 2 (JRII) trials was to expand upon the JRI results by performing chlorine releases on a larger scale. The JRII test series consisted of two phases: the first phase, conducted in 2015, included a simulated urban area through which the cloud would disperse; the urban-like obstructions were removed almost entirely for the second phase, conducted in 2016. A total of 9 trials were performed during JRII: five during phase 1 and four during phase 2.

Pressurized liquid chlorine was released through 6-inch diameter nozzles at different orientations (most of the releases were pointed down towards the ground, but one trial each tested a vertical upward release and one pointed 45-degrees down from horizontal). Total released amounts ranged from 5 to 19.5 tons of chlorine. All trials occurred under low to moderate winds (wind speeds of 2 to 4 m/s) and temperate air. The tests included numerous instruments to record meteorological conditions around the dissemination area, and chlorine concentration at several locations within the urban-like grid and along several arcs up to 11 km downwind of the release.

2.16.2 Test Series Grouping and Rating

The Jack Rabbit II test series involved the release of large quantities of chlorine, liquefied under pressure and discharged downwind through a 6-inch diameter orifice. The resulting cloud dispersed through a simulated urban area and then flat and unobstructed terrain. The test series therefore fits in the following categories:

- Material: Toxic
- Release Type: Flashing Jet
- Dispersion Area: Complex terrain

The release of large quantities of a pressurized liquid is a scenario that typically needs to be modeled in every siting study; however, the release directions (up, down, and angled down) are not common in siting scenarios. On the other hand, the presence of multiple obstructions downwind of the release is unique among flashing jet release experiments and useful for model validation ("Relevance" rating = 4). Chlorine is not a fluid to be considered in LNG facility siting; however, it is a highly toxic material ("Material" rating = 3). The release flow rates and gas concentrations measured along the outer arcs are consistent with typical toxic dispersion scenarios ("Scale" rating = 5).

In every field scale test series, replicating the same test conditions (including the weather) is extremely difficult, therefore, the repeatability of field scale experiments is inherently limited ("Repeatability" rating = 2). The measurement data is of high quality and was subjected to rigorous quality control and analysis. Only peak concentration values were obtained from the project repository[6]; however, additional data including time traces should be available to interested parties ("Data quality/availability" rating = 4).

Overall, the JRII series is rated at 3.6, which is above the "acceptable" threshold; therefore, the JRII series is considered suitable for inclusion in the toxic dispersion MVD.

2.16.3 Ambient Conditions

The meteorological array for the JRII trials included 49 portable weather instrumentation data systems (PWIDS), each including a propeller-vane wind monitor, temperature/humidity sensor, and data logger. With the exception of tower-mounted units, the PWIDS recorded ambient conditions at 2 m above ground; the sampling rate was 1 Hz, and the data was averaged over 10 seconds intervals. Three towers were deployed, each carrying PWIDS at 2, 4, 8, 16 and 32 m above ground. The location of the meteorological instrumentation is shown in Figure 2.16-1.

Ambient data were collected before, during, and after the dissemination. The reported values for each trial represent the mean of all the tripod PWIDS data recorded from the start of the dissemination until 60 minutes after [28].

[6] https://www.uvu.edu/es/jack-rabbit/, last accessed on June 16, 2020.

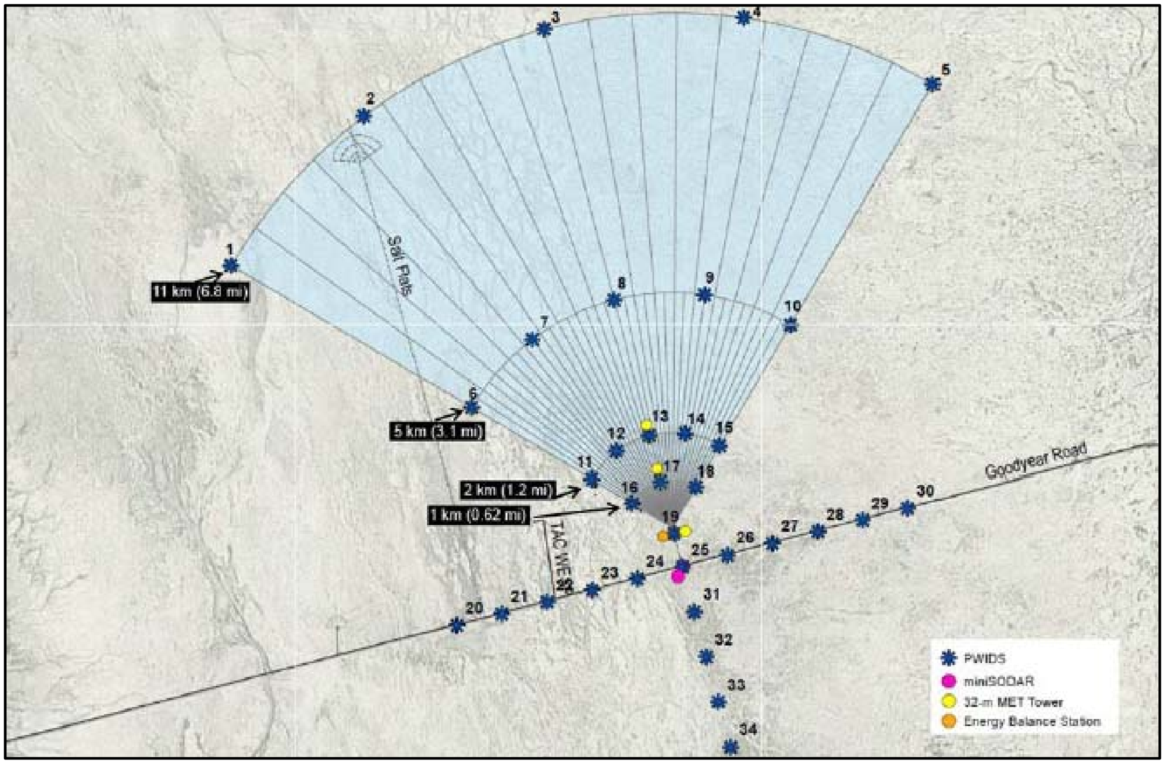

Figure 2.16-1. Location of the JRII meteorological instrumentation [54].

2.16.4 Discharge System

The discharge system consisted of a storage tank (5.64 m long and 1.37 m diameter) placed at the center of a 25 m diameter concrete dissemination pad, which was itself located near the center[7] of a 122 m by 183 m elevated gravel pad, as shown in Figure 2.16-2. The concrete pad had a 1-inch lip around its perimeter, to contain any liquid collecting onto its surface. The simulated urban area structures (identified as "Mock Urban Dispersion Area" in the figure) were placed on the gravel pad.

The tank was equipped with a total of 4 discharge ports with 6-inch penetrations: vertical down, vertical up, horizontal, and 45-degrees down from horizontal, as shown in Figure 2.16-3. The tank was elevated in such a way that the downward-facing release location would be 1 m above ground, placing the tank centerline approximately 1.7 m above

[7] Nicholson et al. [28] reported that the center of the dissemination pad was located 91 m from the upwind edge of the gravel pad, or 0.5 m from its center.

ground. The release was started by triggering a set of explosive bolts on the selected port. Figure 2.16-4 shows a photograph taken during a vertical release trial.

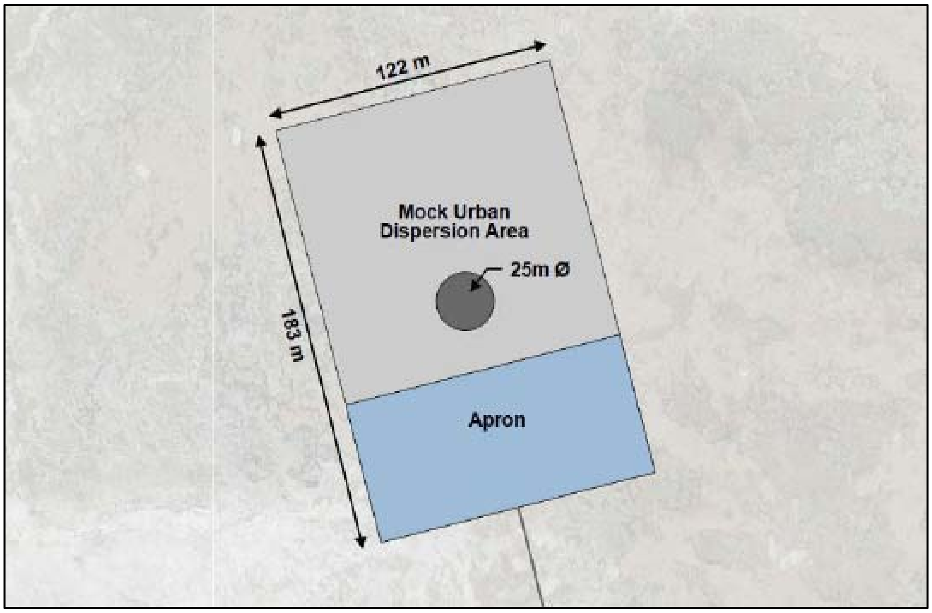

Figure 2.16-2. Layout of the Jack Rabbit II release and urban dispersion area [54].

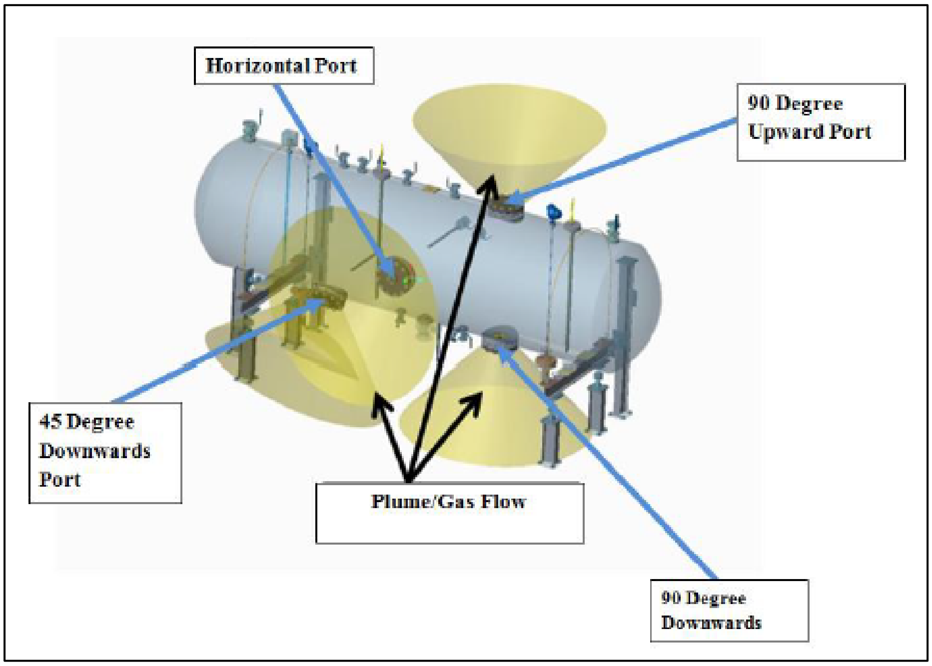

Figure 2.16-3. Schematic of the JRII chlorine disseminator [54].

Figure 2.16-4. Photograph of the dissemination tank during the vertical chlorine release in trial No. 8 [22].

Pressure and temperature in the tank were measured throughout the trial, and load cells were used to track the liquid mass in the tank during the discharge.

No significant rainout was observed from the chlorine trials; some degassing from the ground and other anomalies which could suggest rapid phase transition (i.e., sudden vaporization of pockets of liquid) indicated that some liquid chlorine may have deposited on the ground, however, this amount is believed to be negligible [53].

2.16.5 Dispersion Area

The simulated urban area used in the JRII phase 1 trials consisted of a combination of 86 conex containers (between 5.48 and 12.19 m long, and 2.44 m tall), set up for each trial as shown in Figure 2.16-5. Some of the containers were stacked vertically to simulate a tall structure. The urban area also included two rolling trailers (5.46 x 2.74 m) set up individually in a housing and office configuration and used for interior cast infiltration measurements. Finally, a few vehicles (fire trucks, cars, and one ambulance) were placed at various positions on the urban test grid.

The modular trailers and several of the conex containers were equipped to measure cloud infiltration. Indoor gas migration is outside the scope of the model evaluation for vapor dispersion in LNG facilities; therefore, indoor measurements performed during the JRII trials are not considered in this MVD. For simplicity, all trailers and containers will be assumed to be impermeable to air and gas flow.

2.16.6 Instrumentation

The Jack Rabbit trials included instrumentation for chemical detection as well as video and photographic documentation of the release and vapor cloud dispersion.

Chemical detection occurred within the simulated urban area and along the edges of the gravel pad (as shown in Figure 2.16-5 above), and also along concentric arcs with radii of 200 m, 500 m, 1 km, 2 km, 5 km and 11 km from the source (shown in Figure 2.16-6 through Figure 2.16-8). Most of the instrumentation spanned an arc of 90° around the array centerline (345° from North), but some instruments were placed crosswind and upwind up to 200 m from the release location, to track any retrograde creep of the dense cloud.

Given the focus on low gas concentrations as the typical thresholds for toxic hazards, all JRII measurement arcs included in this MVD. As discussed in section 1.1, only the sensors and arcs with peak concentrations below 1% are included in the SPM calculations; however, all data points are included in the MVD spreadsheet and in any graphical comparisons of model predictions versus experimental measurements.

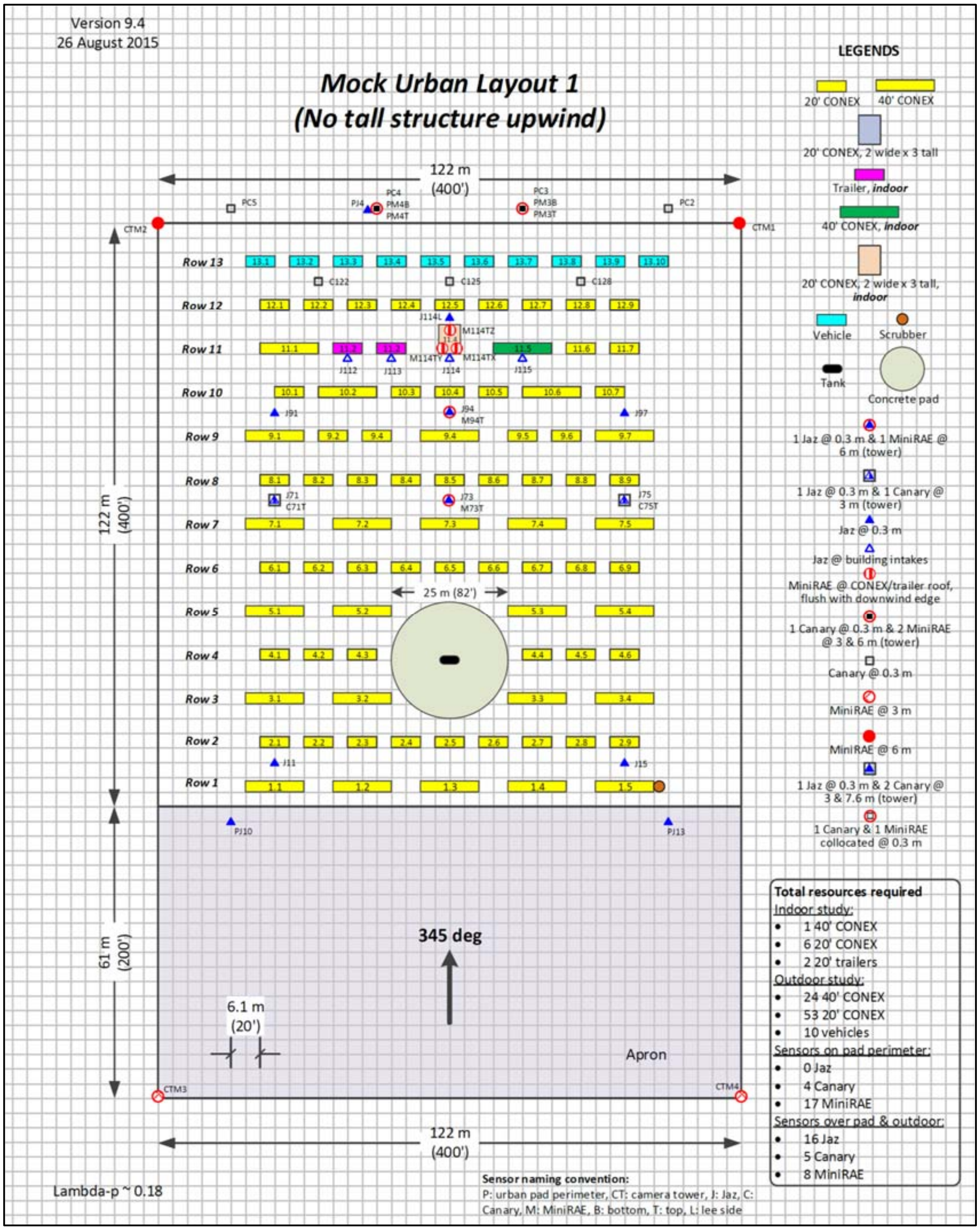

Figure 2.16-5. JRII urban area layout No. 1 (from JRII Mock Urban Plan, version 9.4, dated 26 August 2015 as obtained from project website[8]).

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[8] https://www.uvu.edu/es/jack-rabbit/

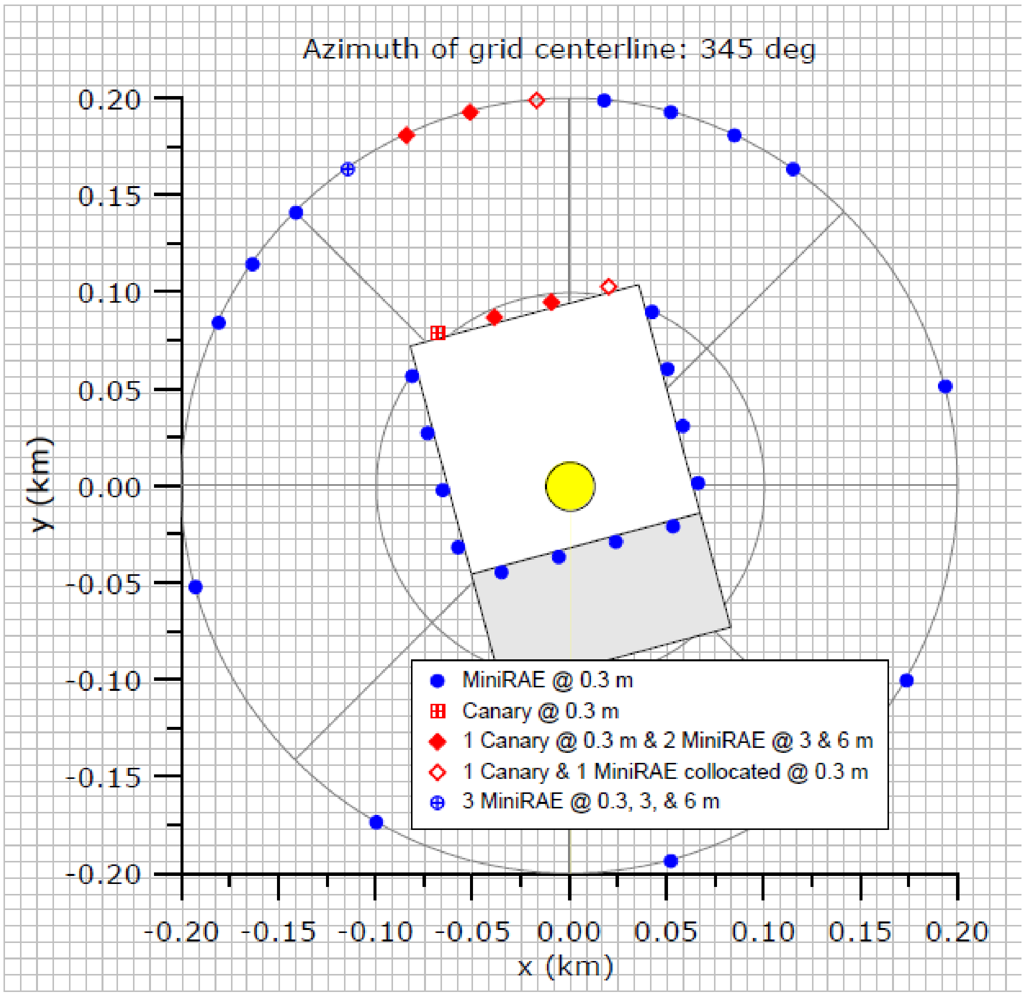

Figure 2.16-6. Overview of the JRII instrumentation layout (near field) (from JRII Urban Test Plan, version 9.1, dated 24 July 2015 as obtained from project website).

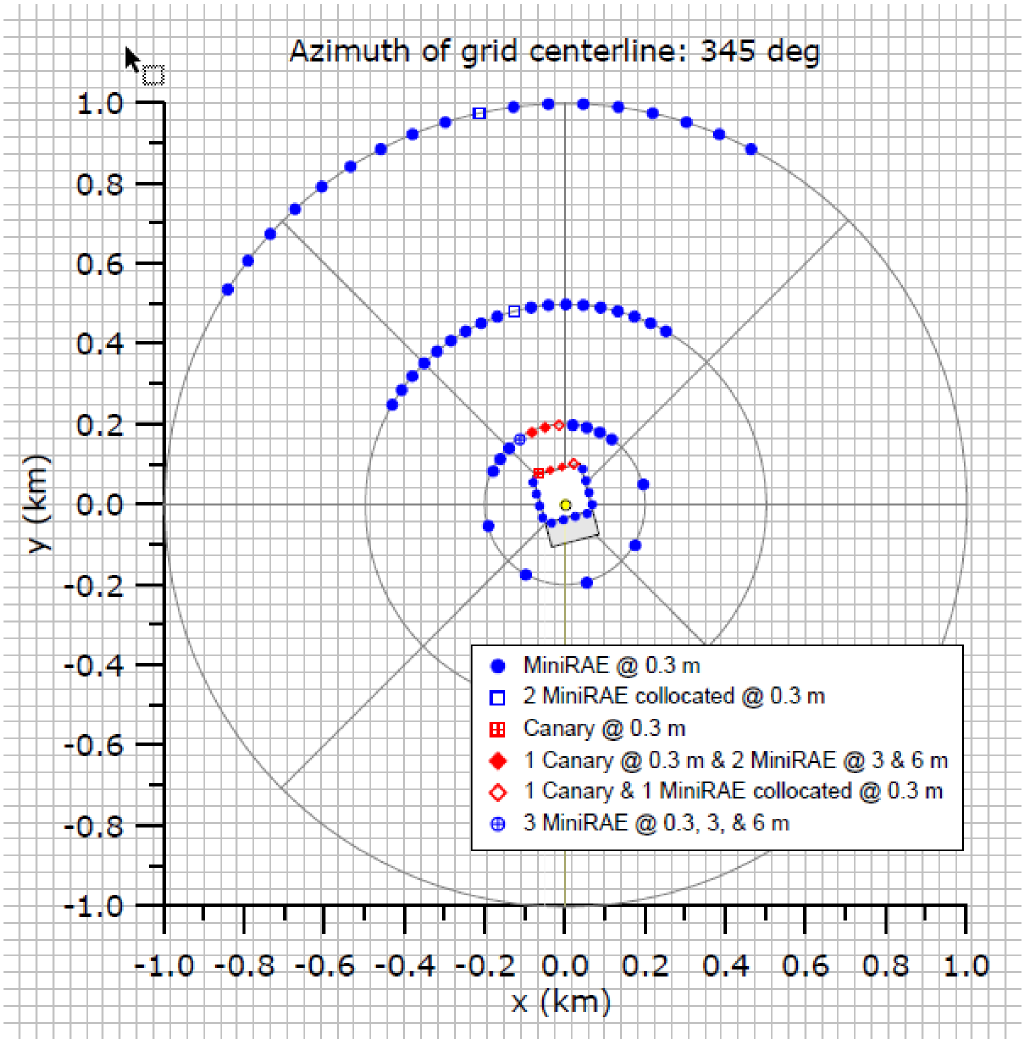

Figure 2.16-7. Overview of the JRII instrumentation layout (up to 1 km) (from JRII Urban Test Plan, version 9.1, dated 24 July 2015 as obtained from project website).

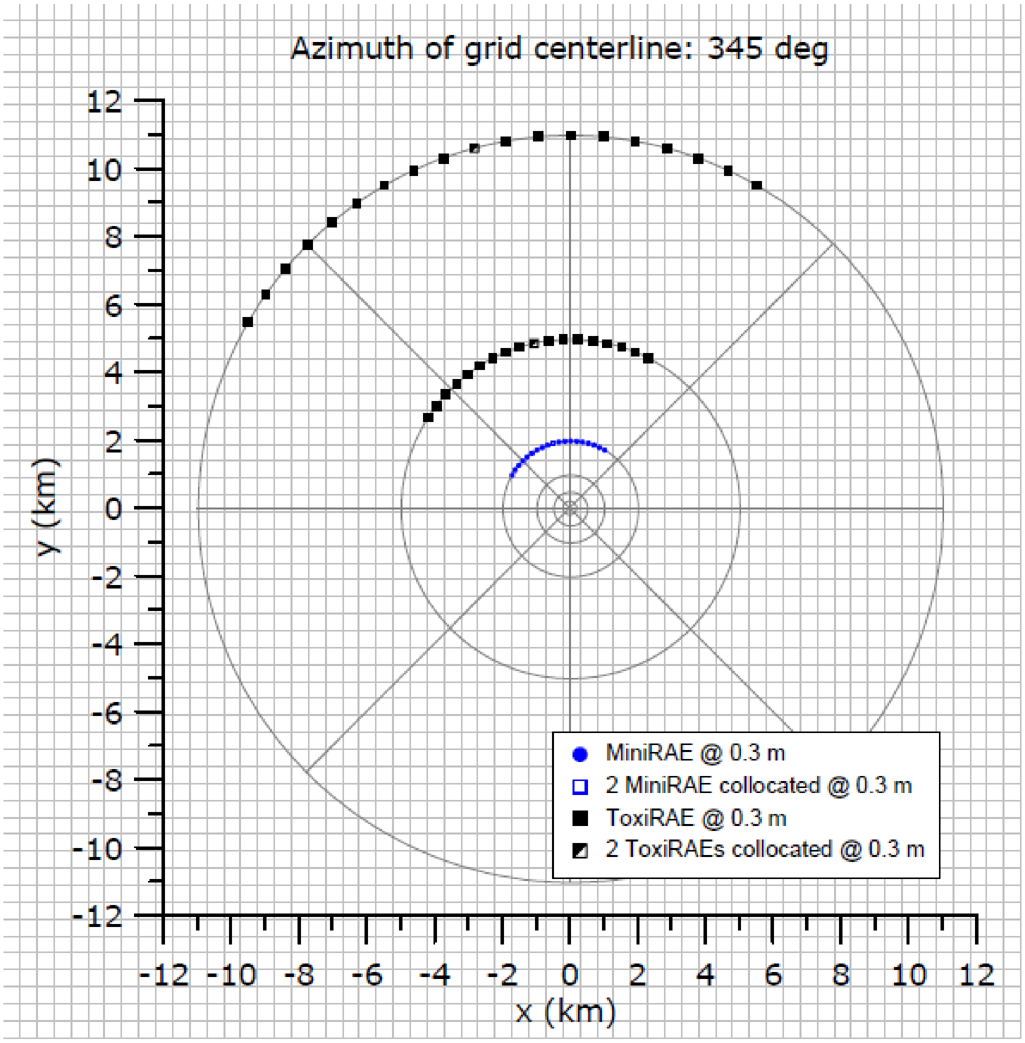

Figure 2.16-8. Overview of the JRII instrumentation layout (far field) (from JRII Urban Test Plan, version 9.1, dated 24 July 2015 as obtained from project website).

The chlorine detection instrumentation included over 200 detectors of different types, as described in detail by Nicholson et al. [28]. Each detector type spanned a different range of concentrations; the detector distribution was arranged to optimize the measurement accuracy. The placement of individual detectors in each trial is provided in the accompanying spreadsheet.

2.16.7 Experimental Uncertainty

The test series report by Nicholson et al. [28] includes limited information on the accuracy of the various instrumentation. Therefore, for the purpose of estimating uncertainty bands in the MVD, all gas concentration measurements in the JRII series are assumed to have 20% uncertainty.

2.16.8 Test Series Observations and Comments

The JRII trials consisted primarily of downward releases impinging onto the ground. As previously discussed, downward releases are of limited relevance to LNG facility siting scenarios; however, since the JRII test series is currently the only one available involving dispersion of a jet release through an urban-like environment, several trials from these series are included in the MVD. A summary of the trial parameters is provided in Table 2.16-1, as listed by Byrnes et al. [56]. A more complete set of data for each test is included in the model validation spreadsheet.

Table 2.16-1. Jack Rabbit II trial parameters

Test No.	Release Orientation	Spill Rate [kg/s]	Spill Duration [s]	Wind Speed [m/s]	Atm. Stability Class
JRII 2	Down	166.3	49	4.2	D
JRII 3	Down	125.3	36	3.9	D
JRII 4	Down	162.1	43	2.3	D
JRII 5	Down	166.1	50	2.7	D
JRII 7	45° down	113.3	80	4.5	D
JRII 8	Up	51.3	177	2.2	F

The thermodynamic properties of chlorine most frequently needed for dispersion modeling are included in the MVD spreadsheet for each trial. These should be used in models which do not have a species database, or do not include the released material.

2.16.9 Time Averaging

The time resolution of the measurements during each trial was reported as 0.1 s (1 s for trial 1) for the dissemination tank and 2 s for the chlorine concentration measurements. Therefore, the “short time average” for the JRII simulations is set to 2 s.

The data obtained from the project repository does not include instrument time traces, but only peak measured concentrations and the time at which they occurred (relative to the start of the release). Therefore, long averaging time data cannot be defined for these trials. Table 2.16-2 lists the short averaging times for the JRII trials included in the MVD.

Table 2.16-2. Time averaging for the JRII trials.

Trial	Short time avg.
JRII 2	2 s
JRII 3	2 s
JRII 4	2 s
JRII 5	2 s
JRII 7	2 s
JRII 8	2 s

2.16.10 Test Series Sensitivities

The JRII phase 1 trials were used in a modeling effort, summarized by Gant et al. [57], who identified several areas of uncertainty regarding model inputs for these trials. The sensitivity cases specified below are based on a review of the test series data and the previous modeling efforts.

2.16.10.1 Source Term

The source term for the JRII trials consisted of a flashing liquid jet; uncertainty exists regarding the conditions of the stream before it reached the discharge port: release flow rate calculations assuming a metastable liquid (i.e., no flashing inside the tank) were found to overpredict the measured release rate, whereas calculations that allowed flashing before the orifice tended to underpredict the measured flow rate.

Additional uncertainty was identified regarding whether rainout occurred, particularly for releases impinging onto the ground. Spicer and Miller [58], for example, reviewed one of the downward release trials and estimated that approximately 35% of the released material could have rained out. Given the different source term sub-models available in different models (including some that may not have a built-in source term model at all), the base case is defined using the metastable liquid discharge calculation and neglecting rainout; sensitivity cases are specified to include rainout, and to assume a two-phase discharge (either with or without rainout).

The release rate was well characterized through load cell measurements, therefore no sensitivity cases are specified for the release rate.

2.16.10.2 Wind Speed

Wind speed was observed to vary significantly during several of the JRII trials. Since most atmospheric dispersion models assume steady wind conditions, sensitivity cases are specified for high and/or low wind speeds.

2.16.10.3 Atmospheric Stability

Sensitivity cases for atmospheric stability are specified, where the ambient conditions (wind speed, cloud cover, etc.) produced uncertainty in the representative Pasquill-Gifford class.

2.16.10.4 Roughness Length

The roughness length of the terrain surrounding the test site was estimated as 0.01 m [59]. Given the uncertainty associated with this value and the effect of surface roughness on atmospheric dispersion, sensitivity cases are specified that span one order of magnitude around the base value.

2.16.10.5 Temperature, Pressure and Humidity

No sensitivity cases to ambient temperature, pressure or relative humidity are specified for the JRII trials, given the small fluctuations and uncertainties in the data.

2.16.10.6 Material Properties

The JRII series consisted of releases of pure chlorine. Models that include chlorine in their species database should use the built-in properties in their simulations; models that do not include chlorine should use the thermophysical properties listed in the accompanying spreadsheet. No sensitivity cases are specified.

2.16.10.7 Summary of Sensitivity Cases

Based on the discussion above, the model validation efforts should include the sensitivity cases listed in Table 2.16-3 and Table 2.16-4. If one or more sensitivity cases cannot be run, for example, due to hard-coding of certain parameters in a model, an explanation should be provided in the model questionnaire.

Table 2.16-3. Base case and sensitivity cases for the Jack Rabbit II test series (1/2).

Parameter	Case	JRII 2	JRII 3	JRII 4
Source term	Base	Flashing jet, no rainout	Flashing jet, no rainout	Flashing jet, no rainout
	S1	Flashing jet, with rainout	Flashing jet, with rainout	Flashing jet, with rainout
Release Rate	Base	166.3 kg/s	125.3 kg/s	162.1 kg/s
Release Duration	Base	49 s	36 s	43 s
Wind Speed (at 2 m height)	Base	4.2 m/s	3.9 m/s	2.3 m/s
Surface Roughness Length	Base	0.01 m	0.01 m	0.01 m
	R1	0.003 m	0.003 m	0.003 m
	R2	0.03 m	0.03 m	0.03 m
Atmospheric Stability	Base	D	D	D
	A1	-	-	E
Ambient Temperature	Base	22.7°C	22.5°C	22.5°C
Ambient Pressure	Base	0.86 atm	0.86 atm	0.86 atm
	P1	1 atm	1 atm	1 atm
Relative Humidity	Base	33.6%	30.3%	26.9%
Stream Composition	Base	Chlorine = 100%	Chlorine = 100%	Chlorine = 100%

Table 2.16-4. Base case and sensitivity cases for the Jack Rabbit II test series (2/2).

Parameter	Case	JRII 5	JRII 7	JRII 8
Source term	Base	Flashing jet, no rainout	Flashing jet, no rainout	Flashing jet, no rainout
	S1	Flashing jet, with rainout	Flashing jet, with rainout	Flashing jet, with rainout
Release Rate	Base	166.1 kg/s	113.3 kg/s	51.3 kg/s
Release Duration	Base	50 s	80 s	177 s
Wind Speed (at 2 m height)	Base	2.7 m/s	4.5 m/s	2.2 m/s
Surface Roughness Length	Base	0.01 m	0.01 m	0.01 m
	R1	0.003 m	0.003 m	0.003 m
	R2	0.03 m	0.03 m	0.03 m
Atmospheric Stability	Base	D	D	F
	A1	E	-	E
Ambient Temperature	Base	22.2°C	18.9°C	14.8°C
Ambient Pressure	Base	0.86 atm	0.86 atm	0.86 atm
	P1	1 atm	1 atm	1 atm
Relative Humidity	Base	26.5%	56.2%	26.5%
Stream Composition	Base	Chlorine = 100%	Chlorine = 100%	Chlorine = 100%

2.17 Kit Fox

Experimental campaign	Kit Fox (KF)
Test dates:	August 1995
Test location:	Frenchman Flat, Nevada
Number of tests:	52
Tests performed by:	Desert Research Institute and Western Research Institute
Brief description:	Carbon dioxide released vertically at low velocity, with dispersion over flat terrain. Artificial roughness elements were introduced to approximate an industrial facility, at 1/10 scale. Two sets of roughness elements distributions were tested.
References:	Western Research Institute, 1998 [60], [61] Hanna and Steinberg, 2001 [62]
Data confidentiality:	Open (based on publicly available data)
Model validation category	
Material:	Non-Toxic
Release Type:	Low-momentum
Dispersion Area:	Unobstructed
Test series rating	
Overall:	**3.2**
Relevance:	4
Material:	3
Scale:	3
Repeatability:	2
Data Quality/Availability:	4
Included in MVD:	**Yes**

2.17.1 Description

The Kit Fox (KF) test series consists of 52 releases of carbon dioxide (CO_2) dispersing through an array of obstacles intended to represent an industrial site at 1/10 of full scale [62]. CO_2 was released upwards from ground level, at flow rates of approximately 1.6 to 4 kg/s through a 2.25 m^2 area. The release duration varied between approximately 20 seconds (puff) and 3-7 minutes (continuous). CO_2 concentration measurements were performed at several locations and elevations along four rows, at 25, 50, 100, and 225 m downwind of the release.

2.17.2 Test Series Grouping and Rating

The Kit Fox test series involved the release of gaseous carbon dioxide from a ground-level opening measuring 1.5 m by 1.5 m. The resulting cloud dispersed over flat terrain; however, two arrays of small obstacles were added to approximate the roughness of an industrial site and neighboring areas, at a 1/10 scale. For the purpose of categorizing the test series, the obstacle arrays do not represent an “obstruction” or a “complex geometry”. The test series therefore fits in the following categories:

- Material: Non-Toxic
- Release Type: Low-momentum
- Dispersion Area: Unobstructed

The ground-level source term behaves similarly to the vapor clouds from liquid spills, which represent required siting scenarios. Additionally, the roughness arrays are intended to approximate the effect of structures and equipment in industrial facilities. Therefore, the Kit Fox series is considered more than relevant to the purpose of this MVD (“Relevance” rating = 4). Carbon dioxide is not a material used in LNG facilities; however, the use of CO_2 to produce dense gas clouds in scaled experiments is well established (“Material” rating = 3). The scaling factor of 1/10 is considered acceptable (“Scale” rating = 3).

In every field scale test series, replicating the same test conditions (including the weather) is extremely difficult, therefore, the repeatability of field scale experiments is inherently limited (“Repeatability” rating = 2). Measurements were performed at four different downwind locations, and each location included several sensors distributed crosswind and at different elevations. The MDA database includes data for each measurement sensor, from both the weather and dispersion arrays (“Data quality/availability” rating = 4).

Overall, the Kit Fox series is rated at 3.2, which meets the “acceptable” threshold; therefore, the Kit Fox series is included in the toxic dispersion MVD. Note that the Kit Fox series is also included in the flammable dispersion MVD [2] and was previously included in the Modeler’s Data Archive [21] as well as in model developers’ internal validation efforts ([12], [42], [63]).

2.17.3 Ambient Conditions

Meteorological instruments were installed on five towers, plus wind vanes at six other locations. Towers were located inside the roughness arrays, as well as on the flat desert surface outside of these areas.

A 24 m tall meteorological tower measured temperature, wind speed and wind direction, and relative humidity at multiple elevations. All data was recorded every 10 seconds (0.1 Hz frequency). The temperature and wind velocity measured by a tower located 20 m upwind of the release location were used to calculate the atmospheric boundary layer parameters for each trial. The wind speed and direction for each trial were obtained from measurements at 2 m above ground, at a weather station 50 m downwind of the release location, averaged over approximately a 1-minute interval.

2.17.4 Discharge System

CO_2 gas was released vertically at a nearly constant rate from a 1.5m x 1.5m area source near the middle of the scaled industrial site. CO_2 was stored at ambient temperature and approximately 125 psig pressure [60]. The discharge piping ran underground and was connected to a release box, measuring 1.5 m x 1.5 m x 1 m deep, placed such that the top of the box would be flush with the terrain. A porous insert was placed within the release box to help distribute the CO_2 flow and obtain a homogeneous vertical velocity at the top surface. Three RTD sensors measured the CO_2 temperature inside the box. A schematic of the discharge system is shown in Figure 2.17-1.

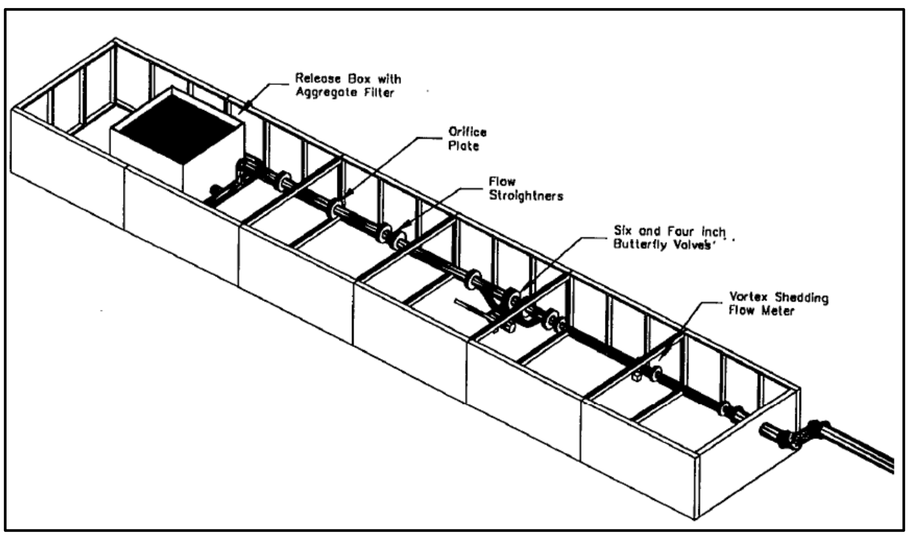

Figure 2.17-1. Schematic of the Kit Fox discharge system [60].

The discharge flow rate was measured by a vortex shedding flow meter with an accuracy of 1% of full rated flow, or 0.075 kg/s. A second flow rate measurement was provided by a 4.5-in diameter orifice in the discharge line. The two sets of measurements are listed in the WRI report [60] and show very good agreement (within 2-3%).

2.17.5 Dispersion Area

The entire experimental set-up was intended to represent an industrial site at about 1/10 of full scale. For that purpose, three sets of obstacles were installed to develop:

- A Uniform Roughness Area (URA) array, with surface roughness representative of the areas surrounding an industrial facility;
- An Enhanced Roughness Pattern (ERP) array, which simulated the actual industrial facility; and
- A row of spires, to “trip” the boundary layer and accelerate its development.

The URA roughness array was constructed of 6,600 rectangular sections of plywood perpendicular to the mean flow direction (corresponding to 230° from North); each element was 0.8 m wide by 0.2 m tall, and the elements were spaced 2.4 m downwind and 2.4 m laterally. The URA array spanned a length of 314 m (in the direction of mean flow) and a width of 120 m (centered on the release location. The leading edge of the URA was 89 m upwind of the release location.

The ERP roughness array was constructed of 75 square plywood baffles, also perpendicular to the mean flow direction; each baffle was 2.4 m wide by 2.4 m tall, and the baffles were spaced 8.5 m downwind and 6.1 m laterally. The ERP array spanned a length of 85 m (in the direction of mean flow) and a width of 39 m (centered on the release location. The leading edge of the ERP was 50 m upwind of the release location. The ERP elements were removed during the 33 experiments that comprised Kit Fox trials 6-8.

A row of 38 spires was placed, perpendicular to the mean flow direction, at the leading edge of the URA. Each spire consisted of a vertical panel, 4.88 m tall and tapering in width from 47.6 cm at the base to 12.1 cm at the top. The spires were spaced 3.25 m apart and spanned the full width of the URA.

Figure 2.17-2 shows the layout of the roughness elements relative to the release location. Note that both URA and ERP elements were staggered from one row to the next, to avoid channeling flow between rows.

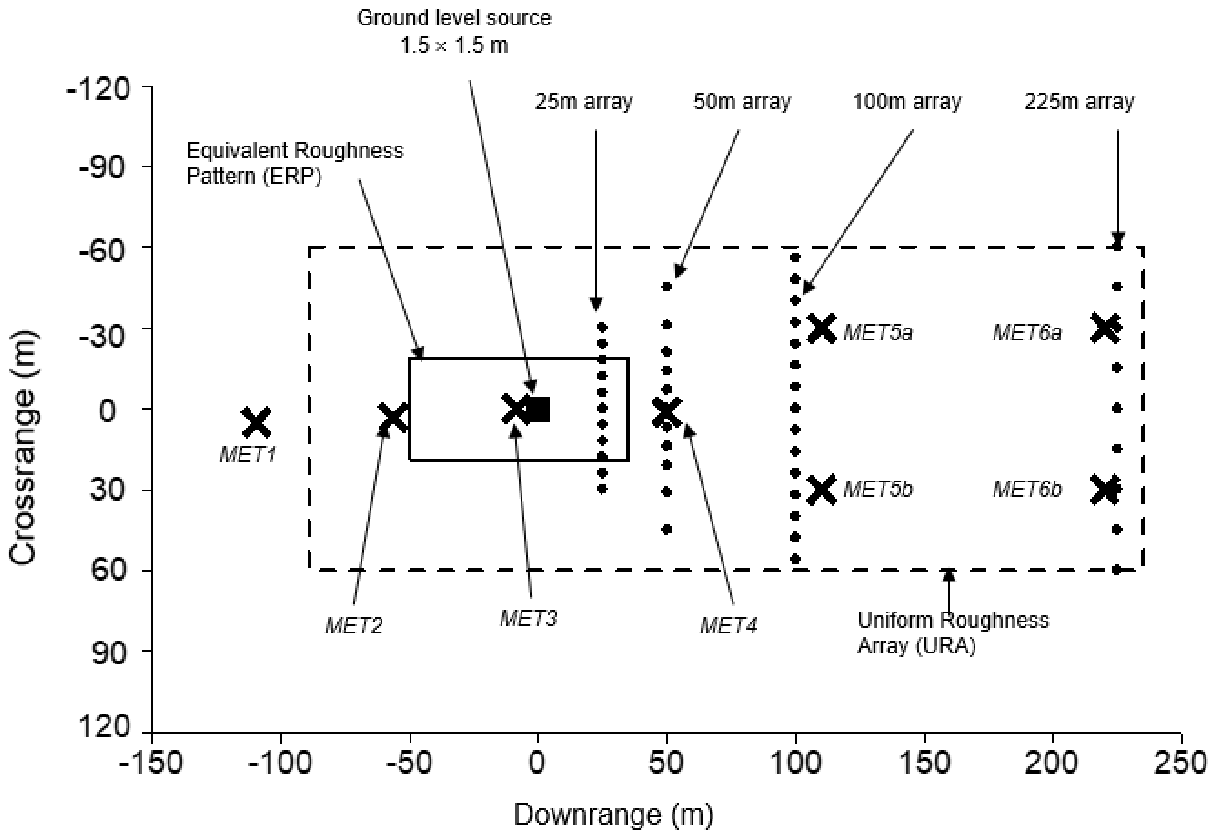

Figure 2.17-2. Schematic of the Kit Fox dispersion area (adapted from [21]).

2.17.6 Instrumentation

The Kit Fox trials used both high-concentration (up to 150,000 ppm) and low-concentration (up to 20,000 ppm) solid-state infrared carbon dioxide sensors. All CO_2 sensors recorded gas concentration at 1 Hz.

A total of 84 sensors were placed in four downwind rows (25, 50, 100, and 225 m); most of the sensors were placed near the ground (0.3 m elevation along the nearest row, 0.5 m elevation along the other rows), while others were mounted on towers at elevations between 0.6 and 10 m. The position of each sensor during the Kit Fox trials is provided in the accompanying spreadsheet.

2.17.7 Experimental Uncertainty

The manufacturer's reported accuracy for the CO_2 sensors is 1% of full-scale; however, the error analysis during pre-test calibration showed uncertainties up to approximately 20%. Therefore, an experimental uncertainty of 20% is used in the MVD.

2.17.8 Test Series Observations and Comments

The Kit Fox test series included both short-duration (puff) and long-duration (continuous) releases. Only continuous releases are considered here, as they more accurately reflect the type of scenarios required for LNG facility siting.

Not all the trials performed during the Kit Fox test series produced useful data, due to changes in wind direction carrying the cloud outside the measurement area. Based on a review of the test series report, 8 of the 18 continuous releases provided sufficient data and thus are included in this MVD. A summary of the test parameters for these 8 trials is provided in Table 2.17-1. A more complete set of data for each trial is included in the model validation spreadsheet.

Table 2.17-1. Kit Fox test parameters

Test No.	Spill Rate [kg/s]	Spill Duration [s]	Wind Speed [m/s]	Atmospheric Stability Class	Roughness Blocks
KF 5-3	3.9	120	2.6 @ 2 m	D	ERP + URA
KF 5-4	3.7	120	2.2 @ 2 m	E	ERP + URA
KF 6-4	1.8	120	4.1 @ 2 m	D	URA only
KF 6-5	1.9	120	3.2 @ 2 m	E	URA only
KF 6-6	2.1	180	2.3 @ 2 m	E	URA only
KF 6-9	1.5	300	1.8 @ 2 m	F	URA only
KF 7-3	1.7	180	3.0 @ 2 m	E	URA only
KF 8-8	1.6	120	3.4 @ 2 m	E	URA only

The thermodynamic properties of CO_2 most frequently needed for dispersion modeling are included in the MVD spreadsheet for each trial. These should be used in models which do not have a species database, or do not include the released material.

2.17.9 Time Averaging

The data included in the MDA database, which is used in this MVD, consists of the calibrated data at 1 Hz frequency. The short averaging time is therefore 1 s for each trial.

The long averaging time is set to the duration of the release.[9] Table 2.17-2 summarizes the short and long time averaging for the KF trials.

Table 2.17-2. Time averaging for the Kit Fox trials.

Trial	Short time avg.	Long time avg.
KF 5-3	1 s	120 s
KF 5-4	1 s	120 s
KF 6-4	1 s	120 s
KF 6-5	1 s	120 s
KF 6-6	1 s	180 s
KF 6-9	1 s	300 s
KF 7-3	1 s	180 s
KF 8-8	1 s	120 s

2.17.10 Test Series Sensitivities

The Kit Fox test series was included in previous model evaluation efforts. However, no sensitivity studies were performed to evaluate the effects of uncertainties in the model input parameters. The following sensitivity cases are based on a review of available data.

2.17.10.1 Source Term

CO_2 was introduced in gaseous form and at low velocity; the flow rate was measured by two independent methods, with good agreement. Therefore, no sensitivity cases are specified for the release rate or other source term characteristics.

2.17.10.2 Wind Speed

No sensitivity cases are specified to wind speed.

[9] It should be noted that the MDA lists a long averaging time of 20 s for all Kit Fox trials.

2.17.10.3 Atmospheric Stability

Sensitivity cases for atmospheric stability are specified, for trials where the ambient conditions (wind speed, cloud cover, etc.) produced uncertainty in the representative Pasquill-Gifford class.

2.17.10.4 Roughness Length

Surface roughness in the KF trials was affected by design, by the roughness arrays (ERP and URA). The roughness due to the URA alone was calculated by WRI as 0.03 m, with an uncertainty of approximately 10%. The roughness due to the combined ERP and URA configuration was calculated as 0.3 m. The calculated roughness values define the base case for each trial; sensitivity cases are then defined for roughness lengths reduced by the 10% uncertainty.

2.17.10.5 Temperature, Pressure and Humidity

No sensitivity cases to ambient temperature, pressure or relative humidity are specified for the Kit Fox trials, given the small fluctuations and uncertainties in the data.

2.17.10.6 Material Properties

The KF trials released pure CO_2. Models that include CO_2 in their species database should use the built-in properties in their simulations; models that do not include CO_2 should use the thermophysical properties listed in the accompanying spreadsheet. No sensitivity cases are specified.

2.17.10.7 Summary of Sensitivity Cases

Based on the discussion above, the model validation efforts should include the sensitivity cases listed in Table 2.17-3 and Table 2.17-4. If one or more sensitivity cases cannot be run, for example, due to hard-coding of certain parameters in a model, an explanation should be provided within the model questionnaire.

Table 2.17-3. Base case and sensitivity cases for the Kit Fox test series (1/2).

Parameter	Case	KF 5-3	KF 5-4	KF 6-4	KF 6-5
Source term	Base	Low-momentum gas	Low-momentum gas	Low-momentum gas	Low-momentum gas
Release Rate	Base	3.9 kg/s	3.7 kg/s	1.8 kg/s	1.9 kg/s
Release Duration	Base	120 s	120 s	120 s	120 s
Wind Speed (at 2 m height)	Base	2.6 m/s	2.2 m/s	4.1 m/s	3.2 m/s
Surface Roughness Length	Base	0.3 m	0.3 m	0.03 m	0.03 m
	R1	0.27 m	0.27 m	0.027 m	0.027 m
Atmospheric Stability	Base	D	E	D	E
	A1	E	F	-	D
Ambient Temperature	Base	33.1°C	31.4°C	36.7°C	36.0°C
Ambient Pressure	Base	0.89 atm	0.89 atm	0.89 atm	0.89 atm
	P1	1 atm	1 atm	1 atm	1 atm
Relative Humidity	Base	15%	16%	14%	14%
Stream Composition	Base	CO_2 = 100%	CO_2 = 100%	CO_2 = 100%	CO_2 = 100%

Table 2.17-4. Base case and sensitivity cases for the Kit Fox test series (2/2).

Parameter	Case	KF 6-6	KF 6-9	KF 7-3	KF 8-8
Source term	Base	Low-momentum gas	Low-momentum gas	Low-momentum gas	Low-momentum gas
Release Rate	Base	2.1 kg/s	1.5 kg/s	1.7 kg/s	1.6 kg/s
Release Duration	Base	180 s	180 s	300 s	120 s
Wind Speed (at 2 m height)	Base	2.3 m/s	1.8 m/s	3.0 m/s	3.4 m/s
Surface Roughness Length	Base	0.03 m	0.03 m	0.03 m	0.03 m
	R1	0.027 m	0.027 m	0.027 m	0.027 m
Atmospheric Stability	Base	E	F	E	E
	A1	F	E	D	D
Ambient Temperature	Base	35.4°C	34.0°C	37.9°C	36.7°C
Ambient Pressure	Base	0.89 atm	0.89 atm	0.89 atm	0.89 atm
	P1	1 atm	1 atm	1 atm	1 atm
Relative Humidity	Base	14%	14%	10%	15%
Stream Composition	Base	CO_2 = 100%	CO_2 = 100%	CO_2 = 100%	CO_2 = 100%

2.18 Lathen/EEC

Experimental campaign	Lathen (EEC)
Test dates:	October 1988 – September 1989
Test location:	Lathen, Germany
Number of tests:	58
Tests performed by:	TüV Norddeutschland and Risø
Brief description:	Pressurized propane releases with different configurations, including: horizontal and vertical jets; no-momentum cyclone source; a mobile jet source; and a pure gas source. Obstacles were placed in different configurations (straight line or arc) and concentration measurements were performed both in front and behind the obstacles.
References:	Nielsen and Jensen, 1991 [64] Nielsen and Ott, 1996 [23]
Data confidentiality:	Open (based on publicly available data)
Model validation category	
Material:	Toxic
Release Type:	Flashing Jet
Dispersion Area:	Obstructed
Test series rating	
Overall:	**3.6**
Relevance:	5
Material:	4
Scale:	4
Repeatability:	2
Data Quality/Availability:	3
Included in MVD:	**Yes**

2.18.1 Description

The Lathen test series, also known as BA-Propane or EEC (therefore identified as EEC throughout this report), consists of over 50 propane releases with different configurations, including: horizontal and vertical jets; no-momentum cyclone source; a mobile jet source; and a pure gas source. The release rates were on the order of 0.2-3 kg/s, for a duration of approximately 3-5 minutes. Barriers were placed in different configurations (straight line or arc), and concentration measurements were performed both in front and behind the obstacles.

2.18.2 Test Series Grouping and Rating

The Lathen (EEC) test series involved the release of propane, liquefied under pressure and discharged downwind through an orifice of approximately 0.6-inch diameter. The resulting cloud dispersed over flat terrain, but barriers were placed approximately 50 m from the release to obstruct the cloud dispersion. The test series therefore fits in the following categories:

- Material: Toxic
- Release Type: Flashing Jet
- Dispersion Area: Obstructed

The release of pressurized liquids through orifices, with dispersion affected by obstructions (e.g., vapor barriers) is a common scenario for siting studies ("Relevance" rating = 5). Propane is used as a refrigerant (pure or mixed with other hydrocarbons) in many LNG liquefaction facilities, therefore, the dispersion of propane releases is frequently modeled in siting studies; it is also considered a toxic material, however, the toxic hazards are always enveloped by the flammable hazards ("Material" rating = 4). The release flow rates and concentration measurement distances are smaller than typically modeled, however, several EEC trials resulted in measured gas concentrations within the range of interest for toxic dispersion modeling ("Scale" rating = 4).

In every field scale test series, replicating the same test conditions (including the weather) is extremely difficult, therefore, the repeatability of field scale experiments is inherently limited ("Repeatability" rating = 2). Limited information is available on the instrumentation and quality of the data recorded during the EEC trials, but the REDIPHEM database includes data for each measurement sensor, reported at 1 s intervals ("Data quality/availability" rating = 3).

Overall, the EEC series is rated at 3.6, which is above the "acceptable" threshold; therefore, the EEC test series is considered suitable for inclusion in the toxic dispersion MVD. Note that the EEC trials are also included in the flammable dispersion MVD [2].

2.18.3 Ambient Conditions

Ambient conditions (wind speed and direction, turbulence and air temperature) were recorded for each trial from instrumentation mounted on a set of 6 m tall masts. In some cases, however, the wind measurements were missing, and the speed and direction were obtained from a separate station which logged 10-min average values of speed and direction. Prior to each release, the ambient humidity and temperature were measured with a hand held psychrometer, and a note was made on the cloud cover [23].

2.18.4 Discharge System

At least four different gas sources were used in the Lathen experiments, as described by Nielsen and Ott [23] and shown schematically in Figure 2.18-1:

1. A jet source which released pressurized liquid propane through a nozzle to generate a flashing jet. In some of the trials, the nozzle was pointed in the vertical direction. No liquid pool formed on the ground.
2. A cyclone release source, with no net momentum. About 33% of the liquid material separated inside the cyclone and formed a pool on the ground.
3. A mobile jet source, which released a jet directed towards the ground. The release rates were lower than for the fixed jet source, and little rainout was observed.
4. A pure gas source obtained by evaporating the liquified propane inside a large reservoir and allowing the evaporated gas to exit at the top. The release pressure and temperature of this source were not measured.

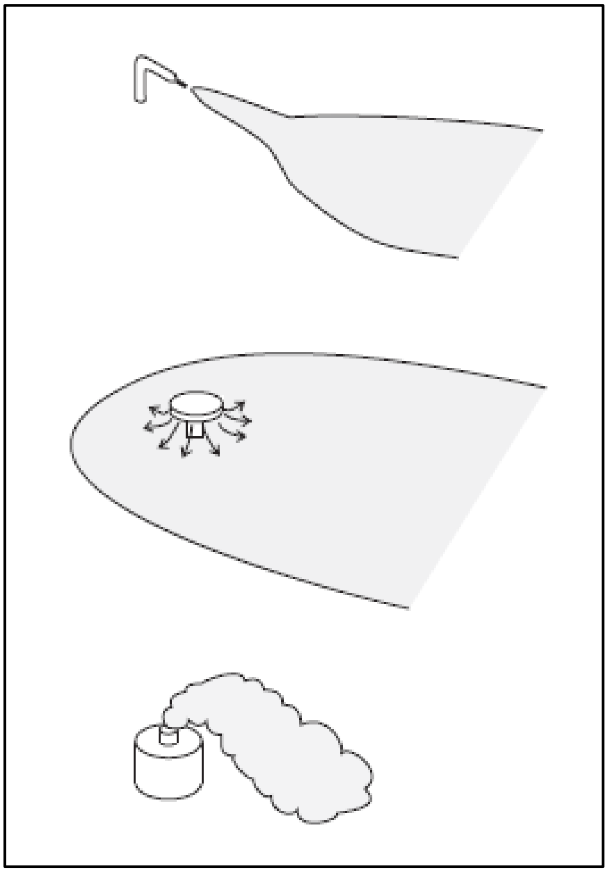

Figure 2.18-1. Schematic of the EEC discharge systems (types 1, 2 and 4, respectively, from top to bottom) [23].

Given the large number of low-momentum releases available from other test series, the focus for the EEC series was placed on jet releases. All EEC jet releases included in this database occurred from a 0.6-in (15.5 mm) diameter orifice, oriented horizontally downwind at 0.5 m above ground.

2.18.5 Dispersion Area

The EEC trials were aimed at evaluating the effect of solid barriers on the dispersion of dense gas clouds; the test series was designed to study gas flow over a linear or curved wall or between two parallel walls. Hence, the test series was intended to be flexible in the type of release, placement of barriers and instrumentation.

The gas cloud was expected to be flat and wide, so the barriers consisted of long stretches of 2 m high heavy curtains. The various curtain configurations were placed approximately 50 m from the release. Before each trial, the curtains were mounted only on the part of the obstacle configuration which was exposed to gas based on the wind direction. Sometimes, only every other curtain in the obstacle lines was mounted, giving a 50% overall porosity. The curtains were designed to be removed during the experiment by pulling a wire, with the intent to obtain a comparison of dispersion with and without obstacles, for the same source term and weather. The variable configuration is not considered relevant to siting studies; however, the use of barriers to control vapor cloud dispersion is currently quite common in LNG facilities, therefore, several EEC trials with barrier removal are included in the MVD. However, only data prior to the removal of the barriers is used for model comparisons.

2.18.6 Instrumentation

A total of 44 catalytic and IR sensors were used to measure propane concentration during the EEC trials. These measurements were performed near ground level in a flexible array, whose arrangement was varied depending on the trial. The catalytic gas sensors were reported to have a response time of approximately 10 seconds, even though data was sampled at 1 Hz.

Gas concentration measurements (in addition to temperature, wind speed, wind direction and turbulence) were also performed on the meteorological masts, which were placed upwind and downwind of the walls, perpendicular to the expected wind direction; the concentration measurements were at 1, 2, and 4 m above ground. Figure 2.18-2 shows a schematic of the barrier and mast layout for two of the test configurations. Given the flexible arrangement of the trials, the user is strongly encouraged to review the instrument location in the MVD spreadsheet for each trial.

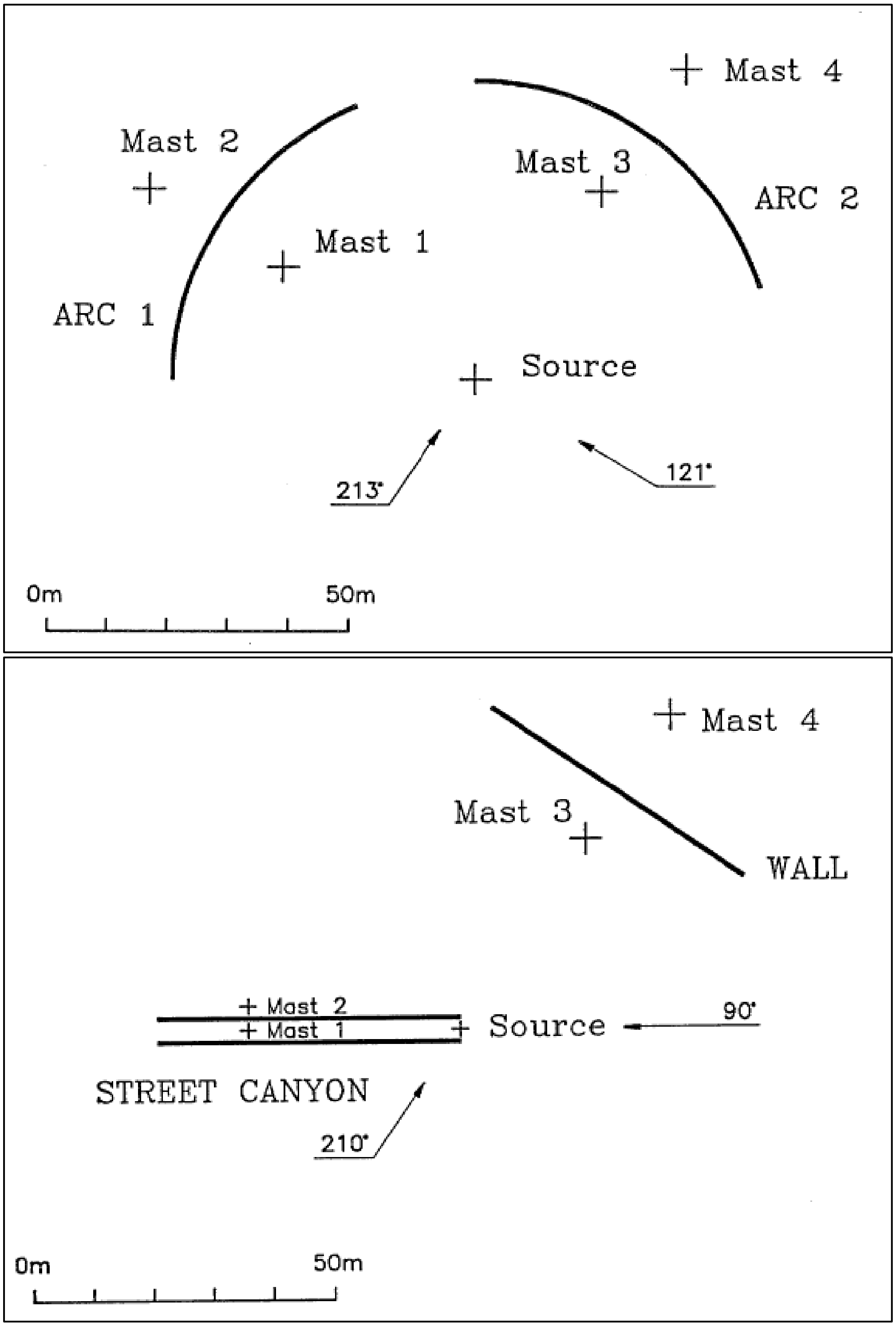

Figure 2.18-2. Schematic of two EEC test configurations: (top) May 1989; (bottom) August-September 1989 [64].

2.18.7 Experimental Uncertainty

No information was found in the available references regarding the uncertainty of the gas concentration measurement. Therefore, an overall experimental uncertainty of 20% is specified in the accompanying spreadsheet.

2.18.8 Test Series Observations and Comments

The REDIPHEM database includes data from 51 trials form the EEC series, including information regarding the discharge, barrier and instrumentation layout. Only a subset of the EEC trials is included in this MVD. Specifically, the focus was placed on trials involving horizontal jet releases and obstructed dispersion. Additionally, it must be noted that for trials during which the barrier was removed, only data prior to the barrier removal was considered. A summary of the test parameters is provided in Table 2.18-1. A more complete set of data for each test is included in the model validation spreadsheet.

Table 2.18-1. Lathen (EEC) test parameters

Test No.	Release Rate [kg/s]	Release Duration [s]	Wind Speed [m/s]	Atm. Stability Class	Barriers
EEC 07	2.9	200	4.3 @ 3.3 m	D	Curved (removed at 90 s)
EEC 08	2.9	250	4.2 @ 6 m	C	Curved, 50% porous (removed at 120 s)
EEC 17	2.9	160	3.9 @ 3.3 m	D	Curved (removed at 90 s)
EEC 18	2.9	180	4.4 @ 3.3 m	D	Curved, 50% porous (removed at 120 s)

As shown in the accompanying spreadsheet, the EEC sensors were not placed along arcs or lines; however, their placement was such that they could be grouped into a discrete set of arcs by ranges of distances (i.e., all sensors within a 10 m deep arc were grouped together, at a nominal arc distance equal to the center of the band). This approach allows arc-wise maxima and SPMs to be calculated for the EEC trials.

The thermodynamic properties of propane most frequently needed for dispersion modeling are included in the MVD spreadsheet for each trial. These should be used in models which do not have a species database, or which do not include the released material.

2.18.9 Time Averaging

Data from the EEC trials is available as part of the REDIPHEM database, where it is presented as 1 Hz time traces. However, the short averaging time is set to 10 s, to match the response time of the catalytic sensors. Long averaging times are not considered meaningful for trials where the barrier was removed before the end of the release, as that action clipped the tail end of the dispersing cloud. The averaging times are listed in Table 2.18-2.

Table 2.18-2. Time averaging for the Lathen (EEC) trials.

Trial	Short time avg.	Long time avg.
EEC 07	10 s	-
EEC 08	10 s	-
EEC 17	10 s	-
EEC 18	10 s	-

2.18.10 Test Series Sensitivities

No previous model evaluation efforts were found that included the EEC trials. Therefore, the following sensitivity cases are based on a review of available data.

2.18.10.1 Source Term

The source term consisted of a flashing jet of propane at known conditions. No rainout was reported. The release rate was reportedly consistent across multiple trials. Therefore, no sensitivity cases to the source term are specified.

2.18.10.2 Wind Speed

No sensitivity cases are specified to wind speed.

2.18.10.3 Atmospheric Stability

Sensitivity cases for atmospheric stability were specified, where the ambient conditions (wind speed, cloud cover, etc.) produced uncertainty in the representative Pasquill-Gifford class.

2.18.10.4 Roughness Length

The surface roughness was estimated from wind profiles measured in the absence of obstacles or gas release. The REDIPHEM database lists the value as 0.006 m. Given the lack of information on the derivation of this value or its uncertainty, sensitivity cases are specified to span one order of magnitude across the base case.

2.18.10.5 Temperature, Pressure and Humidity

No sensitivity cases to ambient temperature, pressure or relative humidity are specified for the EEC trials, given the small fluctuations and uncertainties in the data.

2.18.10.6 Material Properties

The EEC trials released liquefied propane. Models that include propane in their species database should use the built-in properties in their simulations; models that do not include propane should use the thermophysical properties listed in the accompanying spreadsheet. No sensitivity cases are specified.

2.18.10.7 Summary of Sensitivity Cases

Based on the discussion above, the model validation efforts should include the sensitivity cases listed in Table 2.18-3. If one or more sensitivity cases cannot be run, for example, due to hard-coding of certain parameters in a model, an explanation should be provided in the model questionnaire.

Table 2.18-3. Base case and sensitivity cases for the Lathen (EEC) test series.

Parameter	Case	EEC 07	EEC 08	EEC 17	EEC 18
Source term	Base	Flashing jet, no rainout	Flashing jet, no rainout	Flashing jet, no rainout	Flashing jet, no rainout
Release Rate	Base	2.9 kg/s	2.9 kg/s	2.9 kg/s	2.9 kg/s
Release Duration[10]	Base	90 s	120 s	90 s	120 s
Wind Speed	Base	4.3 m/s @ 3.3 m	4.4 m/s @ 6 m	3.9 m/s @ 3.3 m	4.4 m/s @ 3.3 m
Surface Roughness Length	Base	0.006 m	0.006 m	0.006 m	0.006 m
	R1	0.001 m	0.001 m	0.001 m	0.001 m
	R2	0.01 m	0.01 m	0.01 m	0.01 m
Atmospheric Stability	Base	D	C	D	D
	A1	-	D	-	-
Ambient Temperature	Base	12.0°C	15.0°C	15.0°C	16.0°C
Ambient Pressure	Base	1 atm	1 atm	1 atm	1 atm
Relative Humidity	Base	72%	37%	55%	60%
Stream Composition	Base	Propane = 100%	Propane = 100%	Propane = 100%	Propane = 100%

[10] Until barrier removal, where applicable

2.19 Maplin Sands

Experimental campaign	Maplin Sands (MS)
Test dates:	1980
Test location:	Maplin Sands, England
Number of tests:	34
Tests performed by:	Shell Research Ltd.
Brief description:	LNG and LPG spills onto water; unobstructed vapor cloud dispersion over water.
References:	Stewart et al., 2016 [25] Colebrander and Puttock, 1984 [65] Puttock et al., 1982 [66] Ermak et al., 1989 [33]
Data confidentiality:	Open (based on publicly available data)
Model validation category	
Material:	Non-Toxic
Release Type:	Spill
Dispersion Area:	Unobstructed
Test series rating	
Overall:	**0**
Relevance:	0
Material:	
Scale:	
Repeatability:	
Data Quality/Availability:	
Included in MVD:	**No**

2.19.1 Description

The Maplin Sands test series consisted of 34 spills of liquefied gases (LNG and LPG) onto water; they were conducted at the Maplin Sands site, an area of tidal sands in the estuary of the river Thames. The vapor clouds produced by the evaporation of the liquid spills were tracked as they dispersed over water; Figure 2.19-1 shows a schematic of the spill area and measurement arcs. Both continuous and instantaneous releases were carried out.

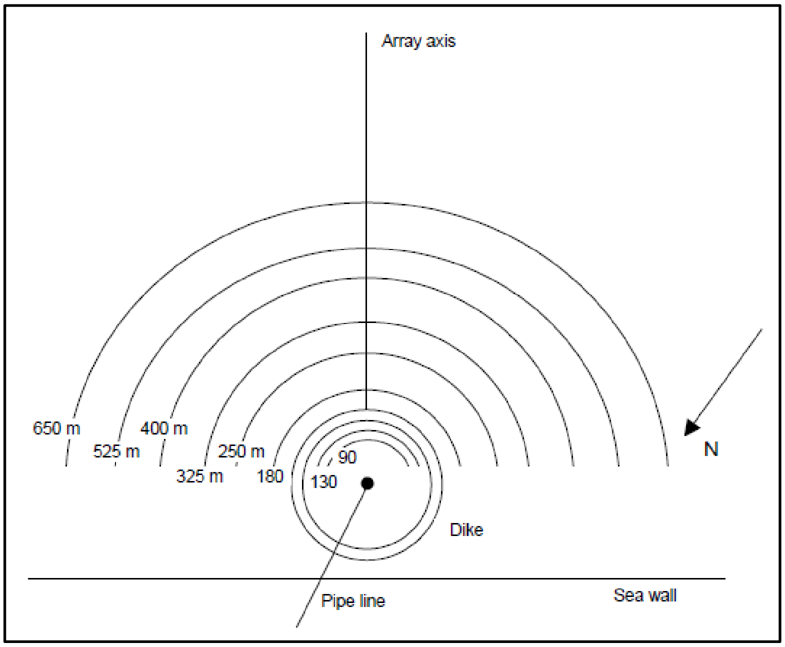

Figure 2.19-1. Maplin Sands spill area and measurement arcs [25].

2.19.2 Test Series Grouping and Rating

The Maplin Sands trials considered for this MVD consisted of spills of LNG onto the water surface. The resulting clouds dispersed over open water, with no obstructions. The test series therefore fits in the following categories:

- Material: Non-Toxic
- Release Type: Spill
- Dispersion Area: Unobstructed

LNG is not toxic, and the peak concentrations measured are above 1% at all measurement arcs. Therefore, the Maplin Sands trials included in the MVD are not relevant to the purpose of this database ("Relevance" rating = 0). The Maplin Sands test series is not included in the toxic dispersion MVD.

2.20 Mock Urban Setting Test (MUST)

Experimental campaign	Mock Urban Setting Test (MUST)
Test dates:	September 2001
Test location:	Dugway Proving Ground
Number of tests:	68
Tests performed by:	Defense Threat Reduction Agency (DTRA)
Brief description:	Pressurized propylene released from a continuous point source or a series of puffs. Vapor cloud dispersed through shipping containers designed to mimic an urban landscape. Propylene concentrations and temperatures measured throughout the urban landscape.
References:	Biltoft, 2001 [67] Yee and Biltoft, 2004 [68]
Data confidentiality:	Open (based on publicly available data)
Model validation category **Material:** **Release Type:** **Dispersion Area:**	 Non-Toxic Gas Jet Complex Geometry
Test series rating **Overall:** **Relevance:** **Material:** **Scale:** **Repeatability:** **Data Quality/Availability:**	 **3.4** 4 2 5 2 4
Included in MVD:	**Yes**

2.20.1 Description

The Mock Urban Setting Test (MUST) was conducted at the U.S. Army Dugway Proving Ground (DPG) Horizontal Grid test site in September 2001. The stated objective was to "acquire meteorological and dispersion data sets at near full-scale for use in urban dispersion model development and validation" [67]. The MUST design consisted of a regular 12 by 10 array of conex shipping containers intended to produce urban-scale roughness over a 200 m^2 area.

Pressurized gaseous propylene (C_3H_6) was released at flow rates between approximately 150 and 225 L/min (i.e., as a tracer gas) from a nozzle pointed horizontally at a height between 0.15 and 2.7 m above ground. The release duration varied between approximately 4 and 133 minutes. The tracer gas dispersion was measured using fast-response photoionization detectors (PIDs), placed at multiple locations throughout the array. A total of 68 trials (63 continuous releases and 5 multiple puff releases) were performed.

2.20.2 Test Series Grouping and Rating

The MUST trials consisted of numerous tracer gas releases of propylene, dispersing through an array of shipping containers intended to approximate the effect of dispersion through an urban area. The test series therefore fits in the following categories:

- Material: Non-Toxic
- Release Type: Tracer
- Dispersion Area: Complex Geometry

Tracer gas releases of toxic streams are not frequently included in LNG facility siting studies; however, the dispersion of gas through a complex geometry is a scenario of particular interest for model validation purposes, given the relative scarcity of such data ("Relevance" rating = 4). Propylene is not a material found in LNG facilities ("Material" rating = 2). The dimensions of the test area and the measured concentrations are consistent with typical toxic dispersion studies ("Scale" rating = 5).

In every field scale test series, replicating the same test conditions (including weather) is extremely difficult, therefore, the repeatability of field scale experiments is inherently limited ("Repeatability" rating = 2).

The MUST trials included numerous high-frequency (10-50 Hz) concentration measurement instruments. The data is available from the MDA database. The overall quality and availability of data is considered more than acceptable ("Data quality/availability rating = 4).

Overall, the MUST series is rated at 3.4, which exceeds the "acceptable" threshold; therefore, the MUST test series is considered suitable for inclusion in the toxic dispersion MVD.

2.20.3 Ambient Conditions

A wide variety of weather instrumentation was used to document the ambient conditions during the MUST trials. These included tethersonde flights to measure wind and thermodynamic profiles up to several hundred meters above ground, and sonic anemometers and thermometers to provide temperature, wind, and turbulence profiles both upwind, downwind and within the conex array. Solar and terrestrial radiation were also measured.

Six Portable Weather Information and Display System (PWIDS) stations, consisting of a tripod-mounted propeller-vane wind monitor and a temperature/humidity sensor (at 2 m) were positioned around the test grid at distances of several kilometers from the release area, to characterize the undisturbed temperature, humidity, and flow fields around the MUST site. The sampling rate for the PWIDS was 1 Hz and the data was averaged over 15-minute intervals.

2.20.4 Discharge System

The propylene release system consisted of three cylinders manifolded together and connected to a mass flow controller. The mass flow controller released a controlled flow of propylene to a PVC pipe with a diameter of 5 cm, as shown in Figure 2.20-1.

Six different tracer release position types were used: (A) 1 m upwind of a conex face; (B) centered in the narrow alley between conex container ends; (C) centered in the intersection between four conexes; (D) on a conex roof; (E) upwind of (outside) the array; and (F) on the road between conex long sides.

In any given trial, the discharge pipe could be oriented horizontally while positioned on a 15 cm tall wire wheel, as shown in the picture: this configuration was used for releases at ground level or on top of a container. In some trials, the pipe was mounted vertically on a tripod.

Figure 2.20-1. MUST propylene dissemination pipe [67].

The continuous release scenarios used flow rates ranging from 150 to 225 L/min; the release rates were controlled to within +/-2%.

2.20.5 Dispersion Area

The test site is mostly flat with sparse brush vegetation and a few sand dunes (4-6 m tall) approximately 1 km north of the test grid. The surface roughness length – outside of the conex array – was estimated to be 2-4 cm [67].

The MUST trials included an urban dispersion area of approximately 200 m^2 formed by an array of 12 x 10 conex containers, each measuring approximately 12.2 m long, 2.42 m wide and 2.54 m tall. The location of the MUST array is shown graphically in Figure 2.20-2 and the conex positions are shown in Figure 2.20-3. It should be noted that the container spacing was not exactly regular due to testbed constraints; the actual coordinates and alignment angles (yaw and tilt) of each container are listed, for each trial, in the accompanying spreadsheet.

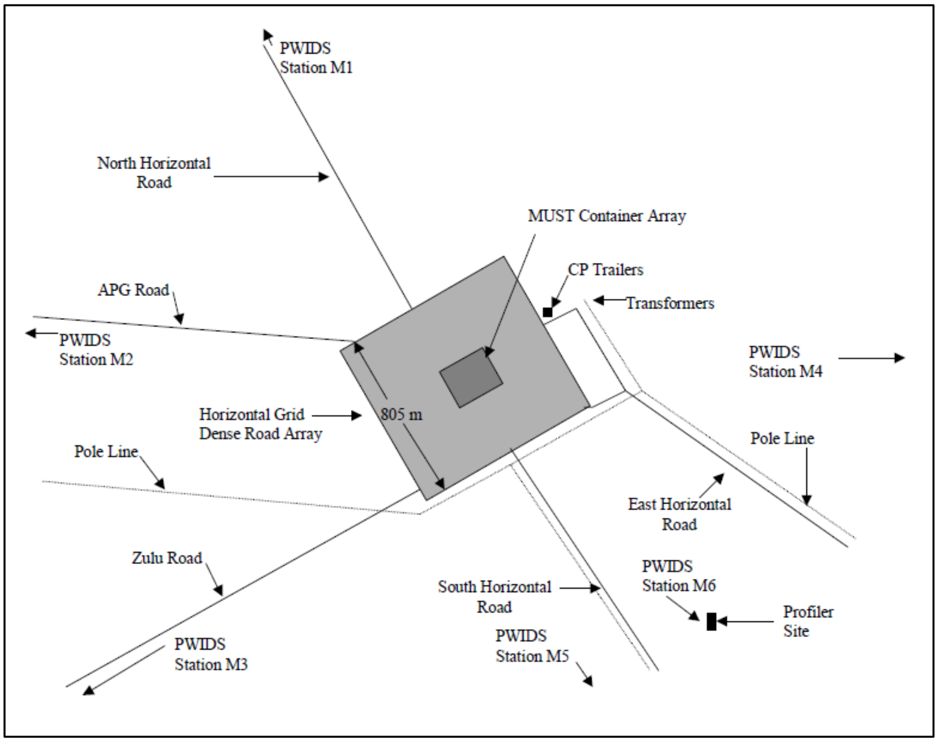

Figure 2.20-2. Layout of the MUST container array and surrounding area [67].

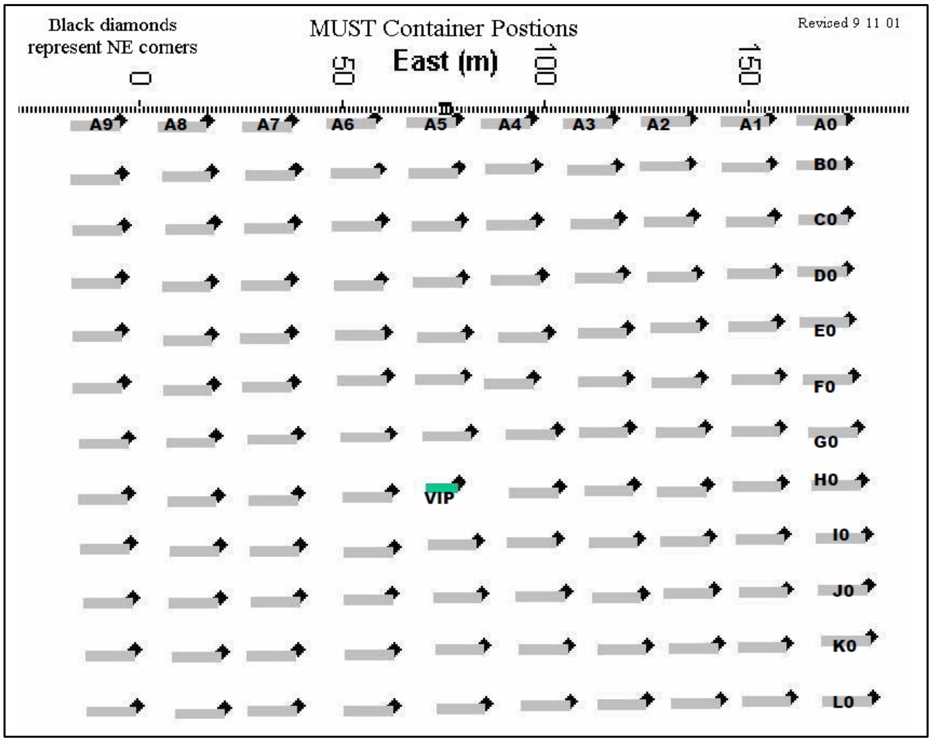

Figure 2.20-3. MUST conex positions [67].

2.20.6 Instrumentation

A total of 74 high-speed digital photoionization detectors (PIDs) and ultraviolet ion collectors (UVIC) was used to measure the propylene concentration during the MUST trials. The placement of the concentration sensors in relation to the containers is depicted in Figure 2.20-4. The coordinates of each instrument, during each trial, are provided in the accompanying spreadsheet.

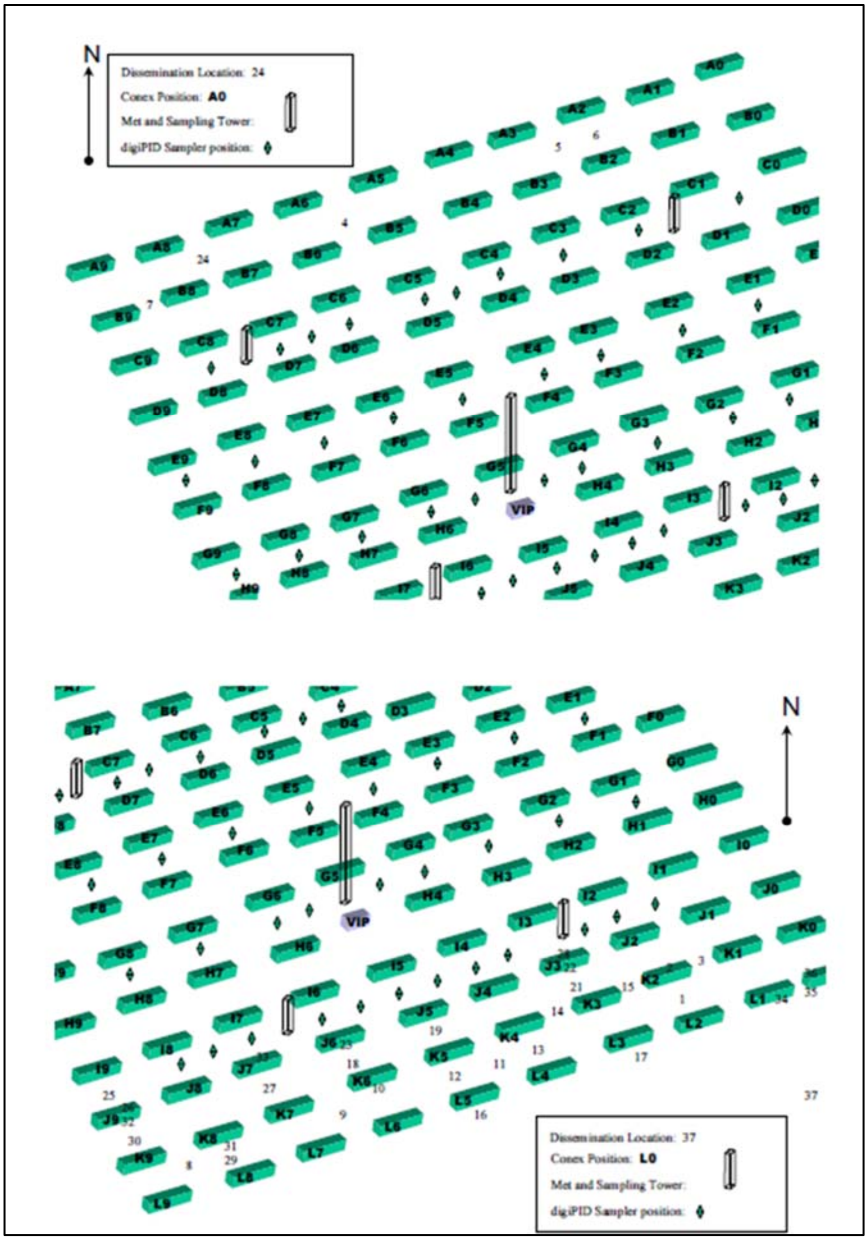

Figure 2.20-4. Instrumentation Location

A total of 48 DPIDs were placed on the 32 m towers and on stands at 1.6 m above ground, along 4 sampling lines. A total of 26 UVICs were placed throughout the conex array: 6 were mounted on each of four 6 m tall towers throughout the array; one was placed in the wake of a container and one was placed near a PID for instrument comparison. The detectors were calibrated together.

The use of PIDs was considered optimal for large downwind sampling distances, because gas molar concentrations at those distances were expected to range from 0.5 to 500 ppm, well within the PID calibrated operating range of 0.04 to 1000 ppm [67]. The UVICs were calibrated over a range of 0.01 to 1000 ppm. Both sets of instruments were sampled at 50 Hz.

2.20.7 Experimental Uncertainty

No information was found in the available references regarding the uncertainty of the gas concentration measurement. Therefore, an overall experimental uncertainty of 20% is specified in the accompanying spreadsheet.

2.20.8 Test Series Observations and Comments

The MUST test series is in the MDA database, including information regarding the discharge, ambient conditions and instrumentation layout. Only a subset of the MUST trials is included in this MVD, selected among the 21 trials evaluated by Yee and Biltoft [68]. A summary of the release parameters is provided in Table 2.20-1. A more complete set of data for each test is included in the model validation spreadsheet.

Table 2.20-1. MUST test parameters

Trial Sequence No.	Trial Name	Location	Position	Height [m]	Duration [min]	Rate [L/min]
MUST-4	2671934	25	F	1.8	15	200
MUST-5	2672033	27	F	1.8	15	200
MUST-15	2682320	26	D	2.7	15	225
MUST-19	2692157	36	D	2.7	15	225
MUST-20	2692223	34	A	1.3	15	225
MUST-21	2692250	37	E	1.3	17	225

2.20.9 Time Averaging

Data acquisition during each trial was performed at a frequency of 50 Hz for the dispersion stations. For consistency with most other datasets included in this MVD, the short time averaging was set to 1 s by applying a 1-s running average to the raw data. Given the very long release duration, aimed at obtaining near-steady concentration measurements, the long time averaging data was obtained by applying a running average with a window of 300 seconds instead of the full release duration (typically greater than 10 minutes). The short and long averaging times for the MUST trials included in this MVD are listed in Table 2.20-1.

Table 2.20-2. Time averaging for the MUST trials.

Trial	Short time avg.	Long time avg.
MUST-4	1 s	300 s
MUST-5	1 s	300 s
MUST-15	1 s	300 s
MUST-19	1 s	300 s
MUST-20	1 s	300 s
MUST-21	1 s	300 s

2.20.10 Test Series Sensitivities

Even though the MUST trials are included in the MDA database, only limited cases of model comparison to these trials are available in the literature – namely, Hanna et al. compared the CFD model FLACS to the field test data [12], and a multi-model comparison was performed against wind-tunnel scale trials that replicated the MUST setup, as part of the COST Action 732 project [69]. However, neither modeling effort included sensitivity cases to model input parameters. Therefore, the following sensitivity cases are based on a review of available data.

2.20.10.1 Source Term

The source term consisted of a metered release of gaseous propylene through a high-accuracy meter. Therefore, no sensitivity cases to the source term are specified.

2.20.10.2 Wind Speed

No sensitivity cases are specified to wind speed, given the small fluctuations and uncertainties in the data.

2.20.10.3 Atmospheric Stability

The base cases for atmospheric stability were set according to the Monin-Obukhov lengths calculated by Yee and Biltoft. Sensitivity cases for atmospheric stability were specified, where the ambient conditions (wind speed, cloud cover, etc.) produced uncertainty in the representative Pasquill-Gifford class.

2.20.10.4 Roughness Length

The surface roughness length outside of the conex area was estimated by Biltoft as 0.02-0.04 m; a later paper by Yee and Biltoft [68] listed the roughness length as 0.045 ± 0.005 m. The base case is therefore set to 4 cm. Given the strong effect of the containers on the wind profile, the surface roughness length of the site is not expected to have a significant effect on the gas dispersion; nonetheless, a sensitivity case is specified to a smaller surface roughness (1 cm).

2.20.10.5 Temperature, Pressure and Humidity

No sensitivity cases to ambient temperature, pressure or relative humidity are specified for the MUST trials, given the small fluctuations and uncertainties in the data.

2.20.10.6 Material Properties

The MUST trials released gaseous propylene. Models that include propylene in their species database should use the built-in properties in their simulations; models that do not include propylene should use the thermophysical properties listed in the accompanying spreadsheet. No sensitivity cases are specified.

2.20.10.7 Summary of Sensitivity Cases

Based on the discussion above, the model validation efforts should include the sensitivity cases listed in Table 2.20-3 and Table 2.20-4. If one or more sensitivity cases cannot be run, for example, due to hard-coding of certain parameters in a model, an explanation should be provided in the model questionnaire.

Table 2.20-3. Base case and sensitivity cases for the MUST test series (1/2).

Parameter	Case	MUST-4	MUST-5	MUST-15
Source term	Base	Tracer gas	Tracer gas	Tracer gas
Release Rate	Base	5.92 g/s	5.92 g/s	6.66 g/s
Release Duration	Base	900 s	900 s	900 s
Wind Speed (at 4 m height)	Base	1.63 m/s	2.69 m/s	4.55 m/s
Surface Roughness Length	Base	0.04 m	0.04 m	0.04 m
	R1	0.01 m	0.01 m	0.01 m
Atmospheric Stability	Base	F	F	F
	A1	-	-	E
Ambient Temperature	Base	29.29 C	29.53 C	26.74 C
Ambient Pressure	Base	1 atm	1 atm	1 atm
Relative Humidity	Base	N/A	N/A	N/A
Stream Composition	Base	Propylene = 100%	Propylene = 100%	Propylene = 100%

Table 2.20-4. Base case and sensitivity cases for the MUST test series (2/2).

Parameter	Case	MUST-19	MUST-20	MUST-21
Source term	Base	Tracer gas	Tracer gas	Tracer gas
Release Rate	Base	6.66 g/s	6.66 g/s	6.66 g/s
Release Duration	Base	900 s	900 s	900 s
Wind Speed	Base	2.98 m/s	2.63 m/s	3.38 m/s
Surface Roughness Length	Base	0.04 m	0.04 m	0.04 m
	R1	0.01 m	0.01 m	0.01 m
Atmospheric Stability	Base	F	F	F
	A1	E	E	E
Ambient Temperature	Base	23.44 C	23.81 C	23.32 C
Ambient Pressure	Base	1 atm	1 atm	1 atm
Relative Humidity	Base	N/A	N/A	N/A
Stream Composition	Base	Propylene = 100%	Propylene = 100%	Propylene = 100%

2.21 Porton

Experimental campaign	Porton (HF)
Test dates:	August 2000
Test location:	Porton, England
Number of tests:	12
Tests performed by:	Risø National Laboratory
Brief description:	Pressurized jet releases of anhydrous hydrogen fluoride, dispersing over sloped terrain, under a wide range of ambient conditions. Designed to evaluate the influence of HF thermodynamics on cloud dispersion.
References:	Ott and Jørgensen, 2001 [70] Trégourès et al., 2001 [71]
Data confidentiality:	Open (based on publicly available data)
Model validation category	
Material:	Toxic
Release Type:	Flashing jet
Dispersion Area:	Unobstructed
Test series rating	
Overall:	**3.0**
Relevance:	4
Material:	2
Scale:	4
Repeatability:	3
Data Quality/Availability:	3
Included in MVD:	**No**

2.21.1 Description

The Porton (HF) test series consists of 12 anhydrous hydrogen fluoride releases designed to evaluate potential buoyancy effects due to HF thermodynamics on the dispersion of the vapor cloud – particularly, enhanced mixing and/or cloud liftoff. HF was released for 3 minutes, at rates of approximately 0.1 kg/s. The cloud dispersed over unobstructed but slightly sloped terrain, with low vegetation. HF concentration measurements were performed at distances up to 2 km from the source.

2.21.2 Test Series Grouping and Rating

The Porton test series involved the release of anhydrous hydrogen fluoride (HF), liquefied under pressure and discharged downwind through a small orifice. The resulting cloud dispersed over unobstructed but slightly sloped terrain. The test series therefore fits in the following categories:

- Material: Toxic
- Release Type: Flashing Jet
- Dispersion Area: Unobstructed

The release of pressurized liquids through orifices, with dispersion affected by terrain features is a very common scenario for siting studies, therefore, the HF trials are relevant to the purpose of this MVD ("Relevance" rating = 4). However, HF is not a material found in LNG facilities; additionally, HF presents peculiar thermodynamic properties that are not representative of any other fluid typically found in LNG facilities ("Material" rating = 2). The release flow rates are smaller than typical siting scenarios, but the measured concentrations are within the range of interest for toxic dispersion ("Scale" rating = 4).

In every field scale test series, replicating the same test conditions (including the weather) is extremely difficult, therefore, the repeatability of field scale experiments is inherently limited ("Repeatability" rating = 2). No information is available to determine the accuracy of most of the instrumentation. The REDIPHEM database includes data for each measurement sensor, reported at 1 s intervals. Therefore, the overall quality and availability of the data, for the purpose of this MVD is considered acceptable ("Data quality/availability" rating = 3).

Overall, the HF test series is rated at 3.0, which meets the "acceptable" threshold. Given the availability of higher rated test series that fit the same categories, the Porton trials are not included in the toxic dispersion MVD.

2.22 Prairie Grass

Experimental campaign	Prairie Grass (PG)
Test dates:	July-August 1956
Test location:	O'Neill, Nebraska
Number of tests:	70
Tests performed by:	Air Force Cambridge Research Center
Brief description:	Neutrally buoyant, horizontal tracer releases of sulphur dioxide dispersing over flat terrain.
References:	Barad, 1958 [72], [73] Haugen, 1959 [74] Hanna et al., 2004 [12] Mazzoldi et al., 2008 [75]
Data confidentiality:	Open (based on publicly available data)
Model validation category	
Material:	Toxic
Release Type:	Tracer
Dispersion Area:	Unobstructed
Test series rating	
Overall:	**3.6**
Relevance:	5
Material:	2
Scale:	5
Repeatability:	2
Data Quality/Availability:	4
Included in MVD:	**Yes**

2.22.1 Description

The Prairie Grass test series consisted of 70 tracer gas releases of sulphur dioxide (SO_2) dispersing over flat terrain. The purpose of the series was to "determine the rate of diffusion of a tracer gas as a function of meteorological conditions" [72]. SO_2 was released horizontally at 0.46 m above ground level (1.5 m in a few of the trials), at flow rates of approximately 0.1 kg/s for 10 minutes; gas concentration measurements were performed at five arcs, 50, 100, 200, 400, and 800 m downwind of the release, at an elevation of 1.5 m above ground.

2.22.2 Test Series Grouping and Rating

The Prairie Grass (PG) test series involved tracer gas releases of sulphur dioxide at small rates (no more than 0.1 kg/s) from a horizontal tube close to the ground. The resulting cloud dispersed over flat terrain. The test series therefore fits in the following categories:

- Material: Toxic
- Release Type: Tracer
- Dispersion Area: Unobstructed

Tracer releases of toxic streams are not frequently included in LNG facility siting studies ("Relevance" rating = 2). Sulphur dioxide is a material sometimes considered as a toxic hazard in these studies ("Material" rating = 5). The dimensions of the test area and the measured concentrations are consistent with typical dispersion studies ("Scale" rating = 5).

In every field scale test series, replicating the same test conditions (including the weather) is extremely difficult, therefore, the repeatability of field scale experiments is inherently limited ("Repeatability" rating = 2).

Measurements were performed at four different downwind locations, and each location included several sensors distributed crosswind and at different elevations. Data from each sensor is available from the MDA database; the overall quality and availability of data is considered more than acceptable ("Data availability" rating = 4).

Overall, the PG series is rated at 3.6, which exceeds the "acceptable" threshold; therefore, the PG series is considered suitable for inclusion in the toxic dispersion MVD. This conclusion is consistent with the inclusion of the PG series in the Modeler's Data Archive [21] as well as in model developers' internal validation efforts [12], [42], [63], [75].

2.22.3 Ambient Conditions

Wind speed and direction were measured by cup anemometers at two different locations: one was located 25 m west of the release location and the other 450 m North and 30 m West of the source. Both instruments were 2 m above the ground. Data was sampled from 10 minutes before to 10 minutes after the release, and averaged over the entire sampling period.

2.22.4 Discharge System

Sulfur dioxide was stored as liquid in a tank and vaporized before passing through a pressure regulator and an adjustable valve before being discharged horizontally from a 2-inch diameter pipe at 0.46 m above ground (in six of the trials, the release height was adjusted to 1.5 m). Figure 2.22-1 shows a schematic of the SO_2 generator. The release rate was set to no more than 0.1 kg/s and was observed to vary no more than 5-10% during each trial.

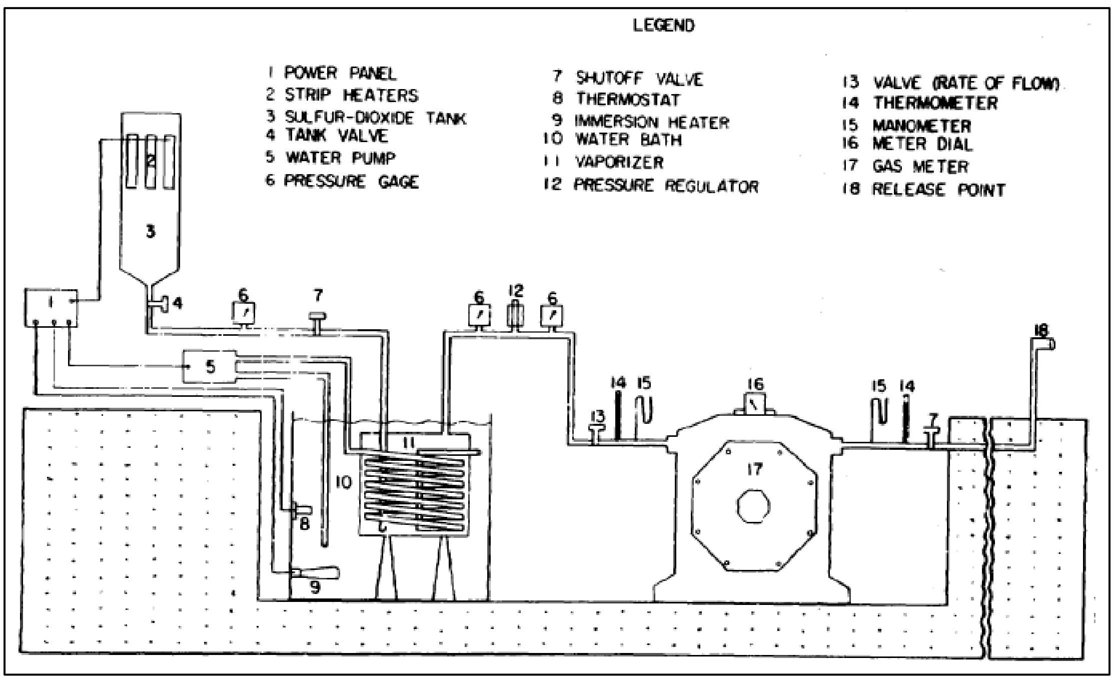

Figure 2.22-1. Schematic of the Prairie Grass dissemination system [60].

2.22.5 Dispersion Area

The terrain at the test site was mostly flat with a slight rise towards the southeast, as shown in Figure 2.17-2. The terrain was covered with grass, which was mowed prior to the experiments and remained low and uniform throughout the test series. No buildings were located within 300 m of the release location, and the dissemination equipment was placed in a dugout upwind of the source.

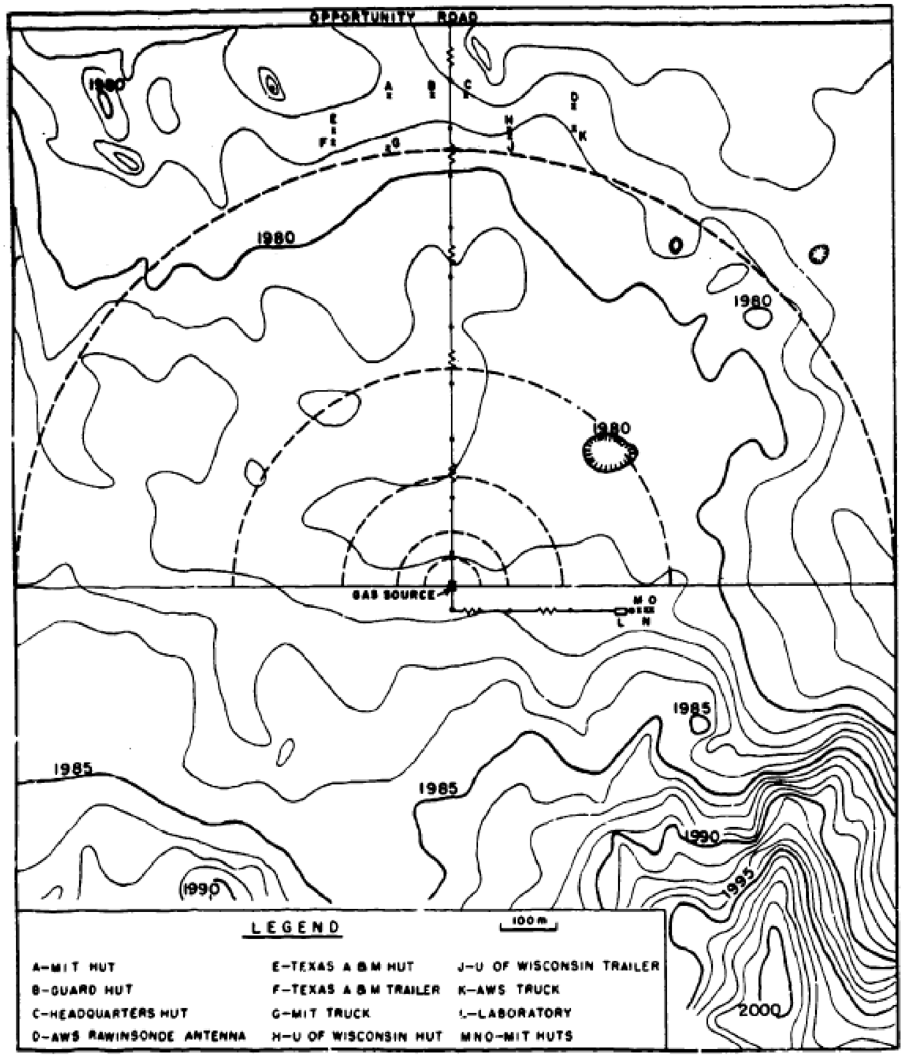

Figure 2.22-2. Schematic of the Prairie Grass dispersion area [60].

2.22.6 Instrumentation

The gas concentration measurements were performed along five arcs at 50, 100, 200, 400 and 800 m from the release; each arc formed a semicircle centered on the release location, spanning from 90 to 270 degrees relative to North. Most measurements were performed at a height of 1.5 m above ground, with six lightweight metal towers positioned along the 100 m arc to measure samples at nine heights (0.5, 1.0, 1.5, 2.5, 4.5, 7.5, 10.5, 13.5, and 17.5 m). The receptor spacing was every two-degrees on the inner four arcs, and every one-degree on the outer 800m arc.

The instrumentation for gas concentration measurements consisted of midget impingers; each impinger contained 10 ml of hydrogen peroxide solution, so that sulfuric acid would be formed as air with sulfur dioxide was drawn into the impinger. Therefore, the impingers measured the cumulative amount of SO_2 at their respective locations over the 10-minute sampling time. As such, no time traces of tracer gas concentration are available, but only long time averaged values.

It should also be noted that the gas concentration measurements reported for the PG trials are in mg/m^3; for consistency with other trial data and most model outputs, the values listed in the accompanying spreadsheet were converted to volumetric concentrations (m^3/m^3) using the SO_2 density at ambient conditions.

2.22.7 Experimental Uncertainty

No information was found in the available references regarding the uncertainty of the gas concentration measurement. Therefore, an overall experimental uncertainty of 20% is specified in the accompanying spreadsheet.

2.22.8 Test Series Observations and Comments

The MDA database includes data from 66 Prairie Grass trials. Only a subset of 5 PG trials is included in this MVD, to limit the total number of trials in the database: each of the selected trials reported a peak SO_2 concentration above 200 ppm at the nearest arc and above 2 ppm at the farthest arc. A summary of the test parameters is provided in Table 2.22-1. A more complete set of data for each test is included in the model validation spreadsheet.

Table 2.22-1. Prairie Grass test parameters

Test No.	Spill Rate [g/s]	Release Duration [min]	Wind Speed [m/s]	Ambient Temperature [C]
PG-17	56.5	10	3.3	27.4
PG-32	41.4	10	2.2	22.9
PG-36	40.0	10	1.9	18.9
PG-53	45.2	10	2.3	17.4
PG-66	43.1	10	3.3	20.2

2.22.9 Time Averaging

The PG gas concentration measurements were obtained from impingers that sampled the SO_2 concentration over a period of 10 minutes. Given the concentration measurement method, short-time averaging is not possible; the long averaging times are equal to the instrument sampling period, as listed in Table 2.22-2.

Table 2.22-2. Time averaging for the Prairie Grass trials.

Trial	Short time avg.	Long time avg.
PG-17	N/A	600 s
PG-32	N/A	600 s
PG-36	N/A	600 s
PG-53	N/A	600 s
PG-66	N/A	600 s

2.22.10 Test Series Sensitivities

No sensitivity cases to model input parameters were found in publicly available comparisons of model predictions to the PG trial data [12], [75]. Therefore, the following sensitivity cases are based on a review of available data.

2.22.10.1 Source Term

The source term consisted of a metered release of gaseous SO_2. Therefore, no sensitivity cases to the source term are specified.

2.22.10.2 Wind Speed

No sensitivity cases are specified to wind speed given the lack of data on potential wind fluctuations.

2.22.10.3 Atmospheric Stability

The atmospheric stability was not included among the Prairie Grass data or listed in the reports; therefore, the base case was determined based on available information. Sensitivity cases were also specified for each trial, given the uncertainty on the representative Pasquill-Gifford class.

2.22.10.4 Roughness Length

The surface roughness length for the PG trials was reported as 0.006 m [49]. Given the lack of information on the surface roughness in the original test series reports, sensitivity cases spanning an order of magnitude around the reference value are specified for this MVD.

2.22.10.5 Temperature, Pressure and Humidity

No sensitivity cases to ambient temperature, pressure or relative humidity are specified for the PG trials, given the lack of data on potential fluctuations.

2.22.10.6 Material Properties

The PG trials released gaseous SO_2. Models that include SO_2 in their species database should use the built-in properties in their simulations; models that do not include SO_2 should use the thermophysical properties listed in the accompanying spreadsheet. No sensitivity cases are specified.

2.22.10.7 Summary of Sensitivity Cases

Based on the discussion above, the model validation efforts should include the sensitivity cases listed in Table 2.22-3 and Table 2.22-4. If one or more sensitivity cases cannot be run, for example, due to hard-coding of certain parameters in a model, an explanation should be provided in the model questionnaire.

Table 2.22-3. Base case and sensitivity cases for the PG test series (1/2).

Parameter	Case	PG-17	PG-32	PG-36
Source term	Base	Tracer gas release	Tracer gas release	Tracer gas release
Release Rate	Base	56.5 g/s	41.4 g/s	40.0 g/s
Release Duration	Base	600 s	600 s	600 s
Wind Speed (at 2 m height)	Base	3.33 m/s	2.21 m/s	1.86 m/s
Surface Roughness Length	Base	0.006 m	0.006 m	0.006 m
	R1	0.001 m	0.001 m	0.001 m
	R2	0.01 m	0.01 m	0.01 m
Atmospheric Stability	Base	E	F	F
	A1	D	E	E
Ambient Temperature	Base	27.44 C	22.93 C	18.94 C
Ambient Pressure	Base	1 atm	1 atm	1 atm
Relative Humidity	Base	N/A	N/A	N/A
Stream Composition	Base	SO_2 = 100%	SO_2 = 100%	SO_2 = 100%

Table 2.22-4. Base case and sensitivity cases for the PG test series (2/2).

Parameter	Case	PG-53	PG-66
Source term	Base	Tracer gas release	Tracer gas release
Release Rate	Base	45.2 g/s	43.1 g/s
Release Duration	Base	600 s	600 s
Wind Speed	Base	2.28 m/s	3.33 m/s
Surface Roughness Length	Base	0.006 m	0.006 m
	R1	0.001 m	0.001 m
	R2	0.01 m	0.01 m
Atmospheric Stability	Base	F	E
	A1	E	D
Ambient Temperature	Base	17.39 C	20.19 C
Ambient Pressure	Base	1 atm	1 atm
Relative Humidity	Base	N/A	N/A
Stream Composition	Base	SO_2 = 100%	SO_2 = 100%

2.23 Thorney Island

Experimental campaign	Thorney Island (TI)
Test dates:	1984
Test location:	Thorney Island, UK
Number of tests:	26
Tests performed by:	UK Health and Safety Executive and National Maritime Institute
Brief description:	Low momentum releases of Freon 12/nitrogen mixture.
References:	Stewart et al., 2016 [25] McQuaid and Roebuck [1] McQuaid [2]
Data confidentiality:	Open (based on publicly available data)
Model validation category **Material:** **Release Type:** **Dispersion Area:**	 Non-Toxic Low momentum gas Unobstructed
Test series rating **Overall:** **Relevance:** **Material:** **Scale:** **Repeatability:** **Data Quality/Availability:**	 **2.6** 3 1 4 2 3
Included in MVD:	**Yes**

2.23.1 Description

The Thorney Island test series took place at a former Royal Air Force station at Thorney Island, in the United Kingdom. The tests consisted of low-momentum releases of a Freon 12/Nitrogen mixture. The vapor clouds dispersed over mostly flat terrain. Figure 2.23-1 shows a schematic of the release area and measurement array.

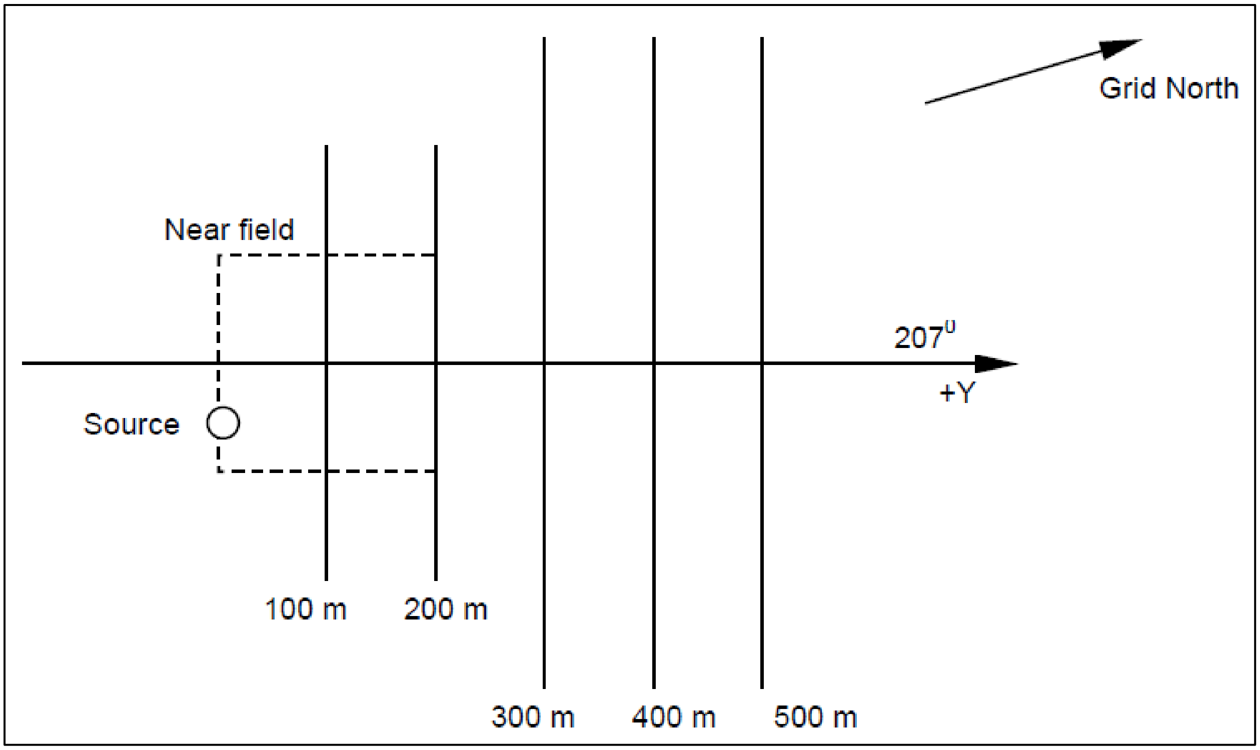

Figure 2.23-1. Thorney Island release area and measurement array [25].

2.23.2 Test Series Grouping and Rating

The Thorney Island trials consisted of releases of a mixture of Freon 12 and nitrogen. In some of the trials, the gas mixture was held at atmospheric pressure and temperature in a tall cylindrical container, whose side walls were suddenly released, allowing the dense gas to slump to the ground and disperse. In other trials, the mixture was introduced upwards from the ground and impinged onto the bottom side of a horizontal plate, thus spreading radially. In both cases, the gas cloud then dispersed over flat terrain, with no obstructions. The test series therefore fits in the following categories:

- Material: Non-Toxic
- Release Type: Low momentum
- Dispersion Area: Unobstructed

The dispersion of low-momentum dense clouds is a frequently modeled scenario, albeit from different source configurations than those tested at Thorney Island ("Relevance" rating = 3). Mixtures of Freon 12 and nitrogen are not toxic and not used in LNG facilities ("Material" rating = 1). The dimensions of the cloud as well as the dispersion measurement area are consistent with typical studies ("Scale" rating = 4).

In every field scale test series, replicating the same test conditions (including the weather) is extremely difficult, therefore, the repeatability of field scale experiments is inherently limited ("Repeatability" rating = 2). The overall quality and availability of data from the Thorney Island trials is considered acceptable for the purpose of this MVD ("Data quality/availability" rating = 3).

Overall, the Thorney Island series is rated at 2.6, which is below the "acceptable" threshold. However, given the limited availability of test data on low-momentum releases with multiple gas concentration measurements below 1%, the Thorney Island trials are included in the toxic dispersion MVD.

2.23.3 Test Series Observations and Comments

Two trials from the Thorney Island test series were included in the LNG spills database; the same trials are included in the current MVD, to provide continuity for models previously evaluated against that database. Table 2.23-1 lists the main test parameters for the trials included in the toxic dispersion MVD. A more complete set of data for each test is included in the model validation spreadsheet; the data included in the spreadsheet was obtained from the LNG spills database. Additional information on these trials can be found in the references listed in the summary table for the Thorney Island test series.

Table 2.23-1. Thorney Island test parameters.

Test No.	Spill Rate [kg/s]	Spill Duration [s]	Wind Speed [m/s]	Atm. Stability Class
TI-45	10.7	455	2.3	E-F
TI-47	10.2	465	1.5	F

The thermodynamic properties of the Freon-12/nitrogen mixture most frequently needed for dispersion modeling are included in the MVD spreadsheet for each trial. These should be used in models which do not have a species database, or do not include the released materials.

2.23.4 Time Averaging

The LNG spills database includes Thorney Island data based on 30-second running averages. Therefore, the only time averaging included for these trials is set to 30 s, as summarized in Table 2.23-2.

Table 2.23-2. Time averaging for the Thorney Island trials.

Trial	Long time avg.
TI-45	30 s
TI-47	30 s

2.23.5 Test Series Sensitivities

The boundary conditions and source data for the base case is the same as in the LNG spill database [25]. The sensitivity cases are specified based on a review of the test series references and the DEGADIS model evaluation report by FERC [20].

2.23.5.1 Source Term

The Thorney Island trials involved the release of gas and the release rate uncertainty was estimated to be 2% [76]. Therefore, no sensitivity to the source term is required.

2.23.5.2 Wind Speed

The wind speed data during the Thorney Island trials in the MVD did not present sufficient uncertainty or variability to warrant sensitivity analysis [20]. It should however be noted that McQuaid reported an approximately 20% decrease in wind speed as well as a noticeable swing in wind direction during TI-47, which may have caused a larger lateral spread of the cloud.

2.23.5.3 Atmospheric Stability

For both trials included in the MVD, FERC performed sensitivity studies to atmospheric stability varying between E (moderately stable) and F (stable) [20]. For consistency, the same sensitivity cases are specified in this MVD.

2.23.5.4 Roughness Length

The Thorney Island trials were conducted on an abandoned airfield and a surface roughness of 0.01 m was specified in the MDA [4]. Other studies estimated surface roughness lengths between 0.001 m and 0.025 m. Given the wide uncertainty associated with this parameter and the significant impact it can have on gas dispersion, sensitivity cases are specified with an upper bound of 0.03 m and a lower bound of 0.001 m; the base case is 0.01 m, as specified in the MDA.

2.23.5.5 Temperature, Pressure and Humidity

No sensitivity cases to ambient temperature, pressure or relative humidity are specified, given the small fluctuations and measurement uncertainties.

2.23.5.6 Material Properties

The Thorney Island trials released a gaseous mixture of Freon-12 and nitrogen, in a known composition. Models that include these components in their species database and allow the use of mixtures should use the built-in properties in their simulations; models that do not include both components, or that do not allow mixtures, should use the thermophysical properties for the mixture listed in the accompanying spreadsheet. No sensitivity cases are specified.

2.23.5.7 Summary of Sensitivity Cases

Based on the discussion above, the model validation efforts should include the sensitivity cases listed in Table 2.23-3. If one or more sensitivity cases cannot be run, for example, due to hard-coding of certain parameters in a model, an explanation should be provided in the model questionnaire.

Table 2.23-3. Base and sensitivity cases for the Thorney Island trials in the MVD.

Parameter	Case	TI-45	TI-47
Source term	Base	Impinging gas jet	Impinging gas jet
Release Rate	Base	10.67 kg/s	10.22 kg/s
Release Duration	Base	455 s	465 s
Wind Speed (at 10 m height)	Base	2.3 m/s	1.5 m/s
Surface Roughness Length	Base	0.01 m	0.01 m
	R1	0.001 m	0.001 m
	R2	0.03 m	0.03 m
Atmospheric Stability	Base	F[11]	F
	A1	E	E
Ambient Temperature	Base	13.1 C	14.3 C
Ambient Pressure	Base	1 atm	1 atm
Relative Humidity	Base	100%	97.4%
Stream Composition (v/v)	Base	Freon-12 = 32% Nitrogen = 68%	Freon-12 = 32% Nitrogen = 68%

[11] Most dispersion models cannot specify "intermediate" atmospheric stabilities such as E-F, therefore, the more stable value is selected as the base case and the other value as a sensitivity.

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