Model Evaluation Protocol for Toxic Dispersion

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EXECUTIVE SUMMARY

The safe siting of LNG facilities requires project developers to evaluate the potential consequences to the public and public property from accidental loss of containment and release of hazardous materials (e.g., flammable and/or toxic). These consequences include: pool, jet or flash fires; vapor cloud explosions; toxic gas exposure; and catastrophic vessel failures. Calculating the distance to which hazardous conditions may extend for each type of scenario requires the use of computational models.

This document presents the model evaluation protocol (MEP) for toxic dispersion models. Given the significant similarities between the dispersion of flammable and toxic materials, the toxic dispersion protocol retains significant information from the flammable dispersion MEP, including several validation data sets.

The scope of the toxic dispersion MEP is to define an objective and transparent methodology to determine the ability of a model to accurately simulate toxic dispersion scenarios in the context of LNG facility siting. The protocol itself is intended to be a guidance document which outlines the tasks required by the petitioner and the reviewer. Specifically, it provides guidance to the petitioner regarding:

- Information to be submitted (e.g., user guide, technical references, etc.);
- Scenarios to be simulated for validation (including any sensitivity analysis); and
- Feedback that should be expected once the evaluation is completed (e.g., whether the model is accepted or not, restrictions on the applicability of the model, or validation factors to be applied to the modeling results).

The protocol also provides guidance to the evaluator, including:

- Requirements that an evaluator must meet to be qualified;
- Tasks to be performed during the evaluation; and
- Reporting requirements.

The toxic dispersion MEP presented in this document follows the general model evaluation methodology previously described by Gavelli et al. [1] as well as the flammable dispersion MEP [2], and includes the following tasks:

1. Scope of the evaluation
2. Evaluator qualifications
3. Model description
4. Scientific assessment
5. User-oriented assessment
6. Verification
7. Validation, which includes:

   a. Model Validation Database (described in a separate report) with:
      i. Datasets for model validation
      ii. Key variables and physical comparison parameters
      iii. Statistical performance measures
      iv. Acceptability criteria
   b. Sensitivity analysis
   c. Qualitative performance assessment
   d. Quantitative performance assessment
8. Model Evaluation Report, which includes:
   a. Summary of the evaluation (i.e., steps 4 through 7 above)
   b. Best practice guidance
   c. Recommendations for improvement

1 Introduction

The safe siting of LNG facilities requires project developers to evaluate the potential consequences to the public and public property from accidental loss of containment and release of hazardous materials (e.g., flammable and/or toxic). These consequences include: pool, jet or flash fires; vapor cloud explosions; toxic gas exposure; and catastrophic vessel failures. Calculating the distance to which hazardous conditions may extend for each type of scenario requires the use of computational models.

Assessing the quality of models, especially those used to evaluate the consequences of hazardous scenarios on the public, has long been a concern to regulatory bodies. This concern led, over time, to the development of several protocols to evaluate models in a consistent and transparent manner. In the context of LNG facility siting, a model evaluation protocol (MEP) and model validation database (MVD) were developed in 2007 [3] to address the modeling of vapor dispersion from LNG spills.

This document presents the model evaluation protocol for toxic dispersion models. The MEP presented in this document is aimed at evaluating models for the dispersion of toxic releases from a range of different release scenarios, including spills as well as pressurized releases. Given the many similarities between the dispersion of flammable and toxic streams, the current protocol retains significant information from the flammable dispersion MEP, including several validation data sets.

The following subsections provide a brief discussion of the different toxic dispersion scenarios considered in this MEP; the main physical phenomena that affect their outcome; and a brief summary of the types of models most frequently used for toxic dispersion simulations.

1.1 Toxic Dispersion Scenarios

When a loss of containment occurs in a pipe or vessel containing a toxic but not flammable fluid[1], a toxic exposure hazard exists in areas where the toxic cloud's concentration equals or exceeds the threshold concentration. PHMSA siting studies currently rely upon the Acute Exposure Guideline Levels (AEGLs) maintained by the United States Environmental Protection Agency (EPA) for toxic thresholds. Toxic hazards depend on both concentration and exposure time, therefore AEGLs are calculated for exposure periods ranging from 10 minutes to 8 hours; the toxic threshold for the same consequence decreases with increased exposure time. In siting studies, the exposure

[1] The potential hazards of releases of materials that are flammable were discussed in the flammable dispersion MEP.

time is set equal to the release duration which is typically 10 minutes for cases with no liquid rainout, and 60 minutes for cases with liquid rainout, due to continued evaporation from the liquid pool. In all cases, a longer exposure time will result in a more conservative hazard calculation (i.e. lower concentration threshold).

Toxic scenarios can be quite different from one another and not all models can accurately simulate each type of scenario. The following subsections define some broad categories for grouping toxic dispersion scenarios, in order to provide some high-level explanation of the differences that may be encountered. By design, this grouping is consistent with the one used to categorize data sets in the flammable dispersion MVD.

1.1.1 Materials

LNG facilities may utilize or produce several different toxic materials or mixtures, such as acid gas or heavy hydrocarbon condensates. Each stream has specific thermophysical properties (density, enthalpy, etc.); the main distinction with respect to toxic dispersion modeling is between gaseous releases (e.g., acid gas) and liquid streams (e.g., condensates) which may result in significant rainout fractions.

1.1.2 Release Type

The characteristics of the release can have a significant effect on the toxic dispersion hazards. There are numerous parameters affecting the release, including: pressure, temperature and phase of the fluid prior to the release; hole size, shape and elevation; etc.

For the purpose of this MEP, releases are grouped into three categories based on how the release mechanism influences the cloud dispersion:

1. Low-momentum releases are those in which the material is introduced into open air with negligible net momentum in any direction. Therefore, the toxic cloud dispersion is driven solely by the wind, gravity and obstacles. The most frequent examples of low-momentum toxic releases encountered in LNG facility siting are:
    a. Spills: liquid releases from low pressure storage or large-bore holes, which result in significant rainout. The liquid fraction is typically collected and conveyed to a dedicated retention area.
    b. Catastrophic releases: volumes of liquid or gas released instantaneously from the sudden disappearance of a storage vessel's walls. The material contained in the vessel is free to expand in all directions, with zero net initial momentum.
2. Momentum-driven releases are those in which the material is introduced into open air with sufficient net momentum in one direction to drive the initial dispersion of

the cloud. The most common momentum-driven release scenarios encountered in LNG facility siting are:

a. Gas jets: releases of pressurized gaseous material through a hole on the order of a few inches diameter. In most practical cases for LNG facility siting, the gas pressure is high enough to result in choked flow conditions and a sonic discharge.
b. Liquid jets: releases of pressurized liquid material through a hole on the order of a few inches diameter. As the liquid exits the hole, it tends to atomize into a spray of droplets which then progressively evaporate as the jet expands and entrains ambient air. In some cases, part of the spray may settle onto the ground before all droplets have evaporated: the deposited liquid fraction is called "rainout" and can effectively create a new source of vapor of the "spill" type. In most practical cases, the liquid prior to release is at temperatures higher than the normal boiling point; therefore, upon discharge to atmosphere, a fraction of the release immediately flashes to vapor while the rest atomizes into a droplet spray as just described: this type of release is commonly known as a "flashing jet" or "flashing and jetting" scenario.

3. 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 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, etc. Tracer releases are not common at LNG facilities, however, since experimental data focuses on low concentrations in the far field, some cases are appropriate for evaluating toxic dispersion models.

1.1.3 Dispersion Areas

Once a cloud is formed, it begins to disperse driven by its own source momentum (if any) and the wind, and it interacts with the terrain and any obstacles or obstructions it encounters. In actual facility siting, every terrain and facility layout has a different effect on the cloud; for the purpose of combining general effects, however, the following three categories are defined:

1. Unobstructed terrain: flat terrain without any obstacles or obstructions. While this case is clearly an approximation since terrain is rarely flat and every facility introduces obstacles and obstructions to air and gas flow, it is a very frequently used approximation. In fact, even the simplest models can handle dispersion over flat terrain (in many cases, flat is the only terrain a model can simulate);

additionally, in many scenarios[2] an unobstructed dispersion case results in longer (i.e., conservative) hazard distances than an obstructed one.

2. Obstructed terrain: flat terrain with one or more obstacles located downwind of the release, for the specific purpose of obstructing the cloud and redirecting the dispersion.
3. Complex geometry: any combination of a realistic (i.e., non-flat) terrain, obstructions due to facility components (e.g., piping, equipment, structures), and one or more obstacles to control cloud dispersion (e.g., vapor barriers). Complex geometry is the most realistic type of dispersion area but also the most challenging for models to simulate accurately.

1.2 Phenomena Affecting Toxic Dispersion

Given the wide range of toxic dispersion scenarios that can be encountered in an LNG facility siting study, toxic dispersion models need to account for several phenomena. What follows is a brief overview; interested readers can find more details in the published literature, for example in the Center for Chemical Process Safety (CCPS) book "Guidelines for the use of vapor cloud dispersion models" by Hanna et al. [4].

1.2.1 Material Properties

The thermodynamic properties of the released material have a significant impact on the behavior of the toxic cloud; therefore, they should be built into the model or allowed to be specified by the user. Given the potentially large pressure and temperature ranges as well as the possibility of phase change, variable properties are preferred over constant properties. Material properties can be included as tabulated values that can be interpolated by the solver, or as mathematical functions.

Mixtures of components are frequently encountered in siting studies, therefore, models should be capable of tracking the dispersion of vapor mixtures, either by performing multicomponent dispersion calculations or by defining a pseudo-component with the properties of the mixture.

1.2.2 Source Term

The ability to calculate the source term for a toxic dispersion scenario is not a requirement for a dispersion model; in fact, several dispersion models do not include a source term submodel, instead opting for the user to calculate the necessary parameters by other

[2] This is not a universal rule: for example, flow channeling due to terrain or obstruction layout has been shown to result in longer dispersion distances than unobstructed dispersion.

means and enter them as a “pseudo-source”. The evaluation of source term models is included in a separate MEP.

Whether a model includes a source term submodel or not, it should still be capable of accounting for the properties and physical characteristics of the source (or pseudo-source), such as:

- Temperature;
- Density;
- Phase;
- Composition (i.e., pure fuel or fuel/air mixture);
- Vapor generation rate;
- Source area, elevation and direction;
- Source momentum.

1.2.3 Ambient Conditions

The behavior of a dispersing cloud depends heavily on the ambient conditions into which it is released. Dispersion models should therefore be able to account for the effects of ambient temperature, wind speed and atmospheric turbulence on the evolution of the cloud. Relative humidity can also affect gas dispersion, both due to the change in air density and to the potential for water vapor condensation (“fog”) and re-evaporation.

The ability to model the effects of the atmospheric boundary layer (e.g., through surface roughness and Pasquill-Gifford stability classes) on the dispersion of dense clouds is critical. Wind direction is also important, particularly for models simulating dispersion in complex geometry or scenarios in which the wind direction is not aligned with the momentum of the release.

1.2.4 Cloud Dispersion

Several different mechanisms come into play as a toxic cloud is formed and begins to disperse, including:

- Gravity-driven spreading, including terrain effects;
- Advection by the wind;
- Mixing due to turbulence at the cloud/air interface;
- Turbulence suppression due to dense cloud stratification;
- Cloud/obstacle interaction (e.g., vapor holdup by barriers);
- Mixing due to obstacle interaction;
- Heat transfer from the ground;
- Water vapor condensation (fog) and evaporation.

Toxic dispersion models should be capable of accounting for as many of these effects as possible, either through numerical solution of physical equations or specific submodels.

1.2.5 Averaging Times

Every dispersion model solves one or more equations that represent an approximation of the physical phenomena. Part of the approximation includes the time interval over which the stochastic fluctuations of the physical phenomena are averaged. Since toxic dispersion hazards are typically associated with prolonged exposure (particularly at the concentrations of interest in siting studies), long time averaging is generally more appropriate in this case whereas short time averaging is considered conservative.

1.3 Toxic Dispersion Model Types

There are numerous models available to calculate toxic dispersion hazards for LNG facility siting, both commercially distributed and freely available. Each model has specific capabilities, solution methods, etc. For the most part, current models fall within one of the categories described below.

It is important to note that the toxic dispersion MEP presented in this document is intended to be applicable to any dispersion model, whether it fits within one of these categories or not (e.g., shallow-layer models).

1.3.1 Screening Tools

Screening tools are the simplest type of models. They typically solve one or more algebraic correlations based on experimental data obtained under very specific conditions. Screening tools are extremely quick to run and in some cases can be quickly developed in-house from published references. However, they are very limited in their applicability and can usually solve only the simplest scenarios.

1.3.2 Integral Models

Integral dispersion models solve a set of semi-empirical differential equations to calculate the dispersion of the cloud. These models typically calculate the bulk cloud properties (gas concentration, temperature, velocity, etc.) at a given distance from the source and then apply similarity profiles to define the cloud properties on a plane perpendicular to the direction of travel.

Integral models can have a broad range of applicability and have been widely used for consequence modeling of toxic dispersion scenarios in various areas, including LNG facility siting. Integral models are more complex than screening tools, yet can run very quickly on most personal computers. Setting up toxic dispersion simulations using an integral model typically requires a small set of input parameters and limited modeling expertise. However, integral models are often limited in their ability to simulate complex scenarios, for example dispersion in the presence of obstacles or complex terrain, wind not aligned with the release direction, etc.

1.3.3 Computational Fluid Dynamics (CFD) Models

CFD models solve the time-dependent equations of fluid flow (the Navier-Stokes equations) over a discretized, three-dimensional domain. The Navier-Stokes equations are solved coupled with turbulence closure models and other equations (e.g., conservation of species for mixtures, heat transfer to/from solid boundaries) as dictated by each specific scenario.

Assuming the resolution of the discretized domain is adequate, CFD models provide the most detailed solution of a toxic dispersion scenario among all model types. There are no general limitations to the type of scenarios that can be modeled with a CFD tool. However, the price for this versatility and level of detail is the need for a certain level of expertise with modeling in order to properly set up and run a CFD simulation, as well as the computing time and resources necessary to perform the simulation. Therefore, CFD models are often not best suited for studies that require numerous simulations.

2 Model Evaluation Protocol

The scope of the toxic dispersion MEP is to define an objective and transparent methodology to determine the ability of a model to accurately simulate toxic dispersion scenarios in the context of LNG facility siting. The protocol itself is intended to be a guidance document which outlines the tasks required by the petitioner and the reviewer. Specifically, it provides guidance to the petitioner regarding:

- Information to be submitted (e.g., user guide, technical references, etc.);
- Scenarios to be simulated for validation (including any sensitivity analysis); and
- Feedback that should be expected once the evaluation is completed (e.g., whether the model is accepted or not, restrictions on the applicability of the model, or validation factors to be applied to the modeling results).

The protocol also provides guidance to the evaluator, including:

- Requirements that an evaluator must meet to be qualified;
- Tasks to be performed during evaluation; and
- Reporting requirements.

The toxic dispersion MEP presented in this document follows the general model evaluation methodology previously described by Gavelli et al. [1] and implemented in the flammable dispersion MEP [2]. It includes the following tasks:

1. Scope of the evaluation
2. Evaluator qualifications
3. Model description
4. Scientific assessment
5. User-oriented assessment
6. Verification
7. Validation, which includes:
    a. Model Validation Database, with:
        i. Datasets for model validation
        ii. Key variables and physical comparison parameters
        iii. Statistical performance measures
        iv. Acceptability criteria
    b. Sensitivity analysis
    c. Qualitative performance assessment
    d. Quantitative performance assessment
8. Model Evaluation Report, which includes:
    a. Summary of the evaluation (i.e., steps 4 through 7 above)
    b. Best practice guidance
    c. Recommendations for improvement

Note that the model validation task, including the validation database, is discussed in a separate document [1]. This allows the validation data sets, statistical performance measures and acceptability criteria to be updated as more information becomes available (e.g., new experimental data sets or results from model evaluations) without requiring a complete revision of the model evaluation protocol.

The following sections provide more detailed information on the various tasks included in the toxic dispersion MEP.

2.1 Scope of the evaluation

The scope of the toxic dispersion MEP is to evaluate models that calculate the extent of toxic dispersion hazards (i.e., AEGL thresholds) from accidental releases of toxic materials or mixtures including toxic components. The objective of the evaluation is to allow the regulatory body (i.e., PHMSA) to determine whether a given model should be approved or rejected for use in toxic dispersion modeling in the context of LNG facility studies. Additionally, the evaluation should allow the regulatory body to specify any restrictions on the use of an approved model, as well as any "validation factors" to be applied to the modeling results. Comparing models against one another and establishing rankings of preferred models are not objectives of this model evaluation protocol.

Each model evaluation is specific to a single model and to a single version of that model. As a new version is released, a new model evaluation must be conducted; however, a goal of this protocol is to minimize the time required to evaluate minor model updates. Section 3.4 will define what constitutes a minor, major, or significant change, and describe the submittal process for an expedited review of minor model updates.

As discussed in section 1.3, this MEP is applicable to a wide variety of models. Therefore, some of the model validation cases or information requested may not be applicable to the specific model being evaluated; in that case, a brief note can be used to explain the exception.

2.2 Evaluator qualifications

Most of the existing protocols specify that the reviewer should be a third party, in order for the review to be objective and independent. The downside of this requirement is that a truly independent reviewer may not have the same level of knowledge and expertise as the model developer in the following areas:

- Accidental release scenarios, particularly in the context of LNG facility siting;
- Physics of atmospheric dispersion, particularly for dense clouds;

- Numeric solutions of atmospheric dispersion problems, particularly for the same type of model being reviewed;
- Capabilities and limitations of the model being reviewed.

It should also be noted that PHMSA's Advisory Bulletin ADB-10-07 [5] states that "The model developer or an independent body may complete the MER[…]". However, this statement is in conflict with the stated objective of this MEP, which is to ensure an objective and transparent model evaluation process. Allowing the model developer to perform the evaluation would inevitably raise objectivity concerns, therefore, a suitably qualified third-party is considered necessary. As such, the following requirements apply to the individual (or group) performing a model evaluation under this protocol:

- The evaluator may not be associated with the model developer or with any of the model distributors. Prior association is acceptable, provided that there is no current or foreseeable collaboration that may raise concerns of objectivity;
- The evaluator must have recognized expertise with the physics of atmospheric dispersion of toxic releases;
- The evaluator must have recognized expertise with consequence modeling, and specifically with the same type of model (e.g., box, Gaussian, semi-empirical, CFD, etc.) as the one being evaluated. Direct experience with the model being evaluated is not required, however, it is desirable.

It is important to note that the use of a third-party evaluator does not mean that the model evaluation process needs to occur "in a vacuum". On the contrary, the evaluator should be encouraged to seek support from the model developer or other model experts as needed in order to ensure a thorough evaluation; any information obtained from sources beyond the Model Description Questionnaire (MDQ) should be properly documented in the Model Evaluation Report (MER).

2.3 Model description

The first step in the evaluation of a specific model is to familiarize with the model itself. Therefore, the evaluation begins with a description of the model, which should include:

- Model name, the version being evaluated and its release date;
- Contact information for the model developer or a designated representative;
- Brief description of the model, including:
    - Model type;
    - Areas of application (including any areas outside of the scope of this MEP, such as flammable dispersion, pool/jet fires, vapor cloud explosions, etc.);
    - Theoretical background;
    - Numerical solution methods

- Brief description of the types of toxic dispersion scenarios the model can simulate (e.g., liquid spills, flashing jets, flat terrain) and for which approval is being sought;
- The operating systems (e.g., Windows, MacOS, Linux) on which the software can be installed, and the types of hardware (e.g., desktop, workstation, tablet) required to run the model;
- An estimate of the simulation set up and run times for a typical toxic dispersion scenario, and of the time and training required for a user to achieve a competent level of mastery of the model;
- Brief description of the data input and output capabilities, including whether a graphical user interface (GUI) is available to set up the simulations and whether a graphical postprocessing package is included to visualize the results;
- List of references including user manuals, technical references and select peer-reviewed publications that further describe the model and its capabilities.

The information needed for the model description should be provided by the petitioner, who should be closely associated with the model developer or otherwise highly knowledgeable about the model. In order to ensure consistency of information across models, a model description questionnaire (MDQ) is included in appendix to this MEP to guide the respondent step-by-step to provide the requested information.

2.4 Scientific assessment

The main purpose of the scientific assessment is to verify that the model is built on scientifically solid foundations, so that if it is able to correctly predict a given scenario, it does so for the “right” reasons. Therefore, the scientific assessment seeks to answer the following questions:

- Does the model include the physical phenomena relevant to the atmospheric dispersion of toxic materials? Specifically:
    - Does it accept source terms from the release types described in section 1.1.2, or define the source term in the model?
    - Does it account for the properties of the atmospheric boundary layer (wind speed, atmospheric stability, surface roughness, etc.)?
    - Does it account for dense cloud effects (gravity driven spreading, turbulence reduction, etc.)?
    - Does it account for buoyancy and the transition from dense cloud to passive dispersion?
    - Does it account for wind direction?
    - Does it account for obstacles, obstructions, or complex geometries?
- Are the governing equations for these phenomena based on published or accepted science?

- Does the model implement numerical methods based on published/accepted practices to solve these equations accurately?
- What are the sources of uncertainty in the modeling results?

The scientific assessment is based on a review of information provided in the MDQ and should rely heavily on published material (technical reports, peer-reviewed papers, etc.) to allow a thorough and efficient review. As stated in section 2.1, the reviewer needs to have a strong understanding of the physics and mathematics of toxic dispersion scenarios, as well as the numerical methods and approximations used by the type of model being reviewed.

While the scientific assessment is mostly a qualitative exercise, it may also include a quantitative task known as “feature testing”. This task is aimed at testing the performance of a single feature of the model, consisting of setting up a simplified scenario, performing the simulations and reviewing the results to verify that the tested feature operates as expected. An example of feature testing could address the dispersion of a downward impinging jet in zero wind. Feature testing is not dissimilar from the verification task (see section 2.6) but it is less complicated. Feature testing is not required but may be requested by the reviewer; in that case, the modeling would be performed by the model developer and the results submitted as supplemental information.

Once the scientific assessment is completed, a summary report for this task should be prepared and include:

- A summary of the scientific basis of the model and an evaluation of its adequacy for toxic dispersion scenarios in LNG facilities. The summary should highlight the model capabilities and limitations with respect to toxic dispersion scenarios;
- A discussion of the results of any feature testing (if applicable);
- A brief discussion of potential areas for improvement of the scientific basis of the model.

2.5 User-oriented assessment

The user-oriented assessment focuses on the usability of the model. Therefore, it seeks to evaluate the following:

- Level of expertise required to run the model;
- User-oriented documentation (e.g., Installation, User Guide) and help;
- User interface (graphical or command line);
- Tutorials or examples;
- Pre- and post-processing interfaces;
- Modeling options (availability and guidance);

- Simulation set-up (user-friendliness and guidance);
- Warning and error messages;
- Output data (availability and format);
- Computing requirements and time.

The user-oriented assessment will be based on information provided in the MDQ. Direct experience with the model by the evaluator would be useful for the completion of this task, as it would provide independent user feedback. The findings of the user-oriented assessment, including recommendations for improvement, will be summarized and included in the model evaluation report.

2.6 Model Verification

Verification is the process of ensuring that the implementation of a model is consistent with its theoretical basis as reviewed during the scientific assessment. The purpose of verification is to demonstrate that the coding of equations, algorithms, submodels and databases is correct. There are several potential approaches to code verification, including:

- Checks for internal consistency (mass or flux balances);
- Modeling of simple scenarios for which analytical solutions are available;
- Examining code behavior for limiting conditions;
- Method of manufactured solutions;
- Comparison with results from ensemble of other models.

Model verification can be a very demanding task, often complicated by confidentiality issues that prevent full access to the code of proprietary models. Therefore, most existing model evaluation protocols consider model verification as a "passive" task - that is, responsibility is placed on the model developer to submit evidence of verification to the reviewer. The same approach is followed in this MEP: the reviewer will rely upon evidence of verification provided by the petitioner and examine it to ensure it is adequate. A summary of the model verification task, including the source of information, will then be included in the model evaluation report.

2.7 Model Validation

Model validation is the process of comparing the predictions of a model against experimental data relevant to the types of scenarios that the model is intended to predict. As discussed in earlier protocols [6], "validation" in the true sense of the word cannot be accomplished by simply comparing a model against a finite number of scenarios; what can be accomplished is an "evaluation", which establishes enough confidence in a model to expect that it will perform in an acceptable manner when applied to similar scenarios. For consistency with the majority of published literature, the comparison of a model with experimental data will be called “validation” but will be understood to refer to the data sets included in the validation database.

The scope of validation for a toxic dispersion model is to assess its performance in predicting the extent of toxic dispersion hazards from release scenarios consistent with those encountered in LNG facility siting. The performance assessment includes the following components:

- Sensitivity analysis;
- Uncertainty quantification;
- Qualitative evaluation;
- Quantitative evaluation.

The model validation task, including the validation data set and the statistical performance measures, is described in detail in “Model Validation Database for Toxic Dispersion” by Gavelli and Hendrickson [7].

2.8 Model Evaluation Report

The Model Evaluation Report (MER) represents the final product of a model evaluation, and the only part of the evaluation that will be made publicly available. The objectives of the MER are to:

- Provide regulators with the information they need to determine whether to approve or reject a model, and to set any conditions or limitations on its use;
- Convince all stakeholders that the model review was conducted in an objective and independent manner.

Therefore, the MER needs to include sufficient information to allow the reader (for example, staff from a regulatory agency, model developer and users, or any other interested person) to understand the review process and the results. An example of information that should be summarized in the MER is provided in ADB-10-07 [5].

The MER will include three sections as described below.

2.8.1 Summary of the evaluation

The main section of the MER consists of a summary of the model evaluation effort, which includes the following:

- Evaluator qualifications
- Model description

- Scientific assessment
- User-oriented assessment
- Verification
- Validation, including:
  - Modeled data sets
  - Sensitivity analysis
  - Qualitative performance assessment
  - Quantitative performance assessment
  - Conditions for acceptance of the model

Most of the model evaluation tasks involve a qualitative assessment and have been described only in general terms in this document, so that the same protocol could be applied to a wide range of models. Similarly, the structure and contents of the MER are only described in broad terms. The choice of which information and level of detail to include in the MER is left to the model evaluator, who should ensure that the MER meets its stated objectives. As a result, the regulatory review process may include a request for more data or further analysis before making a determination on the acceptability of the subject model.

In general, each section in the MER summary should include the following:

- A brief description of the purpose of the task;
- A list of the information provided by the petitioner, including the MDQ, memos/emails and published references;
- A discussion whether the model meets or falls short of the requirements of the task. Note that each task typically includes several subtasks, each with specific requirements. For example, the scientific assessment evaluates the physical models, governing equations and the numerical methods included in the model; the physical models are then broken down into several submodels (dense gas dispersion, atmospheric boundary layer profiles, etc.). The MER should describe the model's capabilities and limitations with as much granularity as necessary to make a determination on its applicability to toxic dispersion scenarios.

It is recommended that a draft of the MER be shared with the petitioner, to provide them with an opportunity to clarify potential areas of concern or disagreement prior to the public release of the document.

2.8.2 Best practice guidance

Most toxic dispersion models include several user-selectable parameters, ranging from boundary conditions (wind, temperature and turbulence profiles) to source term (type, release rate, duration, etc.) and solver options (time step, grid size, compressibility, parallel processing, etc.). Model results tend to change as these parameters are varied, which may produce inconsistent results across users. Therefore, it is important for the MER to indicate which parameters were used in the model validation effort, as well as which parameters should be considered acceptable in toxic dispersion modeling for facility siting purposes.

The choices made for any user-selectable model parameter in the MVD simulations should be considered the "best practice" for toxic dispersion and should ideally be used consistently in any toxic dispersion modeling for LNG facility siting. Where applicable, options and parameter values that are not considered acceptable for toxic dispersion modeling of LNG facilities should also be listed.

Deviations from best practice guidance (e.g., using a computational mesh inconsistent with those used for the model validation, or changing "default" parameters) when submitting simulations for regulatory approval of a siting study may "void" the model approval for that specific study and require the user to provide additional evidence that the model's predictions may still be considered acceptable.

2.8.3 Recommendations for improvement

Model improvement is not a stated purpose of this MEP; however, the model evaluation process may identify performance gaps or other opportunities to improve a model's performance. Since model improvements may ultimately lead to more accurate facility siting studies, any observations made during the model evaluation, which could lead to an improvement in the capabilities of a model to accurately predict the toxic dispersion hazards, should be identified and explained in the MER. It is important to note that these are only recommendations, therefore, the model developer should not be required to act on them as a condition for the approval of future versions of the model.

3 Guidance on Preparing and Submitting a Model Evaluation Application

The various components of the model evaluation protocol for toxic dispersion hazards have been discussed in this document and the toxic dispersion model validation database [7]. This section provides some additional guidance to petitioners preparing a model evaluation application.

3.1 Model Description Questionnaire

The model description questionnaire (MDQ) is provided in the appendix and is also available as a fillable PDF by request to PHMSA. The scope of the MDQ is to facilitate both the submission and review processes, as well as to ensure consistency of information across model evaluations. This scope is accomplished by asking a series of specific questions on each task of the model evaluation.

Petitioners should follow the guidance provided with the MDQ; if any portions of the MDQ are unclear, PHMSA may be contacted for clarification. In order to facilitate the review, the MDQ responses should be clear and complete but concise. Where applicable, a copy of peer-reviewed publications or external reports that are referenced should be submitted for evaluation.[3] Any confidential information submitted with the MDQ should be clearly labeled as such, to prevent disclosure in the MER.

If the space provided in the MDQ for a response is not sufficient, a separate document may be submitted which includes all the answers requiring additional space. Each response should be clearly identified by their respective question number.

The MDQ and all listed references should be submitted in electronic form as text searchable PDF files.

It is important to note that the MDQ is a work-in-progress that is expected to evolve as more and more models are reviewed and questions may be added, deleted or clarified accordingly. Therefore, constructive feedback on the MDQ (or any other part of the MEP) is always encouraged.

[3] The section(s) of interest should be indicated in each response to streamline the review.

3.2 Model Validation Results

In addition to the MDQ, model evaluation applicants need to submit the results from the comparison of their model against the model validation database. All information necessary to set up and run the simulations for the MVD scenarios (including the prescribed sensitivity cases) is provided in the MVD report [1] and associated spreadsheet[4]. Any request for clarification on the MVD may be submitted to PHMSA.

The simulation results should be entered into the MVD spreadsheet for each trial. The spreadsheet will automatically generate graphical and tabulated comparisons between the model predictions and experimental measurements. The spreadsheet will also automatically calculate the statistical performance measures for each trial and for groups of similar trials, and will compare the results to the current acceptability criteria. It should be noted that, as discussed in the MVD, the acceptability criteria are indicative values and not pass/fail values. The MVD spreadsheet, filled out with the modeling results, should be submitted in electronic form as a Microsoft Excel file, as part of the model evaluation application.

The input and output files for each simulation included in the model validation (i.e., both the base case and any sensitivity runs) should be provided in native format as part of the application. If use of the model requires a license, a license suitable for model evaluation purposes should be provided to the model evaluator, for a period of time sufficient to complete the review.

In order to facilitate the model evaluation and the compilation of the best practice guidance, the petitioner is encouraged to prepare a written report that describes the modeling performed during the validation effort. The report should discuss:

- Modeling parameters or options used in the simulations, including an explanation of the selections made and a discussion of acceptable/not acceptable selections;
- The reasons for omitting any trials and/or sensitivity cases from the study (if applicable);
- A discussion of any observed trends, inconsistencies in the results, or other model behavior that could adversely affect the results of the evaluation.

[4] “Toxic dispersion MVD – rev#.xlsx” or “Toxic dispersion MVD – Scaled - rev#.xlsx” as discussed in the MVD

3.3 MER Feedback

Once the model evaluation is complete, the petitioner should receive a draft version of the MER for review and comment. This is an opportunity for the people with the most detailed knowledge of the model to address and clarify potentially inaccurate observations (e.g., due to missing or unclear submittal information, or other reasons).

The petitioner should take full advantage of this opportunity to provide additional clarity so the final MER is as accurate as possible. The petitioner should recognize that significant changes to the overall evaluation at this stage will be unlikely or could result in significant delays to the process; therefore, petitioners are strongly encouraged to be as detailed and forthcoming as possible in their initial submittal.

3.4 Petition for Approval of New Model Versions

As indicated in section 2.1, each model evaluation is specific to one version, which means that as a new version is released, a new petition for approval must be filed. The time and effort required to prepare a new petition and to complete a new evaluation are generally incompatible with the development cycle of most modern modeling tools. This can unduly restrict the use of new model versions, particularly in the case of changes that do not affect the hazard being modeled (i.e., toxic cloud dispersion). Therefore, a goal of this MEP is to allow for an expedited, yet diligent, review process for new versions of already approved models, provided only “minor” changes have occurred since the most recent approval.

3.4.1 Minor Changes

Minor changes include the following categories:

- Modification of the Graphic User Interface;
- Expansion of compatible hardware support;
- Other changes aimed at improving usability and/or performance, without affecting the solution of toxic dispersion scenarios;
- Modification of sub-models that are not relevant to toxic dispersion (e.g., combustion)

The changes introduced with a new model version are considered minor if they produce no “significant” differences in model validation predictions, as measured by point-wise concentrations as discussed below.

3.4.2 Major Changes

Major changes include:

- Any categories listed in section 3.4.1, which result in significant differences in model validation predictions;
- Any changes to the governing equations, species properties, numerical solver, or modeling assumptions for the solution of toxic dispersion scenarios.

3.4.3 Significant Differences

For toxic dispersion modeling, a difference in model validation prediction, as measured by point-wise concentrations, is considered significant if the absolute difference between the currently approved model prediction and the updated model prediction varies more than one order of magnitude below the measured concentration (i.e. with a measured concentration of 0.1%, model predictions cannot vary more than 0.01%).The threshold for a “significant difference” may be reevaluated as new model versions are submitted for approval, to ensure it is adequate.

3.4.4 Model Evaluation for New Versions with Only Minor Changes

Since minor changes introduce no significant differences between the new version and the currently approved version of a model, both the petition and the evaluation process can be greatly simplified. The petition for approval of a new model version with only minor changes will consist of the following:

1. Submitting a short report describing all changes made to the model since its previous approval;
2. Simulating a subset of the cases in the toxic dispersion MVD (the “test cases”) with the new version of the model, and performing a point-wise comparison between the predicted values from the new version and the currently approved version, to demonstrate that no significant differences occur. The subset of cases to be run is listed in Table 3-1;
3. Submitting the tabulated point-wise comparison and the model input and output files, in native electronic form, for the test cases. The model evaluator will need to be granted short-term access to the new and currently approved versions of the model.

The model evaluator will then review the submitted information to verify that the new version only introduces minor changes.

Table 3-1 Test cases for expedited evaluation of new model versions.

Test Cases	Alternatives[5]
BA-Hamburg DA0501	BA-Hamburg DA0120
FLADIS 25	
Jack Rabbit II 8	
Kit Fox 5-4	Goldfish 1
Thorney Island 45	

3.4.5 Model Evaluation for New Versions with Major Changes

If a new version of an approved model introduces any major changes, the petition for approval would follow the same procedure discussed in section 2 for a new model, including simulating all cases in the MVD. All changes introduced with the new version must be properly documented; submitting a change-log document is recommended. In order to facilitate the preparation of the documentation, as well as the model evaluation, the petitioner may utilize the previous MDQ and highlight any responses affected by these changes.

[5] The alternative test cases are included for models that do not have the capability of simulating one or more of the test cases (e.g., integral models that cannot simulate the effect of obstructions)

BIBLIOGRAPHY

[1] F. Gavelli, B. Hendrickson, C. Marsegan, and J. Piekarz, "Model Validation Database for Flammable Releases," Blue Engineering and Consulting, 03903-RP-002, Aug. 2020.

[2] F. Gavelli, B. Hendrickson, C. Marsegan, and J. Piekarz, "Model Evaluation Protocol for Flammable Dispersion," Blue Engineering and Consulting, 03903-RP-003, Oct. 2020.

[3] M. J. Ivings, S. F. Jagger, C. J. Lea, and D. M. Webber, "Evaluating vapor dispersion models for safety analysis of LNG facilities," Health and Safety Laboratory, MSU/2007/04, 2007.

[4] S. R. Hanna, P. J. Drivas, and J. C. Chang, *Guidelines for use of vapor cloud dispersion models*, 2nd ed. New York: Center for Chemical Process Safety of the American Institute of Chemical Engineers, 1996.

[5] Pipeline and Hazardous Materials Safety Administration, *Liquefied Natural Gas Facilities: Obtaining Approval of Alternative Vapor-Gas Dispersion Models*. 2010.

[6] M. J. Ivings, S. E. Gant, S. F. Jagger, C. J. Lea, J. R. Stewart, and D. M. Webber, "Evaluating vapor dispersion models for safety analysis of LNG facilities, 2nd Edition," Fire Protection Research Foundation, MSU/2016/27, Sep. 2016.

[7] F. Gavelli and B. Hendrickson, "Model Validation Database for Toxic Releases," Blue Engineering and Consulting, 03903-RP-004, Dec. 2020.

Appendix – Model Description Questionnaire

The purpose of this Model Description Questionnaire (MDQ) is to gather the information necessary to properly evaluate a toxic dispersion model. The MDQ provides a guided template aimed at facilitating the submittal of information by the petitioner and at streamlining the review by the model evaluator. The questionnaire should be compiled by the petitioner, which is typically the model developer or a third party with deep knowledge about the model being submitted.

The toxic dispersion MDQ is based on the questionnaire developed by Ivings et al. [3], [6] for the LNG vapor dispersion MEP, adapted to account for the broader scope of the current protocol. The MDQ is model- and version-specific; therefore, all information should refer to a single version of the model and – where applicable – each sub-package (e.g., materials database, or porosity sub-model). When the questionnaire is prepared for a new version of a model previously evaluated under this MEP, all questions must be answered as for a model never previously evaluated. In fact, providing answers to all questions in each submitted version of the MDQ will facilitate the review; changes from the previous version can be highlighted (e.g., with shaded text, different color, underline, etc.) to streamline the process.

The MDQ includes an Annex section, which attempts to further clarify the scope of each question. The preparer is advised to review the Annex before filling out the questionnaire.

Model Description Questionnaire for

Model Name

Version

Submitted for the purpose of

Evaluation

for

Toxic Dispersion Modeling

Prepared and submitted by: Name

Affiliation

Completed on: Date

1. General Information

1.1 Name of model

1.2 Version number and release date

1.3 Model developer

1.4 Version history

1.5 Model heredity

1.6 Model description

1.7 Areas of application

1.8 List of documents supplied

2. Scientific Assessment

2.1 Type of Model

○ Screening ○ Integral ○ CFD ○ Other

Additional information:

2.2 Scenario Components

2.2.1 Material Properties

Database:

○ DIPPR ○ REFPROP ○ Built-in ○ Other

Material Properties:

○ Constant ○ f(T) ○ f(T,P)

Additional information:

2.2.2 Source Term

Release Type:

○ Liquid Spill	☐Calculated	☐User-specified	☐N/A
○ Pressurized Gas Release	☐Calculated	☐User-specified	☐N/A
○ Pressurized Liquid Release	☐Calculated	☐User-specified	☐N/A
○ Catastrophic Release	☐Calculated	☐User-specified	☐N/A

Release Flow:

○ Steady ○ Time-dependent

Additional information:

2.2.3 Ambient Conditions

☐Temperature ☐Humidity ☐Wind speed

☐Ground temperature ☐Solar radiation ☐Surface roughness

☐Pasquill-Gifford class ☐Monin-Obukhov length

Atmospheric Boundary Layer Profiles:

☐Wind ☐Turbulence ☐Temperature

Stability classes allowed:

☐A ☐B ☐C ☐D ☐E ☐F ☐G

Minimum wind speed allowed:

Additional information:

2.2.4 Dispersion Area

☐Unobstructed ☐Obstructed ☐Complex Geometry

Additional information:

2.2.5 Boundary Conditions

☐Temperature ☐Wind speed ☐Wind direction

☐Steady ☐Fluctuating

☐Inflow (wind) ☐Outflow (pressure boundary) ☐Symmetry ☐Other

Additional information:

2.3 Physical processes modeled

2.4 Mathematical formulation of the problem

2.5 Solution method

○ Algebraic ○ ODE ○ PDE ○ Other

Computational Grid:

☐Structured ☐Unstructured ☐Adaptive

☐Multi-block ☐N/A

Additional information:

2.6 Output variables

Calculated:

☐Concentration ☐Temperature ☐Velocity

☐Density ☐Turbulence

Derived:

☐Dose

Temporal basis:

☐Steady-state ☐Peak values ☐Time history

Additional information:

2.7 Planned scientific developments

3. User-Oriented Assessment

3.1 Computer environment

3.1.1 Hardware

☐Workstation ☐Desktop/Laptop ☐Tablet ☐Other

Additional information:

3.1.2 Operating System

☐Linux ☐Windows ☐MacOS/iOS

Additional information:

3.1.3 Auxiliary Software Required

3.1.4 Programming Language(s)

3.2 Installation Procedure [ref.]

3.3 User interface [ref.]

3.4 Internal databases [ref.]

3.5 Simulation Set-Up

3.5.1 Geometry Definition

☐CAD import ☐Manual build

Additional information:

3.5.2 Data Input

☐Graphical User Interface ☐Input file(s) ☐Command line

Additional information:

3.5.3 Modeling Guidance

☐User Manual ☐Online Help ☐Training

Additional information:

3.5.4 Input Data Checks

3.6 Running the Simulations

3.6.1 Solver Options

☐Compressible ☐Incompressible

☐Time-dependent ☐Steady-State

Additional information:

3.6.2 Warnings and Error Messages

3.6.3 Run Time

3.7 Simulation Output

3.7.1 Output Variables and Formats

3.7.2 Simulation Files Structure

3.8 Interfacing to Other Models / Software

3.8.1 Program Suite

3.8.2 Source Model Packages

3.8.3 CAD/GIS/FEA/Other Model Interfaces

3.9 Customization

3.10 Status and Availability

3.10.1 Maturity of the Model

○ Widely Used ○ New ○ Research Tool

Additional information:

3.10.2 Dissemination [ref.]

3.10.4 Licensing Options

○ Commercial ☐Term license ☐Perpetual license ☐Purchase

○ Free ☐Open Source

○ Proprietary

○ R&D

Additional information:

3.10.5 Contact Information for Licensing

3.11 Users

3.11.1 Current Users

3.11.2 User Knowledge Requirements

3.11.3 Simulation Set-up Time

3.11.4 Technical Support

3.11.5 Training

3.12 Planned user-oriented developments

4. Model Verification

4.1 Internal Verification Procedures

4.2 QA Procedures and Certifications

5. Model Validation

5.1 Previous Validation

5.2 Previous Sensitivity Studies

5.3 Validation Against the Toxic Dispersion MVD [ref.]

5.3.1 MVD Trials Modeled

○ All ○ Partial Set

Trials excluded:

Additional information:

5.3.2 Solver(s) Used

5.3.3 Grid Independence

5.3.4 Modified Input Parameters

5.3.5 Sensitivity Cases

6. Administrative

Model Developer – Point of Contact

Name:

Organization:

Position:

Email:

Phone:

Petitioner – Point of Contact

Name:

Organization:

Position:

Email:

Phone:

Qualification: developer; user; other

Petitioner – Additional Contact

Name:

Organization:

Position:

Email:

Phone:

Qualification: developer; user; other

Petitioner – Additional Contact

Name:

Organization:

Position:

Email:

Phone:

Qualification: developer; user; other

Annex to the Model Description Questionnaire

This annex is intended to clarify what information and level of detail are expected in the questionnaire. A fillable PDF version of this MDQ is available upon request to PHMSA; should additional space be needed to answer one or more questions, the full response can be included in a separate document, properly labeled to identify the question(s) being answered.

Electronic copies of all references listed in the MDQ should be included with the submittal package; the files should be in PDF format, preferably text-searchable.

It should be noted that some questions may appear similar (e.g., if the same question is relevant to more than one section of the questionnaire); all questions should be answered, to streamline the review process.

General Formatting

- Questions followed by "[ref. only]" indicate that only the reference(s) should be provided, rather than a long response. All references should be formatted according to one of the common scientific formatting standards (e.g., IEEE); the same reference format should be used throughout the MDQ. Where applicable, the reference should include the pages or sections pertinent to the question being answered, to facilitate the review.
- Questions that included pre-populated response options can be of 3 types:
  1. Where each option is preceded by a checkbox (☐), one or more options (i.e., all that apply) may be selected by checking the respective box;
  2. Where each option is preceded by a radiobutton (◯), only one option may be selected by checking the corresponding button;
  3. Where multiple rows of selectable options are available, the first option in each row (together, the first column of options) is preceded by a radiobutton; this means that only one may be selected, by checking the corresponding button. For the selected row, any of the other options (preceded by checkboxes) may be selected as applicable by checking the respective boxes.

1. General Information

This section is concerned with information of a general nature. It is also used to define the reference version of the model. In this section, responses should be made explicitly in the spaces provided.

1.1 Model Name: Include both full name and acronyms

1.2 Version number and date: List the model version being evaluated. This must be the same version discussed in the MDQ and used to simulate the MVD cases. Include the version numbers for any sub-models or packages included with the current model version.

1.3 Model developer: Include company name and address. The point of contact information will be provided in section 6.

1.4 Version history: Indicate the first version of the model, with the year of release (to establish the overall maturity of the model) and provide a chronological list of model versions previously released (going back no more than 10 years). For each previous model version, list the respective version numbers for any sub-models or packages. Indicate any regulatory approvals received for earlier versions of the model.

1.5 Model heredity: Describe earlier models from which the current model originated (e.g., as a "spin-off" or via a name change), if any.

1.6 Model description: Provide a general description of the model (e.g., from the introduction to the User Manual or other background documents). Actual text is preferred to a reference, in this case.

1.7 Areas of application: Indicate the types of toxic dispersion scenarios that can be modeled. Include the types of releases (spills, jets, etc.), materials (LNG, pure hydrocarbons, mixtures, etc.) and phase (gas, liquid, two-phase), and dispersion areas (flat, obstructed, "3D"). Briefly list other types of scenarios (e.g., fires, explosions, etc.) that do not pertain to the scope of this MEP.

1.8 List of documents supplied: Include all the documents referenced in this questionnaire. Place the main references (e.g., user manual, technical reports and other important publications) at the start of the list. The suggested format for each document is: *[No.] Reference (Authors, Year, Title, Publication); Summary*, where:

[No.] is the sequential document number in the list

Reference (...) is the reference for the document. A consistent format should be used, preferably according to one of the main scientific reference formats.

Summary is a one-sentence summary description of the document and its relevance to the questionnaire (e.g., "technical reference discussing the atmospheric dispersion solver", or "peer-reviewed publication describing the validation of version X against the Y test series").

A copy of all referenced documents must be submitted in electronic format with the MDQ. Each document must be labeled as Authors – Year, consistent with the labeling used to answer this question.

Any documents that should be considered confidential must be identified as such by:

- Including the "CONFIDENTIAL" label between [No.] and Reference (...)
- Including the "CONFIDENTIAL" label at the end of the file name for the submitted electronic copy

2. Scientific Assessment

This section evaluates the physical and mathematical basis of the model. Short answers are sought in the MDQ, supplemented by reference documents that would provide as much detail as possible. The information should include, where possible, statement of the assumptions that have been made in defining a given aspect of the model.

2.1 Type of Model: Refer to the categorization of dispersion models included in the MEP in making the selection. Additional information (e.g., RANS, LES, etc. for CFD models) may be also provided.

2.2 Scenario components: Describe the capabilities of the model regarding the various components of a toxic dispersion scenario.

2.2.1 Material properties: Select the appropriate option for the materials database. If "Built-in" or "Other" is selected, describe which materials are included and the source of data. Describe if the model uses the ideal or real gas law to calculate changes in material properties (e.g., density, viscosity, specific heat, etc.), or if they are kept constant. Discuss whether materials not in the model database can be added (e.g., via user functions) and whether mixtures are allowed.

2.2.2 Source term: Check the box next to each type of source term the model can simulate and, for each, indicate whether the model includes a built-in source term calculator (e.g., pool vaporization, flashing jet, etc.) or needs the user to perform the calculation externally and enter the source data.

For each source term that is calculated internally, describe the model used and provide reference documents. Describe if the source term can account for different source sizes (e.g., an elongated trench vs. a circular sump) and time-dependent inputs (e.g., from a spreading pool, pressurized line blowdown, etc.).

Discuss whether the vapor dispersion model can include liquid spills of two-phase releases in the simulation or it requires the source to be fully evaporated before dispersion modeling can initiate.

2.2.3 Ambient Conditions: Describe whether the model is capable of calculating atmospheric boundary layer profiles, and for which variables (e.g., wind speed, turbulence, temperature). Describe which inputs are required (e.g., Pasquill-Gifford class, roughness length, Monin-Obukhov length, cloud cover, etc.). Describe if the ambient conditions are fixed throughout a simulation or can be time-dependent.

Discuss whether wind direction can be different from the release direction (for horizontal pressurized releases).

2.2.4 Dispersion Area: Check the box next to each type of dispersion area the model can simulate. Note that "obstructed" refers to scenarios where one or a few simple obstacles (e.g., walls or barriers) are present, whereas "complex geometry" indicates scenarios in which topography or complex obstructions (e.g., piping, structures and equipment) affect the dispersion. If applicable, describe the sources of data that can be imported to create the complex geometry within the model, and whether an internal CAD package is available to create a geometry "from scratch".

2.2.5 Boundary Conditions: Check the box next to each type of boundary conditions available for dispersion modeling, if applicable, and provide a brief description of their function and limitations.

2.3 Physical processes modeled: Provide information on the physical processes taken into account within the model – not through external calculations (e.g., source term, in some cases). The list should include:

- Phase change of the release (e.g., if built-in source term models can simulate the pool or flashing jet evaporation), aerosols, rainout;
- Fluid dynamics and mass transfer (e.g. entrainment, diffusion, deposition, interaction with obstacles, gravity-driven flow, etc.)
- Species thermodynamics
- Heat transfer modes, sources/sinks
- Dense gas behavior, transition to passive dispersion
- Compressible or incompressible flow
- Heat transfer to/from solid boundaries
- Turbulence models (if applicable)

If a model includes the capability to simulate a certain type of scenario (e.g., dispersion over obstructed terrain) but that capability is not yet fully developed, the questionnaire response should indicate so, in order to optimize the reviewer's time as well as to prevent incomplete capabilities from adversely affecting the overall evaluation of the model.

2.4 Mathematical formulation of the problem: Describe how the mathematical problem is formulated, including:

- The governing equations (e.g. conservation relations)
- Independent and dependent variables
- Boundary conditions
- Any approximations made to the equations (e.g., RANS), including the parameterization of terms in the equations
- The final equations solved, i.e. following non-dimensionalization, transformations, etc.

A brief description supplemented by reference to one or more technical documents is considered an appropriate answer.

2.5 Solution method: Select the appropriate solution method and computational mesh structure (if applicable). Describe how the mathematical problem is solved, especially the numerical methods employed (spatial and temporal discretization, coupled or segregated solver, etc.). This should include an indication of parameters needed to achieve a certain accuracy (e.g. CFL number, grid refinement, convergence criteria, etc.).

Discuss whether the solver uses a single processor or parallel processing; if both options are available, discuss how the solution may be affected (a limited set of sensitivity cases may be appropriate).

2.6 Output variables: Describe the output variables available from the model, both directly, as in the dependent variables of the governing equations, as well as those derived from the primary variables. Select any derived variables that may be calculated. Describe whether time histories of output variables are saved or only peak (or steady-state) values.

Discuss time-averaging: can it be specified by the user, or is it fixed? If it is fixed, are the results representative of long- or short-time averaging?

2.7 Planned scientific developments: Briefly list any scientific developments of the model currently planned (e.g., expanded set of physical scenarios, faster solver, etc.)

3. User-oriented Assessment

This section is concerned with the practical aspects of the model, i.e. all aspects of how the model is operated and used to solve specific problems. Some of this information will be contained in the User Manual or other similar documentation.

3.1 Computer environment: Evaluates the hardware and software associated with running the model.

3.1.1 Hardware: Select the hardware platform(s) on which the model runs. Add any additional information that may be valuable to the reviewer.

3.1.2 Operating System: List the operating systems supported on each of the available hardware platforms. Add any additional information that may be valuable to the reviewer.

3.1.3 Auxiliary Software: List any additional software required to run the model, including for set-up and post-processing (e.g. compilers, proprietary graphics packages, etc.).

3.1.4 Programming Language(s): List the programming languages used to write the computer code.

3.2 Installation procedure [ref.]: Refer to the "installation manual" or "user manual" to describe the procedure to install the model on a given computer platform.

3.3 User interface [ref.]: Refer to the "user manual" or other document to describe how simulations are set up, run and the results extracted.

3.4 Internal databases [ref.]: Refer to a technical document to describe the databases included with the model (e.g., material properties, sub-grid turbulence generation, etc.). The document should describe the function and use of each database, and whether they can be modified or overridden by the user. If no published reference is available, provide a detailed response.

3.5 Simulation Set-Up

3.5.1 Geometry Definition: Describe if the model includes options to build the geometry "from scratch" and/or to import it from external CAD formats. List the CAD formats that can be imported, if any, and discuss if the import requires third-party packages or scripts not included with the model suite. Enter "N/A' if not applicable.

3.5.2 Data Input: Describe if a GUI is available and/or data needs to be supplied in separate files, to be read by the model at run time. A brief response, supplemented by a reference to the user manual or other detailed document, is recommended.

3.5.3 Modeling Guidance: Describe any modeling guidance available (within the program itself, in the accompanying documentation, or through training) on choosing appropriate input data, including “default” values and acceptable ranges. This can include grid size, time step, turbulence or other submodels, wind, boundary conditions, etc.

3.5.4 Input Data Checks: Describe any checks performed by the model on the data values being used, to determine whether the values are valid (e.g. fall within a sensible range or the range of validity within the model) and consistent with regulatory requirements for dispersion studies.

3.6 Running the model

3.6.1 Solver Options: Describe each solver option available to run a toxic dispersion simulation (e.g., single processor/parallel solver, compressible/incompressible, along wind dispersion, etc.) and how each affects the simulation.

3.6.2 Warnings and Error Messages: Provide information on the warnings and error messages produced by the model while running. Explain when an error message may be “overlooked” and when it indicates a critical problem with a simulation set-up or solution.

3.6.3 Run time: Estimate the time to run different types of scenarios, assuming the most common platform used for the model.

3.7 Simulation Output

3.7.1 Output Variables and Formats: Describe the variables that can be displayed and the formats used to display them. For example, are tabular and graphical outputs available? Can the output be easily imported into a spreadsheet for plotting? Is a 3D post-processing package available within the model, or is the output compatible with commonly used third-party packages?

3.7.2 Simulation Files Structure: Outline how cases run are identified, i.e. does the output file contain input data, can the output files be given identifiable names; also, how the cases run are organized, e.g. can the output file be anywhere in the directory structure of the user; and finally, how accessible previous runs are, including whether several cases can be loaded at once.

A brief response supplemented by a reference to the user manual or other document is recommended

3.8 Interfacing to other models and software

3.8.1 Program Suite: If the dispersion model is one of several programs linked together, describe the other models included in the suite and whether the dispersion model's input and/or output are tied to any of these models (e.g., a pool vaporization model whose output automatically creates the source term for the dispersion model).

3.8.2 Source Term Package: Describe which external source term software packages may be used to generate the input data for the model (e.g., SOURCE5 for DEGADIS before 2010).

3.8.3 CAD/GIS/FEA/Other Model Interfaces: Describe any other external software package that may interface with the model being evaluated, such as:

- CAD models that allow 3D terrain or engineering structures to be imported into the model
- GIS models that allow the dispersion results to be exported and overlaid onto a site map
- FEA models that allow the dispersion results to be exported and provide boundary conditions for structural analysis (e.g., temperature onto a structural element exposed to cryogenic conditions from an LNG release)

3.9 Customization: Describe if the model allows customization (e.g., subroutines, user functions, etc.) to expand its capabilities or to handle special cases. Discuss in detail if any customization was used in the MVD validation cases, including any sensitivity cases run to compare the customized runs with the "default" runs.

3.10 Status and availability of model

3.10.1 Maturity of the Model: Check the box that best fits the model:

- "Widely used" is for commercial models with at least 50 users worldwide, outside of the developer's staff, otherwise check the "New Model" box
- "Research Tool" indicates a model for academic or government research
- "Internal" is a model for internal company use or for use by others but only on company projects (e.g., FRED before circa 2018)

Describe if there are any specific modules, outside the "standard" program, necessary to run toxic dispersion scenarios. Discuss if any such modules were used in any of the validation cases submitted with this application.

3.10.2 Development Status: Describe if the model is being actively maintained and developed. How often are new versions being released?

3.10.3 Dissemination [ref.]: Provide a list of references to journal papers and conference presentations where the model (or some of its features) were described. Limit to 10 references.

3.10.4 Licensing Options: Check the relevant box(es).

3.10.5 Contact Information for Licensing: Provide contact details for obtaining the model, if applicable.

3.12 Users

3.11.1 Current Users: Provide the approximate overall number of users worldwide and their general distribution (e.g. USA, Europe, Asia, etc.). Describe the type of users (e.g. researcher, safety engineer, risk analyst, design engineer).

3.11.2 User Knowledge Requirements: Describe the knowledge requirements in various disciplines (fluid dynamics, thermodynamics, programming, computers, etc.) for a successful user. Also, indicate whether experience in hazard and risk analysis is required to run the model correctly.

3.11.3 Simulation Set-Up Time: Estimate the time required by an average user to set up a typical simulation. The estimate should be based on a properly trained, but not expert, user.

3.11.4 Technical Support: Describe the types of support available to a user on a day-to-day basis (e.g. on-call Help Desk, tech support email, FAQ page, etc.). Discuss whether tech support is provided for free, as part of the software license, or as an additional fee.

3.11.5 Training: Describe the availability of training for users. How frequent? Is it included with the license fee, or extra? Is it offered by the developer or third parties? Discuss if specialized training is regularly provided for toxic dispersion modeling, and specifically for PHMSA-regulated studies.

3.12 Planned user-oriented developments: List any user-oriented developments of the model currently planned (e.g., new GUI, faster graphical post-processor).

4. Model Verification

This section is concerned with activities to ensure that the mathematical model is translated accurately into its computer implementation, as well as with the quality assurance procedures adopted during the development of the software.

4.1 Internal Verification Procedures: Describe the verification procedures followed during the model development, including:

- Comparison against analytical solutions
- Accuracy of mass/momentum/energy conservation equations
- Comparison of alternative solution methods
- Verification of internal databases

Include any relevant references that discuss the model verification procedures in more detail.

4.2 Quality Assurance Procedures: Describe the QA procedures followed during the model development. List any QA certifications (e.g., ISO 9000) obtained prior to or during the development of the current version, and valid throughout the development period.

5. Model Validation

This section is looking to gather information on previous model validation efforts, either for earlier versions of the model or for different MEPs.

5.1 Previous Validation: Describe any previous model validation efforts (relevant to the scope of this MEP); describe which test series and trials were modeled, and summarize the results (or list relevant documents that provide such information). Discuss whether these validation efforts were part of an earlier MEP, part of a multi-group exercise, or internal efforts.

For each previous validation effort, indicate which model version was tested; if an earlier version was used than the one being submitted, discuss the relevant differences.

5.2 Previous Sensitivity Studies: Describe any previous model sensitivity studies (relevant to the scope of this MEP); discuss the purpose (i.e., which parameters were tested) and summarize the results (or list relevant documents that provide such information). Discuss whether these sensitivity studies were part of an earlier MEP or independent.

5.3 Validation Against the Toxic Dispersion MVD [ref.]: This section describes the model validation effort produced for the current application. The preparation of a model validation report (MVR) detailing the modeling assumptions and results is highly recommended; in that case, provide a reference to the report in this space and in the following subsections.

5.3.1 MVD Trials Modeled: Check the applicable box. If an MVR is provided, refer to the appropriate section; otherwise, provide a detailed explanation for each MVD trial that was not modeled.

5.3.2 Solver(s) Used: Indicate which solver options (e.g., parallel, compressible, etc.) were used to simulate the trials in the MVD. If an MVR is provided, refer to the appropriate section; otherwise, provide detailed explanations for any trials that did not use the default options. Describe any sensitivity cases run to compare the results using different solvers or solver options.

5.3.3 Grid Independence: Describe how "grid independence" of the modeling results was ensured. If an MVR is provided, refer to the appropriate section; otherwise, discuss the assumptions made for grid sensitivity cases and the results.

5.3.4 Modified Input Parameters: Indicate whether any input parameters were changed from the values provided in the MVD spreadsheet (e.g., Pasquill-Gifford class, material properties, etc.). If an MVR is provided, refer to the appropriate section; otherwise, explain the reasons for any changes and discuss the results.

5.3.5 Sensitivity Cases: Indicate whether any of the sensitivity cases specified in the MVD were not run or were run with different input parameters than specified. Describe any user-selected sensitivity cases run in addition to those listed in the MVD, if any. If an MVR is provided, refer to the appropriate section; otherwise, provide a detailed discussion.

6. Administrative Information

Enter the contact information for each person who contributed to the questionnaire or the model validation effort. The contact person should be listed first, followed by the principal contributors, etc.