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Performance metrics for evaluating liquefied natural gas, vapor dispersion models

Frank A. Licari [a,b,*]

[a] *United States Department of Transportation, Pipeline and Hazardous Materials Safety Administration, Pipeline Safety Office, Washington, DC, USA*
[b] *Mary Kay O'Connor Process Safety Center, 2009 International Symposium, College Station, TX, USA*

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ABSTRACT

New performance metrics are necessary to quantify the inherent margins of safety[1] in vapor dispersion models for liquefied natural gas (LNG) spills. Currently, vapor dispersion model calculations in the 49 Code of Federal Regulations, Part 193 as well as Standard 59A of the National Fire Protection Association (2001 edition) reduce the lower flammability limit (LFL) of methane in air by a safety factor of two (to 50% LFL) to ensure that flammable vapors do not extend beyond an LNG facility's property line during an LNG spill. Yet, neither document explicitly states the additional distance or the additional confidence level this existing safety standard creates to separate the public from LNG vapors at 100 percent LFL within the facility vs. 50 percent LFL at the facility property line.

Although researchers have successfully validated how vapor dispersion models calculate conservative buffer (exclusion) zones, their collective work did not readily explain to the general public the inherent margins of safety in these models. Havens and Spicer developed correlations to demonstrate how well DEGADIS[2] predictions compared with field testing measurements in the late 80s (Havens & Spicer, 1985). Their research also confirmed that peak gas concentrations exceeded time averaged measurements during some field trials as well as DEGADIS predictions. Then Hanna, Chang, and Strimaitis (1993) explained how several vapor dispersion models could be compared by calculating geometric mean bias and geometric variance and shared these validation results with the public. The works of the Havens and Hanna teams were also influential in explaining why the maximum concentration of methane in air at the property limits of an LNG facility should be 50 percent of its lower flammability limit during an LNG spill. Eleven years later, Chang and Hanna discussed how the relationships between fractional bias, geometric mean bias, geometric variance, and normalized mean square error could explain vapor dispersion model over and under prediction (Chang & Hanna, 2004). Despite these successful efforts, there has been reluctance to embrace vapor dispersion model results, because exclusion zones are not described as creating margins of safety (i.e. additional separation distance) or higher confidence levels (i.e. a likelihood of being correct) that protect the public.

This paper proposes an improved performance metric to evaluate the validity of vapor dispersion models and a statistical methodology to determine the confidence level and the inherent margin of safety in calculating vapor dispersion exclusion zones. Descriptions of the new metric and methodology are presented in this document for the DEGADIS vapor dispersion model, together with example calculations.

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1. Introduction

A new performance metric and a corresponding statistical methodology are presented in this paper, which may be helpful in evaluating dispersion models and explaining the results of a validation exercise. However, this new metric and its methodology by themselves do not constitute a comprehensive model validation or evaluation. They, like all performance metrics, are purely another means to judge whether an LNG vapor dispersion model predicts

* United States Department of Transportation, Pipeline and Hazardous Materials Safety Administration, Pipeline Safety Office, Washington, DC, USA. Tel.: +1 202 366 5612; fax: +1 202 366 4566.
E-mail address: licarifa@usa.com

[1] In this paper, margin of safety is an occupational safety phrase, and it is expressed as a ratio.

[2] DEGADIS is a dense gas, vapor dispersion model that was developed in collaboration with the Gas Research Institute and the University of Arkansas. The United States Department of Transportation adopted DEGADIS in its LNG facility siting regulations within Part 193 of the 49 Code of Federal Regulations.

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exclusion zone distances (or gas concentrations) with an adequate margin of safety and an acceptable level of confidence. The remainder of this paper describes how performance metrics for vapor dispersion models have evolved in recent years and how a new metric complements prior research in this field.

2. Historical perspective of performance metrics for vapor dispersion models

In the late 1980s, Havens and Spicer began the first efforts to validate LNG vapor dispersion models by developing statistically meaningful correlations between DEGADIS predictions and field test observations (Havens & Spicer, 1985). They evaluated results from LNG tests conducted by the American Gas Association and Shell, and in their work to document the strength of DEGADIS correlations, they also illustrated how peak, gas concentration measurements exceeded time averaged results in many tests. These findings acknowledged the challenges in creating correlations with high confidence levels as well as the potential uncertainties for predicting flammable gas concentrations.

Then in 1993, Hanna et al. performed comparative validations of fifteen models (Hanna et al., 1993). Their research constructed plots of the geometric mean variance vs. geometric mean bias for gas concentrations of vapor dispersion models and created visual representations of each model's variance within a 95 percent confidence level and its range of over and under prediction. These models were then grouped by instantaneous, passive, and continuous releases to depict the strengths of each model's predictions against observed gas concentrations during field tests. Hanna et al. clearly illustrated how each model's performance in predicting gas concentrations typically falls within a factor of two compared to actual field observations. Using the ratios of gas concentration predictions to observed measurements, residual plots of HGSYTEM were created to illustrate trends related to distance, wind speed, and atmospheric stability. In their conclusions, the authors appropriately acknowledged that the performance of vapor dispersion models could vary by 50 percent from one site to another due to "natural or stochastic variability in the atmospheric diffusion phenomena." Another milestone in the application of performance metrics and the validation of vapor dispersion models had been achieved.

When Europe completed its SMEDIS (Scientific Model Evaluation of Dense Gas Dispersion Models) project, Carissimo et al. published its evaluation of twenty eight vapor dispersion models in 2001 (Carissimo et al., 2001). This report utilized the performance metrics which Hanna et al. had previously established and also proposed that vapor dispersion models be evaluated by their fractional results – the percentage of gas concentration predictions between 50 and 200 percent of observed test measurements (a factor of ½ to 2 of observed results). Using these performance metrics, the authors concluded integral models, like DEGADIS, performed well with no complex effects [boundary conditions like severe terrain and obstacles] to mitigate or aggravate normal atmospheric dispersion. Furthermore, all models were better at predicting arcwise results [rather than pointwise] corresponding to centerline, maximum gas concentrations. Thus, SMEDIS researchers confirmed conventional wisdom that simple integral models would be valuable tools in calculating vapor dispersion exclusion zones without complex effects.

In 2004, Chang and Hanna completed an extensive study of statistical techniques for evaluating air quality models (Chang & Hanna, 2004). They confirmed commonly held views that good vapor dispersion models have 50 percent of their vapor dispersion predictions within a factor of ½ and 2 of observed test measurements. Chang and Hanna recognized that models may be tailored to specific vapor dispersion applications and explained at length how statistical techniques should be selected to complement the correlation of test results to air quality model predictions. Properly understanding and characterizing the relationships between predictions and observed test measurements were critical to selecting an appropriate performance metric for the task. In their view, screening the predictions and observed measurements and performing exploratory data analyses were essential tasks in identifying a reasonable performance metric. Knowing whether observed results were within a factor of two, five, or ten of predictions was an elemental step in the model validation process. Using data sets with at least twenty data points was equally important to achieve statistically valid conclusions.

To date, performance metrics for evaluating vapor dispersion models have been valuable scientific tools for validating how well these models predict gas concentrations measured during field trials. Researchers have developed statistical and analytical methodologies which accurately characterize the strengths of numerous models and describe how such models should be used. However, regulatory agencies and the public require a slightly different performance metric to explain how well vapor dispersion models safeguard communities from LNG vapors at 100 percent LFL within the facility vs. 50 percent LFL at the facility property line. A new performance metric and statistical methodology is needed to describe the additional distance and/or confidence level that an LNG vapor dispersion exclusion zone creates to separate the public from the hazards of flammable LNG vapors.

3. Novel performance metric for evaluating LNG vapor dispersion predictions

Considering the limitations of existing performance metrics for LNG vapor dispersion models, this paper proposes a new metric and statistical methodology for calculating vapor dispersion predictions and exclusion zones at an LNG facility. To his credit, Havens developed ratios of predicted to observed gas concentrations for the Burros and Maplin Sands LNG tests (Havens, 1992). However, Haven's work did not determine the minimum margin of safety and corresponding confidence level that NFPA 59A[3] and 49 CFR Part 193 create, when a vapor dispersion exclusion zone extends beyond 100 percent LFL to 50 percent LFL at an LNG facility's property line. The notional concept of a minimum margin of safety with confidence (*MSWC*) for a vapor dispersion model and its predictions is explained here and applied in several examples.

In principle, a margin of safety (Ms_i) for a dispersion model prediction may be defined by the simple ratio of the prediction (distance or gas concentration) to the observed measurement during a field trial (reference Eq. (1) in the Appendix). However, numerous LNG spill tests have confirmed that atmospheric conditions, local terrain, and testing error create a significant variance in the accuracy of measuring a flammable gas concentration at an observed distance. Furthermore, the inherent modeling and computational errors that are intrinsic to both source term and vapor dispersion models provide additional error. Consequently, the concept of a dispersion model's margin of safety is no longer a single value. On the contrary, it becomes a range of Ms_i values similar to Table 1 (refer to Havens, 1992 paper and Table 10) that may be illustrated by the normal distribution curve in Fig. 1.[4]

[3] The 49 CFR Part 193 selectively incorporates portions of the 2001 edition of the National Fire Protection Association Standard 59A (NFPA 59A), for calculating vapor dispersion exclusion zones at LNG facilities.

[4] The histogram in Fig. A.5 indicates the data set in Table 1 resembles a normal distribution.