A new integral dispersion model based on one-dimensional turbulence theory

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A new model for atmospheric dispersion is presented. The model solves the conservation of mass, momentum and energy, which is typical of most integral models but uses a simple theory based on one-dimensional turbulence to describe air entrainment instead of the highly empirical set of air-entrainment functions common to most integral models. The model agrees well with data from both dense gas and passive experiments without the arbitrary transitions between entrainment functions necessary in typical integral models.

Introduction

Atmospheric dispersion modeling is a critical step in evaluation of risk due to releases of toxic and flammable chemicals. Because the accuracy of the predicted risk depends directly on the accuracy of the selected dispersion model, it is important to use a dispersion model that accurately models the transport phenomena occurring during atmospheric dispersion. On the other hand, reasonable computational cost is required in order to thoroughly evaluate the potential risk posed by chemical release at a full petrochemical (or similar) facility. The class of dispersion models commonly referred to as "Integral Models" is frequently used to analyze risk at chemical and petrochemical facilities because they offer an attractive combination of accuracy and low computational cost.

Within most integral dispersion models the pollutant dilution rate (or air entrainment rate) is described by a set of empirical functions, and transition criteria are used to select between the entrainment functions. Coefficients for the air entrainment functions and the values of the transition criteria are then determined based on comparison with data from experimental dispersion experiments via "tuning" or regression exercises (Woodward, 1995). Consequently, integral models based on identical theories may yield significantly different predictions depending on the data which model developers used to determine the entrainment function coefficients and transition criteria values. Furthermore, models that rely on tuning to empirical data may be limited in their predictive capability because important fundamental phenomena may be masked (Lucas, 1976).

In this work a new integral dispersion model is presented based on simple turbulence theory, avoiding the need for transition functions or model tuning. Predictions are compared with data from two classical dispersion experiments (Prairie Grass and Burro) to illustrate the predictive power of the model.

Theory

Integral Models

Integral models are thus classified because they determine the plume centerline concentration profile by numerically integrating one-dimensional expressions for the conservation of mass, momentum and energy along the plume centerline. Concentration profiles in the other two dimensions are typically based on an assumed distribution of the form

$$f(\zeta) = \exp\left[-\left(\frac{\zeta}{b_\zeta}\right)^m\right] \quad (1)$$

where ζ is the dimension of interest and b_ζ is based on the estimated plume width or height. The exponent m determines the "sharpness" of the concentration profile in the ζ dimension, with a value of 2 corresponding to a Gaussian profile. This exponent is typically an empirical function of the plume density and distance (or time of travel) from the source.

The proposed model solves the system of one-dimensional equations by the Kutta-Merson numerical integration method. The concentration profiles proposed by Webber, et al. (1992) are used for the remaining two dimensions. Because the solution strategy and concentration profiles used in the proposed model are common to most integral models the reader is directed to the work of previous authors for further details (see for example Havens, 1988; McFarlane, 1991; Ott, 2001; Webber, 1992; Witlox, 1999).

Air Entrainment

The mass change of the plume with respect to downwind distance is determined exclusively by the rate air enters the pollutant, also known as the air entrainment rate (E), i.e.,

$$\frac{d\dot{m}}{dx} = \text{E.} \quad (2)$$

The air entrainment rate is therefore arguably the most critical aspect of an integral dispersion model, as it directly determines the rate of dilution and therefore the predicted downwind concentration profile of the plume. A typical integral model uses a complicated system of empirical entrainment correlations to describe air entrainment due to some combination of the following:

- Jet flow
- cross-wind flow
- ambient entrainment in the near-field
- dense gas effects, including separate functions to describe the entrainment through the top and side of the plume
- ambient entrainment in the far-field

Typical integral models assign criteria to determine when each entrainment function applies, often based on the plume velocity, density, or Richardson number, and tuned to experimental dispersion data. Some models use smoothing functions to avoid discontinuities that occur when switching between entrainment mechanisms (Witlox, 1994; Woodward, 1993). Most models switch to some form of the highly empirical Gaussian dispersion model (Turner, 1994) once the plume has become "passive", typically determined by the lack of significant density and velocity differences between the plume and the surrounding atmosphere.

This complex set of empirical functions and switching criteria may be eliminated if a more fundamental explanation of the cause of air entrainment is relied upon. It is the author's opinion that mixing of air and pollutant occurs during dispersion via two mechanisms:

- diffusion resulting from a concentration gradient
- turbulent mixing

As is frequently done, the former phenomenon is assumed to be negligible when compared to the significant mixing that occurs due to the latter. The latter phenomenon may be driven by the existing turbulence in the atmosphere, or by shear originating from a velocity differential, or both. Ricou and Spalding (1961) investigated turbulent mixing arising from a velocity differential using turbulent jets in quiescent atmospheres. They determined that air entrainment in jets (E_{jet}) occurs as a result of shear-induced turbulence along the jet edges and proposed the following relation to describe the resulting entrainment rate:

$$E_{jet} = c_o[\dot{m}\rho_{air}\|u\|]^{0.5} \quad (3)$$

where

$\dot{m}$ = mass flow rate of the jet

c_o = empirical constant, suggested by Ricou and Spalding as 0.282

ρ_{air} = density of air

$\|u\|$ = velocity magnitude of the jet

Extension of this formulation to jets in non-quiescent atmospheres must take into the angle between the jet and the wind, θ, and the wind speed, u_w, i.e.,

$$E_{jet} = c_o[\dot{m}\rho_{air}|\|u\| - u_w \cos\theta|]^{0.5} + c_o[\dot{m}\rho_{air}|u_w \sin\theta|]^{0.5}. \quad (4)$$

Note that the work of Ricou and Spalding indicates that it is the turbulence that drives the air entrainment, and the shear caused by the velocity difference is simply the mechanism for generating that turbulence. In the atmosphere turbulence is present due to wind shear and temperature gradients; yet it is still only the turbulence that drives air entrainment and not the mechanisms of generating that turbulence. Therefore, if a velocity that characterizes the atmospheric turbulence is known, the formulation of Rico and Spalding may be extended to describe the entrainment rate due to atmospheric turbulence ($E_{ambient}$):

$$E_{ambient} = c_o[\dot{m}\rho_{air}v]^{0.5}. \quad (5)$$

In this work the characteristic velocity, v, is assumed to be proportional to the atmospheric turbulent kinetic energy.

The total entrainment rate, E, is the sum of the turbulent mixing mechanisms:

$$E = E_{jet} + E_{ambient}. \quad (6)$$

This simple formulation is advantageous because it contains no smoothing functions or criteria to switch between entrainment functions, and contains no "tuning" coefficients eliminating the need to fit the model to experimental data.

Model Accuracy

Experimental Uncertainty

Obtaining an accurate description of a real plume's concentration profile is a difficult task. Concentration measurements are made via an array of point source sensors deployed in a configuration that will hopefully pick up key readings, the most critical of which is the centerline concentration. Unfortunately, the actual plume centerline and the position of sensors within the plume during an experiment are poorly defined. Therefore, an array with too few sensors may not read the peak plume concentration due to fluctuations in wind direction or a poor guess at the plume centerline elevation. An array with too many sensors is not only cost prohibitive, it may actually increase the bulk plume turbulence and therefore dilution rate as the plume flows through the network of sensors. In either case, reported concentrations will often be below the actual peak plume concentration at the sensor's downwind distance. This is further exacerbated by current limitations of sensor technology, such as response time and sampling frequency, which also increase the uncertainty of reported time-averaged concentrations. When these difficulties are properly understood, the following conclusions may be made:

1. The uncertainty of concentration measurements from experimental dispersions *may* be large and will almost certainly be skewed towards under-measurement of the actual peak concentration
2. A strong predictive model will tend to over-predict measured concentrations and normally only under-predict measured concentrations within the published uncertainty of the sensor combined with the uncertainty of the input parameters used in the model.

Comparison with Experimental Data

Model performance was tested by comparison of centerline concentration predictions with peak measured concentrations for the historical experimental dispersion tests, summarized in Table 1. The mean bias (*MG*) and mean variance (*VG*) are reported for both test sets as recommended by Hanna, et al. (1996), defined as follows:

$$MG = \exp\left[\frac{1}{N}\sum_{i=1}^{N} \ln\left(\frac{1}{F}\right)\right] \quad (7)$$

$$VG = \exp\left[\frac{1}{N}\sum_{i=1}^{N} \ln\left(\frac{1}{F}\right)^2\right] \quad (8)$$

However, mean bias is a poor indicator of overall model performance since it tends to favor models which both over and under predict, as will be seen later, instead of models which consistently slightly over-predict observed data. For this reason model performance was primarily determined based on histograms of the ratio of predicted to observed peak concentrations:

$$F = \frac{Predicted\ Concentration}{Observed\ Concentration}. \quad (9)$$

Simulations were also performed in a commercially available integral dispersion model (PHAST v6.7) for comparison purposes.

Prairie Grass Trials

During the Prairie Grass trials small jets of sulfur dioxide were released over a wide range of weather conditions. Due to the small size and low velocity of the jets most integral dispersion models transition to "passive" air entrainment rather quickly, and the dilution rate is typically predicted based on the Gaussian dispersion model using model coefficients derived, in fact, from the Prairie Grass data. The dilution rate in the proposed model, however, relies heavily on the estimated turbulent kinetic energy of the atmosphere. Thus the Prairie Grass trials are an excellent test of the validity of our simple turbulence-based entrainment theory. Model inputs and observed concentrations were taken from the *Modelers' Data Archive* (Chang, 2010).

As shown in Figure 1, the proposed model predicts within a factor of two (F between 0.5 and 2.0) for more than 70% of the data, over-predicts approximately 30% of the data by more than a factor of two, and under-predicts by more than a factor of two for less than 1% of the data. The proposed model has a mean bias of 0.61, indicating an average tendency to over predict

concentrations, and a mean variance of 2.0. On the other hand, PHAST has a tendency to severely over predict (*MG* = 0.4, *VG* = 3.5), with more than 60% of concentration predictions exceeding an *F* value of 2.

Burro Trials

The Burro experiments involved pools of LNG during weather conditions ranging from unstable to slightly stable. Dense, low-lying plumes evolved from the pools and thus model developers typically use the Burro trials to validate the dense gas functions in their dispersion models. Input parameters and observed concentrations were taken from several reports describing the tests (Ermak, 1988; Koopman, 1982; Morgan, 1984).

The proposed model predicts concentrations within a factor of two for 80% of the data and exceeds an *F* value of 2 for approximately 20% of the data (Figure 2). The mean bias and variance for the data set are 0.71 and 1.56, respectively, again indicating an average tendency to somewhat over-predict concentrations. Special consideration should be given to the results of trial 8, shown in Figure 3, as more than half of the predictions exceeding an *F* value of 2 occur for this trial. During trial 8 an abnormally low and wide plume was observed which bifurcated, presumably the result of low wind speeds permitting the plume to be affected more by vapor density than the weather. Concentration data indicate that the plume veered to the right, and by the second row of sensors (140 m) the right lobe of the plume was beyond the extent of the sensor array. Given that the concentration of the right lobe of the plume initially exceeded the left lobe by nearly a factor of 2, the reported concentrations which all correspond to the left lobe undoubtedly under-represent the actual peak plume concentrations, and therefore model predictions of the centerline concentration should exceed reported values for all but perhaps the first row of sensors.

PHAST results for the Burro trials indicate the commercial model has a tendency to over-predict concentrations in the near-field and under-predict far-field concentrations, creating the bimodal distribution seen in Figure 2. This bias is also visible from the parity plot (Figure 4) and a sample plot of concentration vs. distance, shown in Figure 5 and Figure 6 for trials 7 and 9, respectively. This bias, however, is not readily apparent from the mean bias and variance values (*MG* = 0.8, *VG* = 1.73), showing the importance of relying on additional statistical metrics when evaluating a model's performance. PHAST predicts concentrations within a factor of two for 70% of the data, exceeding an *F* value of 2 for 24% of the observations. It is interesting to note that the best performance of PHAST seems to occur for trial 8 (Figure 3), although the reported values for this trial are expected to be significantly lower than actual plume peak concentrations, as discussed above.

Conclusions

The turbulence-based integral dispersion model described in this work has several key strengths:

- Air entrainment is described by two simple functions
- The model does not use "tuning" coefficients commonly found in most integral models
- The model does not use arbitrary criteria or smoothing functions to transition between air entrainment functions

Performance metrics indicate that the proposed model is a good predictor of downwind concentrations for both the passive gas Prairie Grass trials and dense gas Burro trials, with an average tendency to somewhat over-predict reported observations. Further validation efforts are currently on-going and will be presented in the future.

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Table 1. Summary of Prairie Grass and Burro dispersion test sets

Test Set	Year	Material	Source Type	Rows of Sensors	Sensor Downwind Distance (m)	Sensor Elevations (m)	Analyzed Runs	Data Points
Prairie Grass	1956	Sulfur dioxide	Continuous jet	5	50 to 800	1.5; 9 elevations (0.5 m to 17.5 m) along 100 m arc	44	212
Burro	1980	LNG	Boiling pool	4	57 to 800	1, 3, 8	8	29

Figure 1. Histogram of model performance based on data from the Prairie Grass trials.

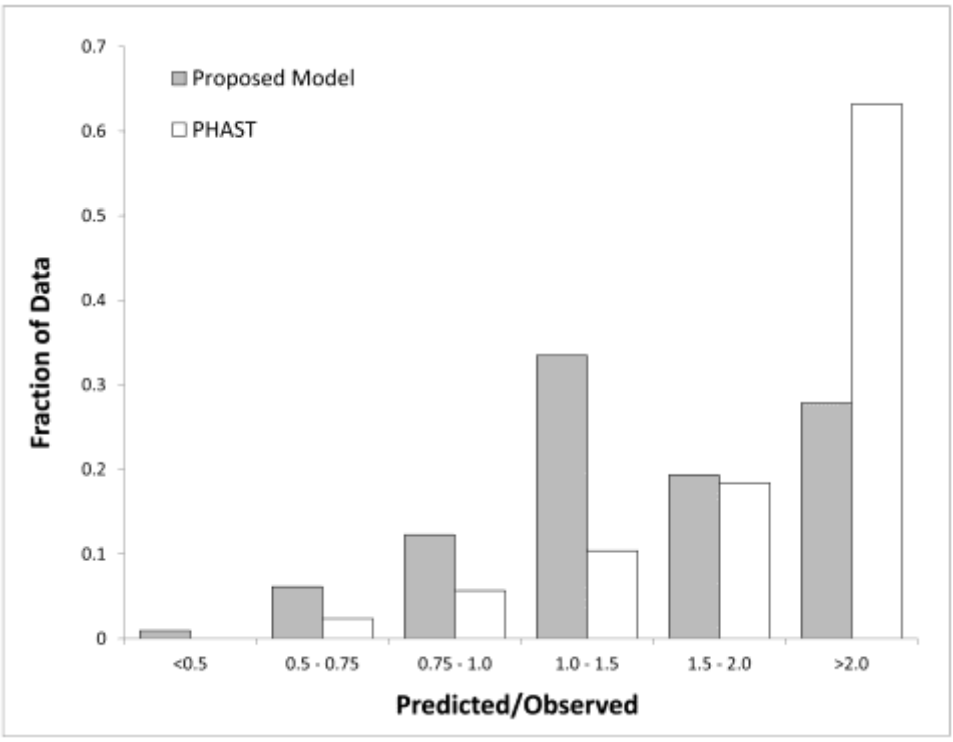

Figure 2. Histogram of model performance based on data from the Burro trials.

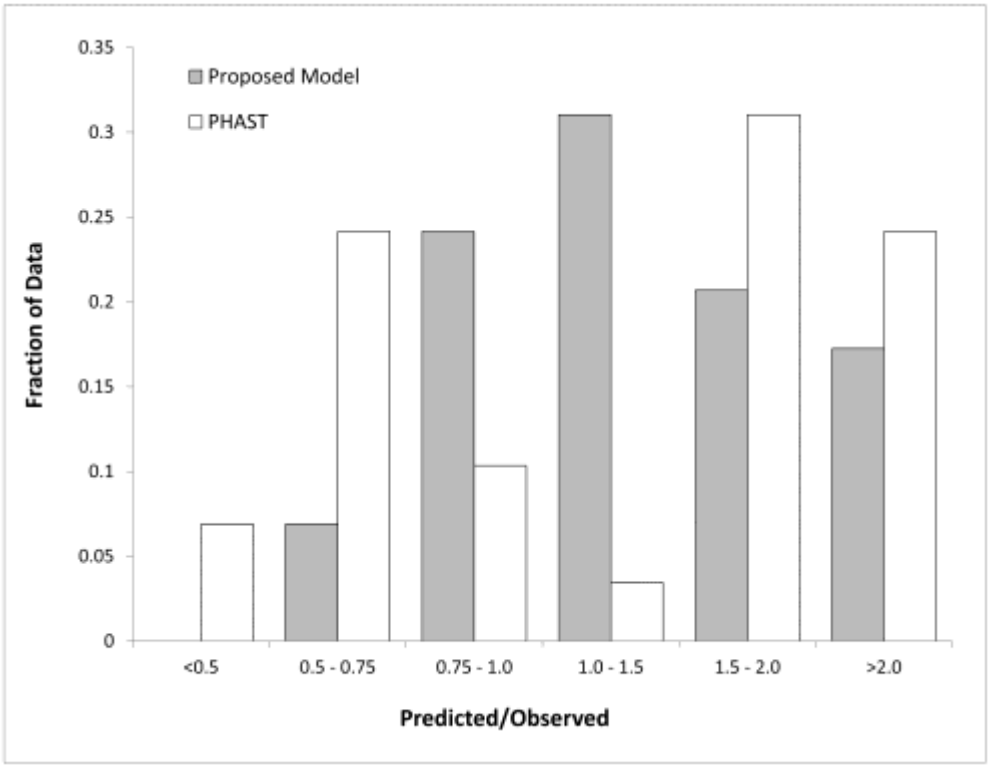

Figure 3. Plume centerline concentrations vs. distance for Burro trial 8.

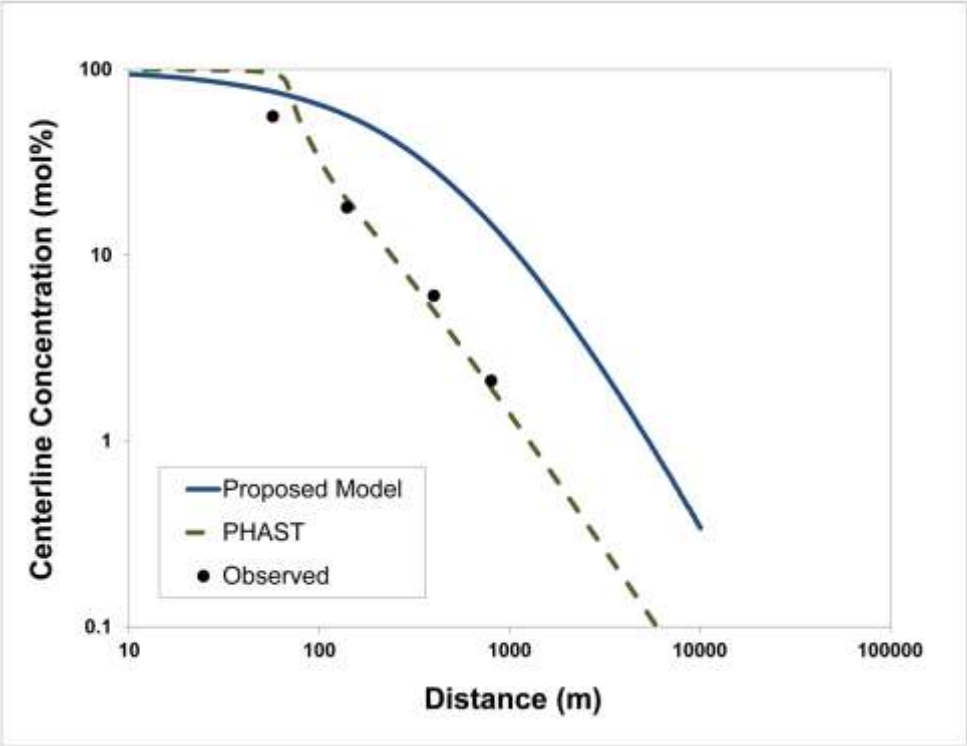

Figure 4. Comparison of data from the Burro trials with model predictions.

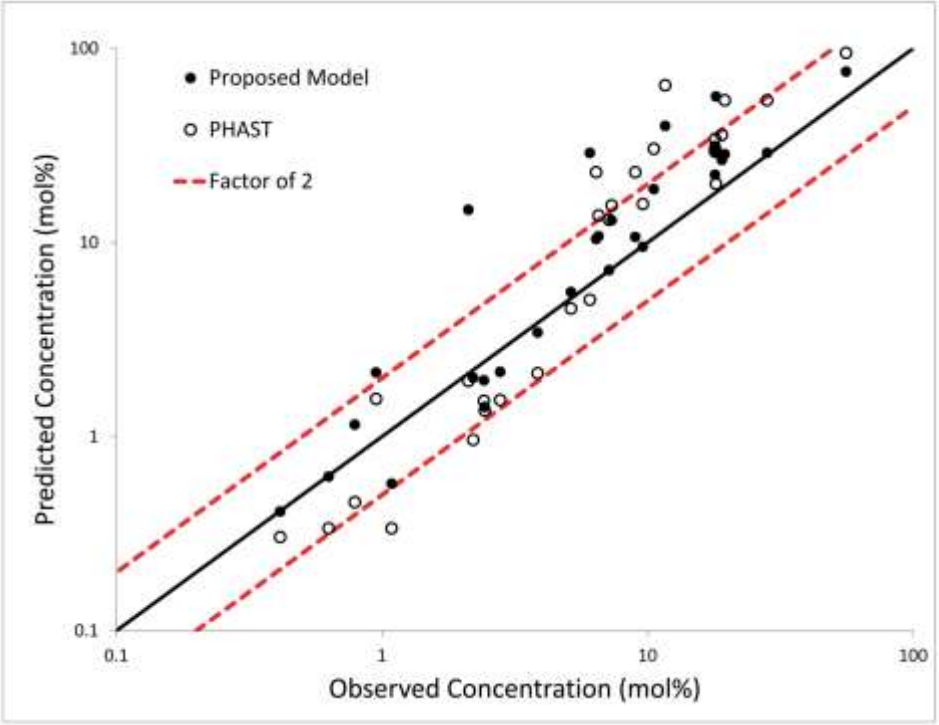

Figure 5. Plume centerline concentrations vs. distance for Burro trial 7.

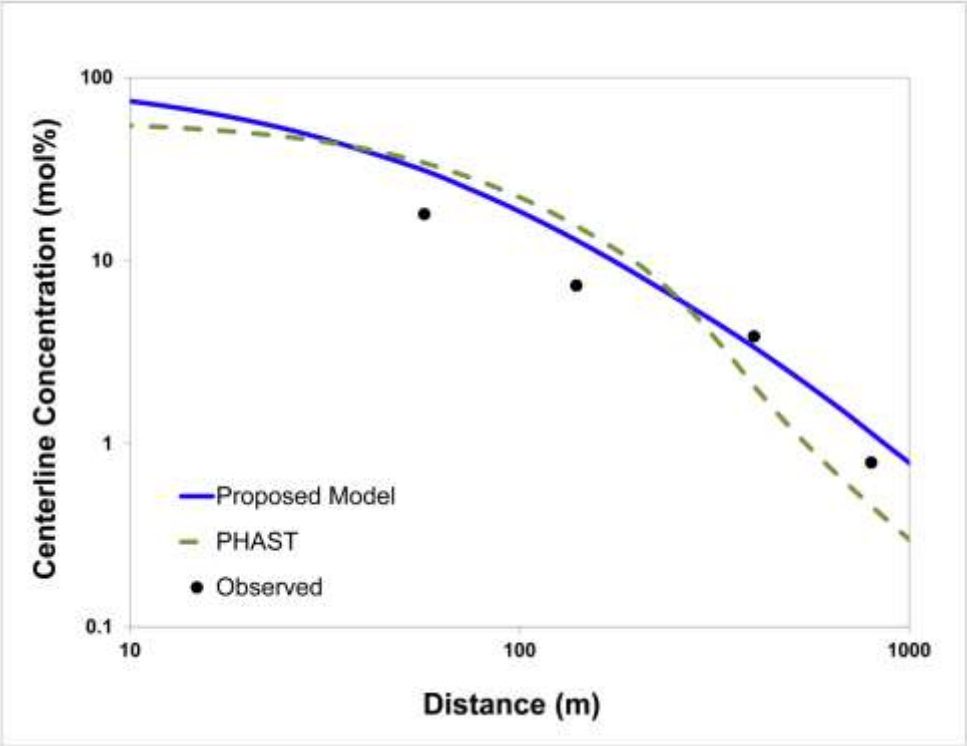

Figure 6. Plume centerline concentrations vs. distance for Burro trial 9.