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AN EVALUATION OF FOUR BOX MODELS FOR INSTANTANEOUS DENSE-GAS RELEASES

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SUMMARY

Four box models for instantaneous hazardous gas releases have been evaluated with data from the Burro field scale tests and also laboratory scale experiments performed at the University of Arkansas. The models are the OME model, the DENS1 model, the SLAB model and the BOX model. The BOX model, developed during this study, incorporates the proposed equation for translational speed by Wheatley and Prince (ref. 1), of a dense gas cloud. The models are evaluated using statistical measures similar to the interim guidelines on air quality model evaluation given by the United States Environmental Protection Agency. The non parametric bootstrap resampling procedure, which is relatively new method, was used to obtain confidence limits on the various statistical measures. In predicting ground level concentrations, the SLAB model performed well in all atmospheric conditions and calm conditions; and the BOX model showed a similar performance in unstable cases, neutral cases and calm conditions. The DENS1 model predictions of the cloud speed under all the conditions are in good agreement with observations.

INTRODUCTION

Modeling episodic releases of hazardous or toxic materials is a rapidly evolving field, driven by the efforts of industry to prevent and mitigate such incidents, as well as public concern that is beginning to be reflected in regulatory requirements. The production, transportation and storage of large quantities of heavy, explosive or poisonous gases may present serious hazard to the public.

The process of model development is not complete until it can be shown that the model agrees with observations. Havens (ref. 2) showed that the few dense gas dispersion models available in 1978 produced concentrations that varied over one or two orders of magnitude. Even complex models show considerable uncertainty due to input errors and the stochastic nature of the atmosphere. Prior to 1980, air quality model evaluations were often conducted on an arbitrary, ad hoc basis.

In response to the inconsistent and arbitrary model performance evaluations that were typical of the earlier period, and the need for standardized model evaluation procedures generated by the United States (U.S.) Clean Air Act and

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it's amendments, both the Electric Power Research Institute (EPRI) and the U.S. Environmental Protection Agency (EPA) sponsored workshops on air quality model performance evaluations. The Department of Energy (DOE) and the American Meteorological Society (AMS) also sponsored workshops in model evaluation procedures (ref. 3). As a result of the recommendations of the workshops, EPA produced interim guidelines on procedures to be followed in evaluating air quality models (ref. 4). Hanna and Drivas (ref. 5) presented a list in which the predictions of hazardous gas dispersion models are evaluated using the results of the recent comprehensive field experiments. In most cases, only rudimentary statistical measures are employed and confidence limits are not calculated.

Other researchers (e.g., ref. 6) have further refined the above EPA methods and proposed schemes for estimating confidence intervals. A point to be noted is that none of the model evaluation studies discussed above use the EPA procedures. Instead a typical study contains plots of observed and predicted ground level contours, graphs of peak concentrations versus distance, or tables of observed and predicted distance to a safe health criteria.

Although a number of dense gas dispersion models are available very few are calibrated and evaluated using field experiments. Most of the models use ad hoc assumptions, and it is only recently that attempts are being made to develop models and calibrate and evaluate them using field data.

Therefore, the purpose of this study is to evaluate four hazardous release models using field data. Instantaneous dense gas releases are considered because these situations have not received much attention in model evaluation studies. To the best of our knowledge a detailed model evaluation of instantaneous dense gas dispersion models using the EPA guidelines (ref. 4) has not been reported in the literature.

MODELS USED

A number of models were reviewed before a decision was made as to which models would be appropriate for a comparison and evaluation study. Some of these models were OME (ref. 7); DENS1 (ref. 8); SLAB (ref. 9); HEGADAS (ref. 10); and RVD 2.0 (ref. 11). The OME, DENS1 and SLAB models were chosen due to their applicability to the instantaneous dense gas release scenario. The front-end model, HEGABOX was not readily available to run HEGADAS model for instantaneous releases. A simple model BOX was developed during this study and is used in the evaluation process.

Ontario Ministry of the Environment (OME)

The portable computing system for use in toxic gas emergencies was developed by the Ontario Ministry of the Environment and contains information on a number of priority chemicals that may be involved in emergencies. In the present system, the heavy gas model can only be used for instantaneous releases. The model used is a simple box model with provision for treating liquid droplets in the gas cloud. The cloud is assumed to translate in the direction of, and with the speed of the ambient wind (measured at a height of 10 m) (ref. 7). The model neglects edge entrainment and assumes a value of 0.4 for the vertical entrainment coefficient. The value of constant K in the gravity slumping equation is taken to be 1.0 (ref. 12). It is our understanding that the OME model is undergoing major changes. The OME model has been used in Canada, USA and Europe.

DENS1

This model was developed by Meroney and Lohmeyer at the Colorado State University at Fort Collins (ref. 8). The model is a numerical box model. Entrainment is assumed to occur from both the top and edge of the cloud. The coefficients of edge and top entrainment, α and β, respectively, can be specified to be between 0.0 and 1.0. The behavior of the box model algorithm is critically dependent on the entrainment constants used. For calm release data, the authors of the model suggest the value of 0.1 for both α and β. This model uses a cloud arrival time related to distance by a fraction of the average undisturbed wind speed over cloud depth. The authors suggest that the cloud be advected along with the wind speed at half the cloud's height.

SLAB

SLAB is a computer model that simulates the atmospheric dispersion of a denser than air vapor release developed at the Lawrence Livermore National Laboratory (ref. 9). The SLAB model is based upon averaged forms of the conservation equations for mass, momentum, energy and species. Additional equations are included for the equation of state (ideal gas law) and the cloud dimensions. Turbulent mixing of the cloud with the ambient atmosphere is treated by using the entrainment concept which specifies the rate of air flowing into the cloud. There is also a submodel to treat the rate of ground heating of the cloud when the cloud is cooler than the ground. SLAB uses a logarithmic vertical profile for the ambient downwind velocity.

BOX

The model is based on the analytical solution of equations representing the behavior of a cylindrical cloud for an instantaneous dense gas release. The top and edge entrainment velocities are based on the work by Fay (ref. 13). The entrainment coefficients α and β were evaluated in this study using Thorney Island data sets 6 and 7 (ref. 14). The edge entrainment turned out to be zero and the top entrainment coefficient is 0.03 for the releases having the ratio of height to diameter of cloud as unity. The translational speed of cloud U_C for the slumping phase is computed using:

$$U_C = 0.8\ U_w \left[1 - \frac{\sqrt{1+\Delta_o'}}{\sqrt{\hat{v}+\Delta_o'}} \right] \tag{1}$$

where, U_w is wind speed, $\hat{v}$ is the ratio of cloud volume at time t and initial volume and Δ_o' is the initial density difference between cloud and environment relative to the air density. This equation is from the work of Wheatley and Prince (ref. 1).

DATA SETS USED FOR MODEL EVALUATION

Data sets used for evaluating hazardous release models should be representative of the conditions the model is designed to simulate. The data should be accurate, precise, and complete. They should be gathered at places and over time intervals to which the model pertains. For many statistical procedures, it is desirable to maintain independent data sets for development and for evaluation. Model evaluation should be conducted using data not used in the development of the model.

For the purpose of this study two data sets were selected. The first data set is based on the work of Koopman et al. (ref. 15) involving liquified natural gas (LNG) releases ranging from 24 to 39 m^3. Trials 3, 8 and 9 were used covering unstable, neutral and stable atmospheric conditions. A brief description of each trial is given below:

Burro Trial 3

The spill volume for this experiment was 34 m^3 and the average wind speed was 5.4 m/s. The Pasquill stability class was C and the atmospheric conditions were unstable.

Burro Trial 8

The spill volume was 28.4 m^3 and the average wind speed was 1.8 m/s. The Pasquill stability class was E. The atmospheric conditions were slightly stable.

Burro Trial 9

The spill volume was 24.2 m^3 and the average wind speed was 5.7 m/s. The Pasquill stability class was D and the atmospheric conditions were neutral.

The second data set is from the work of Havens and Spicer (ref. 16). They conducted a set of laboratory experiments. These experiments involved instantaneous releases of right circular cylindrical volumes of heavy gas (Freon-12/air) with initial volumes ranging from 0.034 m^3 to 0.531 m^3 and specific gravities ranging from 2.2 to 4.2. Releases with initial height-to-diameter ratios of 0.4, 1.0, and 1.57 are reported. The gas concentration measurements provide data describing the rapidly slumping, laterally expanding gas cloud. These were calm air, instantaneous heavy gas releases and the gravity spread and dilution data. Five experiments were selected from the series of experiments performed. These were selected such that three have similar specific gravities of gas used, although different initial volumes, and the other two have difference specific gravities of the gas used and different initial volumes. All five experiments were chosen such that the height-to-diameter ratios were 1.0, to be consistent with the conditions of the calibration procedure of the BOX model.

STATISTICAL MEASURES FOR COMPARING MODELS

In order to determine if one model is significantly better than another, it is necessary to use performance measures. Performance measures give estimates of the discrepancy between predictions and observations. They may be classified as magnitude of difference measures, and correlation or association measures. In this paper, the following five statistical measures are used based on the work by Fox (ref. 17), EPA (ref. 4) and others:

1) Bias or mean error (ME)
2) Fractional bias (FB)
3) Fractional variance (FS)
4) Normalized mean square error (NMSE)
5) Coefficient of determination (r^2)

A brief description of each of the above statistical measures follows. Let C_p be the predicted concentration and C_o the measured concentration at time t for the purpose of defining ME, FB, FS, NMSE and r^2.

Model Bias

Many of the performance statistics characterize the behavior of the model residual, defined as the observed concentration minus the estimated concentration. For example, model bias is defined as the value of the model residual averaged over an appropriate range of values. Large over- and underestimations may cancel in computing this average. The desired value of the model bias is zero.

$$\mathrm{Bias} = \overline{C_p - C_o} \qquad (2)$$

The normalized or fractional bias of the mean concentrations (FB) could be written as:

$$\mathrm{FB} = \frac{2(\overline{C_p} - \overline{C_o})}{(\overline{C_p} + \overline{C_o})} \qquad (3)$$

where $\overline{C_p}$ and $\overline{C_o}$ are the mean predicted and observed concentrations respectively. FB varies between -2 and +2, with a desired value of zero. A similar parameter, the fractional variance (FS) can be defined using the variance of the predictions and observations:

$$\mathrm{FB} = \frac{2(\sigma^2_{C_p} - \sigma^2_{C_o})}{(\sigma^2_{C_p} + \sigma^2_{C_o})} \qquad (4)$$

Model Precision

Model precision refers to the average amount by which estimated and observed concentrations differ as measured by a different type of residual than that used for bias, that is the absence of an algebraic sign. While large positive and negative residuals can cancel when model bias is calculated, the unsigned residuals comprising the precision measures do not cancel. Thus, they provide an estimate of the error scatter about some reference point. This reference point can be the mean error or zero error. Two types of precision measures are the noise, which delineates the error scatter about the mean error, and the gross variability, which delineates the error scatter about zero error.

The performance measure for noise is either the variance of the residuals, σ_d^2, or the standard deviation of the residuals, σ_d. The performance measure for gross variability is the mean square error, or the root-mean-square-error. For our study, a modified performance measure, the normalized mean square error will be used. Supplementary analyses for model precision should include confidence limits.

Normalized Mean Square Error

This performance measure emphasizes the scatter in the entire data set and is defined as the normalized mean square error (NMSE):

$$\mathrm{NMSE} = \frac{\overline{(C_p - C_o)^2}}{\overline{C_o}\;\overline{C_p}} \qquad (5)$$

The normalization by $\overline{C_o}\;\overline{C_p}$ assures that the NMSE will not be biased towards models that overpredict or underpredict. Smaller values of NMSE denote better model performance.

Correlation Analyses

Correlation analyses involve parameters calculated from linear least squares regression and associated graphical analyses. A value of 'r' closer to 1.0 implies good model performance. The numerical results constitute quantitative measures of the association between estimated and observed concentrations. The graphical analyses constitute supplementary qualitative measures of the same information. The correlation is estimated by the parameter 'r' which is given by:

$$r = \frac{(C_p-\overline{C_p})\;(C_o-\overline{C_o})}{\sigma_{C_p}\sigma_{C_o}} \qquad (6)$$

CONFIDENCE LIMITS

The various statistics calculated contain a finite number of observations and corresponding model predictions. Since these observations and predictions can be assumed to be a part of an infinite distribution of samples, we must ascertain the confidence in our estimates of the above mentioned statistics.

Bootstrapping is one way of doing this (Efron (ref. 18), Hanna (ref. 6)). In essence, the bootstrap procedure entails the random resampling from the original sample set, with replacement. Thus any number (say "n") of new samples sets of the same size as the original data set can be generated. The values of the observed and predicted data points are picked independent of each other and not as pairs. From these new "n" samples sets, n values of the required statistic can be calculated. These can be used to form a cumulative distribution function of the statistic. Confidence limits based on any required degree of certainty can than be calculated from this distribution function. This procedure can be applied to any statistic and the 95 percent confidence interval is usually estimated. In this paper confidence limits are estimated on NMSE, FB, FS and the correlation r.

RESULTS AND DISCUSSION

The four models were run using input data from three Burro trials and five laboratory experiments reported by Havens and Spicer. The concentration and the distance traveled by the cloud were computed as a function of time. The predicted values were compared with the corresponding observations and the statistical measures ME, FB, FS, NMSE, r^2, percent of predictions within a factor of two of the observed values (Fa2) and confidence limits on NMSE, FB, FS and correlation coefficient were computed. The results are given in Figures 1 and 2 and tabulated in Tables 1 through 8.

Burro 3

Figs. 1(a) and (b) show the graphs for the two runs, i.e., concentration vs. time; and distance traveled vs. time. From the graphs it is quite obvious that the SLAB and BOX models predict the concentration in time much better than the other two models, OME and DENS1. From Fig. 1(b), it can be seen that the BOX model predicts the distance traveled for a given time (speed of the cloud) in a much superior manner than any of the other models being considered. The DENS1 model underestimates, and the SLAB and OME models overestimate the speed of the cloud by a great extent.

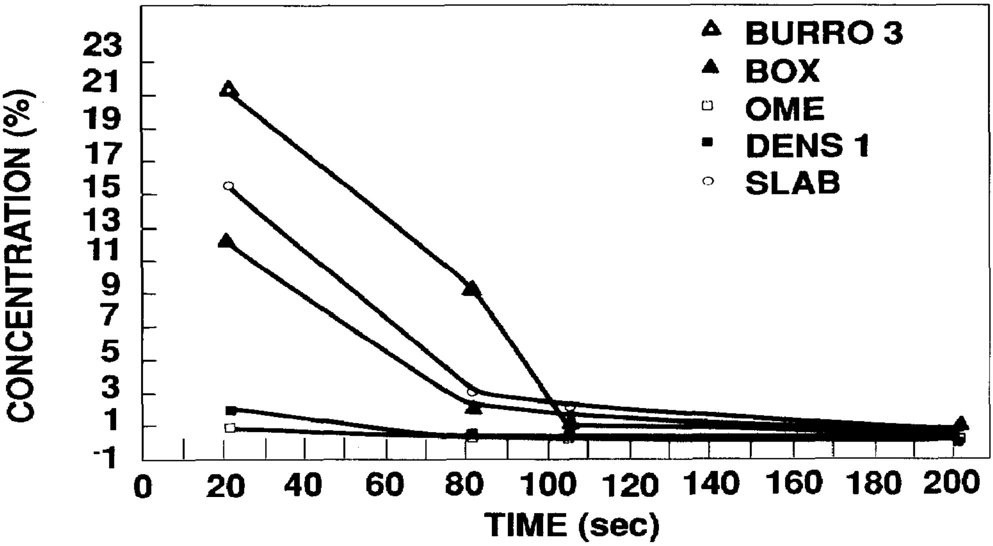

Figure 1(a). **A Comparison of Observed (BURRO 3 Data) and Predicted Concentrations with Time**

The reason for the BOX model underpredicting the concentration may be due to greater dilution of the cloud by the air entrainment mechanism. The SLAB model on the other hand predicts the concentration very well, but simulates a faster cloud speed than observed.

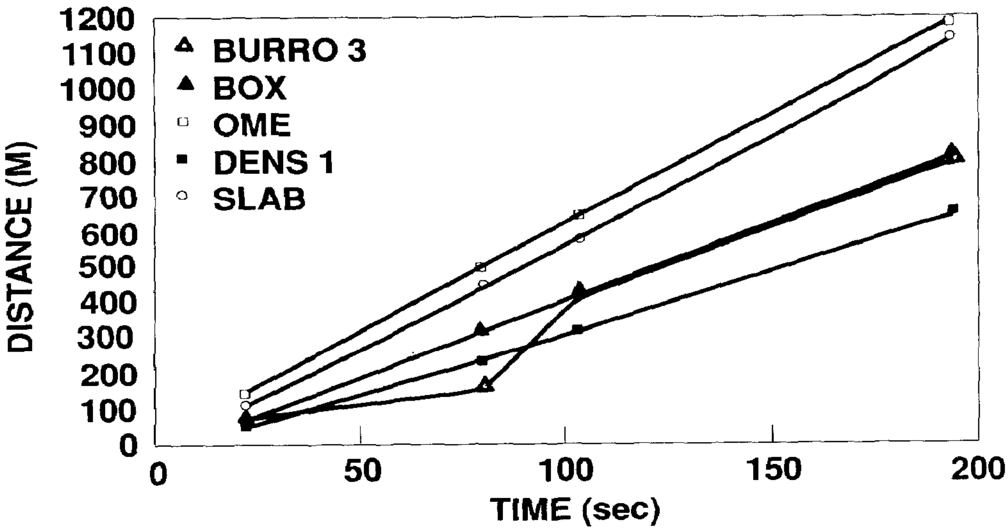

Figure 1(b). **A Comparison of Models with BURRO 3 Field Data for Distance Travelled by the Cloud**

The statistics given in Table 1 lead to the same conclusions. For example, in Table 1(a) the correlation and Fa2 for the BOX and SLAB models are the highest and the NMSE, FB, FS, are the lowest. On the other hand, in Table 1(b), the correlation is the highest for the BOX and DENS1 models, while the NMSE, FB and FS are the lowest. Also, the confidence limits on the parameters in Table 1 estimate values of the NMSE, FB, and FS nearer to zero for the BOX and SLAB models than the other two. Similarly, from Table 1(b), the confidence limits on the FB, FS, and NMSE estimate lower values for the BOX and DENS1 models than the other two. It must be mentioned here, that the need to adopt more than one or two statistical parameters is quite obvious. One or two parameters may not give any definite conclusion or may not be able to differentiate between model performance. For example, in Table 1(a), the correlation and bias do not display any wide disparities, and it is not clear as to which model is really superior. But the NMSE, Fa2, FB and FS, help in differentiating between the model performances.

TABLE 1

STATISTICAL MEASURES FOR EACH MODEL (BURRO 3 DATA)

TABLE 1(a): TIME vs. CONCENTRATION

MODEL	MEAN	SIGMA	BIAS	NMSE	COR	Fa2	FB	FS
BOX	3.92	4.69	-3.95	1.11	.95	.75	.67	.58
OME	.21	.34	-7.66	75.45	.93	.00	1.90	1.85
DENS1	.45	.74	-7.42	32.59	.92	.00	1.78	1.68
SLAB	5.13	5.99	-2.75	.46	.95	.50	.42	.34

CONFIDENCE LIMITS

	NMSE	FB	FS	COR
BOX	0.24 - 4.55	-0.40 - 1.20	-0.67 - 1.73	.78 - 1.0
OME	32.33 - 667.75	1.86 - 1.99	1.76 - 1.99	.90 - 1.0
DENS1	13.55 - 441.22	1.70 - 1.98	1.52 - 1.99	.89 - 1.0
SLAB	0.14 - 2.67	-0.62 - 0.97	-1.11 - 1.57	.77 - 1.0

TABLE 1(b): TIME vs. DISTANCE

MODEL	MEAN	SIGMA	BIAS	NMSE	COR	Fa2	FB	FS
BOX	385.00	264.42	35.75	.04	.98	0.75	-.97	.09
OME	610.00	383.62	260.75	.39	.97	0.50	-.54	-.28
DENS1	296.50	213.98	-52.75	.11	.98	1.00	.16	.30
SLAB	552.28	373.44	203.02	.28	.97	0.75	-.45	-.25

CONFIDENCE LIMITS

	NMSE	FB	FS	COR
BOX	.00 - 0.62	-0.56 - .01	-0.94 - 0.82	.83 - 1.0
OME	.19 - 1.99	-1.03 - -.41	-1.24 - 0.57	.80 - 1.0
DENS1	.07 - 0.23	-0.26 - .29	-0.71 - 1.01	.83 - 1.0
SLAB	.13 - 1.56	-0.90 - -.34	-1.20 - 0.66	.80 - 1.0

Burro 8

This trial was performed in low wind speeds and slightly stable conditions. It can be seen from Tables 2(a) and (b), that only the SLAB model predicts the concentration as a function of time well. The other 3 models perform poorly. But from Fig. 2(b) and Table 2(b), it can be seen that the BOX and DENS1 models predict the cloud travel distance in time better than the other models. One reason for the BOX model predicting such low concentrations could be attributed to greater cloud dilution, when in practice, there is minimal dilution under stable conditions.

TABLE 2

STATISTICAL MEASURES FOR EACH MODEL (BURRO 8 DATA)

TABLE 2(a): TIME vs. CONCENTRATION

MODEL	MEAN	SIGMA	BIAS	NMSE	COR	Fa2	FB	FS
BOX	0.74	0.72	-15.85	43.17	.997	.00	1.83	1.84
OME	0.17	0.21	-16.42	203.79	.976	.00	1.96	1.95
DENS1	0.16	0.19	-16.43	213.33	.988	.00	1.96	1.96
SLAB	10.04	10.59	-6.56	0.54	.999	.75	0.49	0.49

CONFIDENCE LIMITS

	NMSE	FB	FS	COR
BOX	9.60 - 66.1	1.66 - 1.84	1.48 - 1.87	.987 - 1.0
OME	96.01 - 454.1	1.95 - 1.98	1.92 - 1.98	.960 - 1.0
DENS1	101.30 - 392.4	1.96 - 1.97	1.93 - 1.97	.979 - 1.0
SLAB	0.11 - 0.9	.27 - 0.57	-0.41 - 0.63	.996 - 1.0

TABLE 2(b): TIME vs. DISTANCE

MODEL	MEAN	SIGMA	BIAS	NMSE	COR	Fa2	FB	FS
BOX	438.1	358.8	88.9	.09	.997	1.0	-.23	-.21
OME	657.5	512.4	308.3	.63	.998	0.5	-.61	-.56
DENS1	302.3	260.9	-47.0	.04	.994	1.0	.14	.10
SLAB	573.5	537.3	224.3	.57	.994	1.0	-.49	-.60

CONFIDENCE LIMITS

	NMSE	FB	FS	COR
BOX	.03 - .16	-.35 - -.16	-.33 - -.03	.995 - 1.0
OME	.38 - .98	-.80 - -.56	-.66 - -.37	.996 - 1.0
DENS1	.01 - .12	.05 - .26	-.07 - .48	.989 - 1.0
SLAB	.12 - .90	-.57 - -.33	-.75 - -.24	.989 - 1.0

Burro 9

The atmospheric conditions for this trial were neutral. Tables 3(a) and (b) show that the BOX and SLAB models predict the concentration as a function of time better than the other two, although BOX is slightly superior than SLAB. The BOX and DENS1 models predict the cloud downwind travel distance in time better than the other two models (Table 3(b)).

TABLE 3

STATISTICAL MEASURES FOR EACH MODEL (BURRO 9 DATA)

TABLE 3(a): TIME vs. CONCENTRATION

MODEL	MEAN	SIGMA	BIAS	NMSE	COR	Fa2	FB	FS
BOX	5.32	7.34	-.53	1.01	.66	.25	.10	-.62
OME	.28	.47	-5.60	26.97	.63	.00	1.82	1.56
DENS1	.76	1.29	-5.10	8.13	.63	.00	1.54	1.00
SLAB	11.27	12.72	5.42	2.01	.75	.75	-.63	-1.10

CONFIDENCE LIMITS

MODEL	NMSE	FB	FS	COR
BOX	.45 - 5.1	-.51 - 1.33	-1.85 - 1.67	.45 - 1.0
OMER	9.35 - 1122.3	1.64 - 1.99	-0.49 - 1.99	.41 - 1.0
DENS1	2.11 - 573.9	1.13 - 1.99	-1.28 - 1.99	.41 - 1.0
SLAB	.05 - 3.5	-1.03 - .22	-1.90 - .49	.54 - 1.0

TABLE 3(b): TIME vs. DISTANCE

MODEL	MEAN	SIGMA	BIAS	NMSE	COR	Fa2	FB	FS
BOX	407.08	291.37	57.8	.06	.968	.75	-.15	.03
OME	641.25	415.02	292.0	.49	.965	.75	-.59	-.36
DENS1	301.25	220.70	-48.0	.09	.978	.75	.15	.27
SLAB	549.40	391.80	200.1	.29	.976	.75	-.45	-.30

CONFIDENCE LIMITS

MODEL	NMSE	FB	FS	COR
BOX	.002 - .89	-.58 - -.001	-1.07 - .68	.824 - 1.0
OME	.252 - 2.33	-1.02 - -.443	-1.34 - .31	.819 - 1.0
DENS1	.055 - .29	-.22 - .296	-.78 - .86	.851 - 1.0
SLAB	.137 - 1.53	-.80 - -.299	-1.23 - .30	.853 - 1.0

Thus from the Burro series of trials, it can be seen that the BOX and SLAB models are the better models for predicting downwind concentration as a function of time. The OME and DENS1 models assume great dilutions and hence predict much lower concentrations. The BOX and DENS1 models incorporate superior treatments of the cloud translational speed and hence predict the downwind location of the cloud in time better than the other two models.

Havens/Spicer 1-5

Figs. 2(a) and (b) show the graphs for the two runs, i.e., concentration vs. time; and distance traveled vs. time. Tables 4(a) and (b) list the results of the statistics related to the above two runs respectively. A comparison with the results obtained from the other four trials show similar trends and model performance (Tables 5-8). Thus a discussion of the first trial will suffice to describe the other four trials. The reason for the agreement is that the atmospheric conditions for all the trials were the same. The only differences were the initial specific gravities and initial volumes of gas used.

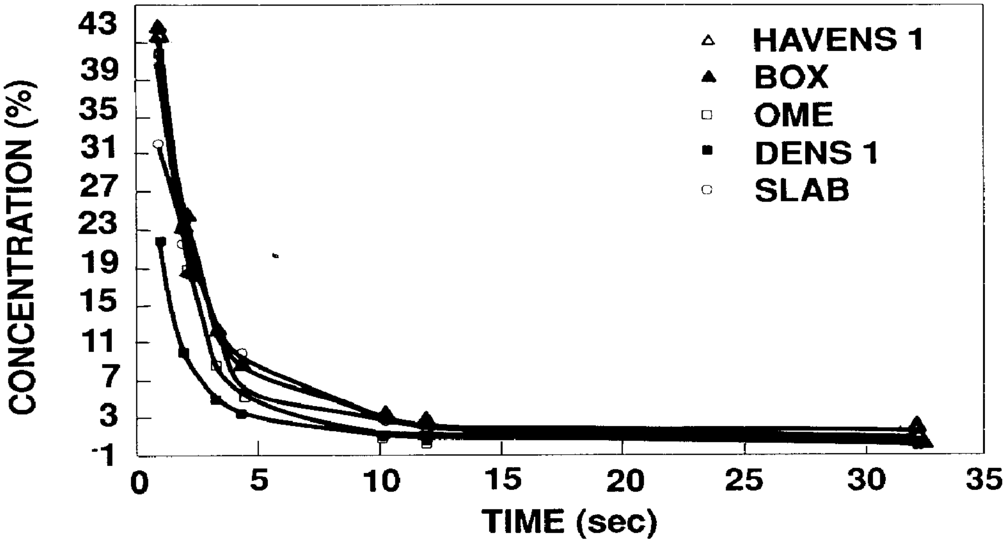

Figure 2(a). A Comparison of Observed (H/S 1 Data) and Predicted Concentrations with Time

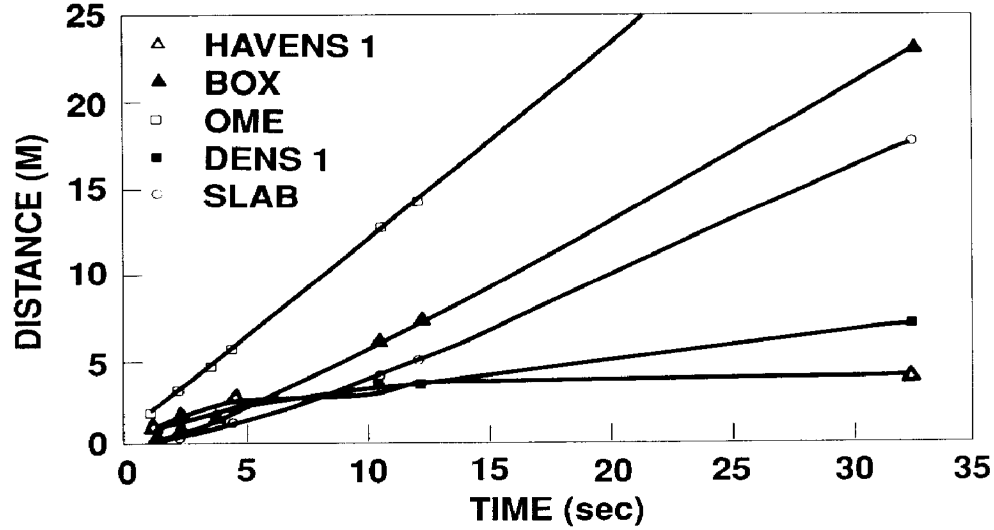

Figure 2(b). A Comparison of Observed (H/S 1 Data) and Predicted Concentrations

TABLE 4

STATISTICAL MEASURES FOR EACH MODEL (HAVENS/SPICER 1 DATA)

TABLE 4(a): TIME vs. CONCENTRATION

MODEL	MEAN	SIGMA	BIAS	NMSE	COR	Fa2	FB	FS
BOX	13.12	14.53	0.99	0.02	.994	.86	-.08	-.032
OME	10.65	14.02	-1.48	0.03	.997	.57	.13	.003
DENS1	5.70	7.08	-6.43	1.31	.997	.29	.72	.661
SLAB	11.23	10.88	-0.90	0.16	.965	.86	.08	.256

CONFIDENCE LIMITS

MODEL	NMSE	FB	FS	COR
BOX	.001 - 0.14	-.22 - .02	-.25 - .02	.953 - 1.0
OME	.004 - 0.43	.05 - .57	-.10 - .21	.967 - 1.0
DENS1	.736 - 2.23	.67 - .93	.60 - .85	.948 - 1.0
SLAB	.017 - 0.36	-.24 - .27	-.22 - .41	.914 - 1.0

TABLE 4(b): TIME vs. DISTANCE

MODEL	MEAN	SIGMA	BIAS	NMSE	COR	Fa2	FB	FS
BOX	5.67	7.44	3.17	3.83	.821	0.57	-0.78	-1.53
OME	11.36	11.69	8.86	6.92	.843	0.29	-1.28	-1.69
DENS1	2.80	1.93	0.30	0.19	.894	1.00	-0.11	-0.63
SLAB	4.19	5.76	1.69	2.66	.796	0.29	-0.51	-1.41

CONFIDENCE LIMITS

MODEL	NMSE	FB	FS	COR
BOX	.42 - 6.1	-1.18 - .17	-1.7 - -0.85	.77 - .993
OME	1.52 - 10.5	-1.49 - -.88	-1.8 - -1.30	.79 - .995
DENS1	.01 - 0.4	-.35 - .14	-1.0 - 0.05	.85 - .994
SLAB	.17 - 4.3	-.99 - .51	-1.6 - -0.46	.74 - .994

TABLE 5

STATISTICAL MEASURES FOR EACH MODEL (HAVENS/SPICER 2 DATA)

TABLE 5(a): TIME vs. CONCENTRATION

MODEL	MEAN	SIGMA	BIAS	NMSE	COR	Fa2	FB	FS
BOX	12.44	17.57	-2.25	.08	.997	.63	.17	.14
OME	12.63	19.44	-2.06	.03	.998	.50	.15	.04
DENS1	14.17	30.86	-0.52	.84	.952	.13	.04	-.42
SLAB	13.46	18.65	-1.22	.05	.993	.63	.09	.08

CONFIDENCE LIMITS

MODEL	NMSE	FB	FS	COR
BOX	.04 - 0.24	.06 - 0.36	-.29 - .20	.97 - 1.0
OME	.01 - 0.68	.08 - 0.71	-.32 - .06	.98 - 1.0
DENS1	.37 - 4.50	-.30 - 1.20	-.51 - .92	.91 - 1.0
SLAB	.02 - 0.36	-.12 - 0.32	-.52 - .13	.94 - 1.0

TABLE 5(b): TIME vs. DISTANCE

MODEL	MEAN	SIGMA	BIAS	NMSE	COR	Fa2	FB	FS
BOX	9.15	8.93	6.00	3.24	.953	0.25	-0.98	-1.45
OME	17.08	13.89	13.92	6.52	.962	0.13	-1.38	-1.63
DENS1	4.24	2.63	1.09	0.21	.978	1.00	-0.30	-0.59
SLAB	6.66	6.55	3.51	1.88	.949	0.25	-0.72	-1.28

CONFIDENCE LIMITS

MODEL	NMSE	FB	FS	COR
BOX	1.78 - 4.66	-1.17 - -0.32	-1.58 - -1.31	.86 - 0.997
OME	4.34 - 8.33	-1.47 - -1.09	-1.72 - -1.56	.88 - 0.998
DENS1	0.12 - 0.26	-0.39 - -0.10	-0.80 - -0.48	.93 - 1.000
SLAB	0.95 - 2.80	-0.94 - 0.00	-1.46 - -1.09	.85 - 0.997

TABLE 6

STATISTICAL MEASURES FOR EACH MODEL (HAVENS/SPICER 3 DATA)

TABLE 6(a): TIME vs. CONCENTRATION

MODEL	MEAN	SIGMA	BIAS	NMSE	COR	Fa2	FB	FS
BOX	19.52	22.46	-5.47	.21	.993	.75	.25	.30
OME	31.69	38.66	6.70	.21	.976	.50	-.24	-.24
DENS1	10.80	14.40	-14.19	1.73	.991	.13	.79	.72
SLAB	21.94	23.02	-3.05	.18	.976	.88	.13	.28

CONFIDENCE LIMITS

MODEL	NMSE	FB	FS	COR
BOX	.02 - .40	.04 - .34	-.05 - .36	.98 - 1.0
OME	.05 - 1.30	-.48 - .10	-.77 - -.13	.94 - 1.0
DENS1	.92 - 3.66	.71 - 1.0	.65 - .88	.98 - 1.0
SLAB	.08 - .45	-.30 - .29	-.30 - .41	.92 - 1.0

TABLE 6(b): TIME vs. DISTANCE

MODEL	MEAN	SIGMA	BIAS	NMSE	COR	Fa2	FB	FS
BOX	7.6	9.55	4.02	2.96	.882	.38	-.72	-1.37
OME	15.11	15.24	11.54	5.91	.909	.38	-1.24	-.16
DENS1	4.75	3.54	1.17	.30	.947	1.00	-.28	-.66
SLAB	4.98	6.62	1.41	1.61	.858	.13	-.33	-1.15

CONFIDENCE LIMITS

MODEL	NMSE	FB	FS	COR
BOX	.46 - 4.87	-1.10 - .32	-1.56 - .68	.81 - .98
OME	1.44 - 8.67	-1.41 - .79	-1.70 - -1.16	.85 - .98
DENS1	.03 - .48	-.46 - -.00	-.92 - -.17	.91 - .99
SLAB	7.42 - 2.94	-.76 - .81	-1.39 - -.11	.78 - .97

TABLE 7

STATISTICAL MEASURES FOR EACH MODEL (HAVENS/SPICER 4 DATA)

TABLE 7(a): TIME vs. CONCENTRATION

MODEL	MEAN	SIGMA	BIAS	NMSE	COR	Fa2	FB	FS
BOX	20.75	23.23	-7.49	.33	.983	.63	.31	.37
OME	24.79	32.95	-3.45	.03	.996	.50	.13	.02
DENS1	8.91	10.47	-19.33	3.65	.990	.00	1.04	1.05
SLAB	17.41	18.25	-10.83	.82	.959	.63	.48	.59

CONFIDENCE LIMITS

MODEL	NMSE	FB	FS	COR
BOX	.03 - .80	.072 - .44	-.15 - .47	.966 - 1.0
OME	.01 - .62	.040 - .71	-.24 - .10	.981 - 1.0
DENS1	1.51 - 7.33	.912 - 1.18	.67 - 1.11	.974 - 1.0
SLAB	.05 - 1.64	.065 - .66	-.15 - .74	.906 - 1.0

TABLE 7(b): TIME vs. DISTANCE

MODEL	MEAN	SIGMA	BIAS	NMSE	COR	Fa2	FB	FS
BOX	11.02	11.31	7.45	3.78	.94	.50	-1.02	-1.46
OME	18.58	17.12	15.00	6.98	.95	.38	-.14	-1.62
DENS1	4.98	3.42	1.41	.29	7.96	1.00	-.33	-.63
SLAB	7.00	8.00	3.63	2.10	.92	.13	-.67	-1.27

CONFIDENCE LIMITS

MODEL	NMSE	FB	FS	COR
BOX	1.44 - 5.56	-1.22 - -.370	-1.61 - -1.19	.858 - .988
OME	3.41 - 9.34	-1.47 - -.995	-1.73 - -1.46	.875 - .990
DENS1	.09 - .41	-.46 - -.090	-.87 - -.35	.918 - .994
SLAB	.56 - 3.39	-.95 - .195	-1.49 - -.82	.840 - .983

TABLE 8

STATISTICAL MEASURES FOR EACH MODEL (HAVENS/SPICER 5 DATA)

TABLE 8(a): TIME vs. CONCENTRATION

MODEL	MEAN	SIGMA	BIAS	NMSE	COR	Fa2	FB	FS
BOX	19.4	23.4	.07	.04	.988	.625	-.004	.018
OME	15.1	23.4	-4.30	.07	.997	.375	.248	.019
DENS1	8.9	12.2	-10.40	1.42	.997	.125	.736	.644
SLAB	16.4	20.5	-2.92	.11	.984	.500	.163	.151

CONFIDENCE LIMITS

MODEL	NMSE	FB	FS	COR
BOX	.01 - .46	-.24 - .19	-.66 - .09	.94 - 1.0
OME	.02 - 4.15	.13 - 1.38	-.16 - .71	.92 - 1.0
DENS1	.72 - 2.77	.67 - 1.10	.27 - .68	.97 - 1.0
SLAB	.04 - .42	-.04 - .43	-.53 - .24	.95 - 1.0

TABLE 8(b): TIME vs. DISTANCE

MODEL	MEAN	SIGMA	BIAS	NMSE	COR	Fa2	FB	FS
BOX	12.01	11.65	8.44	3.98	.944	0.25	-1.10	-1.47
OME	20.75	17.78	17.17	7.47	.953	0.13	-1.40	-1.64
DENS1	4.88	3.15	1.31	0.23	.968	1.00	-.31	-.56
SLAB	8.67	8.72	5.09	2.45	.938	0.25	-.83	-1.32

CONFIDENCE LIMITS

MODEL	NMSE	FB	FS	COR
BOX	2.37 - 5.59	-1.25 - -0.62	-1.61 - -1.36	.862 - .990
OME	4.77 - 9.79	-1.51 - -1.17	-1.73 - -1.56	.884 - .991
DENS1	0.10 - 0.31	-0.42 - -0.13	-0.80 - -0.39	.915 - .993
SLAB	1.33 - 3.51	-1.04 - -0.28	-1.51 - -1.16	.842 - .994

From Figs. 2(a) and (b) and Tables 4(a) and (b), it can be seen that all the models predict the concentration decline with time in the cloud quite well. The BOX model and the SLAB model have high r and Fa2 and low values of NMSE, FB and FS as compared to OME and DENS1 models.

From Fig. 2(b) and Table 4(b), it can be seen that only the DENS1 model predicts the downwind travel distance with time well. This may be due to the fact that the DENS1 model was calibrated using laboratory-scale data and almost similar conditions to these experiments. The OME model far overestimates the cloud speed, while the SLAB model is better than BOX in it's predictions of cloud speed.

As discussed earlier, one advantage of using several statistical measures is that it allows us in evaluating one model over the other. This is important in situations when the coefficient of determination for the models being evaluated is in the same range. A simple computation on percent of predictions within a factor of two of the observed values (Fa2) along with other statistical measures is also useful for practical applications. For example, in predicting concentrations DENS1 model has high values of r and low values of Fa2. However, high values of r and Fa2 and low values of NMSE, FB and FS were obtained in predicting cloud speed from DENS1 model.

CONCLUDING REMARKS

Four box models for instantaneous dense-gas releases were evaluated against field and laboratory data reported in literature. A set of statistical measures were used in determining the performance of each model. From this study, the following points can be made on the performance of models:

A. Prediction of Concentration With Time

1) The BOX model performed well in unstable and neutral atmospheric conditions.
2) The SLAB model did a good job in stable, neutral and unstable atmospheric conditions.
3) The BOX model and the SLAB model produced good concentration estimates under calm conditions.

B. Prediction of Cloud Speed With Time

1) The DENS1 model predictions under all the conditions considered are in good agreement with observed data.
2) The BOX model performed well in stable and neutral atmospheric conditions.

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