

Predictions by Computer Models of Downwind Effects from Instantaneous Releases of Toxic Gases¹

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Introduction

Small towns located on rail or highway transportation routes, or which have chemical industry, oftentimes have a great deal of trouble dealing with the release of toxic gases. By the time they had contacted the shipper, the company responsible or local, state and federal officials to find out the nature of the hazard and what areas to evacuate, it is too late. Many times the general public has already been exposed to the toxic material.

Five computer programs have been developed which will help the appropriate officials to determine the following: 1) The concentration of the toxic gas at any point at any given time after the release. 2) Locates the toxic gas cloud at any given time after release. This program increments distance and gives the concentration of the gas at each downwind distance at a given time after release. 3) Calculate the shape and size and location of the toxic gas cloud at any given time after release. This program plots concentration isopleths. 4) Calculate the concentration with time as the toxic gas passes a fixed point. This could be used to determine the integrated dose that an individual would be exposed to if he did not evacuate. 5) The evacuation zone needed for public safety. This program plots an evacuation zone encompassing an area where the public will be exposed to a concentration that may cause bodily harm. This program also computes the arrival time of the toxic gas cloud and thus allows the determination of the time allowed for evacuation. A book of data including calculations for some common size gas releases and accompanying plastic templates have been developed which can be used with geological survey maps for a rapid determination of evacuation zones.

Equations of the Model

A model equation for the concentration produced at a given time and location downwind following an instantaneous release of a gas has been reported (2) and is expressed as

$$C = \frac{2Q}{(2\pi)^{\frac{3}{2}} \sigma_x \sigma_y \sigma_z} \exp \left[-\frac{1}{2} \left(\frac{x - ut}{\sigma_x} \right)^2 \right] \\ \cdot \exp \left[-\frac{1}{2} \left(\frac{H}{\sigma_z} \right)^2 \right] \exp \left[-\frac{1}{2} \left(\frac{Y}{\sigma_y} \right)^2 \right]$$

¹ The programs are written in the HP-Basic language for the Hewlett Packard 9830A computer equipped with plotter. A list of the programs can be obtained from the authors.

in which C (g/m^3) is the concentration at the surface at the location $x(\text{m})$ downwind from the release on the center line and $y(\text{m})$ lateral displacement perpendicular to the center line, $H(\text{m})$ is the vertical height at which the release occurs; σ_x , σ_y , σ_z (m) are dispersion coefficients referred to the horizontal x and y directions and the vertical z direction; Q (g) is the amount of the release; U (m/s) is the windspeed; and $t(\text{s})$ is the time interval following the release.

The dispersion coefficients σ_x , σ_y , and σ_z are in general complex functions of the weather conditions which are meteorologically classified by six weather stability categories, which are labeled as A through F from the most unstable to the most stable weather category. Weather stability category D is commonly regarded as an average condition which can be generally employed for estimations of the desired type where more detailed weather information is not available and was chosen to be employed as the basis for all of the computations carried out in this investigation.

In a previous paper (1) the authors reported the determination of low order functional approximations for horizontal and vertical dispersion coefficients to apply to a plume produced by a continuously emitting source for all six weather conditions. However, the data reported (2) indicated that these same dispersion coefficients would not apply to instantaneous releases. Values for σ_y and σ_z were reported for only two downwind distances from the source, and it was suggested that σ_x should be about the same as σ_y (2). It was regarded for this application that an adaptation of any of the previously determined approximations for any weather condition which would reasonably agree with the two specified values for weather condition D for both σ_y and σ_z would provide the most favorable estimation to apply to instantaneous releases. It was found that σ_y and σ_z to apply to an instantaneous release under weather condition D could be estimated by the σ_y and σ_z approximations for a continuous source under weather conditions F and E, respectively. The approximation for σ_y was also applied as the approximation for σ_x .

All of the computer programs developed were derived from the reported equation for the downwind concentration with the dispersion coefficients computed by the approximation stated above.

The Programs and their Applications

Program 1: This first basic program was developed to directly calculate the concentration at a specified position and time. This program is used to answer specific questions such as, "Is the emergency vehicle located at the corner of 1st Street and Chestnut Avenue being subjected to a dangerous concentration at this time?"

Program 2: This program developed as a modification of Program 1 will scan over a range of distance at a given time after the release. This program is used to locate the cloud as a variation of concentrations with distance at any given time. The program also has the capability of plotting the concentrations on a selected map scale. An example of the output of this program is presented in Table 1.

Program 3: This program was developed to locate and plot the isopleths or contours of constant concentration for a specified concentration using a range of distance previously determined from application of Program 2. The maximum concentration which can be employed is also obtained from the output of Program 2. This program is used to show the region in which the concentration will exceed a specified value or values. Several isopleths for differing concentrations can be overlaid in the same figure. Exemplary plots of a system of isopleths is shown in Figure 1.

Program 4: This program was developed to scan over time at a fixed position

TABLE I. *Variation of Concentration with Distance*
Amount Released, Q1 = 500 Pounds at Height, H1 = 10 feet or Wind Speed, U1
= 5 M.P.H. Time After Release = 30 Minutes.

DWIND DIST	CONC PPM
2.000	0.000
2.100	0.000
2.200	0.001
2.300	0.558
2.400	13.753
2.500	33.746
2.600	13.010
2.700	1.134
2.800	0.030
2.900	0.000
3.000	0.000

following the release. The concentration is computed with variation of time to indicate the exposure variation with time at that position. An example of the output

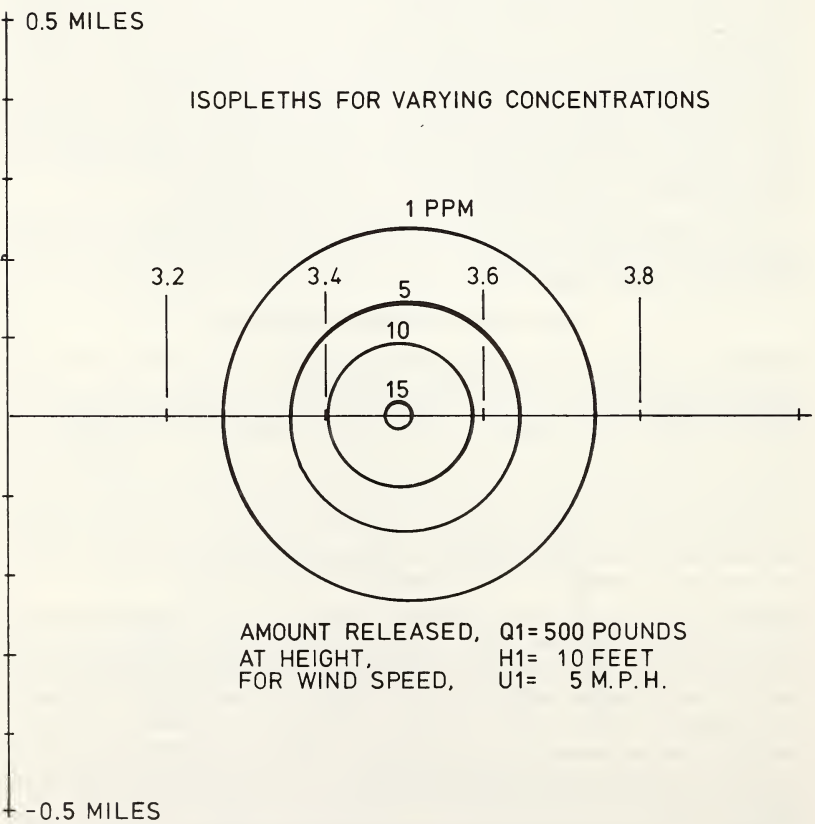


FIGURE 1.

TABLE II. *Variation of Exposure With Time at A Fixed Downwind Location. Amount Released, $Q_1 = 500$ Pounds At Height, $H_1 = 10$ feet for Wind Speed, $U_1 = 5$ M.P.H. for Downwind Distance, $X = 2.5$ miles.*

TIME (MIN)	CONC (PPM)
27.000	0.11
28.000	2.59
29.000	17.77
30.000	33.75
31.000	17.77
32.000	2.60
33.000	0.11

of this program is shown in Table II. This output can be numerically integrated to yield a total exposure a person would encounter at a given location.

Program 5: This program was developed to determine and plot the envelope of the isopleths for a specified concentration but varied over a sequence of times. The region contained within the envelope is exposed at some time to a concentration above the specified value. Two or more envelopes for differing concentrations can be overlaid on the same figure. Exemplary Plots from this program are shown in Figure 2.

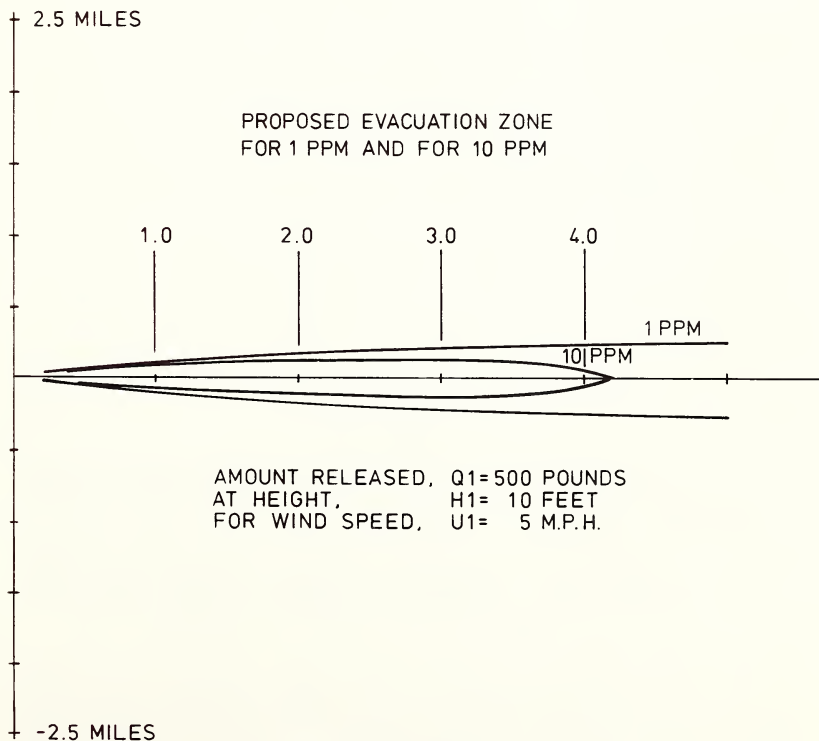


FIGURE 2.

This computer program has a great deal of practical utility. The output could aid authorities in rapidly assessing the area in which an imminent danger existed in the event of a toxic gas release or spill. It would allow them to get an idea of the urgency of the situation, and how much time they had to evacuate the people downwind from the source.

The program allows the user to pre-estimate the most likely size of a toxic gas release in his region, and to plot to scale the size of the downwind area that would be considered for evacuation. This isopleth envelope is drawn by the computer and can be permanently mounted on a plastic template or overlay. The authors have made some templates of this type to the same scale as found on Geological Survey maps. This was done so that the program would have the broadest applicability. With this information at hand an evacuation zone could be rapidly determined and the time allowed for such an evacuation could be obtained from a set of pre-calculated tables. The users of this information would have to know the following parameters: 1) the exact place and time of the toxic gas release, 2) the estimated size of the release, 3) the direction and velocity of the wind, 4) the height above the ground that the release took place. With this input information, the program will calculate: 1) the downwind centerline concentration, P , in parts per million at downwind distance, X , in miles, 2) the arrival time, T , in minutes at downwind distance X , 3) and the lateral displacement, Y , in miles of the toxic gas cloud at some predesignated concentrations. An example of the tabulate output of this program is given in Table III.

TABLE III. *Evacuation Zone Data*

Amount Release, $Q_1 = 500$ Pounds At Height, $H_1 = 10$ Feet for Wind Speed, $U_1 = 5$ M.P.H. Isopleth Envelope = 10 PPM

X(MI.)	T(MIN)	P(PPM)	Y(MI.)
0.500	6.000	1727.033	0.054
1.000	12.000	309.527	0.083
1.500	18.000	115.118	0.102
2.000	24.000	57.526	0.112
2.500	30.000	33.746	0.115
3.000	36.000	21.893	0.109
3.500	42.000	15.219	0.092
4.000	48.000	11.125	0.052
4.500	54.000	8.449	0.000

Literature Cited

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