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INTERNATIONAL CENTRE FOR SCIENCE AND HIGH TECHNOLOGY
c/o INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS 34100 TRIESTE (ITALY) VIA GRIGNANO, 9 (ADRIATICO PALACE) P.O. BOX 586 TELEPHONE 040-224572 TELEFAX 040-224575 TELEX 460449 APH I

SMR/760-7

"College on Atmospheric Boundary Layer and Air Pollution Modelling"
16 May - 3 June 1994

"Guidelines for Use of Vapor Dispersion Models"

S. HANNA
Environmental Research and Technology, Inc.
Concord, Massachusetts
USA

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a sufficient time has elapsed that neighboring puffs overlap each other. This computational problem has been partially solved by Zannetti (1986), who uses trapezoidal-shaped plume segments rather than puffs under certain conditions in his AVACTI model.

While the puff trajectory models are justified from physical arguments, Lewellen et al. (1985) have found that their predictions do not agree with observations much better than the predictions of standard straight-line Gaussian plume models. They used data from the set of experiments at Idaho National Engineering Laboratory (INEL) from which the example in Figure 5-12 was drawn. It is suspected that the uncertainties due to stochastic variability in atmospheric concentrations are responsible for the lack of a significant difference among the models.

5.1.6 Concentration Fluctuations; Averaging and Sampling Time

Discussions of averaging and sampling times (see Figure 2-1) or concentration fluctuations are either non-existent or very minimal in the research reviewed to this point. Some models grossly parameterize this effect by assuming that the ratio of the peak (fluctuating) concentration to the model predicted mean concentration is about two. Chatwin (1982) pointed out that in many cases involving accidental releases of hazardous gases, the maximum short term (~1 sec) concentration is the most important variable to predict. Lung damage from H_2S can occur with one breath if the concentration is sufficiently high, and an explosion of gas from an LNG accident can occur if a spark is struck in a small volume of gas at the flammability limit. According to Chatwin the mean concentration predicted by the model can be irrelevant in these cases, since the probability distribution function (pdf) of concentration fluctuations in the atmosphere is characterized by a standard deviation at least as large as the mean. The relative magnitude of concentration fluctuations ($\sigma_c/\bar{C}$) is the same order as the relative magnitude of velocity fluctuations (σ_u/U) in the atmosphere. The parameters σ_c and σ_u are the standard deviations of turbulent fluctuations in concentration and wind speed, respectively. Thus it is important to predict the upper end of the pdf for the

H_2S and LNG incidents described above. Since Chatwin's article was published, a few other researchers have studied this problem, although we are far from having a comprehensive operational model.

Predictions of models such as DEGADIS or FEM3 can be thought of as ensemble means for certain averaging times. An ensemble mean is defined as the mean over an infinite number of realizations of a given experiment. The averaging time is usually implicit in the data used by the model and in its formulations for treating the input data - for example, if hourly-averaged wind and turbulence observations are used, then the predictions represent a one hour average. If the Pasquill-Gifford-Turner dispersion curves are used, then the predictions represent a 10 minute average, since data from 10 minute periods were used to derive the curves. In the case of instantaneous (puff) models, the predictions represent an ensemble mean only to the extent that a large enough set of experiments (20 or more) was used to derive the model. These experiments should be conducted under the same external conditions (i.e., wind speed, stability, source term). For example, if it were possible to run the Thorney Island experiments long enough that 100 independent time periods (e.g., of ten-minute duration) could be found which all satisfy the following conditions:

$4.8 < u < 5.2$ m/s, $\qquad 65\% < RH < 70\%$

$10^o < T_a < 12^oC$, $\qquad 10^o < T_{surface} < 12^oC$

$-2 <$ net radiation flux < 2 watts/m^2

$(\rho_p - \rho_a)/\rho_a = 2$, $h=10m$, $R=10m$,

then the observed concentration field averaged over these 100 experiments would approach an ensemble average. The reader quickly sees that it is difficult operationally and financially to generate ensemble averages from atmospheric field experiments. A true ensemble would contain an infinite number of individual data points!

Thus the results of a single experiment, or even three or four experiments will likely differ (perhaps by as much as an order of magnitude) from the ensemble mean predictions of the model. If this happens, it is not an indictment of the model but may be a manifestation of the inherent stochastic variability of the atmosphere.

Wind tunnel experiments can be used to study variability, since it is easier to insure repeatability of experiments and thus create a large ensemble of data. On the negative side, the wind tunnel cannot simulate larger scale eddies and other phenomena that contribute to variability in the atmosphere. Furthermore, the laboratory Reynolds number is not high enough to permit the establishment of an inertial subrange like there is in the atmosphere. Meroney and Lohmeyer (1984) conducted extensive studies of dense gas clouds released in a wind tunnel and calculated the concentration fluctuation intensity, $\sigma_C/\overline{C}$, for various source volumes, wind speeds and downwind distances. These results are plotted in Figure 5-14, showing that the average $\sigma_C/\overline{C}$ is about 0.3 in this wind tunnel. In contrast, Hanna (1984) reports observed values of $\sigma_C/\overline{C}$ of 1.5 on the plume centerline and $\sigma_C/\overline{C}$ of 5.0 on the plume edges for a smoke plume released in the atmospheric boundary layer.

The probability distribution function (pdf) of concentration fluctuations in the atmosphere has been studied by several persons (e.g. Wilson, 1982; Hanna, 1984; Lewellen and Sykes, 1985), and all agree that the distribution is non-Gaussian and is skewed towards higher concentrations. For hazardous gas analysis, we are usually interested in the probability $P(C>C_L)$ that the concentration is higher than some limiting value, C_L:

$$P(C>C_L) = \int_{C_L}^{\infty} p(C)\, dC \qquad (5\text{-}56)$$

It has been suggested that the probability distribution function, p(C), can be approximated by a log-normal, clipped normal, or Gamma function. The exponential function is a special case of the Gamma function, and is quite good for intermittent clouds or plumes. The intermittency, I, is defined as the fraction of time that non-zero concentrations are observed at a monitor. For the exponential distribution, $\sigma_C/\overline{C}$ equals one. In this case, the pdf is given by the formula:

$$p(C) = (I^2/\overline{C})\exp(-IC/\overline{C}) + (1-I)\,\delta(0) \qquad (5\text{-}57)$$

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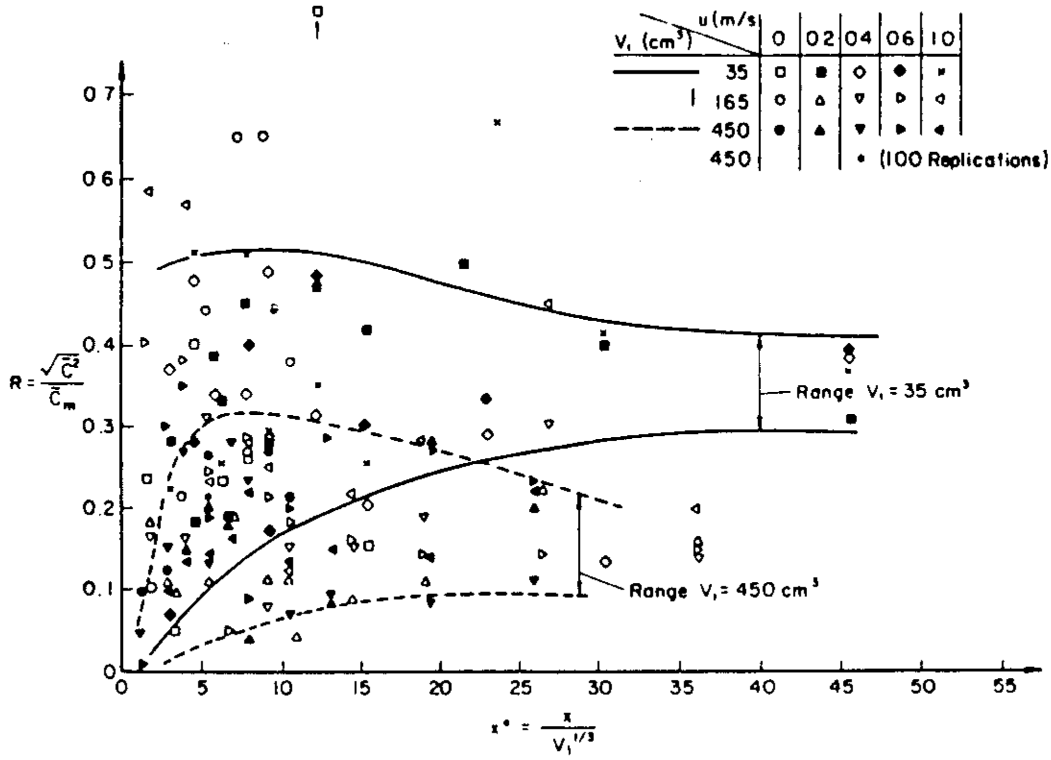

Figure 5-14. Concentration variance ratio, $\sigma_C/\bar{C}$, versus downwind distance, observed by Meroney and Lohmeyer (1984) in a wind tunnel. The source is an instantanteous dense gas cloud.

where the Dirac delta function $\delta(0)$ equals 1.0 at C equal to 0 and equals 0.0 elsewhere. This can be substituted into equation (5-56) to give:

$$P(C>C_L) = I \exp(-IC_L/C) \tag{5-58}$$

Thus if the dispersion model predicts an ensemble mean, $\bar{C}$, of $0.1C_L$, where C_L is the threshold concentration for some health effect, and the intermittency I equals 0.5, then the probability that the instantaneous C will exceed C_L is 0.3%. If the ensemble mean prediction is $0.5C_L$, then this probability is 18%.

The formulas given above are for nearly-instantaneous averaging times. It is clear that the standard deviation of concentration fluctuations, σ_c, will decrease as averaging time T increases. If the integral time scale of the concentration fluctuations is T_I and the autocorrelogram is assumed to be exponential, then the following formulas apply:

$$R(t') = \overline{C'(t)C'(t+t')}/\sigma_c^2 = \exp(-t'/T_I) \tag{5-59}$$

Then

$$\sigma_c^2(T)/\sigma_c^2(0) = 2(T_I/T)(1-(T_I/T)(1-\exp(-T/T_I))) \tag{5-60}$$

where $\sigma_c^2(0)$ refers to the variance for instantaneous averaging time. If T_I has a typical value for the surface layer (about 10 sec), then the ratio of variances for an averaging time of T equal to 60 sec is 0.28. If the averaging time is one hour, the ratio $\sigma_c(3600s)/\sigma_c(0)$ is 0.075. It can be concluded that the fluctuation intensity $\sigma_c/\bar{C}$ for one hour averages in the atmosphere is about 0.1 even if the integral time scale is only a few seconds.

If it is assumed that the equations in the first part of this section produce predictions of ensemble mean concentrations, $\bar{C}$, then the probability of the concentration exceeding any threshold limit, C_L, can be estimated using equations (5-56) through (5-60) for any averaging time and integral time scale.

Equation (5-60) can be used to assess the effects of averaging over distances as well as time. Observed concentrations and health effects always involve some averaging distance. For example, if the integral distance scale of the turbulence is 5m and the averaging distance is 1m, then the ratio $\sigma_c^2(1m)/\sigma_c^2(0)$ equals 0.94.

At the other end of the scale the sampling time or sampling volume can also influence observations. Figure 2-2 illustrates a typical time series, showing that the sampling time, T_s, can be thought of as the total length of time that the instrument is turned on. It is intuitively obvious that the likelihood of more extreme concentrations being observed is increased if the sampling time increases (e.g. notice how several new "record" high and low temperatures are observed at any given weather station each year). The usual definition of any ensemble assumes that the sampling time is infinity. In practice this requirement is considerably relaxed, such that a set of ten dense gas experiments conducted during similar external conditions is assumed to comprise an ensemble. Equation (5-60) can also be used to calculate the variance "missed" by an instrument because it is turned on for a finite sampling time T_s:

$$\sigma_c^2(0,\ T_s)/\sigma_c^2(0,\infty) = 1-2(T_I/T_s)(1-(T_I/T_s)((1-\exp(-T_s/T_I))) \qquad (5\text{-}61)$$

where the first variable inside the parentheses after σ_c^2 is the averaging time and the second variable is the sampling time. Any eddies with time scales much larger than T_I are not detected by the instrument. For example, if T_s is ten times the integral scale T_I, then only 82% of the total possible variance is seen. If both the sampling time T_s and the averaging time T are finite (as they are in any experiment) then the fraction of the total possible variance can be calculated by multiplying equations (5-60) and (5-61) together. An example is given in Figure 5-15 for the special case $T_s/T = 100$ (for example, averaging time could be one minute and sampling time could be 100 minutes). This function clearly defines a "window", with high and low frequency fluctuations filtered out by the finite sampling and averaging times.

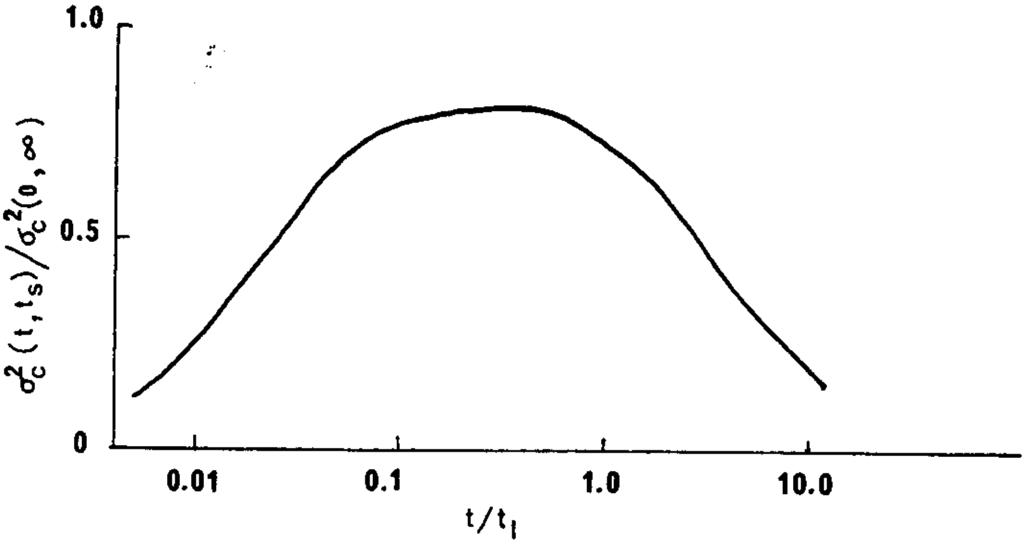

Figure 5-15. Fraction of total possible concentration fluctuation variance from Eqs (5-60) and (5-61), as a function of sampling time T_S, averaging time T and integral time scale T_I. It is assumed that T_S/T_I = 100.

Algorithms for Concentration Fluctuations and Variations of Concentrations with Averaging Time

(First Draft - Jan. 5, 1994; Second Draft - March 23, 1994)
by S.R. Hanna

1) Predictions of Plume Centerline Concentrations at a Given Downwind Distance

Hazardous gas models such as HGSYSTEM can predict the crosswind concentration distribution at distance x from the source for a certain averaging time, T_a. The basic model predictions of the dense gas modules are appropriate for averaging times of about two minutes, which correspond to the field data on which the dense gas algorithms are based. The predictions of the passive gas models generally refer to an averaging time of about 10 or 20 minutes, which is the averaging time for the passive gas field data used in deriving the Pasquill-Gifford-Turner σ_y and σ_z curves. Also, the HGSYSTEM prediction is for an ensemble average--that is, the average of millions of independent realizations of that particular experiment for those specific initial and boundary conditions and other input parameters. Those millions of individual realizations would themselves have a distribution about the ensemble average.

The model predictions of the ensemble average plume centerline concentration, $C_{cl}(x,T_a)$, are not keyed to any particular geographic point--the only restriction is that the downwind distance must be x. But because natural plumes meander or swing back and forth, the ensemble average centerline concentration will drop as averaging time increases, and the position of the centerline may also shift as T_a varies. The effects of averaging time on plumes are thoroughly discussed in the review report by Wilson and Simms (1985).

Consider an ensemble of concentration observations under certain initial and boundary conditions. Then the variation of the distribution of C_{cl} with T_a at a fixed x would be as shown in Figure 1. The box plots indicate key points on the distribution function at each T_a. The dashed line on the figure passes through the mean or median (whichever you prefer) of the distributions. If the model predictions are corrected for averaging time, T_a, the corrected ensemble average concentrations should fall along this dashed line. As averaging time, T_a, approaches 0.0 (i.e. an instantaneous snapshot of the plume), the concentration C_{cl} should approach a value representative of the instantaneous plume.

Concentration on Plume Centerline for Given Averaging Time

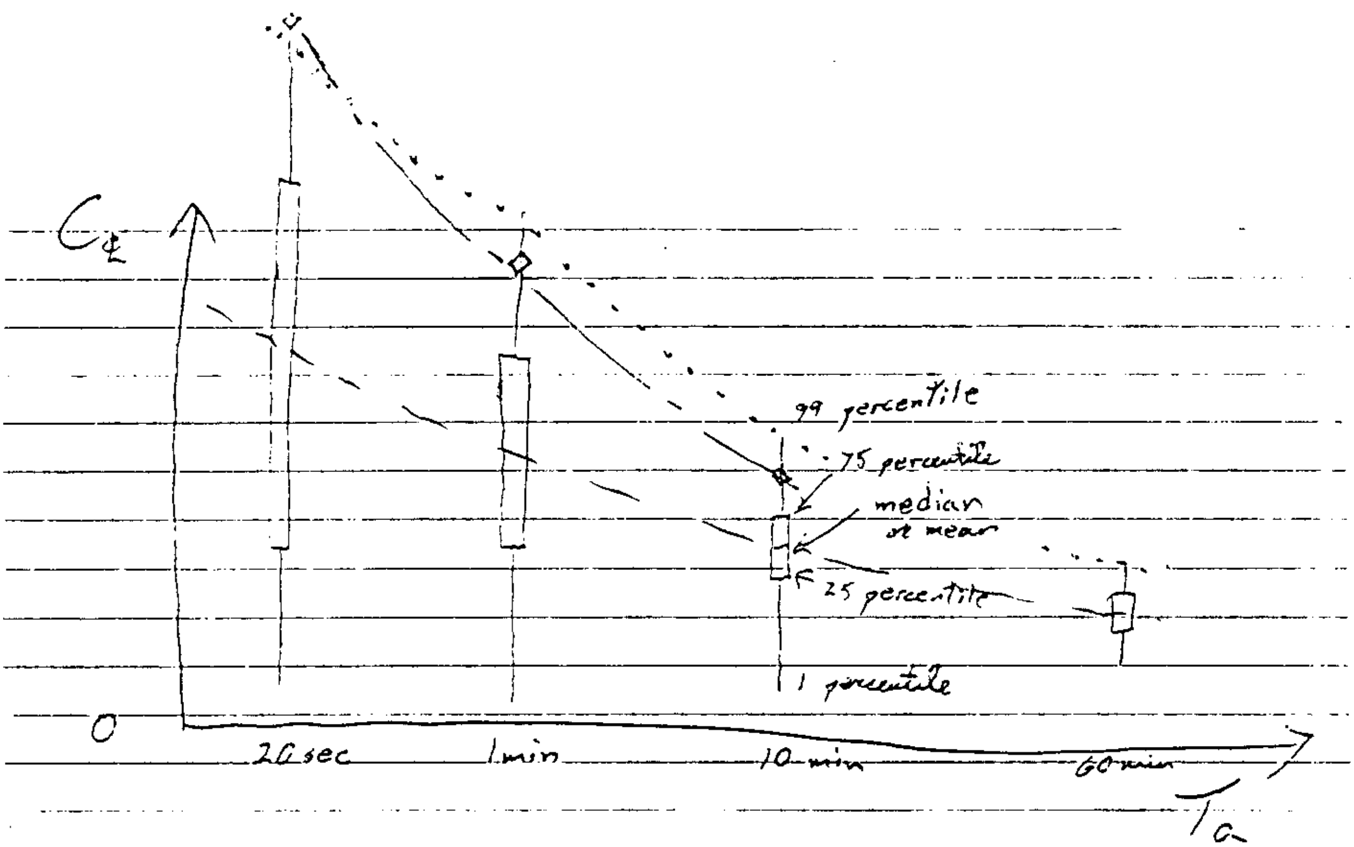

Figure 1. Typical distributions of centerline concentration, $C_{c\ell}$ at a given x, for various averaging times, T_a. The dashed line goes through the means at each T_a, and the dotted line goes through the 99th percentile of each distribution. The dashed-dotted line goes through the maximum at that T_a assuming the sampling time is 60 min.

It should be mentioned that some models such as TRACE are designed to be conservative--i.e., to predict concentrations, C_{cr}, higher than the mean. The descriptions of these models do not specify the quantitative percentile (e.g. the 99th percentile) of the distribution that they are aiming for. However, if a model were designed to predict the 99th percentile at each T_a, the concentration predictions would follow the dotted line in Figure 1. If a model were designed to give the maximum at a given T_a for a given total sampling time (60 min, in this case) the concentration predictions would follow the dash-dot line. In this latter example, the percentile associated with the single maximum concentration would increase as T_a decreases, since the total number of concentration values equals (60 min/T_a).

Parameterizations

Most hazardous gas models that correct for averaging time are attempting to follow the dashed line in Figure 1, even though they do not articulate these conditions. In addition, most models accomplish this correction by applying a $T_a^{1/5}$ power law to the lateral dispersion coefficient, σ_y, due to ambient turbulence.

$$\sigma_y\ (T_{a2}) / \sigma_y(T_{a1}) = (T_{a2} / T_{a1})^{1/5} \quad (1)$$

In order to prevent σ_y from dropping below its known value for instantaneous conditions, which would inevitably happen with equation (1) as $T_{a2} \rightarrow 0$, a "minimum T_{a2}" criterion is usually applied. This is the T_{a2} which would result in σ_y equalling the following values given by Slade (1968) for instantaneous plumes or puffs:

$$\text{Unstable} \quad \sigma_{yI} = 0.14\ x^{0.92} \quad (2)$$

$$\text{Neutral} \quad \sigma_{yI} = 0.06\ x^{0.92} \quad (3)$$

$$\text{Very Stable} \quad \sigma_{yI} = 0.02\ x^{0.89} \quad (4)$$

For neutral conditions, this criterion is satisfied at T_{a2} equal to about 20 seconds, where it is assumed that σ_y for continuous plumes is given by the Briggs-EPA formulas. However this minimum T_{a2} is dependent on what is assumed for (1) distance x, and (2) representative averaging time for the Briggs-EPA formulas. Furthermore, equations (2)-(4) themselves are based on limited data and would have significant uncertainties (say ± 50%).

As a default parameterization, it is recommended that the formulas used by DEGADIS, HGSYSTEM, SLAB, and other models be retained, with the following assumptions:

- The σ_y Briggs-EPA formulas are valid for an averaging time of 20 minutes.
- The "minimum T_a" criterion is 20 seconds.
- Equation (1) is valid for σ_y corrections for T_a.

The models mentioned above assume that the lateral distribution in a dense gas plume is made up of a dense gas core of width W and Gaussian edges with standard deviation, σ_y. The averaging time correction is then applied only to the Gaussian edges. We depart from these models by assuming that the averaging time correlation applies to the entire plume width:

$$C_{ct}(T_{a1})/C_{ct}(T_{a2}) = (T_{a2}/T_{a1})^{1/5} \tag{5}$$

Our analysis (Section 6.1 of Hanna et al., 1993) of field data from the Burro, Coyote, and Desert Tortoise experiments showed that $C_{ct} \propto T_a^{-1/5}$ for many types of dense gas plumes, despite the fact that the DEGADIS, HGSYSTEM, and SLAB models were predicting that the dependency be much smaller (in all cases, the models were predicting that the size of the dense gas core of the plume was relatively large compared to σ_y).

If we were interested in the centerline concentration at a given averaging time at a given percentile as the distribution (see the dotted line on Figure 1), we would need to make an assumption for the form of the distribution. For in-plume fluctuations, a log-normal distribution is applicable (see Hanna, 1984):

$$P(\ell nC) = \int_{-\infty}^{\ell nC} p(\ell nC')\, d(\ell nC') \tag{6}$$

$$p(\ell nC') = \frac{1}{\sqrt{2\pi}\ \sigma_{\ell nC'}}\, e^{-(\ell nC' - \overline{\ell nC'})^2/2\sigma^2_{\ell nC'}} \tag{7}$$

where P is the cumulative distribution function (ranges from 0.0 to 1.0) and p is the probability distribution function.

At small averaging times ($T_a \sim 20$ seconds or less), atmospheric data show that

$$\sigma_{\ell nC}/|\overline{\ell nC}| = 1.0 \tag{8}$$

We will assume that this relation is valid and that $\sigma_{\ell nC}$ decreases as averaging time increases according to the following approximation to Taylor's formula:

$$\frac{\sigma^2_{lnC}\,(T_a)}{\sigma^2_{lnC}\,(20\ \mathrm{sec})} = \frac{1}{1 + T_a/2T_I} \qquad (T_a > 20\ \mathrm{sec}) \tag{9}$$

where T_I is the integral scale for turbulent fluctuations in concentration. For plumes in the atmospheric boundary layer, a default assumption would be

$$\text{Default} \qquad T_I = 300\ \textit{seconds}. \tag{10}$$

With this value of T_I, equations (8) and (9) gives

$$\sigma_{lnC}(\textit{one hour}) = 0.4\ \sigma_{lnC}\,(20\ \mathrm{sec})$$

2) *Predictions of Concentrations at a given Receptor Position*

The discussions in the previous section were concerned with predicted concentrations on the plume centerline or axis, which can shift position with time. For that type of model application, the analyst is concerned only with the maximum plume impact independent of location. Another type of model application would be concerned with the plume impact at a given receptor position, as defined by for example a monitoring site or a critical subset of the surrounding population (say a school or a hospital).

Consider an ensemble of concentration observations from a giver monitoring site. The data are taken from many independent field studies, all with nearly the same ambient conditions (i.e. release rate, wind speed and direction, stability). These observations would show a variation of distribution functions with averaging time as suggested in Figure 2. Note that there are three major differences between Figures 1 and 2:

Figure 1 **Centerline C**	**Figure 2** **Fixed Receptor C**
Median C decreases as T_a increases	Median C is constant with T_a
There are no zeros in C	There are many zeros in C
σ_c is relatively small	σ_c is relatively large

Fixed Monitor Location

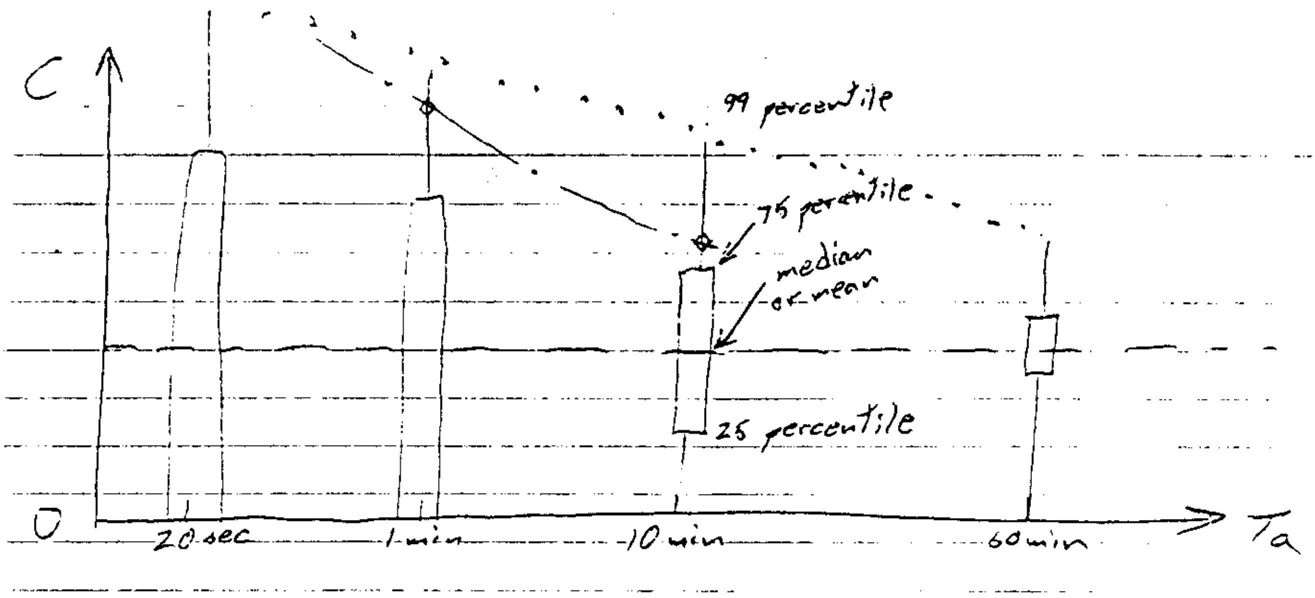

Figure 2. Typical distributions of concentration observed at a given monitor location, for various averaging times, T_a. The dashed line goes through the means at each T_a, and the dotted line goes through the 99th percentile of each distribution. The dashed-dotted line goes through the maximum at that T_a assuming the sampling time is 60 min.

All of these differences are due to the fact that, in the case of Figure 2, the plume can meander away from the receptor, leading to many C = 0 observations at that receptor. In contrast, by definition C_{ct} is always greater than zero in Figure 1.

Often the variation of $_{max}$ with T_a is calculated from data at fixed receptors. A time series C(t) is searched in order to identify the various $C_{max}(T_a)$; for example this was done by us using the field data from the Burro, Coyote, and Desert Tortoise experiments. The resulting C_{max} values would follow the dot-dashed-curve in Figure 2. In that example, the total length of the time series is 60 min (the sampling time T_s). The percentile of C_{max} for each T_a is given by:

$$Percentile/100 = 1 - (T_a/60 \text{ min}) \tag{11}$$

Note that the variation of C_{max} with T_a is greater than the variation of C (fixed percentile) with T_a. From a theoretical point of view, C (fixed percentile) is preferable, but from a practical point of view researchers always seem to work with C_{max}. It is clearly important to at least recognize the difference.

The distribution function that is proposed for the data in Figure 2 must account for the possibility of many zeros. The exponential cumulative distribution function is recommended by Hanna (1984):

$$P(C) = 1 - I \exp(-IC/\overline{C}) \tag{12}$$

$$\sigma_c/\overline{C} = ((2/I) - 1)^{1/2} \tag{13}$$

where I is the so-called intermittency, or fraction of non-zero observations in the total record (I = 1.0 if the plume is always impacting the receptor). A typical value of I in the atmosphere is about 0.2, giving $\sigma_c/\overline{C} = 3$. In the absence of other information, it is recommended that a default value of I = 0.2 be used for very small averaging times, T_a:

$$\left.\begin{aligned} P(C) &= 1 - 0.2 \exp(-0.2C/\overline{C}) & \text{(14a)} \\ \sigma_c/\overline{C} &= ((2/I) - 1)^{1/2} = 3 & \text{(14b)} \end{aligned}\right\} \; as\ T_a \rightarrow 0$$

As averaging time increases to 60 minutes, equation (8) can be used to calculate $\sigma_c^2(T_a)/\sigma_c^2(0)$, again assuming that the integral time scale is 300 seconds and that $\sigma_c/\overline{C} = 3$ at $T_a \rightarrow 0$. "I" can be calculated by inverting equation (13):

$$I = 2/(1 + (\sigma_c/C)^2) \tag{15}$$

The sequence to be followed is given below

Step 1: Calculate $\frac{\sigma_c^2(T_a)}{\sigma_c^2(0)} = \frac{1}{1 + T_a/600 \text{ sec}}$

Step 2: Calculate $I(T_a) = \frac{2}{\left(1 + \left(\sigma_c/\overline{C}\right)^2\right)}$

Step 3: Calculate $P(C) = 1 - I \exp\left(-IC/\overline{C}\right)$

It is assumed that $\overline{C}$ is known and that $\sigma_c/\overline{C}$ ($T_a \rightarrow 0$) = 3 and hence that I ($T_a \rightarrow 0$) = 0.2.

Note: These formulas should not be used at T_a > 3600 sec, since the intermittency, I, would be calculated to exceed 1.0, which is impossible. Instead, use I = 1.0 and $\sigma_c/\overline{C}$ = 1.0 at T_a > 3600 sec.

References:

Hanna, S.R., 1994: The exponential probability density function and concentration fluctuations in smoke plumes. *Bound. Lay. Meteorol.*, **29**, 361-375.

Hanna, S.R., J.C. Chang and D.G. Strimaitis, 1993: Hazardous gas model evaluation with field observations. *Atmos. Environ.*, **27A**, 2265-2285.

Slade, D.H., 1968: Diffusion from instantaneous sources. *Meteorology and Atomic Energy, 1968*, TID-24190, USAEC, 163-175.

Wilson, D.J. and B.W. Simms, 1985: Exposure time effects on concentration fluctuations in plumes. Report No. 47, Dept. of Mech. Eng., Un. of Alberta, Edmonton, Alberta, Canada.