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Dependence of maximum concentration from chemical accidents on release duration

Steven Hanna [a, *], Joseph Chang [b]

[a] Hanna Consultants, 7 Crescent Ave., Kennebunkport, ME 04046, USA
[b] Homeland Security Studies and Analysis Institute, Falls Church, VA, USA

HIGHLIGHTS

- Maximum chlorine concentrations from releases from tanks with fixed mass content are studied.
- Effects of release duration t_d are investigated.
- An analytic formula is derived based on dimensional analysis.
- It is found that t_d has the largest effect near the source.
- At large distances, t_d has little influence and all releases behave like puffs.

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ABSTRACT

Chemical accidents often involve releases of a total mass, Q, of stored material in a tank over a time duration, t_d, of less than a few minutes. The value of t_d is usually uncertain because of lack of knowledge of key information, such as the size and location of the hole and the pressure and temperature of the chemical. In addition, it is rare that eyewitnesses or video cameras are present at the time of the accident. For inhalation hazards, serious health effects (such as damage to the respiratory system) are determined by short term averages (<1 min) of concentrations, C. It is intuitively obvious that, for a ground level source and with all conditions the same (e.g., the same mass Q released), the maximum C near the source will be larger for a shorter than a longer release duration, t_d. This paper investigates the variation with downwind distance, x, of the ratio of maximum C for two time durations of release. Some simplified formulas for dispersion from finite duration releases are presented based on dimensional analysis. A primary dimensionless number of importance is the ratio of the release duration, t_d, to the travel time $t_t = x/u$, at distance, x, where u is wind speed. Examples of applications to pressurized liquefied chlorine releases from tanks are given, focusing on scenarios from the Jack Rabbit I (JR I) field experiment. The analytical calculations and the predictions of the SLAB dense gas dispersion model agree that the ratio of maximum C for two different t_d's is greatest (as much as a factor of ten) near the source. At large distances (beyond a few km for the JR I scenarios), where t_t exceeds both t_d's, the ratio of maximum C approaches unity.

1. Background

Many hazardous gas releases from valve breaks or tank ruptures have a finite time duration, t_d, on the order of a few seconds to several minutes (CCPS/AIChE, 1996). The total mass of material, Q, in the tank or in the pipe is given. A number of dispersion models are available as software packages to assess the downwind concentrations resulting from these releases. For example, Hanna et al. (2008) compared the predictions of six of the more widely-used models using inputs from three major chlorine railcar accidents (Festus, Macdona, and Graniteville). For these large (10–50 ton) releases of chlorine, the important averaging times, T_a, for concentration, C, are a few minutes or less, since more serious health effects occur at such small T_a (Sommerville et al., 2007). One way to determine the variation in maximum concentration C with t_d for a given scenario is a brute force method involving running a model

* Corresponding author.
E-mail address: hannaconsult@roadrunner.com (S. Hanna).

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many times using a range of values of t_d and then choosing the maximum. This can be very time-consuming. A better way to determine the variations in maximum C with t_d is to carry out a set of controlled field experiments with side-by-side (but non-interfering) releases with everything the same except t_d. But field experiments with hazardous substances are expensive and it is difficult to accumulate enough trials under the same conditions required to produce a statistically significant conclusion.

The current paper approaches the estimation of the variation of maximum C with release duration, t_d, by using fundamental similarity formulas for continuous plume dispersion, relative (puff) dispersion, and finite duration releases (e.g., Taylor, 1921; Batchelor, 1950; Pasquill, 1974). These formulas can be written as one-line analytical expressions that can be easily manipulated to show how the maximum C varies as t_d and other inputs vary. Two Jack Rabbit I (JR I) chlorine field experiment trials (see Fox and Storwold, 2011; Hanna et al., 2012) are used as test cases.

It is assumed in the derivations in Section 3 that the fundamental release process (e.g., dense momentum jet, evaporation from liquid pool) is unchanged when comparing concentrations for two values of release duration, t_d. This assumption may not be valid for some release scenarios, such as an initial strong two-phase momentum jet, which may have significant rain-out (deposition of liquid to the surface) and a subsequent period of evaporative release from the liquid pool. In this case the entrainment rates and other processes are different for the two segments of the release.

In the case of flammables, where the concentrations of interest (e.g., LFLs) are a few percent, the results in this paper are valid in the near field as long as the t_d's of interest are associated with the same general release scenario.

If the initial release scenario involves an instantaneous explosion, the concept of two different t_d's is irrelevant, since t_d is always near zero and will be much smaller than the travel times to any distance of interest.

2. Overview of similarity theory of puffs and continuous plumes

In the days before computers, scientists put much thought into the derivation of analytical formulas to describe physical phenomena such as the transport and dispersion of materials released into the boundary layer of the atmosphere. Examples are the seminal papers by Taylor (1921) on dispersion of continuous plumes (one-particle dispersion) and Batchelor (1950) on puffs (two-particle or relative dispersion). Pasquill (1974) reviews this literature and unifies the theory so that it can be applied to time-variable releases, given knowledge of analytical formulas for the spectrum of boundary layer turbulence.

The atmospheric boundary layer is always turbulent and contains a wide spectrum of space or time scales. The material from any type of pollutant release encounters this full spectrum of motion. Depending on the duration of the release, t_d, and its initial size, σ_o, different ranges of this full spectrum have more influence on the turbulent dispersion of the material. Turbulent eddies with sizes much larger than the cloud (plume or puff) do not contribute much to the internal cloud dispersion, since all they do is move the cloud around bodily (e.g., a meandering plume). Pasquill (1974) points out that the range of turbulent eddy scales that affect the dispersion can be understood as a "window", in analogy with signal theory, described as high-pass and low-pass filters.

Gifford (1968) and Hanna et al. (1982) comment that the instantaneous cloud width of a continuous release seen in a downward pointing snapshot at a given downwind distance can be considered equivalent to the width of a single puff at that distance. If more snapshots were taken of the plume in rapid sequence over an averaging time period of T_a, and all snapshots laid on top of each other, the width of the averaged plume will gradually increase as T_a increases. When a large number of cases are considered, the dispersive spread (width) of a time-averaged plume at a given downwind distance is always larger than or equal to the dispersive spread (width) of an instantaneous puff at that distance. Gifford (1968) and Hanna et al. (1982, see Fig. 6.4) present observations of puff and plume widths that demonstrate this difference. The observations show that, depending on the initial cloud size, the wind speed, and the stability, the width of the puff could be as small as 10% of the width of the continuous plume at positions not far from the source.

Batchelor (1950) used similarity theory to suggest a simple relation for the growth of the standard deviation, σ, of a spherical puff. The puff size, as denoted by σ (m), is assumed to increase with time due to turbulence in the inertial subrange, which can be characterized by the eddy dissipation rate ε (m^2/s^3). The variation of σ with travel time, t, is then given by:

$$\sigma^2 = c\varepsilon t^3 \quad (1)$$

where c is a non-dimensional constant that has been determined to be in the range from 0.5 to 2 based on comparisons with field observations.

The Taylor (1921) equation for the growth of continuous plumes is widely used as the basis for current Lagrangian particle dispersion models. It assumes a Lagrangian turbulent time scale of T_L, and gives σ proportional to t at $t << T_L$ and σ proportional to $t^{1/2}$ at $t >> T_L$. Thus, based on the Batchelor (1950) and Taylor (1921) equations, at small to intermediate times of travel, the puff σ is growing at a greater rate (proportional to $t^{3/2}$) than the continuous plume σ (proportional to t). As mentioned above, the puff σ starts out smaller but asymptotically approaches the plume σ at large times of travel.

Gifford (1985) and Gifford et al. (1988) show that the transition in the Taylor (1921) equation to a σ proportional to $t^{1/2}$ regime at large travel times or distances seldom occurs in the many sets of atmospheric observations that they analyzed of horizontal dispersion at scales from 20 to 2000 km (meso to regional scales). They conclude that there are significant magnitudes of horizontal turbulent variations at large time scales (from a few hours up to a day or more). This presence of ever-larger scales of motions causes the lateral standard deviation, σ_y, to continue to increase in proportion to t and not drop off to a $t^{1/2}$ relation.

The vertical dispersion, σ_z, is more strongly influenced than σ_y by stability and by the presence of capping inversions (at the top of the boundary layer or at the tropopause), which limit the vertical extent to which plume or puff material can be spread by turbulent mixing. The daytime boundary layer mixing depth is usually about 1 or 2 km and the tropopause is usually at a height of about 10–15 km. But during the daytime, at times less than about 30 min and distances less than a few km, before the cloud has dispersed throughout the mixed layer, the puff and plume σ_z's follow similar relations as described above for σ_y.

3. Analytical dispersion formulas for puffs and continuous plumes

We are searching for simple analytical dispersion models that can be manipulated to study the ratio of the arc-maximum cloud centerline concentrations predicted for a given scenario for two different release durations, t_{d1} and t_{t2}, where $t_{d1} < t_{d2}$. We shall assume that the total mass of the release, Q, is constant. This would be consistent with a tank of chlorine where different hole sizes lead to different release durations.