Estimating Health Effects of Accidental Releases of Toxic Chemicals such as Chlorine and Ammonia

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Introduction and Background

Toxic chemicals such as chlorine and ammonia can have acute health effects at high concentrations, including destroying lung tissue. This can occur in a few seconds. The health effects do not follow **Haber's law**; i.e. they are not the same for all exposure times for a given dosage (concentration C integrated over time).

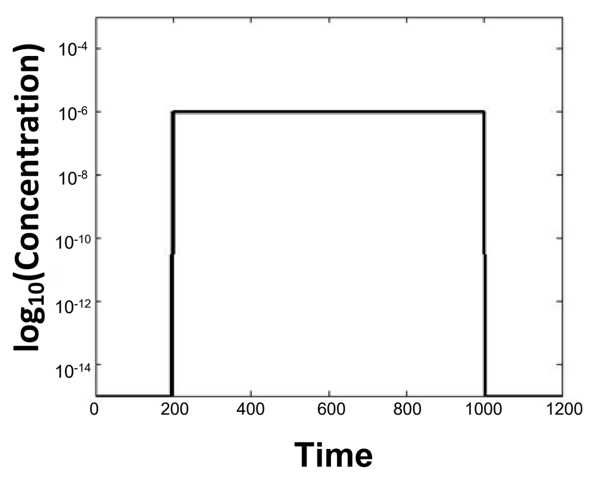
Instead, the **toxic load (TL) formula** should be used as a substitute for dosage. TL says that the health effect is proportional to the integral over time of C^n, where observations[1,2] show that the power law coefficient, n, is between about 2 and 3 for chlorine and ammonia.

$$\text{Toxic Load} = \int C^n dt$$

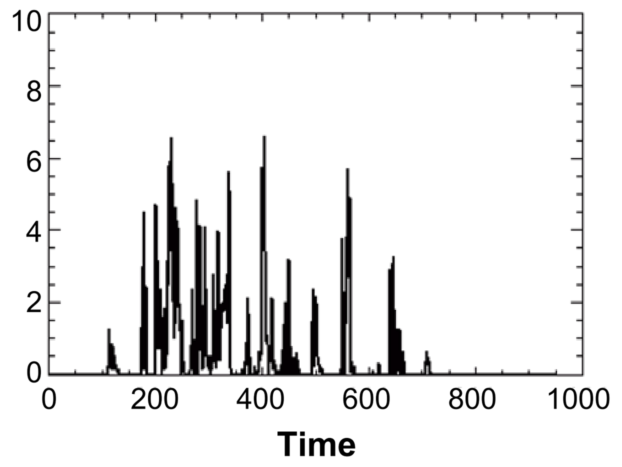
For the same dosage ($D = \int C dt$ = 10 ppm-min), and assuming n = 2, the toxic load TL will be 10 times greater for C = 10 ppm over T = 1 min than for C = 1 ppm over 10 min.

The values for n for many chemicals have been determined in laboratories by exposing animals (sometimes humans) to constant C over different times T. This situation is shown in the left figure below. Of course, in the real atmosphere, C is quite variable due to turbulence and due to time variations in wind direction and emissions (as in the right figure). (the figure is from Platt et al., 2017).

Laboratory Testing Profile



Possible Real-World Profile



Probit formulas for population casualties or incapacitation

Given the toxic load, TL, a probit formula is often used to estimate incapacitation or casualties at certain percentages:

$$Cas(TL) = F[(b/n)\log_{10}(TL/TL_{50})]$$

Where Cas is the fraction of the population receiving the defined health effect at the given TL, F is the standard normalized cumulative distribution function, b is the concentration-based probit slope, and TL_{50} is the defined value for 50 % casualties.

Health Effects Criteria

Various agencies set criteria for health effects of toxic chemicals. The three (AEGL, ERPG, and PAC) below are for non-lethal effects and have similar definitions

- Acute Exposure Guideline Levels (AEGLs)
- Emergency Response Planning Guidelines (ERPGs)
- Protective Action Criteria (PACs)

AEGL-1 is the concentration (expressed as ppm or mg/m^3) of a substance above which it is predicted that the general population, including susceptible individuals, could experience notable discomfort, irritation, or certain asymptomatic nonsensory effects. However, the effects are not disabling and are transient and reversible upon cessation of exposure.

AEGL-2 is the airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape.

AEGL-3 is the airborne concentration above which it is predicted that the general population, including susceptible individuals, could experience life-threatening adverse health effects or death. AEGL's are defined for five averaging times:

Table 1. AEGLs for Chlorine are defined for exposure or averaging times of 10, 30, and 60 minutes, and 4 and 8 hours. Current recommended values are listed in the table below.

	10 min	30 min	60 min	4 hr	8 hr
	ppm	ppm	ppm	ppm	ppm
AEGL 1	0.50	0.50	0.50	0.50	0.50
AEGL 2	2.8	2.8	2.0	1.0	0.71
AEGL 3	50	28	20	10	7.1

In the above table, the chlorine AEGL-3 variation with averaging time follows a C^2 relation. ERPGs are defined similar to AEGLs but are defined only for an averaging time (exposure time) of 60 min. ERPG-1 is 1 ppm, ERPG-2 is 3 ppm and ERPG-3 is 20 ppm.

- Lethal Toxic Load TL_x is defined as the TL where x percent of the population dies.

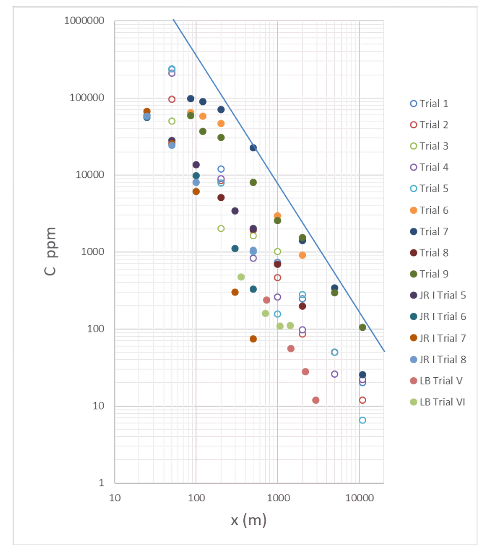
To account for known non-linear effects of chlorine, the toxic load TL and a probit formula are used. Different groups use slightly different values of TL_{50}, n (power law coefficient) and b (probit slope). Also, b varies with the population type and the effect (e.g., lethal, severe, mild). Platt et al. (2017) use the Sommerville et al. (2010) analysis to justify n = 2.75 and b = 6 for lethal effects on the general population. For example, for the general population, TL_{50} = 2.58E+10 min-$(mg/m)^{2.75}$ for lethality. Thus for a chlorine C of 1000 ppm (about 3000 mg/m^3), an exposure time of about 10 min is required to reach TL_{50} .

Real World Examples

The photos below are from two trials during the 2015-2016 Jack Rabbit II field experiment[3]. Each had an 8 ton release of pressurized liquefied chlorine in 30 s. The hole in the tank is at the bottom in the left and in the top in the right figure. As seen in the plot (under the photos) of observed max 3-s C versus distance for the 9 JR II trials, the max C usually exceeded 1000 ppm out to 1 km and exceeded 10 ppm out to 11 km.

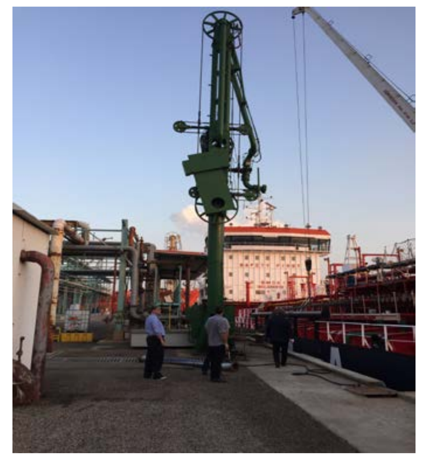
Arc max C (in ppm) versus x for Lyme Bay (LB), Jack Rabbit I (JR I), and Jack Rabbit II (Trials 1 – 9).

Lyme Bay and JR I points are also plotted. They involve 1 to 10 ton releases of chlorine



The straight line represents the -5/3 power law that best fits the max C point at the various x.

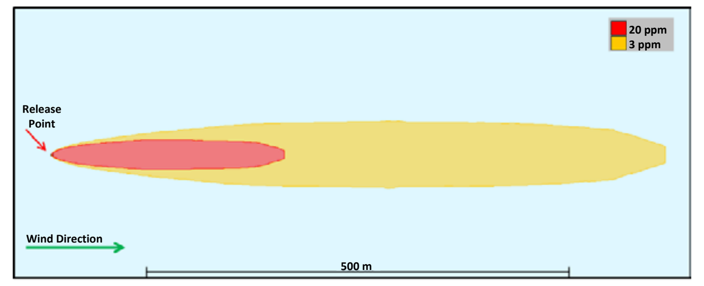
The photos below show an industrial facility handling anhydrous ammonia. Left - The large refrigerated ammonia tank holds about 100,000 tons. Right – The dock and piping system for unloading 6,000 tons from a ship**.**



Modeling Systems

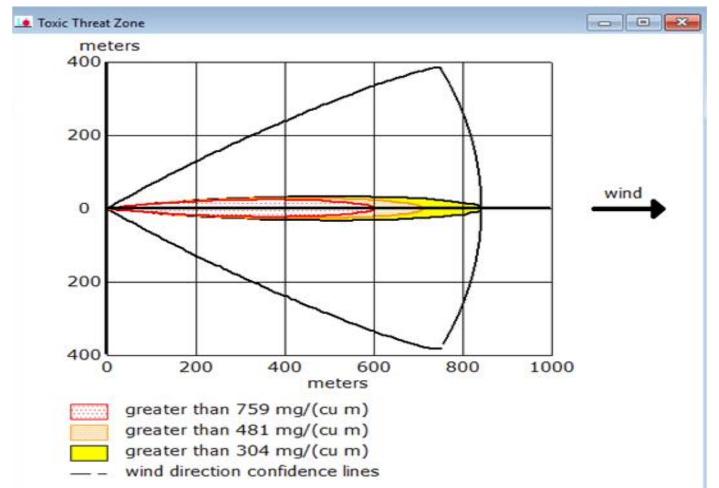
Multiple linked models are used

- Definition of scenario (location/topography/buildings, type of release (magnitude, timing, chemical and physical properties), meteorology, population density maps)
- Emissions model
- Wind flow model
- Transport and dispersion model (produces concentration distribution in time and space)
- Health effects and risk assessment model
  1) For non-lethal, plot predicted AEGL or ERPG concentration contours for the various averaging times (10, 30, 60 min, 4 and 8 hrs for AEGLS and 60 min for ERPGs) on maps. Determine population affected.
  2) For lethal, use Toxic Load formula with the probit model to calculate toxic load for various lethality fractions



To illustrate, the above figure contains maximum 60-min avg C predictions by the DOD's HPAC/SCIPUFF model for a 30 minute-duration one-ton chlorine release. The red area defines C > 20 ppm (ERPG-3); the yellow area defines 3 ppm (ERPG-2) < C < 20 ppm. This plot could be combined with a population distribution map to estimate the numbers of people with possible harmful health effects.

The figure to the right is an ALOHA model output for a 100 kg HCl release, showing 30-min avg C's at several lethality percentage levels (90, 50, and 10). It is seen that the 90 % contour extends to 600 m. The outer fan reflects wind direction uncertainty.



References

1. Platt N, K Luong, J Urban, 2017: Downwind chlorine hazard estimates for the 2015-2016 Jack Rabbit II campaign. Proceedings, 17th Conf on Harmonization of Air Quality Models, Budapest, 4 pp.
2. Sommervile D, J Bray, S Reutter-Christy, R Jablonski, R Shelly, 2010: Review and assessment of chlorine mammalian lethality data and the development of human estimate. Military Operations Research V15 N3
3. Hanna S, J Chang, T Mazzola, 2017: Analysis of variation of concentration with downwind distance and characteristics of dense gas plume rise for Jack Rabbit II 2015 and 2016 chlorine field experiments. Proceedings 18th Conf on Harmonization of Air Quality Models, Bologna, Italy, 4 pp.