SPATIAL DISTRIBUTION OF AN INSTANTANEOUS POINT RELEASE OF A FINITE AMOUNT OF GAS.

Jorge E. Majchrzak, Nestor Fruttero, Diego Roel,
Eduardo Grassi, Enrique Ponce.

Ente Nacional Regulador Nuclear.
Av. del Libertador 8250 (1429),Buenos Aires,Argentina

The risk to human health from exposure to vapors can be assessed by first quantifying an individual's potential exposure to, or dose of, the toxicant of concern. This is followed by a comparison of the exposure with an ascribed hazard determined from a known exposure-response relationship or exposure limit.

Occupational exposures to chemicals occur as a result of inhalation of workroom air contaminated with the vapor or aerosol of the chemical. The first step in the dose assessment process usually involves a determination of the concentration of the toxicant in the air that might be inhaled by the worker. Second, an estimation is made as to how much contaminated air would be inhaled. Next, the amount of toxicant potentially absorbed into the body, transported to potential target organs, and available for physiological response is estimated. The final step in the total assessment process is to compare the estimated potential human dose with the dose response from a toxicological/radiological data base. In the case of inhalation of a toxicant with an established exposure limit, the process needs only to determine the concentration in the workroom air and actual exposure time. Comparison of the workroom air concentration with an established limit,often is considered an adequate inhalation risk assessment.

A simple but usually very conservative approach to inhalation exposure assessment is to calculate the concentration of contaminant in air. The indoor air pollution model (also known as general ventilation model) describes the concentration of contaminant in the workroom air as a balance between the total input of contaminant, and the removal of contaminant from the workroom air by general ventilation with mixing volumes of clean air and the loss of contaminant from the combined sources of absorption, adsorption chemical transformation and radioactive decay.

In addition to the above temporal elements, the modeler also must deal with spatial factors that impact on workplace concentrations of airborne toxicants. It is intuitively obvious to most observers that the aiborne concentrations around point sources in large industrial rooms are much higher near the source, than at more distant locations in the room.In consecuence we can find a gradient of airborne concentration versus distance from the source.

This gradient is inversely proportional to air movement in the room, which in turn is a function of temperature gradients, movement of physical objects within the room and ventilation rate.

A rational approach would be to determine or estimate the rate of contaminant diffusion in a room.

This information is used to determine the subsequent dimensions of a volume around the source in wich the majority of the contaminant concentration would be found relative to the time frame choosed. This conceptual model is the affected volume, and it assumes omnidirectional (random) air movement at any point in the room. Its dimensions are determined by the manner in wich the air contaminant is dispersed from the source.

Diffusion theory is based on the random motion of the diffusing molecules resulting in net movement of the molecules from areas of high concentration into areas of low concentration. The rate at wich the concentration of diffusing particles change with time is equal to the flow into the

region less the flow out. Each flow depends on the flux of particles, or flow per unit area. The flux of particles in a fluid from point to point is directly proportional to the difference in the concentration of the particles, at the two points.

The coefficient of proportionality is called the diffusion coefficient, or D and its value must be determined experimentally.

The relation between flux and the rate of change in the concentration is known as Fick's Law. The mathematical formulation of this physical state of affairs leads to a differential equation called the diffusion equation. The solution is a mathematical expression that gives the concentration of the diffusing substance at every point in the space for every time. For example, if the diffusing substance is initially concentrated on the surface of a permeable membrane that divides a box in two at its center, the solution of the diffusion equation is a family of bell-shaped curves. The center of each curve coincides with the center of the box and as time passes the curve becomes broader and flatter.

There is another way to interpret each bell-shaped curve. Every point on the curve can be considered the probability density for the diffusion of a single Brownian particle from the central membrane in the box. The probability density multiplied by an appropriate measure gives rise to a probability. For the bell shaped curve the appropriate measure is a lenght, it is the distance between two points along the horizontal axis of the graph. The product of that distance and the average height of the bell-shaped curve in the interval between the two points is a probability.

The probability that the Brownian particle will be found in a region of the affected volume at a given time is the area under one of the bell-shaped curves between two vertical lines. Each vertical line passes through one of the two points on the horizontal axis that correspond to the boundaries of the given region in the box. According to this interpretation, the solution of the diffusion equation is not an expression that gives the distribution of molecule concentrations, instead the solution is a probability distribution. A convenient probabilistic measure of the displacement of a Brownian molecule is the root-mean-square displacement, or R.M.S. displacement. The probability that a Brownian particle diffuses at most as far as the R.M.S. displacement away from the central membrane in the box is 0,68; the probability that it travels more than twice as far as the R.M.S. displacement is less than 0.5.

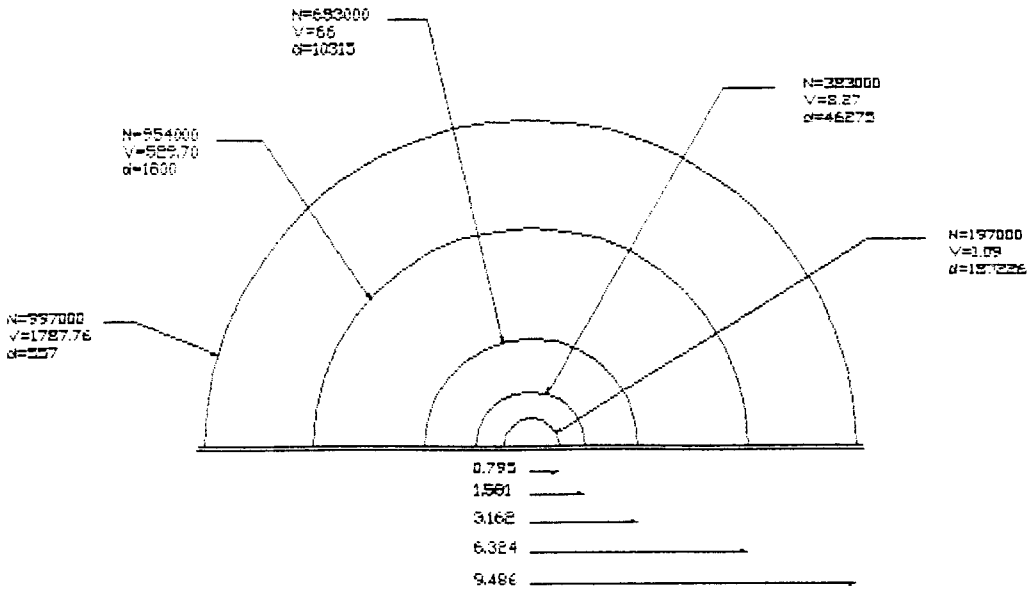
The R.M.S. displacement of a Brownian molecule diffusing away from the membrane in the box is $(2.D.t)^{1/2}$ where D is the diffusion coefficient and t is the time. Thus if a particle diffuses on the average one centimeter in one second, it will require four seconds to diffuse two centimeters and nine seconds to difusse three centimeters. So we can conclude that the radial displacement of a particle diffusing in any direction away from a central point "is not proportional to time, but proportional to the square root of time".

Consider now the instantaneous release of 1.000.000 μCi of a gaseous contaminant from a point source in the center of a large industrial room that has 12 mixing changes of air/hour or 5 minutes/mixing air change. Given 5 min. in an eddy diffusion field (D = 1 m^2/min), the R.M.S. distance from the source containing 68% of the diffusing molecules is calculated from:

$$R.M.S.= (2xDxt)^{1/2} = (2x1m^2/minx5min)^{1/2} = (10\ m^2)^{1/2} = 3,162\ m$$

Thus, approximately 68% of the gas will be within one R.M.S. distance or a 6,324 m diameter sphere. One would find 95% of the gas within 2 R.M.S. distance or within a 12,648 m diameter sphere with the source at the center.The following table was made by calculating the volume and average concentration from the normal probability density for concentric spheres with radii of 1/4, 1/2, 1, 2 and 3 R.M.S. It shows the average concentration of the various volumes around the source, 5 min. after instantaneous release of 1.000.000 "molecules" of gas.

R.M.S.	Ø 1/2 Sph.	Volume(m^3)	Nø Molecules	C=Nø/Volume
1/4= 0,790	1,581	1,0	197.000	187.226
1/2= 1,581	3,162	8,2	383.000	46.275
1 = 3,162	6,324	66,2	683.000	10.315
2 = 6,324	12,648	529,7	954.000	1.800
3 = 9,486	18,972	1787,7	997.000	557



Repeating this procedure for succesive periods of 5 min. we can see how the affected volumes that contains the majority of the contaminant molecules is growing with time, and in consequence diminishing the contaminant concentration (mass/unit volume)

As mentioned above, actual worker exposure or delivered dose results from the time-weighted integration of contaminant concentration and uptake rate. Obviously, concentration modeling alone will not suffice to answer completely questions of how much toxicant was delivered. Ultimately the models or combination of monitoring/modeling must render an acceptable estimation of dose and be validated against measured worker exposure data in various occupational settings.

References:

1- American Conference of Governmental Industrial Hygienists - 1988
Threshold Limit Values and Biological Exposure Indices.

2- Wu, Jhon an J. Schory : "Emissions from spills".
Air Pollution Control Association - Fefruary 1979.

3- Eddy Diffusivities Measured Inside a Light Industrial Building
American Industrial Hygiene Conference - 1985.

4- Lavenda, B.H. : Brownian Motion, Sci. Am. 252 (7) : 70-85 (1985)