

GIS-BASED TOXIC-GAS-VESSEL LEAKAGE, DISPERSION AND SIMULATIONS

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ABSTRACT:

People have been becoming serious of more and more accidents of toxic-gas-vessel leakage and dispersion (TLD) recently. This paper describes a TLD model derived from Gaussian instantaneous leakage model, and then simulates the process of TLD with GIS. When a high-pressure container or vessel breaks, toxic gas (including gasification of high-pressure liquid gas and low-temperature liquid) will leak, and then the gas cloud will disperse in atmosphere. We can calculate the leakage speed of toxic gas, and decide the primary source of dispersion consequently. Assumed that there are N independent equivalent air masses created during the period of leakage, and every air mass subjects to Gausses instantaneous leakage model. Therefore, the effect of TLD is equivalent to the superposition of the N air masses. Thus, the concentration of toxic gas at certain time, location and weather condition can be calculated. After that, concentration isoline can be traced out. We pay more attention to the concentration isolines at half lethal dose, badly injury dose, middle injury dose, and low injury dose. The relevant areas are called death zone, badly injury zone, middle injury zone, and low injury zone respectively. The dispersion trend and affection range can be predicted by illustrating these zones at different time, wind direction and speed. A decision support system of emergency treatment during TLD can be made together with the data of population distribution, traffic, economy, etc. Besides, it provides an analyze tool to forecast or evaluate casualty in TLD.

1. INTRODUCTION

Hazardous chemic products have been used in many industries today. Many accidents, such as explosion, inflammation, dispersion and simulation, may be occurred during storage or transportation of these products. The dispersion of toxic gas takes great damage to people's safety especially.

Toxic gas often stored in vessels or containers. When the vessels or containers broken, toxic gas will be released, and then dispersed in atmosphere. People have been becoming serious of more and more accidents of toxic-gas-vessel leakage and dispersion (TLD) recently. The wide affection range of TLD, different form explosion or inflammation; is even up to several kilometers, and results in thousands of people evacuation, or heavy casualties sometimes. In order to predicting the dispersion trend and affection range of TLD, it is important to simulate the process of TLD on GIS.

2. The MODEL OF TLD

TLD have two stages: leakage and dispersion. When a high-pressure container or vessel broken, toxic gas (including gasification of high-pressure liquid gas and low-temperature liquid) will be leaked, and then the gas cloud will be dispersed in atmosphere. We can calculate the leakage speed of toxic gas, and decide the primary source of dispersion consequently.

I 、 Leakage

The leakage of high-pressure liquid gas and low-temperature liquid obeys Bernoulli's equation. The rate of leakage is ^[1]:

$$Q_0 = C_d A \rho \sqrt{\frac{2(p - p_0)}{\rho} + 2gh}$$

Gasification ratio of high-pressure liquid gas and low-temperature liquid is:

$$K_v = \begin{cases} 0.2 & F_v \leq 0 \\ 0.5F_v & 0 < F_v \leq 0.2 \\ 1 & F_v > 0.2 \end{cases}$$

$$\text{Where } F_v = c_p \frac{T - T_0}{H}$$

Meanings of symbols in formulas above are as follows:

Q_0 —rate of leakage, kg/s;

C_d —modulus of leakage;

A —area of rift, m²;

ρ —density of the liquid, kg/m³;

p_0 —pressure of environment, Pa;

P —pressure of substance before leakage in the vessel,

Pa;

g —acceleration of gravity, 9.8m/s²;

h —height of liquid level above the rift, m;

C_p — specific heat at constant pressure of liquid, J/(kg • K);
 T — temperature of substance before leakage, K;
 T_0 — boiling point at ordinary pressure, K;
 H — heat of vaporization, J/kg.

The leakage rate of high-pressure gas rests with its pressure^[1].
 $Q_0=0.2138 \cdot A \cdot \rho \cdot (M/T)^{0.5}$ when $P_0/P \leq 0.8991$
 $Q_0=0.1717 \cdot A \cdot \rho \cdot (M/T)^{0.5}$ when $P_0/P > 0.8991$

II、Dispersion

Gaussian model is used to describe the dispersion of toxic gas in atmosphere usually. There are two typical cases for Gaussian model: continuous source and instantaneous source. Considering the limited capacity of toxic-gas-vessels, neither of the two cases can be accorded with. We adopt the method of superposition of instantaneous sources to describe TLD. Assumed that there are N independent equivalent air masses created during the period of leakage, and every air mass subjects to Gauss instantaneous leakage model. Therefore, the effect of TLD is equivalent to the superposition of the N air masses. Thus, the concentration of toxic gas at certain time, location and weather condition can be calculated. For instantaneous leakage:^[1]

$$C(x, y, 0) = \frac{2Q_0}{(2\pi)^{1.5} \sigma_x \sigma_y \sigma_z} e^{-\frac{(x-x_0)^2}{2\sigma_x^2}} e^{-\frac{(y-y_0)^2}{2\sigma_y^2}} e^{-\frac{z_0^2}{2\sigma_z^2}} \quad (1)$$

Where:

$C(x, y, 0)$ — Concentration of toxic gas at downwind point(x,y,0)

x_0, y_0, z_0 --Coordinate of every air mass's centre

$\sigma_x, \sigma_y, \sigma_z$ -- Denote the coefficient of diffusion in x, y and z directions respectively.

For actual requirement of succor and evacuate, we are usually concerned with the maximum concentration on the ground.

Therefore we let $y_0=0, z_0=0$. Assumed that the move speed of air mass equate to wind speed, the centre of every air mass lies on the direction of wind, and there is one air mass created every second, that is,

$$x_0 = u \cdot (t - i)$$

Where u is wind speed, t is time after leakage beginning, i is index of the air mass (the 1st air mass is 1, the 2nd air mass is 2, the 3rd air mass is 3, and so on).

Thus, we get the ith air mass's concentration at (x,y,0) after t time of leakage, that is,

$$C(x, y, 0) = \frac{2Q_0}{(2\pi)^{1.5} \sigma_x \sigma_y \sigma_z} e^{-\frac{(x-u(t-i))^2}{2\sigma_x^2}} e^{-\frac{y^2}{2\sigma_y^2}}$$

The superposition of n air masses' concentration at time t is:

$$C(x, y, 0) = \frac{2Q_0}{(2\pi)^{1.5} \sigma_x \sigma_y \sigma_z} e^{-\frac{y^2}{2\sigma_y^2}} \sum_{i=1}^n e^{-\frac{(x-u(t-i))^2}{2\sigma_x^2}} \quad (2)$$

Assumed that total leakage time is T, there are n air masses created after leakage beginning at time t,

$$\begin{cases} n = t & t \leq T \\ n = T & t > T \end{cases}$$

$$c_t = \sum_{i=1}^n e^{-\frac{(x-u(t-i))^2}{2\sigma_x^2}}$$

Let $i = t - i$, ($t \leq T$), then

$$c_t = \sum_{i=1}^n e^{-\frac{(x-u(t-i))^2}{2\sigma_x^2}} = e^{-\frac{(x-u)^2}{2\sigma_x^2}} + e^{-\frac{(x-2u)^2}{2\sigma_x^2}} + \dots + e^{-\frac{(x-nt)^2}{2\sigma_x^2}}$$

$$= e^{-\frac{x^2+u^2}{2\sigma_x^2}} \cdot \frac{1 - e^{-\frac{-tux}{\sigma_x^2}}}{1 - e^{-\frac{-xu}{\sigma_x^2}}}$$

After a series of transformation from equation (2), we get concentration isoline equation at certain concentration C:

$$y = \pm \sqrt{-2\sigma_y^2 \ln \frac{(2\pi)^{1.5} \sigma_x \sigma_y \sigma_z \cdot C}{2Q_0 \cdot C_t}} \quad (3)$$

Where $\sigma_x, \sigma_y, \sigma_z$ are the functions of x, C_t is the function of x and t.

3. SIMULATION

Through above functions, following input parameters needed to simulate the process of dispersion:

Source of leakage: the location of leakage source and its projection point on the ground;

Name of leakage substance: through the name, the properties of leakage substance can be determined, such as state (liquid or gas), density, constant pressure specific heat, boiling point, heat of vaporization, half lethal dose, badly injury dose, middle injury dose, and low injury dose, etc;

Rift of the vessel: including the rift's dimension and shape, height of liquid level above the rift;

Properties of vessel: including the vessel inner pressure and temperature, the weight of substance in the vessel;

Weather conditions: wind speed, wind direction (expression by the included angle between wind direction and eastward axes, like east bias north 250 degrees), stability of atmosphere (involving day/night, sunlight intension, etc);

Landform of accident occurred: champagne, suburb, or urban areas.

All the other parameters can be figured out by these data.

A series of isolines can be traced through equation (3). We pay more attention to the concentration isolines at half lethal dose, badly injury dose, middle injury dose, and low injury dose. The relevant areas are called death zone, badly injury zone, middle injury zone, and low injury zone respectively. The dispersion trend and affection range can be predicted by illustrating these zones on digital map at different time after leakage, certain wind direction and speed. The depth and area of these zones can be calculated similarly.

4. APPLICATION CASE:

Suppose the situation of a chlorine leakage as Tab1:

Symbol	Value	Meaning of the symbol
W	4000kg	Total weight of substances released
A	0.0025 m ²	Area of rift
P	0.8Mpa	Pressure of substance before leakage in the vessel
T	20 °C	Temperature of substance before leakage in the vessel
H	1.5m	Height of liquid level above the rift
u	4.4m/s	Wind speed
--	210°	Wind direction (expression by the included angle between wind direction and eastward axes)
--	Day; Sunlight strong	Atmosphere condition
--	Champagne	Landform of accident occurred

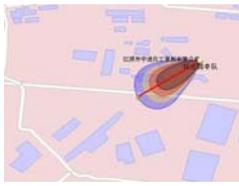
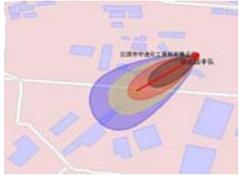
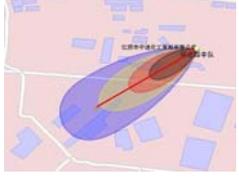
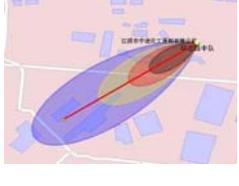
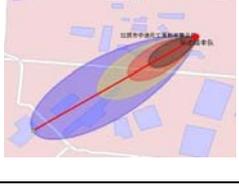
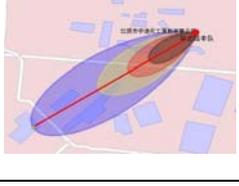
Tab1: leakage initial condition

Some parameters of chlorine queried form a chemical database as Tab2:

Molecular weight (g)	Boiling point (°C)	Saturated vapor pressure (Pa)	Density (g/cm ³)	Heat of gasification (J)
70.9	-34	638	0.00324	2888000
Constant pressure of specific heat (J)	Half lethal dose (g)	Badly injury dose (g)	Middle injury dose (g)	Low injury dose (g)
4970	0.6	1.6	3.2	6.4

Tab2: some parameters of chlorine

We designed a program based on ArcIMS9.2 to simulate the dispersion. All the 4 concentration isolines at different time were illustrated on the map with different colors. Dark red, red, yellow, light blue represented death zone, badly injury zone, middle injury zone, low injury zone respectively. Start from evacuation and succor, depth and area of the zones were used to show the process of dispersion as Tab3.

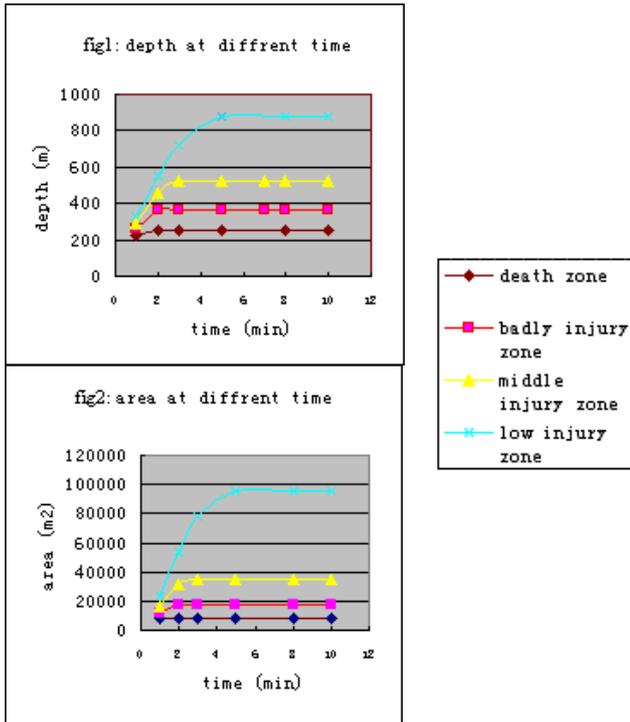
	Zones	Depth (m)	Area (m ²)	Simulation results
1 minute after leakage	Death	226	7701	
	Badly	262	11552	
	Middle	290	15983	
	Low	331	23193	
2 minutes after leakage	Death	256	8709	
	Badly	362	17448	
	Middle	458	30931	
	Low	550	53241	
3 minutes after leakage	Death	256	8709	
	Badly	365	17515	
	Middle	522	35235	
	Low	721	77955	
5 minutes after leakage	Death	256	8709	
	Badly	365	17515	
	Middle	523	35287	
	Low	877	95255	
8 minutes after leakage	Death	256	8709	
	Badly	365	17515	
	Middle	523	35287	
	Low	879	95321	
10 minutes after leakage	Death	256	8709	
	Badly	365	17515	
	Middle	523	35287	
	Low	879	95321	

Tab3: depth and area of every zone at different time

Where:

- Death refers to death zone;
- Badly refers to badly injury zone;
- Middle refers to badly injury zone;
- Low refers to badly injury zone;

According to Tab3, trend line of depth and area at different time were traced out as fig1 and fig2 respectively.



We found that all the depth and area of different zones were almost changeless from 5 minutes to 10 minutes after leakage. This indicated that the dispersion come into steady state at 5 minutes after leakage, like continuous leakage. These illustrations predicted the dispersion trend and affection range preferably. A decision support system of emergency treatment during TLD can be made together with the data of population distribution, traffic, economy, etc. Besides, it provides an analyze tool to forecast or evaluate casualty in TLD.

5. CONCLUSION AND DISCUSSION

This paper describes a toxic-gas-vessel leakage and dispersion model based on Gaussian Model, and gives a method to simulate the process of dispersion. Death zone, badly injury zone, middle injury zone, low injury zone figure different damage to human body respectively. These zones are very

important to decision of succor and evacuation. According to a series of illustrations on digital map at different time after accident occurred, the toxic gas dispersion trend can be well simulated. On the other hand, toxic-gas-vessel leakage is different from instantaneous leakage or continuous leakage, and the illustrations show the difference and relations between them.

Gaussian model describes the behavior of non-heavy gas cloud formed during a hazardous substance leakage, or the far-field diffusion behavior of heavy gas cloud when the gravity's affect disappears, so the TLD model has same restrictions with Gaussian model. But, because the speed of heavy gas dispersion is lower than non-heavy gas's, as the view of safety, we can still use the TLD model to describe a toxic-gas-vessel accident.

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