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The simulation of dangerous gas diffusion in port area

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THE SIMULATION OF DANGEROUS GAS DIFFUSION IN PORT AREA

By

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THE DECLARATION

I certify that all the materials in this research paper that are not my own work has been identified, and that no material is included for which a degree has previously been conferred on me.

The contents of this research paper reflect my own personal views, and are not necessarily endorsed by the University.

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ABSTRACT

Title of Research paper: **The Simulation of Dangerous Gas Diffusion in Port Area**

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With the technical improvement of the shipping industry and the development of the world's energy industry, there are more and more dangerous chemical goods transported by ship in recent decades. From the point of view of safety management, the risks of transporting dangerous chemical goods are increasing because of two reasons: on the one hand, it improves the probability of ship accidents because of the expanding quantity of ship fleets that were designed for transportation of dangerous chemical goods; on the other hand, the consequence of chemical tankers or gas tankers, due to the inflammable and explosive dangerous goods they carried usually have some characteristics in strong corrosion, high toxicity features, can be more serious than other types of ship accident. This thesis is intended to study and analyze the gas diffusion pattern after accidents, especially focusing on gas migration path and concentration distribution after dangerous gas leakage from the ship in the port area. Under the consideration of a suitable model of describing the gas diffusion, through the comparison between results of different parameters in the model, this thesis tries to verify the applicability of the model and clarify the sensitivity of the different parameters in gas diffusion.

The dangerous gas concentration distribution is of importantance for making decides of emergency response acts after leakage accidents, what's most fundamental is to demarcate the poison and fire & explosion danger area of an accident. For the purpose of protecting human health and environment, different countries and regions have set up different ambient air quality standards based on the concentration of the pollutants. These standards are set on the premise of the stationary pollution sources, in other word, they focus on the constant pollutants source rather than the accident leakage pollutants accident. On the basis of the concentration distribution, considering the current ambient air quality standard and environmental toxicology and the time-weighted poison exposure assessment, this thesis discusses the danger area or safety distance of the leakage accident from shipping hazardous materials, so as to provide the support to the decision-making in the emergency response of the accident in the port area.

KEY WORDS: gas diffusion, Gaussian Model, emergency response

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LIST OF ABRREVIATIONS

CERC	Cambridge Environmental Research Consultants
DOT	Department of Transportation
ERG	Emergency Response Guidebook
EPA	Environmental Protection Agency
GIS	Geographic Information System
IMO	International Maritime Organization
LC50	Median Lethal Concentration
LNG	Liquefied Natural Gas
LPG	Liquefied Petroleum Gas
LOC	Level of Concern
MEP	Ministry of Environmental Protection
MEPC	Maritime Environment Protection Committee
MOT	Ministry of Transport
UNCTAD	United Nations Conference on Trade and Development

CHAPTER 1

Introduction

1.1 Background of this research

With the rapid development of industry, more and more amounts of chemicals are put into use. As a result, natural environment and people's living environment has been threatened by the bigger potential risk than ever before on account of emergent environmental pollution incidents occurring more frequently. Not as same as general pollution accident, emergent environmental pollution incidents have no fixed discharge mode and approach, and the pollutants are ferociously discharged within the transient emissions (Liu, 1995).In recent years, the occurrence of emergent environmental pollution incidents showed a tendency of increase and most of the accidents has caused enormous losses to the environment and bring about the repercussions of the society. Emergent environmental pollution incidents, as the important factors of the threat to human health and the damage to the ecological environment, have become a burning concern all over the world. In 2002,at the World Summit on Sustainable Development, present states had agreed that the negative effects should be reduced to minimum in the production and utility of chemicals on the human health and the environment by 2020(UNEP,2013).

It is observed that hazardous chemicals leakage, explosion, diffuse pollution accidents are highly frequent in emergent environmental pollution incidents. Large amounts of chemicals are utilized in the procedures of production, storage and control process in the chemical, energy, oil and other industries. Because of operation error or failures of equipments, chemical leak could threaten the environment safety and human health. In spite of the joint efforts, which have been carried out by all means, to eliminate the accidents, it still can't avoid the accidents. Take China as an example, the emergent environmental pollution incidents since 2000 is visible in the table below:

Table 1：The environmental incidents in China, 2000-2012

	Water pollution incidents	Air pollution incidents	Other pollution incidents	Total
2000	1138	864	409	2411
2001	1096	576	170	1842
2002	1097	597	227	1921
2003	1043	654	146	1843
2004	753	569	119	1441
2005	693	538	175	1406
2006	482	232	128	842
2007	198	141	123	462
2008	198	141	135	474
2009	1011	1533	608	3152
2010	135	157	228	420
2011	39	52	451	542
2012	30	1	511	542

Data source: Wan,2006. MEP China,2008， 2009a， 2010， 2011. China Environment Yearbook, 2012，2013.

Based on the study of safety bureau of United Kingdom Atomic Energy Commission (Data is got by retrieval from the international major hazards incidents database software, MHIDAS CD 1996 version), there were 3440 chemical accidents occurred around the world due to transportation errors (including railway, highway, water transport and pipeline transport) during 1900~1996 years(Wang,2001). According to the main damage classification, the fire damage was far more than others (59.3%), followed by poisoning (21.35%), and the last was corrosion (8.87%) (Wan, 2001). Fire caused the most death and the biggest economic loss, poisoning ranked the second. Vis-a-vis, poisoning is much higher than the fire and corrosion in the number of injured people and the scope of crowd evacuation, that is to say, poisoning has a wide geographical range of influence.

As it can be seen from the numerous cases, emergent environmental pollution incident has the following characteristics: (1) the occurrence is sudden, accidental and transient; (2) the perniciousness is serious; (3) it is difficult of disposal (wan, 2006). Those characteristics (Wan, 2006) are especially obvious in atmospheric pollution accident.

It is universally known as the world's worst industrial disaster (Lin, 2009) that the gas leak from the Union Carbide factory in Bhopal in central India. Attributing to the failure of pesticide plant emergency control valve of an underground tank, more than about 30 tons of toxic liquid methyl isocyanate was leaking in gaseous form in 40 minutes, it took only 1 hour after the leakage, the influenced area reached 40 square kilometers. As a consequence, more than 2,000 people were killed and 50,000 people were caused blindness and hundreds of thousands of people had to be evacuated, which attracted much attention from the entire world. Happened on December 23, 2003 in KaiXian county, ChongQing province in China, an accident caused a gas diffusion which contained a large number of high concentrations of hydrogen sulfide, there were 243 people near the accident location died because of the poisonous hydrogen sulfide, more than 2,000 people were sent into the hospital for medical treatment against hydrogen sulfide poison, more than 65,000 people had to be evacuated and resettle, moreover, the directly economic losses amounted to more than 60 million RMB(Lin, 2009).

In this thesis, the "dangerous goods" means the gas transported by gas carrier and the bulk liquid chemicals except the oil and the inflammable material which is similar to oil. There are more than 30000 kinds of chemicals have been registered in the international maritime organization (IMO) currently. According to the amendment of IBC code adopted in 2012, 754 kinds of chemicals were transported in bulk (IMO, 2012).

1.2 Purpose of this study

In this thesis, gas diffusion simulation after chemical spilling belongs to the category of accident consequence assessment; it is the important content and key technology to develop an emergency response plan of dangerous goods accident. Consequence analysis is an important part of safety assessment, by which people would know more deeply about the accident and enhance safety awareness. The main purpose is to calculate the consequence of accidents in qualitative or quantitative ways, including accident influenced scope, extent of damage and the situation of property damage, casualties and environmental damage; so as to take security measures to reduce the losses of accidents and provide the decision-making basis for the emergency response acts.

This study aims to analyze the concentration distribution of pollutants and danger (fire, explosion and poisoning) area by gas diffusion simulation. To apply an accurate simulation, it is necessary to analyze the gas properties and the accident conditions so that simulation model could be properly chosen. It is different in danger area to determine in different countries which is according to the concentration distribution standards. The method to determine danger area will also be discussed in this thesis.

CHAPTER 2

Literature Review

The distribution of atmospheric pollutants is dependent on the atmospheric transport and diffusion process. Therefore, the atmospheric pollutants diffusion theory is based on the basic theory of atmospheric turbulence diffusion, then conduct the correct mathematical physics simulation on diffusion process. There are two main types (Anderson, 2010) of the basic theory of atmospheric turbulence diffusion: statistical theory and the gradient transportation theory. It is also an approach to simulation by box model derived from experience or other models based on theoretical approaches. Statistical theory research method is to track the movements of individual air micelle which belongs to the Lagrangian method; gradient transportation theory is the Euler method, discussing the fixed point in space on the quality of the mass flux (pollutants concentration) caused by atmospheric turbulence movement.

Gas leakage diffusion model research began in the 1970s (Wang, 2001). In order to study the dangerous gases spread theory and verify the mathematical physical model, in the early 1980s, researchers from Britain, the United States, Germany and other countries completed a series of experimental study of dangerous chemicals leakage diffusion on field represented by the Coyote, Buro and ThorneyIsland, they got the actual concrete data from the real situation (Ding, 1999). In the 1990s, they studied in leakage diffusion conditions of toxic substances, such as liquid ammonia, LNG, LPG and hydrogen fluoride etc., which were mainly based on the field testing procedure of toxic substances leakage. Experimental data was including the source term characteristics (diameter, release of the fluid flow and mass flow rate, etc.) and the surrounding atmosphere environment (wind speed, atmospheric stability). Those data not only provided some initial conditions for calculating, but also provided the validation of numerical model of physical quantities: concentration of hazardous substances, jet velocity, jet temperature, droplet size etc. Because of the model size, personal safety and the uncertainty of the environment, the application scope of this model has its limitations.

It is also active in this field of research till now. So far, there are hundreds of accident assessment models (Zhang, 2006), such as Gaussian model, BM model and SUTTON model, FEM3 model, Box model, ALO2HA model, SLAB model, DEGADIS model etc. Even if each model has its own characteristics, application scope as well as limitations, researchers have a wide range of theoretical basis and experiment tools to analyze the gas leakage diffusion.

With the development of computer technology, the pollutants diffusion model was supported by some software by which large number of computations has been made. To built an emergency environmental system, Geographic Information System (GIS) was introduced to provide some functions for gas diffusion: map loaded, pollution monitoring visualization and concentration isograms visualization etc.(Guo, 2008) GIS can be utilized to predict the direction and scope of pollutant diffusion, moreover, it can show different isoline on request and demonstrate the scope of defined concentration, therefore, it provides reliable support for decision-making of the accident.

CHAPTER 3

The Research of Gas Diffusion

Atmospheric pollutants diffusion is a dynamic process changed with time and space; it accords with the basic pattern of atmospheric diffusion. The chemical gas spreads from the height of the initial release location into the surrounding environment with gas concentration decreasing in accord with time and distance, ultimately, the atmospheric pollutants concentration is equal to the value of background concentration. The distribution of atmospheric pollutants is driven by the atmospheric transport and diffusion process. Therefore, atmospheric pollutants diffusion is based on the basic theory of atmospheric turbulence diffusion from which the different mathematical physics simulations on diffusion process are developed.

3.1 Basic theoretical treatment of gas diffusion

The basic theories of gas diffusion have been developed along the three theoretical systems (Jiang, 2003), namely the gradient transportation theory, the turbulent statistical theory and the similarity theory; the treatments of those theories are on the basis of different physical mechanism, consequentially, they utilize different parameters and different meteorological data respectively, and are built with different assumptions.

3.1.1 Basic processing of the gradient transportation theory

According to Euler method, gradient transportation theory deals with gas diffusion considering that the pollutants distribution occurs in the fluid turbulent flow which can be described by Reynolds equation. There are 9 terms of Reynolds stress (also called the turbulent viscosity) which represent the roles of fluctuation velocity in the whole turbulent motion. Not surprisingly, there are so many unknown terms (more than a dozen) that it is very difficult to solve equations. In order to solve the diffusion equation and deal with air pollutants spreading, using turbulent semi-empirical theory the researchers established relationship between the pulsating quantity and average quantity in the velocity field, so that the unknown terms could be reduced and the equations be closed. This is the basic train of thought of gradient transportation theory to deal with air pollutants spread.

It is a basic assumption of the semi-empirical turbulence theory that momentum flux caused by the turbulent is proportional to the local wind velocity gradient. The proportional coefficient K is the turbulent exchange coefficient, also known as the turbulent diffusion coefficient (Jiang, 2003). If it is measured with mass concentration of diffusion material, the equations can be built as follow:

$$\begin{cases} \overline{\rho u' q'} = -\rho K_x \dfrac{\partial \bar{q}}{\partial x} \\ \overline{\rho v' q'} = -\rho K_y \dfrac{\partial \bar{q}}{\partial y} \\ \overline{\rho w' q'} = -\rho K_z \dfrac{\partial \bar{q}}{\partial z} \end{cases}$$

Kx, Ky, Kz: The proportion coefficient of three directions X, Y and Z;

ρ: The mass concentration of diffusion material;

$\overline{\rho u' q'}$、$\overline{\rho v' q'}$、$\overline{\rho w' q'}$: The wind velocity gradient of three directions;

$\bar{q}$: The average concentration gradient diffusion material;

This is the basic relationship of the gradient transportation theory: there is a linear proportional relationship between the pulsating quantity values of mass concentration of diffusion material and the mass concentration gradient of mass concentration. The minus sign means that it is opposite between the direction of mass transportation and the direction of gradient. This theory is also called the K theory because Kx, Ky, Kz mean the turbulent diffusion coefficient in X,Y,Z directions. There are respectively simplifying and solving ways to following types in practical application: instantaneous point source without wind, continuous point source without wind, instantaneous point source with wind and continuous point source with wind.

The disadvantage of gradient transportation theory (Jiang, 2003) attributes to the turbulent semi-empirical theory which is derived from simulation of molecules. This theory regards the irregular turbulent eddy motion as the molecular thermodynamic movement so as to conduct exchange and transportation of various properties in flow field in the same way as molecular motion. In fact, the simulation is just apparent, there is an essential difference between turbulent eddy motion and molecular thermodynamic movement. Mathematical treatment of molecular processes is on the basis of objective molecular transport model by which it can strictly deduce the relationship between flux and gradient, and the proportionality constant is physical properties of the fluid and approximate to constant. The relationship between flux and gradient is only an assumption in turbulent eddy motion considering that it is impossible to confirm the basic status its mathematical model as strict as molecular process in turbulent eddy transportation, so the linear relationship between flux and gradient in essence is a kind of assumption too. The flow field of surface layer is so complicated that it cannot be illustrated by simple linear relations. As a result, the difference between the flow fields is completely described through the different assumptions and different forms of proportionality constant K. the K value varies with different conditions (even to several orders of magnitude). There are many limits in practical application so it cannot be a universal guideline because it is very difficult to determine the K value.

3.1.2 Basic processing of the turbulent statistical theory

Surface layer atmosphere is always in a state of turbulent motion. In a fully developed turbulent flow, the speed and other characteristics are the random quantity in accordance with time and space; it is so-called that the turbulent motion is highly random. But it has a certain statistical regularity when lots of micelle movements are observed. Turbulent statistical theory describes material diffusion in flow field on basis of the study of statistical properties of turbulence pulsation. Taylor built the relation between concentration distribution standard σ and statistical data of turbulent pulsation in 1921 and established the formula for statistical data of turbulent pulsation and turbulence transverse diffusion coefficient σ_y (which means it quantitatively describes the relationship between Laplace correlation coefficient $R_L(\tau)$ and turbulence transverse diffusion coefficient σ_y). It can calculate the spread variance (towards the origin point) from any starting time to T time frame by following form of Taylor formula:

$$\sigma_y^2 = \overline{y^2}(T) = 2\overline{v'^2}\int_0^T \int_0^t R_L(\tau)\, d\tau dt$$

σ_y : The turbulence transverse diffusion coefficient;

$\overline{y^2}(T)$: The displacement variance of particles which started to spread from the origin point after T period of time in the Y direction;

$R_L(\tau)$: The autocorrelation coefficient of speed v'

As can be seen from this formula, the particle turbulent diffusion scope depends on the turbulent fluctuation velocity variance and the Laplace correlation in constant homogeneous turbulence field. The fluctuation velocity of Laplace correlation coefficient is changed along with the turbulence intensity, and so is the spread scope of the particles.

But Taylor formula describes diffusion coefficient with statistical properties of turbulence pulsation, it cannot be directly used to deal with the simulation of atmospheric diffusion. The properties of the atmospheric turbulence field is mainly determined by the meteorological factors, therefore, in order to apply Taylor formula for practical utilization, it is necessary to express Laplace correlation coefficient with the meteorological parameters. And then, the direct link between diffusion coefficients and meteorological parameters should be established. This is the common starting point of diffusion model (processing by statistical theory) and this characteristic is especially obvious in the application of Gaussian model.

Taylor formula is derived on condition that the atmospheric flow field is uniform and constant, but the actual atmosphere is not in keeping with such conditions. It can be approximated to such situation only when the underlying surface is flat and open, the flow is steady in small scale processing. This makes a lot of restrictions in the applications of this theory. The application beyond this scope needs experience to promote formula and some reasonable amendments.

3.1.3 Basic processing of similarity theory

The theory is applied to the particle diffusion firstly by Monin (1959). Since then, Batchelor (1959, 1964), Gifford (1962) and others promote the turbulent diffusion similarity theory and finally, it become other processing of theory used for simulating atmospheric turbulence diffusion (Jiang, 2003).

The basic assumption of Lagrange similar theory is that the statistical features of fluid particle can be confirmed by the Euler characteristic parameters in surface layer. The parameter is u by which it can characterize the Euler characteristic of flow field in the neutral atmosphere. It needs to consider heat flux when the atmosphere is non-neutrality layer, or be represented by Monin-obukhov length.

As if a particle moves from the origin point, then, the average of vertical displacement is $\overline{Z}$ and the average of horizontal displacement is $\overline{X}$. for particles released from point source z = 0,using dimensional analytical method, it can get the average vertical displacement growth rate of particles which have been released for t time, as follow:

$$\frac{d\overline{Z}}{dt} = bu * \emptyset(\frac{\overline{Z}}{L})$$

b: The universal constant to be confirmed;

The universal function to be confirmed;

u: The Euler characteristic of flow field;

L: Monin-obukhov length;

$\overline{Z}$:The average of vertical displacement.

Under neutral conditions, L→ ∞， $\emptyset = 1$， , the formula type can be simplified to initial results presented by Batchelor in 1959. If the assumption that the corresponding growth rate of the average horizontal displacement is equal to the average wind speed relating to, another form of the formula can be expressed as:

$$\frac{d\overline{X}}{dt} = \overline{u}\ (c\overline{z})$$

c: the constant

When the migration time of particles is t, the average particle diffusion equation depends on the average vertical velocity and the average horizontal velocity. The formula can be solved if the wind profile and the constant are given. So the two formulas above are the foundation of mathematical treatment.

Similarity theory is based on principle of Lagrange similarity hypothesis, so there are two physical models for describing diffusion: firstly, the particle diffusion characteristics are associated with the Lagrange properties. Assume that the Lagrange properties of flow field only depend on the parameters which are used to describe Euler characteristic parameters of flow field, so that the particle diffusion can be connected with the spatial distribution of the surface layer wind speed. Statistical characteristics of particle velocity also confirm Euler characteristic parameters; Secondly, in the surface layer, the parameters used to describe Euler characteristic parameters of flow field are friction velocity u and Monin-obukhov length L (dynamic and thermal effects). The two (u,L) are deduced through dimensional analytical method by similarity theory by which it can be used to describe the spread of the particles.

So far, solutions of diffusion derived from the similarity theory are applied within the surface layer which turbulent viscous force is constant and the thickness is only about a dozen meters. At this altitude, the role of Coriolis effect and other factors must be considered, which would make the dimensional analytical method far more complicate so that it is hardly to get a definitive result (Jiang, 2003).

3.2 The Gas Diffusion Models

The diffusion models were established based on the theoretical treatments mentioned above. In order to calculate the result, models often simplify some conditions, the typical models are introduced as follows:

3.2.1 Gaussian model

Gaussian diffusion model is deduced under the premise of pollutants concentration in accord with normal distribution. The solution of normal distribution can be conducted assuming that diffusion coefficient K is constant. It can also be proved that the probability distribution of particle displacement is normal distribution under the condition of stable and homogeneous turbulence atmosphere from statistical theory perspective. It does not meet those in practical atmosphere, but it has been proved by numerous pollutants diffusion tests in small scale that the normal distribution hypothesis can be used as approximate of real situation.

Gaussian diffusion model includes Gaussian plume model and Gaussian puff model; both of them have their own application domain. But the common applicable conditions are as follow (Ding, 1999):

1. Underlying surface needs to be flat, open and uniform properties;
2. There is no chemical reaction, dry deposition or cleaned by precipitation etc. to attenuate the particles; and there is no relative movement against air;
3. The average flow field is stable and straight, average wind speed and wind direction should not be significantly changed.
4. It is applicable for small scale diffusion (no more than 10-20Km) because the underlying surface, wind speed and wind direction could change significantly beyond certain scope.

3.2.1.1 Gaussian point source plume model

Gaussian plume model is the solution of turbulent diffusion equation in a continuous point source with certain wind speed. The concentration is considered in the steady state for continuous source, which means the discharged pollutants concentration is not changed along with time; it is only a function of spatial coordinates (Wang, 2001). The concentration distribution can be directly deduced by solving the diffusion equation with wind speed:

$$C(x,y,z)=\frac{Q}{2\pi u\sigma_y\sigma}.\exp\left[-\frac{1}{2}\left(\frac{y^2}{2\sigma_y^2}+\frac{z^2}{2\sigma_z^2}\right)\right]$$

C(x,y,z): The concentration of coordinate (x,y,z) (mg/m^3);

Q: The source strength (Kg/s);

u: Wind speed (m/s);

σ : Diffusion Coefficient.

The formula of Gaussian elevated point sources diffusion model under the condition of bounded situation (ground reflection) is as follow:

$$C(x,y,z)=\frac{Q}{2\pi u\sigma_y\sigma}.\exp\left(-\frac{y^2}{2\sigma_y^2}\right).\left\{\exp\left[-\frac{(z-H0)^2}{2\sigma_z^2}\right]+\exp\left[-\frac{(z+\Delta H)^2}{2\sigma_z^2}\right]\right\}$$

H: effective source height (m);

ΔH: lifting height of smoke (m);

If z=0, it is the concentration of ground:

$$C(x,\ y,\ 0,\ H)=\frac{Q}{\pi u\sigma_y\sigma}.\exp\left[-\frac{1}{2}\left(\frac{y^2}{\sigma_y^2}+\frac{H_e^2}{\sigma_z^2}\right)\right.$$

The concentration distribution is as follow: the concentration is close to zero near the source, and then it gradually increases. After reaching maximum at a certain distance, it slowly decreases along with the distance. The concentration is according to normal distribution on the y direction. This model is not only suitable for application of continuous source diffusion, but also can be used for line source and non-point source after reasonable promoting.

3.2.1.2 Gaussian point source puff model

For pollutant gas leakage accident, a large number of poisonous and harmful gases are often released a short time or partitioned in a long time from the sources. The calculation of ground should use Gaussian point source puff model .Assuming that the puffs are independent and continuous, the volume of those puffs increases along the horizontal and vertical direction, so as to simulate how the puffs change along with the location and time considering the wind speed and wind direction.

In the case of no wind or a breeze (u≤1m/s), the atmospheric turbulence and diffusion properties in surface layer are different with the ones when the wind speed is faster than 2m/s. The pollutants spread slowly and it is easy to concentrate highly in certain part of local area. Gaussian point source puff model of no wind is as follow:

$$C(x,y,z,t)=\frac{Q}{(2\pi)^{\frac{3}{2}}\sigma_x\sigma_y\sigma_z}\exp\left[-\left(\frac{x^2}{2\sigma_x^2}+\frac{y^2}{2\sigma_y^2}+\frac{z^2}{2\sigma_z^2}\right)\right]$$

When the point source t is continuous (The source strength is Q (kg/s)), it can assume that the instantaneous puffs are released continuously in T period. And it is reasonable to divide T into several equal periods of time within which a puff is released. The divided period is considered as time marching (for example, 1 min) in which the wind direction, wind speed and stability are supposed to be constant.

To calculate the concentration in a point in space (x, y, z) under the continuous source, it is practicable to superimpose the concentration caused by the instantaneous puffs which is released in time interval ∆T. It is the formula of continuous source puff model without wind after Gaussian point source puff model is integral along the time T:

$$C=\int_0^T \frac{2Q}{(2\pi)^{\frac{3}{2}}\cdot\sigma_x\cdot\sigma_y\cdot\sigma_z}\exp\left(-\frac{R^2}{2\sigma_y^2}\right)\exp\left(-\frac{H^2}{2\sigma_z^2}\right)dt$$

T: integral time (period without wind)(s);

R: the distance to the origin point (m), $R=\sqrt{x^2+y^2}$;

σ_x: diffusion coefficient along the wind direction, $\sigma_x = \sigma_y$

3.2.2 Turbulent closure model

Turbulent closed model was established based on turbulent diffusion equations of pollutants. Though seeking pulsating quantity's (which belong to the characteristic physics quantities of equations.) second-order correlation matrix (first-order closure) or third-order correlation matrix (second-order closure), the independent relationship between matrix and correlated variables could be established so as to close the, then, the solutions of equations can be got. Turbulent kinetic energy closure model is based on the gradient transportation theory, so diffusion is properly only when the plume scale is bigger than the turbulent eddy scale, that is to say, the equation is applicable when pollutants spread range is over several hundred meters. There are several types (Andersson, 2012)of first-order closure model: IM – PACT, the standard model used to simulate the pollution control area and the impact of air quality; INTERA ,a model used to simulate the atmospheric diffusion in complex terrain; PDM, the model used to simulate urban pollution diffusion which the emission source changes along with the time etc. Second-order closure model also have some types: ARAP , a model considering heat buoyancy of flue gas in detail; Arginne, a model used to simulate transfer of water vapor and turbulence effects with humidity and condensation process.

3.2.3 Large eddy model

Large eddy simulation model is a simulation of atmospheric boundary layer studied by Deardorf in the early 1970s. It is a compromise algorithm between direct numerical simulation (DNS) and theoretical model. Physical quantity of fluid field can be artificially divided into large quantity and small quantity with filtering method

(Deardorf, 1970). There are several filters such as BOX filter, Fourier filter and Gaussian filter. Deardorf deeply explore the turbulent motion properties of convective boundary layers and diffusion pattern though effective numerical simulation and laboratory simulation test, and those works had shown the potential of large eddy simulation in studying the subject of convective boundary layers.

The model was continuously developed and amended after 1980 s. Moeng and Wyngaard promoted large eddy simulation method by introducing the pseudo-spectral calculation method into this model and comparing the functions of different filters (Moeng, 1994). Mason investigated the influence of various model parameters on the simulation results in detail, especially the wall effect near the ground which was more careful handled. Schmidt and Schumann researched large eddy model structure and the statistical features of motion in convective boundary layer using high resolution model. Hadfield and Walko applied compressibility of model to simulate simple inhomogeneous influence in the ground. Schumann discussed how topographic relief affected the result of model. It is obvious that the basic method and simple application of large eddy simulation has been conducted successfully, and the basic method of large eddy simulation has been relatively mature. However, this model was not easily to extensively use because of the complexity of the model and the large amount of calculation needed.

3.2.4 Box model

The basic assumptions of Box model is: the spatial scope of pollutants diffusion can be looked as a fixed size box in the simulation of the atmospheric pollutants concentration. The height of this box is mixing layer height from the ground, and the pollutant concentration is equal everywhere in the box. The concentration of the pollutants can be roughly calculated according to the conservation of pollutant mass.

This model can reflect the dynamic pattern of average pollutant concentration along with time. This model can be divided into single box model and multi box model (Wang, 2001).

Single box model is the simplest model to calculate atmospheric quality of a region or a city. It assumes that the region or the city was enveloped by a box which plan view scale is exactly as same as the plane of the region or the city and the height is as high as the mixing layer. The pollutants are uniformly distributed in the box. This model does not consider of the pollutant vertical diffusion coefficient, the change of wind speed along with height and the heterogeneity of pollutant diffusion so the result of signal box model is cursory with large errors.

Two-dimension box model is the improvement of single box model, it splits the box into several parts on the vertical direction and height, and hence it forms a two-dimensional box structure. If the width is also discretization, it can constitute a three-dimensional multiple box model which calculation method is similar with the two-dimensional box model but far more complex.

Multiple box model can reflect the spatial difference of air quality in regional area or urban area which precision is better than single box model. Undoubtedly, it is an effective tool for simulating atmospheric quality.

In 1995, Du proposed that the parameters of the box model can be confirmed by Gaussian diffusion model to comprehensively consider fluctuation distribution of pollutants concentration, pollutants attenuation, pollutants sedimentation process and lateral spread to outside the box of pollutants, and this combination model was applied to *The environment comprehensive treatment plan of Nantong city* and its calculation result is satisfactory. McDonald compared the two-dimensional multiple box steady model and Gaussian model so as to study the sulfur dioxide concentration distribution in Canada in 1996 (Wang, 2001). Shui-yuan Cheng built two-dimensional multiple box steady model in 1998 with the improvement that the direction of wind was simply divided into four directions. After calculating the pollutants concentration of each box in four directions, the average concentration was summation of them which have been weighted on the basis of wind direction frequency. Compared with single box model, the accuracy of this model is improved. But it only summarized the wind direction change as four direction frequencies instead of taking into account of the complexity of the wind direction, wind speed and other meteorological conditions. Such defects make prediction precision be lower than other complex models (Guo, 2008).

There are many other models such as BM model, SUTTON model, FEM3 model, ALO2HA model, SLAB model and DEGADIS model etc. They were developed based on different to deal with the complex conditions of atmospheric environment.

3.3 Diffusion simulation software of gas

The simulation of gas diffusion involves a lot of calculation and complicated boundary conditions. With the progress of computer technology, the task of calculation was dependent on computer more and more. The developers have established many soft -wares which were based on the theories and models mentioned above. The typical examples are as follow:

ADMS model was developed by Cambridge Environmental Research Consultants “to make use of the most up-to-date understanding of the behavior of the lower levels of the atmosphere in easy-to-use computer modeling systems for atmospheric emissions” (CREC, 2015). There are several functions in this model such as modeling dispersion of industrial emissions, managing air quality for urban planning and reviews, modeling road traffic and some industrial sources, managing air quality at airports and Screening model for industrial emissions. As a new generation of stable atmospheric diffusion mode, the latest atmospheric boundary layer and atmospheric diffusion theory is applied to air pollutant diffusion model. Moreover, the up-to-date atmospheric physics theory based on Monin-Obukhov length and boundary layer height (by which it describes the structure of the boundary layer parameters) is also introduced into ADMS.

AERMOD was developed by U.S. Environmental Protection Agency and the Office of Air Quality Planning and Standards. “It is an advanced plume model that incorporates updated treatments of the boundary layer theory, understanding of turbulence and dispersion, and includes handling of terrain interactions” (EPA, 2004). AERMOD system can be used in a variety of sources (including point source, non-point source and volume source), applied to Rural environment and urban environment, flat terrain and complex terrain, ground source and elevated source.

The following table is part of the soft wares:

Table 2: software using to simulate gas diffusion

ADAM	A model considers that how chemical thermodynamics, heat transfer, aerosols and dense gas affect gas diffusion, it is an improvement to Gaussian diffusion model.。
ADMS	A model uses point source, linear source, non-point source, volume source and network source model to simulate pollutants diffusion from the industrial, civil and road traffic pollution sources, and the latest air boundary layer and diffusion theory is applied to this model.
AERMOD	A pollution diffusion model is used to simulate influenced by pollutant emissions, meteorological, topography factor (that is, the concentration of any receptor point is sum of the weighting value of plumes concentration in two kinds of fluid field.).
AFTOX	A kind of Gaussian diffusion model simulates point ,non-point source, continuous and instantaneous high temperature liquid source and

	continuous and instantaneous high temperature gas source diffusion, shows pollutants concentration contour map, calculates the highest concentration of given height and time.
ASPEN	A kind of Gaussian diffusion model assesses annual average concentration of given receptor point within a fixed pollution source, considering the influence of source strength, meteorological condition and population density.
BlueSky	A model is used to predict the influence of smoke diffusion.
CALPUFF	An atmospheric quality assessment system considering of long-distance transport of pollutants and complex meteorological conditions in the unstable meteorological.
CAMEO	A gas diffusion method assesses the influence of pollutant considering fuel characteristics, lighting conditions, fuel conditions and meteorological conditions.
CMAQ	An atmospheric quality model is multiple nested aerodynamic and atmospheric -chemical coupling.
DEGADIS	A model simulates dense gas (or aerosols) dispersion under the condition of u flat topography.
EMIT	A model can effectively and conveniently dispose pollution source storage, editing and calculation, and assess a variety of scenarios.
FLUENT	A model stimulates the diffusion process of rotating machinery, pneumatic noise, point and non-point source.
FLOWSTAR	A model stimulates wind field and turbulent flow field changes in complex boundary layer can be simulated. It can be used to analyze the pollutant diffusion in wind power plant planning, forest wind movement.

HYROAD	A multiple model simulates pollutant discharge and diffusion in roadway.
ISCST3	A diffusion model mainly deals with point source, linear source, non-point source, volume source and open pollutants concentration distribution in the ambient air.
MMSOILS	An exposure assessment model used to charge the receptors influenced by soil intake/inhaled volatile substances and particles in the air, skin contact, drinking water etc.
PLUVUEII	An assess model used to predict source strength of point or non-point source in the condition of dispersion, chemical reaction and optical effect.
SHAOOS	A model used to inverting earth's air based on the law of refraction and ray tracing.

Source: Zou, 2012.

CHAPTER 4

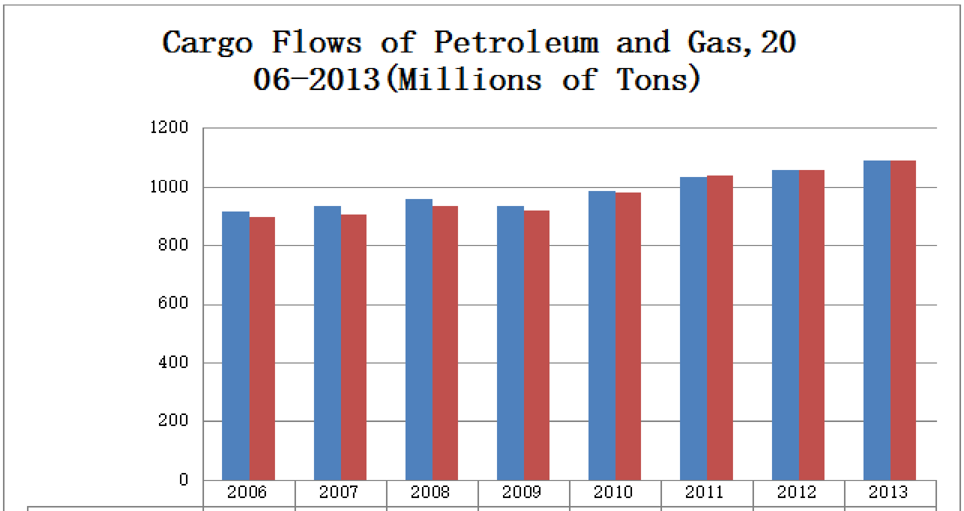
The Simulation of Dangerous Gas Leakage in Port Area

4.1 The necessity of study on gas diffusion in port area

The gas diffusion in port area has its features. Basically, there are three type of gas which may diffuse in port area: the gas leaked from gas carriers or associated pipes, the vapor from liquid chemicals leakage caused by chemical tankers or its associated pipes, the gas or vapor from package. The dangerous goods in package are usually transported by container ship and the transportation account is difficult to known. So the gas carriers and chemical tankers would be analyzed as an example.

4.1.1The increase of ship fleets of gas carriers and chemical tankers

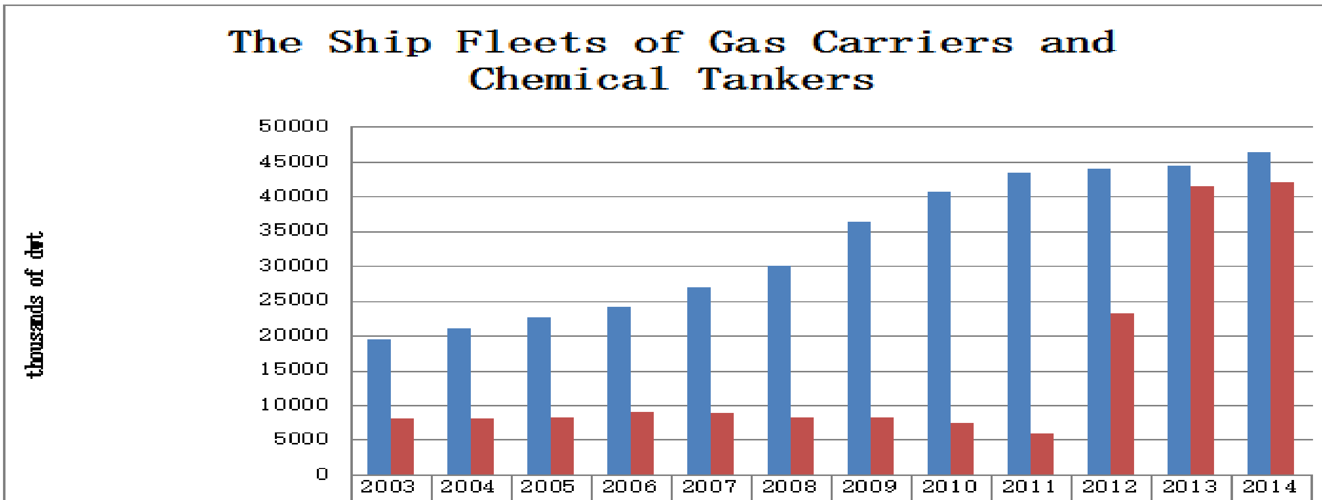
In recent years, with the development of world economy, there are stable increase in the freight volume of liquefied gas, chemicals in bulk and the ship fleets. Although affected by the global financial crisis, the freight volume of natural gas and petroleum products declined in 2008 (Most kinds of the petroleum are dangerous chemicals listed in IBC. It is unsuccessful to confirm freight volume of total dangerous chemicals transported by seaborne, so the freight volume of petroleum products is used to estimate total dangerous chemicals'.), but there is a obvious increment of the freight volume in this decade as shown:



	2006	2007	2008	2009	2010	2011	2012	2013
Goods loaded	914.8	933.5	957	931.1	983.8	1034.2	1055	1088.5
Goods Unloaded	893.7	903.8	934.9	921.3	979.1	1037.7	1055.1	1090.6

Figure1: Cargo Flows of Petroleum and Gas. Source: UNCTAD, 2007,2009,2011,2013.

It is interesting to note that despite the global freight volume fluctuated in recent years, the seaborne transport capacity of gas carriers and chemical tankers has maintained steady growth in same period. According to the statistic data of UNCTND, the increasing trend of transport capacity is as follows:



	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014
Gas carriers	19469	20947	22546	24226	26915	30013	36341	40664	43339	44060	44346	46427
Chemical tankers	8027	8004	8290	8919	8823	8236	8141	7354	5849	23238	41359	42009

Figure 2: The Ship Fleets of Gas Carriers and Chemical Tankers. Source: UNCTAD, 2005,2007,2009,2011,2013,2014

From the point of view of safety management, the expanding ship fleets of gas carriers and chemical tankers make accident probability increase correspondingly. In order to reduce the accident frequency or the consequences of the accident, the advanced technical method must be introduced into the industry of dangerous goods transportation.

4.1.2 The increase of cargo categories and hazard

For the dangerous goods transportation, another risk is that the cargo categories and the hazard are continuously rising. Take dangerous chemicals in bulk as an example, according to the catalogue of IBC, the quantity of cargo categories and X category

(Which is the most hazardous type of chemicals in IBC.) are shown in the table below:

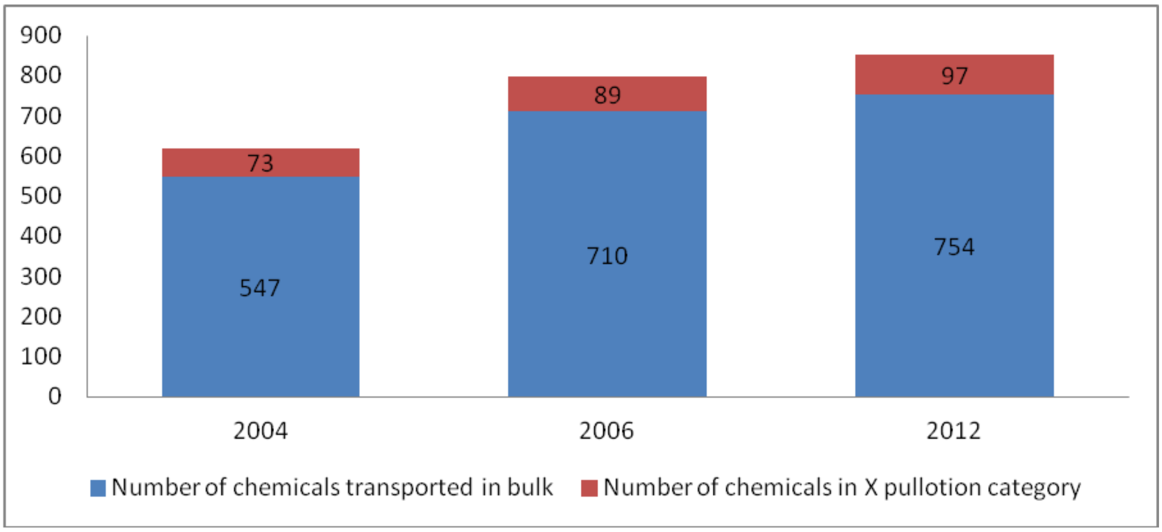


Figure 3: The change of cargo categories in IBC. Source: IMO,2004,2006,2012

From analysis mentioned above, both of the probability of dangerous goods leakage and the consequence are enlarged, thus it is necessary to utilize a more accurate tool to assess accident. It is the reason why the models are introduced to simulate gas diffusion which is one of types of harmfulness after an dangerous chemical leakage.

4.2 The simulation of toxic gas diffusion after chlorine leakage in a port

To understand the effectiveness of the accident model and estimate accident consequences of dangerous goods leakage in the port area, Gaussian point source puff model is used to conduct this simulation.

4.2.1 Accident scenario

Supposed that there is a chlorine gas leak accident in April 2015, the location is one of berths in a port. The port is flat topography near a chemical factory and power plant, their positions are as the chart:

Chart 1: The Location of Sensitive Points

Source: Author.

It is an instantaneous leakage which source strength is 1000 kilograms; the height of leakage source is 3 meters; date: 1000, April 16th,2015; meteorology: t southeast wind which speed is the annual average 4.4 m/s; temperature:35 ℃;cloud cover: 3;the location of the leakage:19°06 'N, 108° 36' E.

4.2.2 The process of simulation

In this simulation, multiple puffs superposition was used. Assuming that constant average wind speed is u, the x axis is parallel to the average wind direction in a fixed space coordinate system. At t = 0,a puff is released from the origin (0, 0,0) moving with the wind and swelling because of diffusion. The center position of puff is (ut, 0, 0) relative to the fixed coordinate system. A moving coordinate system is built when center position of puff is set as the origin. At a point in space (x, y, z) , the concentration after T period caused by the continuous discharge can be equal to the superposition of concentration by instantaneous puffs which was released in time interval △ t that is divided from T (Jiang, 2003).

$$C = \sum_{i=1}^{n} C_i(x, y, z, t - t_i)$$

C: The concentration caused by puff i (mg/m^3);

t: The time from the first puff released（s）;

t_i: The time of puff i released, so $t - t_i$ means the time span after puff i released;

The single puff' contribution to a point can be calculated according to the Gaussian puff model mentioned before.

Based on the given scenario, the diffusion coefficients can be confirmed (MEP China,2009b): within 1000 m from the origin, transverse diffusion coefficients $\sigma x=0.924279x^{0.177154}$, $\sigma y=0.924279y^{0.177154}$; beyond 1000 m from the origin, $\sigma x=0.885157x^{0.232123}$, $\sigma y = 0.885157y^{0.232123}$; vertical diffusion coefficient$\sigma z=0.917595z^{0.106803}$.

Meteorological conditions is particularly important in the simulation of gas diffusion so that the steady wind is a basic premise, namely during the accident, the wind speed and direction is without obvious change. Leakage source strength calculation is also a very important part in the numerical simulation because it directly affects the level of the accident and the security area. In this thesis, the source strength is a hypothesis without detailed calculations:

Table 3： The parameters of leakage source

The	The	Emission	Exhaust gas	Discharge	Displacement	The

leakage	type	rate Q （kg/s）	temperature Ts （℃）	duration(min)	Qv（m^3/s）	height of leakage source H (m)
Chlorine	Point source	3	50	30	1.0	3

Source: Author.

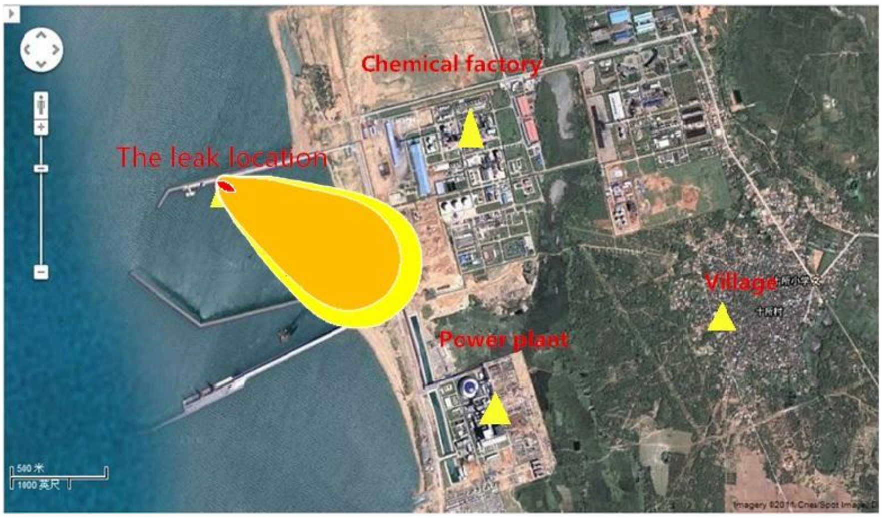
4.2.3 The result of simulation

After an accident, emergency response concerns about the scope of given concentration and the concentration change at control points (such as operation room where persons are near leakage location or the roads nearby), the result of two will be discussed.

4.2.3.1 The scope of given concentration

There are three LOC (Level of concern) used to confirm scopes: 850mg/m^3(red area)，3mg/m^3 (deep yellow area)and 1 mg/m^3 (light yellow area), because they are lethal concentration 50 (LC50), short term exposure high limit and short term exposure low limit of chlorine. The scopes in different time are as follows:

Chart 2: The diffusion scope after 3 min



Source: Author.

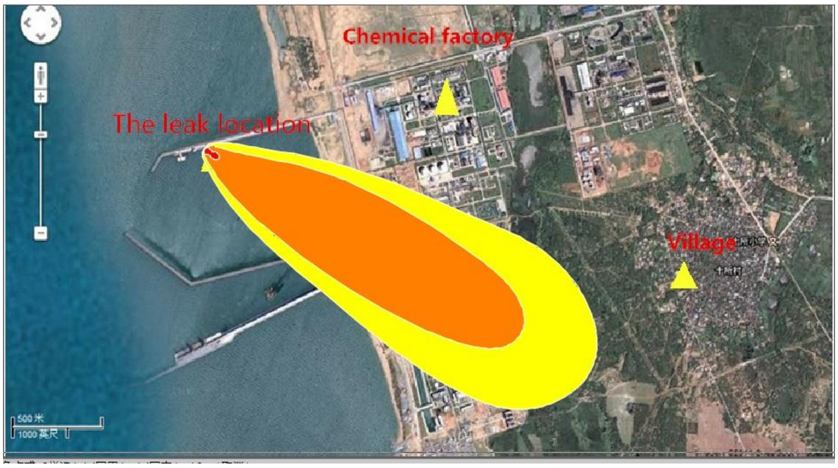
The detailed data are listed:

Table 4: The LOC distances after 3 min

The maximum ground-level concentration (mg/m^3)	The distance of the max ground-level concentration（m）	The length of median lethal concentration（m）	The length of short term exposure high limit（m）	The length of short term exposure low limit（m）
7004.5	38.2	112.4	881.6	974.3

Source: Author.

Chart 3: The diffusion scope after 10 min



Source: Author.

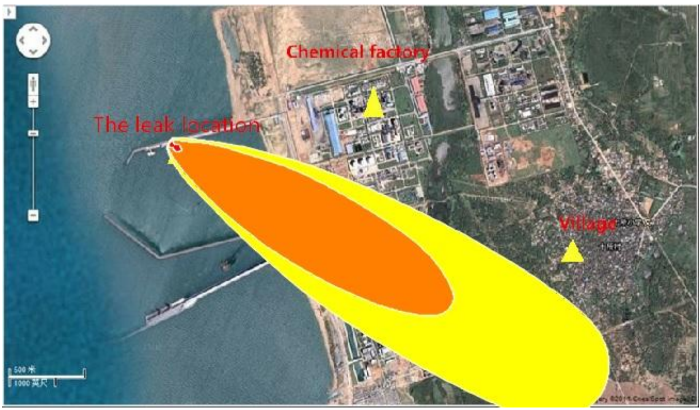
The detailed data are listed:

Table 5: The LOC distances after 10 min

The maximum ground-level concentration (mg/m^3)	The distance of the max ground-level concentration （m）	The length of median lethal concentration （m）	The length of short term exposure high limit（m）	The length of short term exposure low limit （m）
7004.5	38.2	112.4	2072.7	2504.1

Source: Author.

Chart 4: The diffusion scope after 15 min



Source: Author.

The detailed data are listed:

Table 6: The LOC distances after 15 min

The maximum ground-level concentration (mg/m^3)	The distance of the max ground-level concentration （m）	The length of median lethal concentration （m）	The length of short term exposure high limit（m）	The length of short term exposure low limit（m）
7004.5	38.2	112.4	2188.1	3341.8

Source: Author.

4.2.3.2 The concentration change of control points

In the simulation, the control points are set as below: A, the operation room with several operators; B, C, the traffic road corner by which reflect the pollutant concentration distribution of the road nearby; B is also the outer walls of the chemical plant that can assess the effect of gas leak to chemical factory; D, the location of the power plant that can measure the influence to power plants; E, one of the village control point that can monitor the influence to local residents. These points are set to illustrate the result of simulation without detailed audited.

Chart 5: The Location of Control Points

Source: Author.

The concentration trend of each point is as follows:

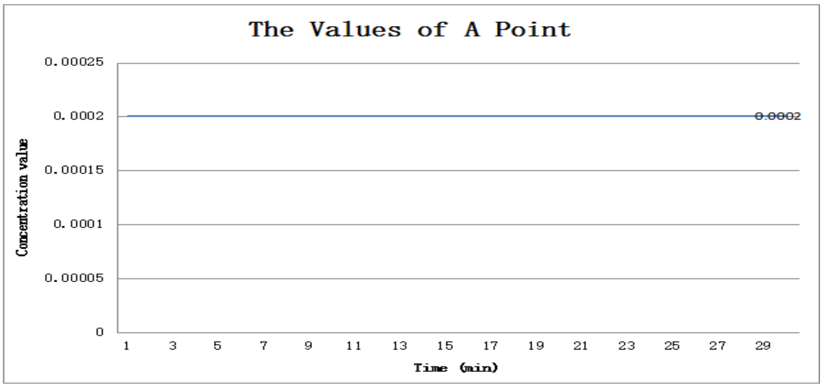


Figure 4: The Values of A Point. Source: Author.

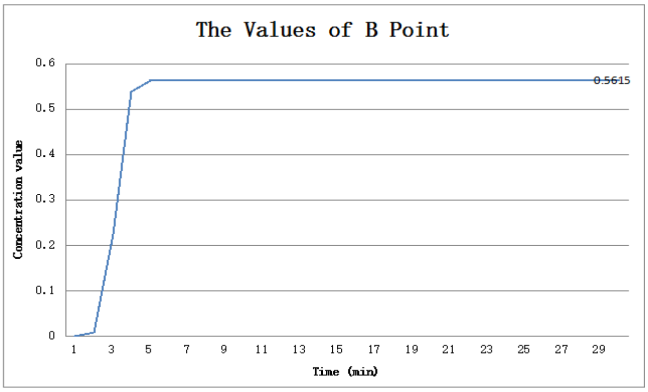


Figure 5: The Values of B Point. Source: Author.

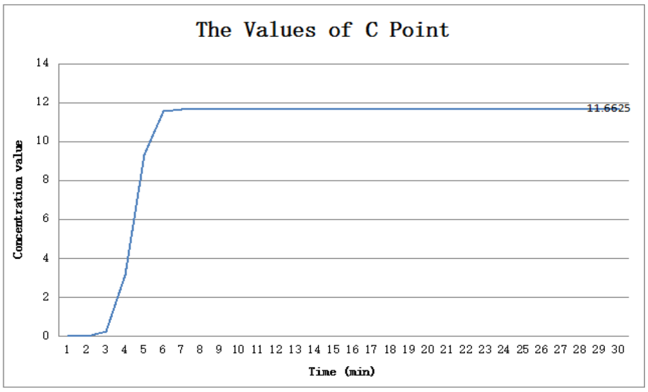


Figure 6: The Values of C Point. Source: Author.

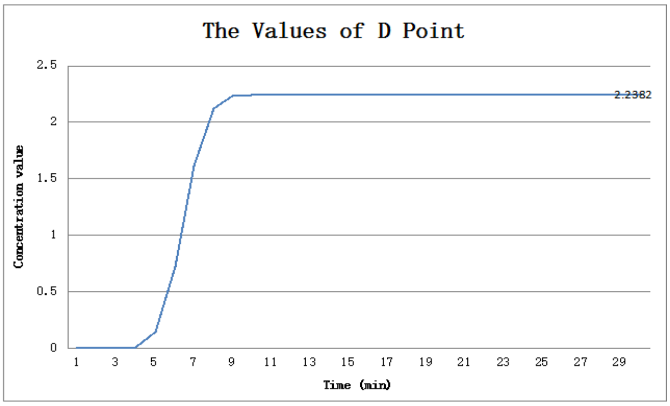


Figure 7: The Values of D Point. Source: Author.

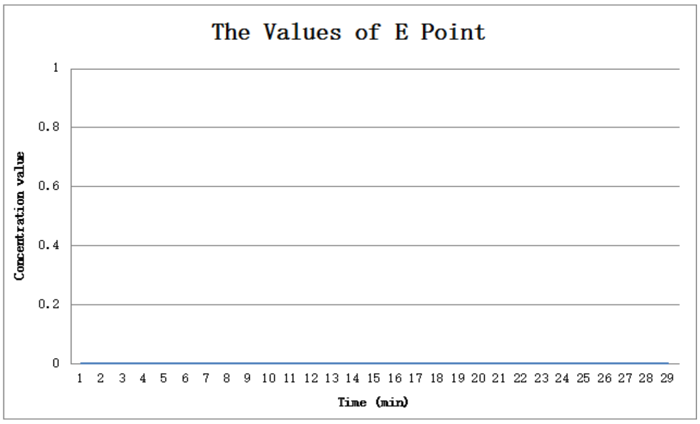


Figure 8: The Values of E Point. Source: Author.

The emergency response can be guided by these data.

4.3 The simulation of fire and explosion

If combustible gas reaches the explosion limit in the air, there would be a violent explosion after touching an open fire. It can produce a great fire ball and the strong thermal radiation causing casualties and property losses. The severity assessment of such accident is as follows (MOT China, 2013):

4.3.1 The fireball radius

The fireball radius is directly proportional to the cube root of the fuel quality:

$$R = 2.9W^{1/3}$$

R: fireball radius (m);

W: the mass of fuel (kg);

4.3.2 The fireball duration

The fireball duration is also directly proportional to the cube root of the fuel quality:

$$t = 0.45W^{1/3}$$

t: fireball duration (s);

4.3.3 The thermal radiation flux endured by the receptor

The thermal radiation flux received by the receptor q(r) can be calculated:

$$q(r) = Q_f R^2 r(1 - 0.058\ln(r))/(R^2 + r^2)^{3/2}$$

Q_f : the radiation flux of fireball surface (W/m^2);

r: the distance from receptor to the center of fireball (m);

4.3.4 The quantity of heat received by receptor

It can be confirmed by:

$$Q(r) = q(r)t$$

$Q(r)$: The quantity of heat received by receptor (J/m^2);

Followed the relationship between heat flux and the damage radius, the casualties radius and building damage radius can be obtained.

4.3.5 The simulation of gasoline vapor cloud explosion

The result of a gasoline vapor cloud explosion in a port:

Table 7: The Result of gasoline vapor cloud explosion

		Items	Values
Basic parameters	1	simulant model	typical
	2	Pool area type	Constant
	3	Pool area(m^2)	600
	4	Pipe diameter (mm)	DN250
	5	Gap area(m^2)	0.05
	6	Fuel	gasoline
	7	Quantity of fuel(Kg)（leakage speed×leakage time）	417.33×600 =250398
	8	Leakage time (S)	600
	9	Heat of combustion (kj/kg)	43687
	10	Density of liquid (kg/m3)	700
		Density of gas (kg/m3)	4.375
	11	Storage pressure (Pa)	300000

	12	Atmospheric boiling point (k)	373
	13	The distance between receptor to the flame surface (m)	29
	14	Combustion efficiency	1
	15	Environmental temperature (K)	298.15
	16	Combustion velocity （kg/s*m^2)	0.02247
	17	The time of exposure to fire (s)	90
Results	1	Leakage speed (kg/s)	417.33
	2	Casualties radius (m)	24.3
	3	Serious injured radius (m)	29.3
	4	Minor injured radius (m)	46
	5	Property loss radius(m)	15.7
	6	Safety distance for person(m)	59.1
	7	Mean flame height (m)	8.4
	8	Thermal radiation flux of receptor(kw/ m^2)	2.6
	9	Thermal radiation flux of flame surface(kw/ m^2)	66.3
	10	Total thermal radiation flux (kw/ m^2)	32267
	11	Casualties thermal radiation flux (kw/ m^2)	8.1
	12	Serious injured thermal radiation flux (kw/ m^2)	5.4
	13	Minor injured thermal radiation flux (kw/ m^2)	2.4

Source: Author.

According to the simulation, the consequences of gasoline vapor cloud explosion are: Casualties radius is 24.3m; Serious injured radius is 29.3m; Property loss radius is 15.7m.

CHAPTER 5

Demarcation of Safe Distance

There are two kinds of hazards after dangerous gas or vapor diffusing: fire and explosion, poisoning. In order to forecast the accident threat, it is necessary to choose a specific parameter used to confirm early warning. How the parameter changes need to be studied so as to decide the safe distance with LOC (level of concern) and take response actions such as: isolate hazard area and deny entry, evacuate or shelter in-place (DOT U.S.,2012). The diffusion concentration is chosen for this purpose.

5.1 The factors that need to be considered

The choice of safe distance for a given situation depends on several factors (DOT U.S.,2012). Firstly, the characters of dangerous goods namely: degree of health hazard, chemical and physical properties, source strength, control of release and rate of vapor movement.

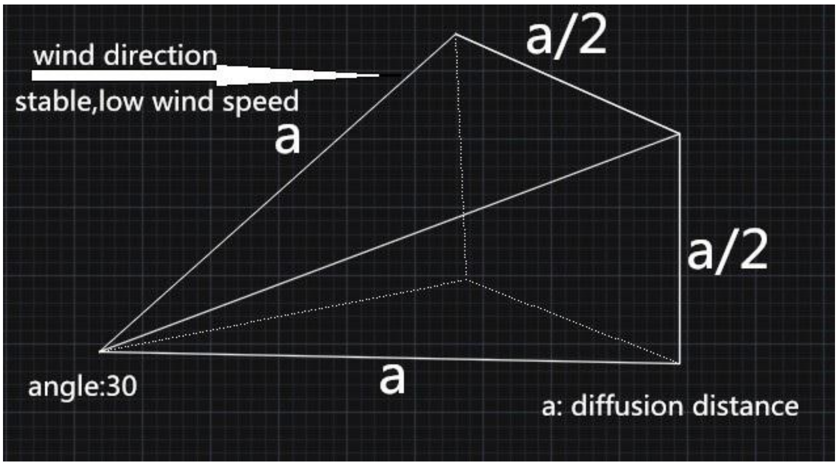
Secondly, the population threatened includes: location, number, time available to evacuate or shelter in-place, ability to control evacuation or shelter in-place, building types and availability and special institutions or populations (such as chemical factory and power plant in the scenario of this thesis.)

Thirdly, weather conditions includes: effect on vapor and cloud movement, potential for change, effect on evacuation or shelter in-place.

5.2 The guideline made by IMO

The Maritime Environment Protection Committee (MEPC) of IMO used to publish a guideline named *Pamphlet of Disposing the Chemical Pollution* to provide the methods which includes how to evaluate the hazard of chemicals leakage. For convenience of response to the chemicals leakage, the pamphlet listed a simple diffusion model by which can estimate the hazardous scope of chemical vapor as well as some roughly calculated data of chemicals as follows:

Chart 6: The simple diffusion model of instantaneous released chemicals



Source: IMO, 2000.

Table 8: The "a" value of some chemicals' hazardous scope (m)

Released Account(t)	Ammonia, Chloroethylene		Butane, Butadiene, Chloroethane, Ethylene, Propane
	Health threatened distance	Fire and explosion distance	Health threatened/ Fire and explosion distance
0.1	1000	200	200
1	2000	400	400
10	5000	1000	1000
100	10000	2000	2000

Source; IMO, 2000.

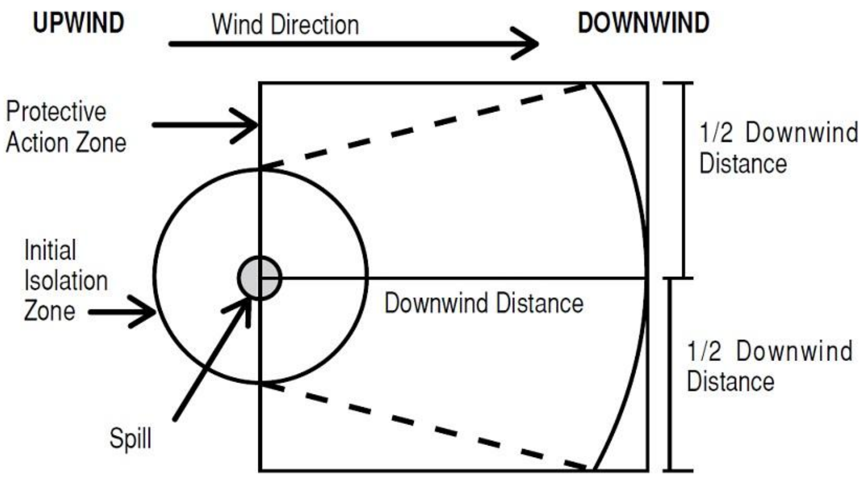
In addition, the measuring apparatus was requested for monitoring the chemical concentration. The combustible gas detector and the oxygen detector was applied to combustible gas detection; flame ionization detector, photo ionization detector, infra-red spectrophotometer should be prepared for poisonous gas leakage.

5.3 Emergency response guidebook (ERG) 2012

ERG (2012 vision), as its self-introduction, is a guidebook for first responders during the initial phase of a dangerous goods/hazardous materials transportation incident developed jointly by Transport Canada (TC), the U.S. Department of Transportation (DOT), the Secretariat of Transport and Communications of Mexico (SCT) and with the collaboration of CIQUIME (Centro de Información Química para Emergencias) of Argentina. The contents of this book include index list of dangerous goods in numerical order of ID number, index list of dangerous goods in alphabetical order of material name, safety recommendations which comprises a total of 62 individual guides and the data of safe distances which are "Initial isolation distances" and "Protective action distances".

The "Initial Isolation Distance" is "*a distance within which all persons should be considered for evacuation in all directions from the actual spill/leak source. It is a distance (radius) which defines a circle (Initial Isolation Zone) within which persons may be exposed to dangerous concentrations upwind of the source and may be exposed to life threatening concentrations downwind of the source*" (DOT U.S.,2012). The "Protective Action Distance" for "*a small spill is 0.5 kilometers (0.3 mile) for a daytime incident and 2.2 kilometers (1.4 miles) for a nighttime incident, these distances represent a downwind distance from the spill/leak source within which Protective Actions could be implemented. Protective Actions are those steps taken to preserve the health and safety of emergency responders and the public. People in this area could be evacuated and/or sheltered in-place"* (DOT U.S.,2012). The two types of safe distance can be shown as follows:

Chart 7: The Safe Distance after Accident



Source: DOT U.S.,2012

5.4 The effects of factors being considered in diffusion process

As mentioned above, there are several factors which can affect the concentration distribution in a diffusion process. To illustrate this effects, how the source strength and the weather condition influence diffusion would be analyzed according to the Gaussian puff model.

Firstly, the distance of chorine leakage is estimated with only one variable----source strength. The other parameters are set as :the height of leakage is 3m;the diameter of emission is 0.5m; the emission duration is 10 min; the temperature is 34 ℃; the atmospheric stability is D level; the wind speed is 1.8m/s; the LOC is LC50(850mg/m^3);according to the source strength, the safety distances of 10min after the leakage are listed in following table:

Table 9: The Result with Changing Source Strength

Emission rate Q (kg/s)	Gas Displacement Qv (m^3/s)	The maximum ground-level concentration (mg/m^3)	The distance of the max ground-level concentration (m)	The length of median lethal concentration (m)
3	1.0	3414.3	91.5	342.0
3	2.0	1223.2	163.0	291.0
3	3.0	615.0	241.3	---
6	1.0	6829.6	91.5	523.0
6	2.0	2445.1	163.8	492.4
6	3.0	1229.7	242.8	432.8
12	1.0	13659.2	91.5	767.4
12	2.0	4890.3	163.8	752.6
12	3.0	2459.4	241.8	724.7

Source: Author.

If in same gas displacement (1.0 m^3/s), the relationship between emission rate and the distance of LC50 is as follow:

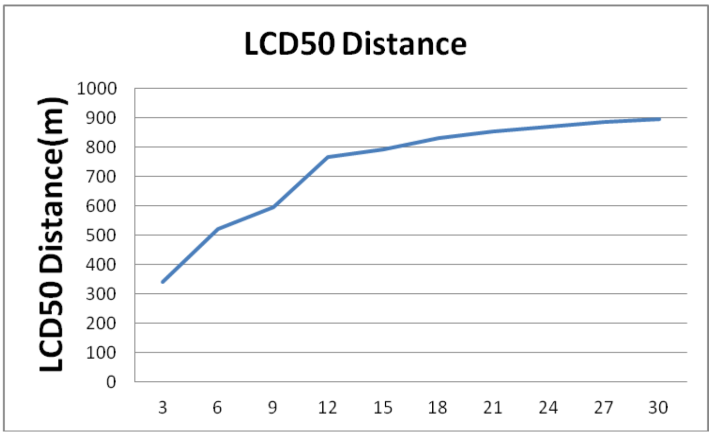


Figure 9: The Change of LC50 Distance with Source Strength Changing..

Source: Author.

Secondly, the safe distance is estimated by other variable----wind speed. The other parameters are set as same as the scenario except the atmospheric stability which depends on both wind speed and solar radiation intensity. The solar radiation intensity is assumed to +2 and the source strength is fixed, emission rate is 12Kg/s and gas displacement is 1 m^3/s, so as to observe the relationship between wind speed and the safe distance (LC50). The safe distance of 10min after the leakage is as follows:

Table 10: The Result with Changing Wind Speed

Wind speed(m/s)	atmospheric stability	The maximum ground-level concentration (mg/m^3)	The distance of the max ground-level concentration （m）	The length of median lethal concentration （m）
1	A-B	17420.7	9.6	64.8
2	B	13241.2	46.4	330.9
3	B-C	14196.6	51.0	335.9
4	B-C	24460.7	35.3	287.6
5	C-D	41821.1	42.7	434.8
6	D	41680.4	49.1	398.7
7	D	36517.9	56.9	365.1

Source: Author.

The trend is more obvious in this chart:

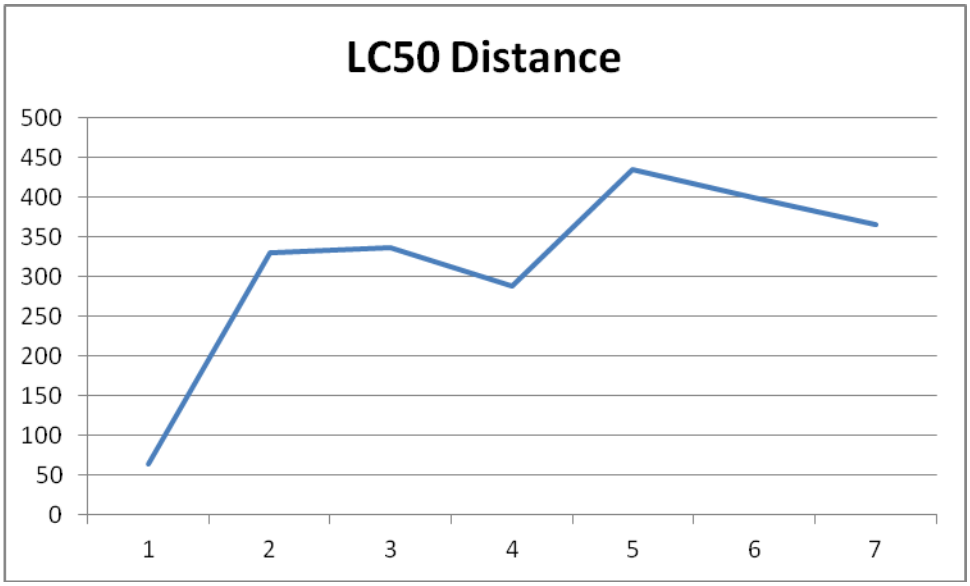


Figure 10: The Change of LCD50 Distance with Wind Speed Changing. Source: Author.

Considering that the wind speed affects movement of the gas puff as well as the atmosphere turbulence, it is more complex than source strength to concentration distribution.

CHAPTER 6

Conclusions

This thesis analyzes the theories of gas diffusion and the risk of air pollution incidents faced by maritime transportation. The simulation of chorine leakage is conducted to estimate the accident consequence and confirm the safe distance. The guidelines and standards are introduced also to compare the emergency response actions advised by different organizations and countries. Taking Gaussian puff model as an example, the effects of influenced factors, such as source strength, meteorological condition and population threatened etc., are roughly discussed. So the conclusions are listed below:

1. The distances according to different LOC are predicable when the data of leakage and weather are provided. Based on a trustworthy simulation, the evacuate scope can be decided more reasonable so as to reduce losses and avoid public panic.

2. It is necessary to pay more attention to gas diffusion in a breeziness or calm wind because of its highly hazardous degree. The pollutants is more difficult to diffuse in a breeziness or calm wind so it may have high concentration in some area for a long period, and the diffusion scope is larger.

3. The empirical data of safe distance is not enough to emergency response because of the complex source strength and weather condition in fact that influence the diffusion process vastly.

4. The fire and explosion distance is much less than poisonous distance because the gap between the low explosion limit level and poisonous LOC is huge when they are transited in same unit.

Some factors are not considered in this thesis that are important for gas diffusion, such as the estimation of source strength, suitable models for different chemical, evaporation rate and water reactive effect which is extremely relevant to port area. To achieve a more precise simulation, these factors need to be researched in future.

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