# Simulation analysis of leakage, diffusion and explosion of ships carrying

# dangerous goods while waiting for lock and mooring

Zhang Jiayi<sup>1</sup>, Qi Le<sup>1</sup>,Liu Jingxian<sup>1,2,3</sup>

 Wuhan University of Technology, School of Shipping, Wuhan 430063; 2. Wuhan University of Technology, Hubei Provincial Key Laboratory of Inland Shipping Technology, Wuhan 430063, Hubei; 3. National Water Transportation Safety Engineering Technology Research Center, Wuhan 430063, Hubei

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### ABSTRACT

In order to minimize the casualties and economic losses caused by dangerous goods leakage accidents caused by dangerous goods ships passing through the Three Gorges ship locks and waiting to be anchored, the article is based on the ALOHA software, which comprehensively considers the volume of dangerous goods passing through the Three Gorges locks, the form of dangerous goods, the form of packaging and Physical and chemical properties and other factors were used to determine the numerical simulation parameters, and numerical simulations were carried out for methanol, 1,2-xylene, and oil and gas in the toxic area, flammable area, and explosion area of the vapor cloud. Combined with the MARPLOT software, the numerical simulation results were fitted to the Three Gorges Waiting Gate. The electronic river map of the anchorage is visualized. And through the analysis of the numerical simulation results, it is proposed that for the leakage accident of methanol, 1,2 xylene and oil and gas, the emergency response warning range should be set at 3000m, 781m and 6300m downwind of the leakage source, so as to effectively guide the danger. The anchoring of the ship before passing the lock is safe.

### **1** Introduction

With the rapid development of the national economy, especially affected by the needs of economic and industrial development, shipping on the Yangtze River has become the main choice for the transportation of chemical dangerous goods. According to the data, the shipping throughput of the Three Gorges Hub will reach 150.58 million tons in 2021, a year-on-year increase of 9.29% and a record high. Among them, the Three Gorges Ship Lock will have a throughput of 146.44 million tons, exceeding 46% of its designed throughput capacity<sup>[1]</sup>. The Three Gorges Ship Lock is basically operated at full capacity. In the original design, the normal number of flights of the Three Gorges Project have four characteristics: high political sensitivity, high security risk, high correlation with people's livelihood and high social concern<sup>[3]</sup>, the research on the safety risks of ships carrying dangerous goods in the waters of the Three Gorges Project.

In the past ten years, the safety of dangerous goods shipping has received extensive attention from the industry and researchers. Some scholars have discussed the market access issues for the shipping of dangerous goods in the Yangtze River<sup>[4]</sup>, transportation process monitoring<sup>[5]</sup>, fire supervision and inspection<sup>[6]</sup>, the management mechanism<sup>[8]</sup>, the safety of dangerous goods ships passing through the lock<sup>[9]</sup>and the safety management problems in the anchorage of the Three Gorges waiting to be locked<sup>[12]</sup>, running strength<sup>[13]</sup>, anchoring method<sup>[14]</sup>, anchorage scale prediction<sup>[15]</sup>and other aspects were discussed and studied, However, there

is a lack of accident analysis during the waiting period.

The average waiting time of dangerous goods ships passing through the locks of Class 1 inflammable and explosive dangerous goods has been shortened from 7 days in 2006 to about 3 days in 2011<sup>[1]</sup>, but in recent years, with the increase of large ships<sup>[12]</sup>, and it is more common for ships to be affected by special meteorology and hydrology when they are waiting for locks. During this period, there are safety risks such as ship anchorage, collision, and damage. Risk<sup>[13]</sup>, once the leakage of dangerous goods, fire, explosion and other accidents due to anchor movement or collision affects the normal operation of the water area of the Three Gorges Project, it will cause serious economic losses and social impacts. Therefore, it is necessary to simulate and analyze the leakage, fire, explosion and other accidents of ships carrying dangerous goods anchored at the Three Gorges waiting lock for emergency needs, and combined with the MARPLOT software to fit the numerical simulation results to the corresponding map, which can quickly and vividly provide reference information to emergency managers.

#### 2. Simulation Design Based on ALOHA Software

ALOHA software is a software for risk analysis and research of the consequences of hazardous chemical leakage accidents. The chemical library of the software contains the physical property information of about 1,000 common hazardous chemicals, and can consider the leakage materials, leakage locations, Atmospheric conditions and other information, the software prompts the input scene information in the form of a dialog box, and can simulate dangerous accidents such as the diffusion, explosion, flash fire, jet fire and other dangerous accidents after the leakage of dangerous goods from ships. After the end, the corresponding calculation results are output in the form of charts and texts. The main process of software accident simulation is shown in Figure 1.



Figure 1 ALOHA-based simulation process for the leakage accident of dangerous goods on ships waiting to be locked

# 3. Determination of Numerical Simulation Parameters for Dangerous Goods Leakage in Ships Waiting for Lock

# 3.1 Determination of leak scenarios

The driving force of liquid leakage is generally pressure, and during the leakage process, the density of the liquid remains unchanged. The leak rate can be determined from the Bernoulli equation of fluid mechanics:

$$Q_0 = C_d A \rho \sqrt{\frac{2(P - P_0)}{\rho} + 2gh}$$

In the formula,  $Q_0$  is the liquid leakage rate, kg/s;  $C_d$  is the dimensionless leakage coefficient,

dimensionless; A is the orifice area,  $m^2$ ;  $\rho$  is the medium density,  $kg/m^3$ ; P is the pressure in the tank,

Pa;  $P_0$  is the external environmental pressure, Pa; h is the height of the liquid level above the orifice, m.

# $(C_d \text{ value } 0.61)$

For the liquid leakage rate under normal pressure, it depends on the liquid level above the crack; for the liquid leakage rate under very pressure, it mainly depends on the difference between the medium pressure in the container and the ambient pressure and the liquid level.

It is assumed that the ship is in the state of the greatest risk, that is, the ship is fully loaded, the damaged position of the ship's compartment is at the lowest point and the liquid level does not decrease with leakage.

# **3.2 Determination of Typical Dangerous Goods**

Since there is no statistical data for the goods waiting to be locked, this paper uses the relevant statistical data of the dangerous goods passing through the Three Gorges Gate to represent the data of the dangerous goods waiting to be locked. According to statistics, the volume of dangerous goods in bulk accounts for about 99% of the total, and the volume of liquids accounts for about 99.5% of the total. Therefore, the selection of typical goods only considers bulk and liquid goods. From 2015 to 2020, the traffic volume of dangerous goods passing through the Three Gorges Gate is shown in

Table 1.

Table 1 2015~2020 Three Gorges Crossing Dangerous Goods Traffic Volume bulk/packaging

bulk/packaging	Liquid volume (10,000 tons)	Solid volume (10,000 tons)	Total volume (10,000 tons)
Bulk	5258.2	0	5258.2
Package	22.2	25.6	47.8
total	5280.4	25.6	5306

According to statistics, from 2015 to 2019, the types of dangerous goods passing through the Three Gorges Ship Lock were sorted according to the volume of transport. Among them, the first 6 types of dangerous goods accounted for 90.5%, namely flammable liquids (diesel, crude oil), gasoline, coal tar pitch, Kerosene, methanol, 1,2-xylene, the physical and chemical properties of the first six dangerous goods are shown in エラー! 参照元 が見つかりません。. The physical and chemical properties such as boiling point, ignition temperature, saturated vapor pressure, and flash point of the first six dangerous goods were compared and analyzed, and gasoline, methanol and 1,2-xylene were selected as the simulation objects. Because gasoline, kerosene, etc. cannot be simulated in ALOHA software mixture, so the propane leak is used instead of the oil and gas leak.

Table 2 Typical Dangerous Goods Physical and Chemical Properties

and al		Elash		Saturated		Boilin	Ignition	
numb	name	noint/	chemical	vapor	explosion	g	temperature/	Density/g/
er	nume	°C	formula	pressure/k	limit	point/	°C	m3
•1		Ū.		Pa		°C	0	

	(33648)							
1	Flammable liquids (diesel, crude oil)	>55	C10-C22	54.8	0.6%~7.5 %	>180	257	0.84~0.86
2	(32001/310 0) Gasoline (61869)	-50~-2 0	C <sub>5</sub> -C <sub>12</sub>	54.8	1.0%~6%	30-220	415~513	0.70~0.78
3	Coal tar	204.4	-	-	>30%	<470	485	1.15~1.25
4	(33501) Kerosene	40	C <sub>11</sub> -C <sub>17</sub>	56	0.6%-5%	180-31 0	223	0.8~1.0
5	(32058) Methanol	8	CH <sub>3</sub> OH	12.3	6%~36.5 %	64.7	473	0.777
6	(33535) 1,2-Xylene	10	C <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>	4.89	1.2%~7%	110.6	535	0.87

# 3.3 Parameter setting

According to the real picture of the anchorage of the hazardous chemicals ship waiting to be locked, the annual average natural environment data released by the local meteorological department, the specific size of the hazardous chemicals ship, and the distribution of the compartments where the hazardous chemicals are stored, the relevant parameters are set in the ALOHA software. The specific parameter value settings are shown in Table 3. Among them, since the ALOHA software can only simulate the leakage of cylindrical or spherical cabins, it is converted into a horizontal cylinder according to the actual volume of the cabin, so the leakage cabin is set as a horizontal cylinder.

Table 3 leakage accident simulation basic parameter table

	_	-		
parameter	Numerical value	parameter	Numerical value	
ambient temperature	24°C	shape	cylinder	
Storage	2000	longth	10m	
temperature	20 C	length		
wind direction	East (E)	Bottom diameter	7m	
wind speed	1.5m/s	loading method	100%	
Relative humidity	75%	Crack size	1m×0.02m	
cloud cover	50%	leak location	10%	
Dangerous species		Methanol, o-xylene, Propane		

### 4. Analysis of Numerical Simulation Results of Dangerous Goods Leakage in Ship Locking

There are four hazard levels built into ALOHA: toxic level of concern, flammable level of concern, thermal radiation level of concern, and overpressure level of concern), which is used to calculate the range of areas for various hazards. ALOHA software divides the red zone, orange zone and yellow zone according to the hazard level standard (the red zone represents the area with the most serious damage, and the orange zone and the yellow zone represent the areas with decreasing damage in turn).

4.1 Analysis of the simulation results of the toxic area of vapor cloud

Toxicity Hazard Levels describe the extent to which a person is harmed by exposure to a chemical gas cloud for a certain period of time. The AEGL value (Acute Exposure Guideline Level, AEGL) is the best acute exposure guideline concentration currently available. It was formulated and published by the National Academy of Sciences based on the data of human and animal research on chemical substances. There are now more than 250 AEGLs for hazardous chemicals<sup>[16]</sup>. The volatilized gas of 1,2-xylene, methanol, and oil and gas leaks quickly combines with the air to form a large area of toxic gas without encountering a fire source. In this paper, the Acute Exposure Guideline Level (AEGL) is used Table 4. index divides the influence scope of toxic gas produced by methanol and oil and gas leakage process. For 1,2-xylene leakage, the toxic gas impact range is divided by health concentration (IDLH). For 1,2-xylene, this standard has only one level, that is, IDLH=900ppm is 1,2-diol Hazardous limits for toluene.

AEGL grade	Display color	Representative area	Description of the degree of danger
AEGL-1	yellow zone	Mildly poisoned area	Persons exposed to this toxic atmosphere will experience discomfort such as loss of feeling, but this phenomenon is temporary and the body can return to normal after
AEGL-2	Orange District	Moderately toxic area	Persons exposed to this toxic atmosphere can experience serious adverse health effects
AEGL-3	red zone	High toxicity area	Persons exposed to this gas can experience life-threatening effects or cause death

The simulation results of the toxic area of methanol, 1,2-xylene, and vapor cloud generated by the leakage of oil and gas in the waiting stage of the ship carrying dangerous goods are shown in Figure 2. Use the MARPLOT software to fit the results simulated by ALOHA to the corresponding locations on the map. The results are shown in Figure 3.



Figure 2 Methanol, 1,2-Xylene, Vapor cloud toxic area from oil and gas leaks



Figure 3 MARPLOT fitting results of methanol, 1, 2 xylene, oil and gas vapor cloud toxic area in the waiting area

The following conclusions can be drawn from the analysis of the above simulation results of the cargo leakage toxic area in the waiting stage of the ship carrying dangerous goods:

(1) The boundary of the third-level toxic area (AEGL-3) of methanol and oil and gas is 737m and 1300m downwind of the leak point respectively. The concentration of methanol and oil and gas in this area can reach 7200ppm and 33000ppm respectively. If there are no protective measures, personnel are exposed In this area, there will be anesthesia, severe poisoning and even death due to respiratory failure. Therefore, in the event of a leakage accident, it is forbidden for people to stay in this area to prevent poisoning and death.

(2) The boundaries of the secondary toxic area (AEGL-2) of methanol and oil and gas are respectively 1500 m and 2200 m downwind of the leak point. The concentrations of methanol and oil and gas in this area are above 2100 ppm and 17000 ppm, respectively, which are at a relatively dangerous level. If people exposed to the area are not evacuated in time, poisoning symptoms such as vomiting and dizziness will occur. People in this area need to be evacuated in time.

(3) The first-level toxic area of methanol and oil and gas (AEGL-1) has a wide range of influence, and the boundaries are 3000m and 4100m downwind of the leakage point. People in this area will experience obvious discomfort if inhaled, but it is not irreversible damage. In the event of an accident, a cordon should be set up to prohibit unrelated persons from entering.

(4) 781m from the leeward side of the 1,2 xylene leakage point is the limit that endangers life, safety and health (IDLH). The concentration of 1,2 xylene in this range is above 900ppm. In this range, human or animal inhalation will cause serious damage. as a result of.

(5) If cargo leakage occurs during the waiting period of the ship carrying dangerous goods, it can be seen from the fitting analysis of the actual map that the serious injury area (red area) of the leaking ship is a non-residential area, and there are fewer ships, personnel and roads. When an accident occurs, the residents in the area should be evacuated immediately, and other ships and personnel should be prohibited from entering the area to avoid irreversible accidents caused by carrying fire sources. The minor injury area (yellow area) has a wide range, including relatively far residential areas, riverside highways and other areas. This area may cause physical discomfort to personnel, which may be caused by the increase in wind speed, wind direction and leakage aperture. The area has expanded, so residents and people in the dangerous area need to organize evacuation.

## 4.2 Analysis of simulation results of vapor cloud flammable area

ALOHA uses 60% LEL (Lower Explosive Limit, LEL) as the flammable level red zone and 10% LEL as the flammable level yellow zone. The degree of danger represented by each level of LEL is shown in Table 5.

Table 5 LEL Risk Levels

LEL rating	Display color	Representative area
LEL10%	yellow zone	flammable area
LEL60%	red zone	Extremely flammable area

From the perspective of vapor cloud flammability, methanol, 1,2-xylene, and oil and gas are all flammable gases. LEL), more than 60% are extremely flammable areas, which will cause deflagration and are very dangerous. The simulation results of the flammable area of the vapor cloud generated by the leakage of methanol, 1,2-xylene and oil and gas in the waiting stage of the ship carrying dangerous goods are shown in Figure 4. Use the MARPLOT software to fit the results simulated by ALOHA to the corresponding locations on the map. The results are shown in Figure 5.



Figure 4 Methanol, 1,2-Xylene, Vapor Cloud Flammable Area from Oil and Gas Spills



Figure 5 MARPLOT fitting results of methanol, 1, 2 xylene, oil and gas vapor cloud flammable area in the waiting area

The following conclusions can be drawn from the analysis of the simulation results of the above simulation results of the flammable influence range of the cargo leakage vapor cloud during the waiting period of the ship carrying dangerous goods:

The highly flammable areas of methanol and 1,2-xylene vapor clouds are 226m and 241m downwind from the leak source, and 130m and 130m from the sidewind, respectively. If there is an ignition source in this area, it is very likely to cause the vapor cloud to burn, causing fire and explosion accidents. In this area, the ignition source should be avoided as much as possible.

The flammable areas of methanol and 1,2-xylene vapor clouds are 732m and 781m downwind from the leak source, and 150m and 200m from the sidewind. , should be used as a warning range for emergency response.

# 4.3 Analysis of simulation results of vapor cloud explosion area

The overpressure hazard level describes the degree of hazard caused by the overpressure of the shock wave generated by the explosion. The range of hazards at different overpressures is given when ALOHA calculates a vapor cloud explosion. The overpressure damage level used by ALOHA is as shown in Table 6:

Overpressure hazard level	Display color	Description of the degree of danger
1.0 psi	yellow zone	broken glass
3.5 psi	Orange District	Persons may be seriously injured
8.0 psi	red zone	building destroyed

The gas pressure generated by the concentration of 1,2 xylene after the leakage cannot reach the explosion condition, so this paper does not simulate 1,2 xylene in terms of vapor cloud explosion. The simulation results of the vapor cloud explosion area generated by the leakage of methanol and oil and gas during the waiting period of the ship carrying dangerous goods are shown in Figure 6 Methanol, Vapor Cloud Explosion Area from Oil and Gas Leak. Use the MARPLOT software to fit the results simulated by ALOHA to the corresponding locations on the map. The results are shown in Figure 7 MARPLOT fitting results of methanol and oil and gas vapor cloud explosion areas in the waiting area.



Figure 6 Methanol, Vapor Cloud Explosion Area from Oil and Gas Leak





The following conclusions can be drawn from the analysis of the simulation results of the above simulation results of the explosion of the cargo leakage vapor cloud in the waiting stage of the ship carrying dangerous goods:

The explosion range of methanol vapor cloud is as follows: an explosion within 154m downwind of the leakage source will cause damage to buildings, an explosion within 170m may cause serious injury to personnel, and an explosion within 289m will cause glass to break. In this range, there are fewer ships, people and roads, so

the impact of severe explosions is less effective.

The explosion range of the oil and gas vapor cloud is: the explosion within 2100m downwind of the leakage source may cause serious injury to personnel, the explosion within 2200m will lead to broken glass, and the impact of the explosion is still very strong, which should be used as a warning range for personnel.

## **5** Conclusion

According to the specific environmental background conditions at the anchorage of the Three Gorges dangerous goods ship waiting to be locked, it is assumed that the ship carrying dangerous goods is in a state of maximum risk, and the ALOHA software is used to simulate the hazard degree of the leakage accident of dangerous chemicals, and the following warning suggestions are obtained. Provide technical guidance for crowd evacuation and emergency rescue decision-making to minimize casualties and economic losses caused by accidents.

If methanol leaks, irrelevant personnel should be prohibited within 3000m downwind of the leakage source, and personnel within 1500m downwind of the leakage source should be evacuated in time, and fire sources should be avoided within 732m downwind and 150m from the leakage source to prevent occurrence of fire fire. To sum up, the downwind direction of 3000m from the source of methanol leakage should be used as the warning range for emergency response.

In the event of leakage of 1,2 xylene, a cordon should be set up within 781m downwind of the leakage source to prevent irrelevant personnel from endangering life, and fire sources should be avoided within 781m downwind and 200m from the sidewind of the leakage source to prevent fires. To sum up, 781m downwind of the 1,2 xylene leakage source should be used as the warning range for emergency response.

If oil and gas leaks, a cordon should be set up within 4100m downwind of the leak source to prohibit irrelevant personnel, and those within 2200m downwind of the leak source should be evacuated in time, and fire sources should be avoided within 6300m downwind and 3000m from the sidewind of the leak source to prevent fire. In the unfortunate event of an explosion, a range of 2200m downwind from the leak source should be used as a warning range for personnel to prevent serious injury to personnel. To sum up, the downwind direction of 6300m from the source of oil and gas leakage should be used as the warning range for emergency response.

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#### About the author

1. Zhang Jiayi, female, master student of Wuhan University of Technology. Her main research direction is traffic environment and security.

Address: Yujiatou Campus, Wuhan University of Technology, No. 1178, Heping Avenue, Wuchang District, Wuhan City, Hubei Province

Postcode: 430063

Contact: 13517116800; E-mail: zhang\_jiayi@whut.edu.cn

2. Qi Le, male, associate professor and master tutor of Wuhan University of Technology, doctor of engineering. His main research directions are transportation engineering, ship traffic flow modeling and simulation.

Address: Yujiatou Campus, Wuhan University of Technology, No. 1178, Heping Avenue, Wuchang District, Wuhan City, Hubei Province

Postcode: 430063

Contact: 13396063826; E-mail: leqiem@s163.com

3. Liu Jingxian, male, professor and doctoral supervisor of Wuhan University of Technology, Ph.D.

Address: Yujiatou Campus, Wuhan University of Technology, No. 1178, Heping Avenue, Wuchang District, Wuhan City, Hubei Province

Postcode: 430063 Contact: 13387581712; E-mail: ljxteacher@sohu.com