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Risk Simulation and Route Optimization for Hazardous Chemical Transportation Based on Gaussian Plume Model

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The boom of chemical industry has made China heavily demanding for hazardous chemicals. In response to this, the security of road transport for hazardous chemicals has become even more important, while in the academic circles, the great challenge is to study how to ensure the security in the course of highway transportation of hazardous chemicals. It is suggested that the consequences of possible accidents occurred in transition be predicted accurately and effectively, by which a safer route can be chosen for transporting these chemicals. The most effective ways of how to reduce the probability of accidents resulting from hazardous chemicals and how to mitigate the consequences of road transport accidents resulting from hazardous chemicals are nothing but choosing an ideal transport route for these. This paper simulates the leakage of dangerous chemicals with the Gaussian plume model to determine its affected area, analyze the key factors affecting the choice of transportation routes and the route tuning objective. There are two problems: how to reduce the road transport risk and how to optimize the transport route for dangerous chemicals. We should settle both of them to provide the clues to improving the security of road transportation for dangerous chemicals.

1. Introduction

Hazardous chemicals are a class of chemicals flammable and explosive and extremely apt to cause personal injury and property losses during storage, transportation and application. In recent years, the burgeoning of the chemical industry has led to a rapid increase in the demand for hazardous chemicals. In response to this, the illegal operation and potential risks during road transportation of hazardous chemicals have also brought the surge in accidents actually occurred in this process. Unlike ordinary traffic accidents, the dangerous chemical has its own natures such as flammability and explosive which determine the particularity of transportation accidents. Traffic accident of dangerous chemicals (Shi, 2018), once occurs, often triggers grave consequences, which pose great threats to people’s lives and properties (Wang et al., 2005). The management of hazardous chemicals should be settled urgently (Thomson, 1999; Wang and Meng, 2012), and even it has aroused the common concern of all interested parties.

Against this background, it is of great significance to analyze the road transport risk of hazardous chemicals, thereby reducing the probability of traffic accidents resulting from hazardous chemicals. In this process, the first thing is to simulate the consequences of transportation accident if it occurs, determine the extent of the areas affected by the accidents possibly occurred in the transportation process of hazardous chemicals, based on which to optimize the transportation routes for such chemicals.

2. Simulation of transport risk of hazardous chemicals

Leakage of hazardous chemicals are often accompanied by the release of harmful gases. The fluidity of the gas determines that the release of continuous toxic gases often brings disaster to much wider extent of areas than other types of accidents. In the analysis of transport risk of hazardous chemicals, a key step is to analyze where and how far the transport accident spreads to. The affected areas of hazardous chemicals are often subjected to a variety of meteorological conditions such as atmospheric temperature and wind speed (Bubbico et al., 2004), as well as climate conditions. Therefore, in the process of road transport of hazardous chemicals,

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the appropriate analytical method must be chosen to determine the affected area of accidents occurred in the transport process of hazardous chemicals (Schweitzer, 2006; Patel and Horowitz, 1994; Barkan et al., 2003; Wang and Sun, 2010; Hwang et al., 2001). The toxic gas flows caused by the leakage of hazardous chemicals are subject to complex and diverse meteorological conditions. In general, they will form a pinniform smoke plume. Since the Gaussian model more applies to calculate the diffusate concentration level in the case when the distribution of diffusate concentrate fits the Gaussian distribution, it is often used to simulate atmospheric diffusion. This study takes into full account the advantages of the Gaussian model and applies it to the road transport risk of hazardous chemicals. It can help simulate and calculate the concentration of toxic gases in the affected area of accidents. The commonly used Gaussian models include two types, i.e. the Gaussian plume model and the Gaussian puff model. Among them, the latter seems to fit well with point source diffusion which lasts for shorter time, that is to say, it more applies to the case when sudden and transient leakage occurs; on the contrary, the former may be better suited to simulate the spread in continuity. Therefore, this paper chooses the Gaussian plume model to study the distribution of toxic substance concentration levels in the affected area.

2.1 Gaussian plume model

Since the Gaussian plume mode features simple and easy to use, visual diffusion effect, high flexibility, it has become one of the most widely used air diffusion models. For example, Ma et al. applied the Gaussian plume model to explore the diffusion caused by the leakage of natural gas (Ma et al., 2017); Wu Kaifeng, Dong He et al. introduced the Gaussian plume model into PM 2.5 pollution in different areas (Wu et al., 2017; Dong et al., 2014); Liu Xinxing et al. traced the liquid nitrogen leakage and diffusion using the Gaussian plume model (Liu and Liu, 2014). This model more applies to the leakage accident where the leakage time of continuous point sources is not less than the diffusion time. The accident occurrence point is usually used as the coordinate origin. This model takes the advection diffusion differential equation as the basis. When the wind speed and the turbulent diffusion coefficient are all constant, the solution of the advection diffusion differential equation normally follows the standard normal distribution. The expression that the Gaussian plume model describes the distribution of pollutant concentration levels in air pollution accidents is:

$$c(x,y,z)=\frac{Q_m}{2\pi\mu\sigma_y\sigma_z}\exp\left(-\frac{y^2}{2\sigma_y^2}\right)\{\exp[-\frac{(z-H)^2}{2\sigma_z^2}]+\exp[-\frac{(z+H)^2}{2\sigma_z^2}]\} \tag{1}$$

Where: x, y, z represent the distance from the origin in the downwind, lateral and windward directions, m; c(x, y, z) represent the concentrations of hazardous substances at the distances of x, y, z x from the origin in the three directions, respectively, mg/m3;*u* represents the average wind speed, m / s; σ_y is the horizontal diffusion coefficient, m; σ_z is the vertical diffusion parameter, m; Q_m is the release rate of harmful substances, mg/s; *H* represents the effective leak source height, i.e. the sum of the original height and its lift height of the leak source, m.

2.2 Parameter setting for Gaussian plume model

Table 1: Pasquill-Gifford-Turner atmospheric stability classification

Speed of wind (m/s)	Daytime sunshine			Cloud amount≤4/8	Cloud amount≤3/8
	Strong	Medium	Weak		
<2	A	A~B	B		
2~3	A~B	B	C	E	F
3~5	B	B~C	C	D	E
5~6	C	C~D	D	D	D
>6	C	D	D	D	D

Table 2: Diffusion coefficient interpolation formula

Atmospheric stability	σ_y	σ_z
A	$0.22(1+0.0001x)-0.5$	$0.20x$
B	$0.16(1+0.0001x)-0.5$	$0.12x$
C	$0.11(1+0.0001x)-0.5$	$0.08(1+0.0002x)-0.5$
D	$0.08(1+0.0001x)-0.5$	$0.06(1+0.0015x)-0.5$
E	$0.06(1+0.0001x)-0.5$	$0.03(1+0.0003x)-1$
F	$0.04(1+0.0001x)-0.5$	$0.016(1+0.0003x)-1$

Since the diffusion of pollutants has a close bearing on atmospheric conditions, it can be graded according to atmospheric stability (He et al., 2016). The commonly used classification methods are shown in Table 1.
In formula (1), the horizontal and vertical diffusion coefficients are calculated according to the Briggs interpolation formula, as functions subject to the distance. The functional relationship is shown in Table 2.

3. Optimization of transport routes for hazardous chemicals

The Gaussian plume model can be used to simulate the consequences of accidents occurred in the transportation process of dangerous chemicals. The area affected by accidents has close concern with the optimization of transport routes, providing the clues to the route optimization. The choice and optimization of routes for transporting hazardous chemicals matter both the area affected by the consequences of accidents and many other factors. Only when we fully consider these factors that may affect route selection can the transport route optimization of dangerous chemicals come true.

3.1 Factors that affect road transport risk of hazardous chemicals

There are manifold factors affecting road transport risk of hazardous chemicals (Zhong, 2018), including route and traffic characteristics, meteorological conditions, population density along the route, traffic volume, characteristics of hazardous chemicals, and vehicle conditions. Among them, the most important factors include the population density within the affected area, route traffic conditions and meteorological conditions, etc.; in the affected area, there are the affected populations in the road and non-road areas and in the relatively dense areas (hospitals, shopping malls, schools, etc.). The traffic conditions mainly include the probability of traffic accidents and the traffic volume. The main impact factors are shown in Table 3.

Table 3: Main Factors Affecting Road Transportation Risk of Hazardous Chemicals

No.	1	2	3	4	5	6	7	8	9
Factor	Hospital	School	Shopping mall	Intersection	Road	Traffic	Temperature	Wind speed	Population

3.2 Route optimization target of hazardous chemicals

To optimize the transport routes for hazardous chemicals, the first thing is to identify the objectives, including how to reduce the probability of accidents, narrow the affected area, and minimize the number of people affected. Among them, the most common factors are how to shorten the transportation distance, compress the driving time and reduce the transportation cost. The multi-objective routes can often achieve a better optimization effect than single-objective routes, but this is limited to ideal conditions only. Under real world conditions, there are often contradictions and games in the process of multi-objective optimization. The route optimization process must allow for the constraints of realistic conditions triaged ruthlessly. After comparison and demonstration, this paper chooses the routes where the freight and the transportation risk between the origin and destination can be minimized to achieve the transport route optimization of hazardous chemicals.

3.2.1 Minimize the freight

The costs incurred during the road transport of hazardous chemicals depend on the driving distance and time. The total time required for the transportation directly determines how much the transportation costs and what are the profits. Therefore, travel duration can indirectly represent economic benefits; the transport mileage of dangerous chemicals represents fuel consumption, the mechanical loss, and the increase and decrease of transportation costs in the whole process, which account for almost the vast majority of the total cost of road transport.

3.2.2 Minimize the transport risk

Many factors such as the historical accident rate of the selected routes for hazardous chemicals in the transportation, the population density along the route, and the meteorological conditions directly affect the transportation risk, as well as the different risk levels. Government regulatory authorities generally focus on the population exposure in the areas surrounding the transportation route for hazardous materials when transporting hazardous chemicals in bulk. They hold main responsibility for planning the transport route of dangerous chemicals with minimal risk, thereby improving the management level of dangerous goods transportation.
Seen from past experience, we should minimize the transportation cost and risk as the departure point for security management of hazardous chemicals, considering the interests of government regulatory authorities, while taking into account the benefits of hazardous chemicals companies. It indeed has a certain practical

significance.

3.3 Route selection for dangerous chemicals

The transport routes for hazardous chemicals can be chosen in many ways. This paper uses the widely used Dijkstra algorithm based on angle improvement (Wang et al., 2009), which has correlation with the fitness in the genetic algorithm. This fitness means to specify a corresponding fitness value for each solution based on the actual proximity. The angle-improved Dijkstra algorithm has a relatively narrow search range, does not cover all road segments. It only aims at partial road segments. It is unnecessary to traverse all the routes in the road network, making the computation quick and easy; the other feature of the algorithm can calculate the fixed value, while genetic algorithm cannot do so.

The following is an example to illustrate how this algorithm is implemented.

The intersections in the road network are abstracted as nodes, and the routes between the intersections as edges. It is assumed that the start point of the traffic flow in the road network is unique and the destination point is also unique. Each road is unidirectional, and in positive direction, it runs from the departure to the destination points. There is a traffic light installed on each intersection. All the nodes in the road network need to be numbered with the departure point marked as A, the destination point as B; there are the option of different routes between departure and destination points. The driver should consider how to select one optimal route in the regional road network that can minimize the transit time and ensure a safe and quick delivery of the dangerous chemical transported by the driving vehicle to the destination. The following input and output models can simplify and solve the problem.

Input:

(1) Road network topology;

(2) All nodes D(i), where *i* represents node *i* in the road network; the weights B(i, j) of all nodes, respectively. As shown in Fig. 1, the original road network can be abstracted into the type of Fig. 2. The circle represents the node and the line represents the edge in Fig. 2.

Output: Set S of the shortest route.

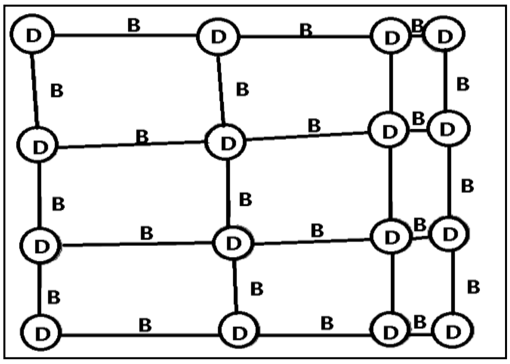

Figure 1: Schematic diagram of nodes and edges in the topology

The algorithm is described as follows:

Step 1. Establish a suitable coordinate system with the departure point A as the origin, the direction from the departure point A to the destination point B as the positive semiaxis of the X-axis. Each element in the topology is weighted;

Step 2. Within the range of positive and negative right angles in the positive direction of the X axis, search all nodes directly connected to the departure point A, and put the qualified node into the set S;

Step 3. Find the node closest to the departure point from the set S, and re-establish a coordinate system with the selected point as the new origin, repeat step 1 to find the child node within positive and negative included angle of 90° along the X-axis positive direction;

Step 4. Traverse all the child nodes, and re-calibrate the weight of any edge directly connected to the node at the moment according to the shortest duration between these nodes.

Steps 3 and 4 should be repeated multiple times until a predetermined destination point is found. After the search, the route corresponding to the sum of the minimum B and D is the shortest one to be sought, while this sum is just the minimum time required for the driver to drive from the departure point to the destination point.

The overall process of the algorithm is shown in Fig. 2.

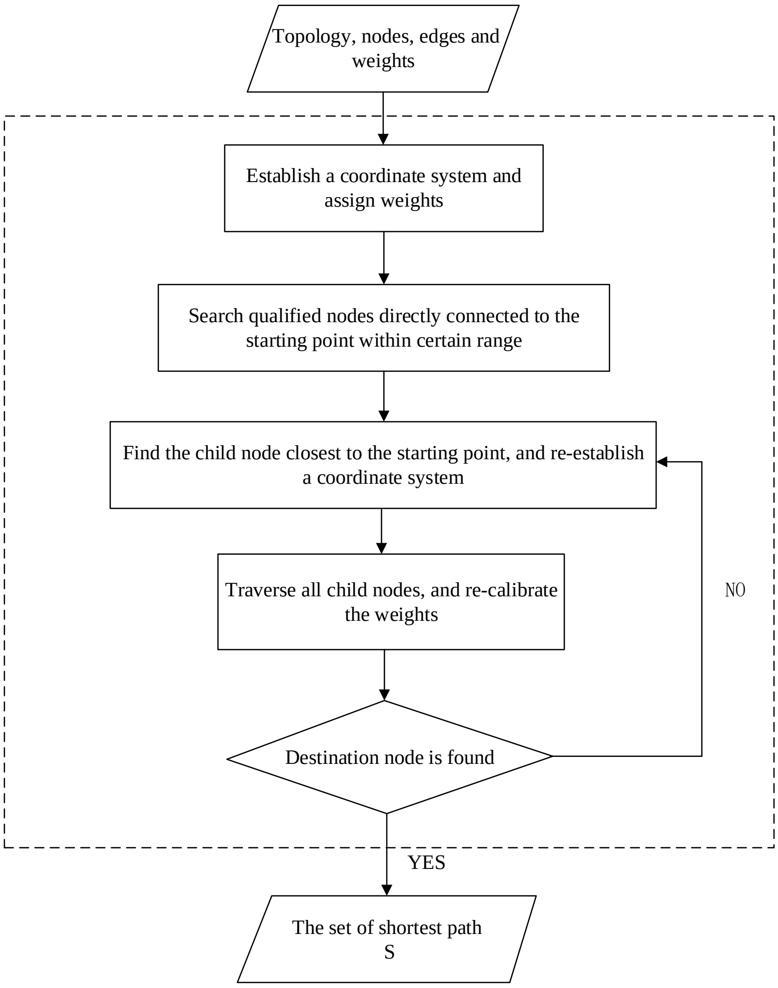

Figure 2: Algorithm flow chart

4. Conclusion

(1) The Gaussian fume model is used to simulate the road transportation risk of hazardous chemicals, and calibrate its parameters so as to achieve more accurate simulation on the possible area affected by the accidents;
(2) Route optimization is also studied hereof, fully involving other factors rather than the area affected by the accident, such as population distribution, meteorological conditions, traffic conditions, etc. in the affected areas, clarify the objectives of route optimization, that is, how to minimize the transportation costs and risk, fully considering the interests of government regulatory authorities and corporations and individuals running dangerous chemicals. The improved Dijkstra algorithm is applied to optimize the transportation route of hazardous chemicals.

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