Environmental Engineering and Management Journal

December 2020, Vol. 19, No. 12, 2187-2196
http://www.eemj.icpm.tuiasi.ro/; http://www.eemj.eu

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OPTIMIZATION OF THE EVACUATION ROUTE IN CHEMICAL PLANTS BASED ON THE DEPTH-FIRST SEARCH ALGORITHM

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Abstract

Optimal evacuation routes are crucial to protect workers' safety when accidental leakage of toxic gas occurs in chemical plants. However, the majority of route optimization focuses on the transport field and few on the evacuation routing optimization in chemical plants. This paper proposes a dynamic evacuation routing optimization method for chemical plants under toxic gas release scenarios. From the complete accident scenario set (CASS) built with wind fields and leakage sources, the leakage probability can be quantitatively represented. Based on the computational fluid dynamics (CFD) simulation, the consequences of toxic gas dispersion including the time-dependent concentration under different leakage scenarios can be obtained. Subsequently, considering the time-dependent toxic gas concentration and exposure time, the dynamic cumulative individual risk (CIR) can be calculated by applying the dynamic dose-response model (DDR). Then according to the simplified evacuation topology, the Depth First Search (DFS) algorithm is employed to define all evacuation routes connected with arcs. With the objective of minimizing CIR, an evacuation route optimization model is proposed and solved by MATLAB. Results demonstrate that the proposed method can hopefully minimize the CIR in chemical plants when they are facing toxic gas release and poisoning risks.

Key words: complete accident scenario set; computational fluid dynamics; Depth First Search; dynamic dose-response model; evacuation routing optimization

Received: January, 2020; Revised final: April, 2020; Accepted: June, 2020; Published in final edited form: December, 2020

1. Introduction

An appropriate evacuation route can reduce losses during evacuation when toxic gas releases in chemical plants (Xi et al., 2016), especially when shelter-in-place fails. Toxic gases usually exist in chemical plants, such as chlorine and ammonia, leakage of such gases may lead to multiple casualties (Li et al., 2012; Xiong et al., 2016; Zhang et al., 2017; Zhu et al., 2009). For example, an anhydrous ammonia release incident at the Millard Refrigerated Services, Alabama, on August 23, 2010, caused one employee injured during evacuation (CSB, 2015). Therefore, a proper evacuation pathway should be identified to reduce losses when gas leakage accidents occur in chemical plants (Dou et al., 2019; Xiong et al., 2016; Zhou et al., 2008).

The evacuation routing optimization problem has aroused interest in many researchers since it is of vital significance to reduce losses when accidents happen (Aziz et al., 2017; Gai et al., 2018; Li, 2009; Liu et al., 2016). Various approaches are proposed and developed to handle routing optimization. In general, they are based on mathematical modeling, simulation, and soft computing (Liu et al., 2016; Zhang et al., 2013). New sights have been brought by soft computing, which is based on intelligent algorithms and effective to solve evacuation problems by stochastic programming methods. As for stochastic programming, appropriate measures are important in

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yielding the best evacuation plan (Yuan and Han, 2009). The number of optimization objectives varies with optimization targets. Setting the minimal evacuation time as objective, a modified Dijkstra algorithm is proposed to solve the optimization model (Yuan and Wang, 2008; Zheng et al., 2019). Improved algorithms based on heuristics are developed to solve multi-objective evacuation routing problems (Gai et al., 2017; Koca et al., 2018; Kou et al., 2013). In large-scale evacuation problems, such as the evacuation of the downtown population in big cities under terrorist attacks, gas leakage or natural disasters, the combinational explosion of routes will increase computation time significantly. Thus, heuristic algorithms are commonly applied to solve such problems (Li and Chen, 2012; Wang et al., 2019).

When there are fewer choices, exhaustive search also called brute-force search is adopted to accomplish the optimization of evacuation routes, which is a very general problem-solving technique and algorithmic paradigm that consists of systematically enumerating all possible candidates for the solution and checking whether each candidate satisfies the problem's statement (Draganov Stojanovski, 2014), but it will be difficult or even impossible to get optimal results due to the huge amount of route combinations in large-scale problems (Uijlings et al., 2013). Thus the exhaustive search is typically used in small scale problems that do not have a large number of potential solutions. A modified exhaustive search method has been carried out to reduce computation costs (Chakrabarti and Kyriakides, 2008; Liu et al., 2016; Uijlings et al., 2013). Since the evacuation routes optimization problem does not have a large number of potential solutions, this paper employs the exhaustive search which is effective in small-scale situations to realize routing optimization. The Depth-First Search (DFS) algorithm, which is an exhaustive algorithm, has been employed to find all evacuation routes in this research.

The time-dependent concentration of toxic gas during dispersion is essential for planning evacuation routes. Simulation of accidental toxic gas leakage has been conducted since the early 1980s, and some numerical models and trails have been developed and used, such as Dense Gas Atmospheric Dispersion (DEGADIS), An Atmospheric Dispersion Model for Denser-Than-Air Releases (SLAB), Area Location of Hazardous Atmospheres (ALOHA), and Unified Dispersion Model (UDM) (Fan et al., 2016; Gerbec et al., 2017; Tauseef et al., 2011; Zhang et al., 2007). These models have been developed based on gas dispersion empirical formulas, though they are time-saving in computation, sometimes simulation results calculated by these models are not accurate enough to meet demands (Gavelli et al., 2008; Havens and Spicer, 2005; Qiao and Zhang, 2010). Whereas the computational fluid dynamics (CFD) simulation method has become one of the most appropriate ways to simulate toxic gas leakage and dispersion, and it has been verified by some experiments (Deng et al., 2012; Gavelli et al., 2008; Huang et al., 2012; Shen and Yu, 2008; Sun et al., 2013; Zhang et al., 2020). In this paper, based on the complete accident scenario set (CASS) (Zhang et al., 2019), time-dependent toxic gas concentration is obtained from CFD. Depending on two parameters: the concentration of toxic materials and the exposure time, the dose-response model has been widely used to evaluate the consequences of a toxic material exposure (Bagheri et al., 2016; Zhang and Chen, 2010).

In this paper, considering the time-dependent chlorine concentration, we combined dynamic dose response (DDR) model with CFD to evaluate the dynamic cumulative individual risk (CIR), and with the purpose of minimizing CIR, a MATLAB script based on the exhaustive search is developed to determine optimal evacuation routes.

The paper is organized as follows: Section 2 introduces the evacuation problem and sheds light on the results of the CFD simulation and the CIR model. Section 3 details the methodology of evacuation route planning. Conclusions are presented in Section 4. The nomenclature is shown in Table 1.

Table 1. Nomenclature

Nomenclature		
Acronym	CFD	Computational Fluid Dynamics
	CIR	Cumulative individual risk
	DFS	Depth First Search
	CASS	Complete accident scenario set
	DDR	Dynamic dose-response
	DEGADIS	Dense Gas Atmospheric Dispersion
	SLAB	An atmospheric Dispersion Model for Denser-Than-Air Releases
	ALOHA	Area Location of Hazardous Atmospheres
	UDM	Unified Dispersion Model
	IR	Individual risk
	HSE	Health and Safety Executive
	SIMPLE	Semi-Implicit Method for Pressure Linked Equations
	erf	Error function
Parameter	m	Toxic concentration index
	A, B	Constants depending on the types of toxic gases
	f	Exposure probability of evacuees to hazardous equipment
	v	Evacuation speed (m/s)
	t_r	Response time of evacuees (s)
Variable	$V = \{v_1, v_2, ...v_n\}$	Set of nodes
	E	Set of arcs
	v_1	Starting node
	v_n	Destination node
	i, j	Node i, j
	x	Abscissa of position (x, y) (m)
	y	Ordinate of position (x, y) (m)
	D_{ij}	Exposure dose when evacuating through arc (v_i, v_j)

	M_{ij}	Decision variable
	k	Leakage scenario
	R	Complete route
	P_r	Probit variable
	P	Individual fatality probability
	P_k	Occurrence probability of scenario k
	I	Total number of leakage scenarios
	t	Exposure time of evacuees (s)
	c_{ij}	Concentration of toxic gas between time t_i and t_j (ppm)
	$D(R)$	Exposure dose on route R
	n	Total number of nodes
	t_i	Time that evacuees enter arc (v_i, v_j) (s)
	t_j	Time that evacuees leave arc (v_i, v_j) (s)
	$IR_k(R)$	Individual risk under leakage scenario k on route R
	$CIR(R)$	Cumulative individual risk on route R under all leakage scenarios

2. Material and methods

2.1. Problem description

Our first case study consists in modeling a Chlor-Alkali plant with a liquid chlorine preparation system, which is a sealed circulation system. The cyclic material is liquid and gas chlorine. The Chlor-Alkali plant has 6 workshops, 12 units, 46 production teams, and 326 workers. Chlorine is highly toxic. That means in case of severe leakage, workers' lives will be seriously threatened.

According to the layout of this chemical plant, an evacuation model is built to simulate the evacuation. The evacuation problem is a network flow problem with certain constraints. To emulate the flow of evacuees, a graph Graph = (V, E) defined with sources and links is proposed to represent the network of the evacuation area. V denotes the set of nodes and E represents the set of arcs. Inside the chemical plant, nodes are used to describe the starting point, crossing roads and the destination point, and segment E show the links between nodes.

Node v_1 near the leakage area is selected as the evacuation starting point. Similarly, node v_n in the safe area is selected as the destination node and all other nodes are intermediate nodes.

Restricted by the layout of roads and installations in the plant, where some nodes cannot be connected. This results in a directed evacuation network with 10 nodes and 15 arcs but first the evacuation area is simplified. The evacuation network topology is shown in Fig. 1.

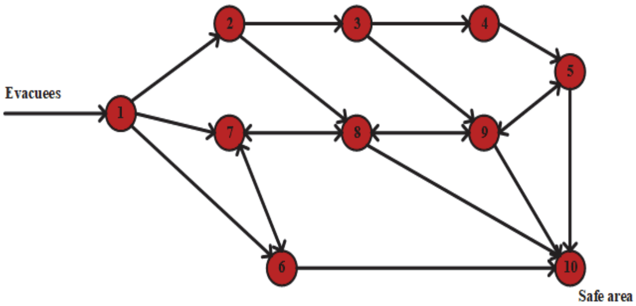


Fig. 1. The evacuation network topology

2.2. CFD simulation and outcomes

A previous CFD simulation is carried out to predict the leakage process of chlorine in this chemical plant (Li et al., 2018). The leakage and dispersion process, as well as the time-dependent concentration of chlorine are obtained from this simulation. The CFD simulation methodology is shown in Fig. 2, which will be described in the following.

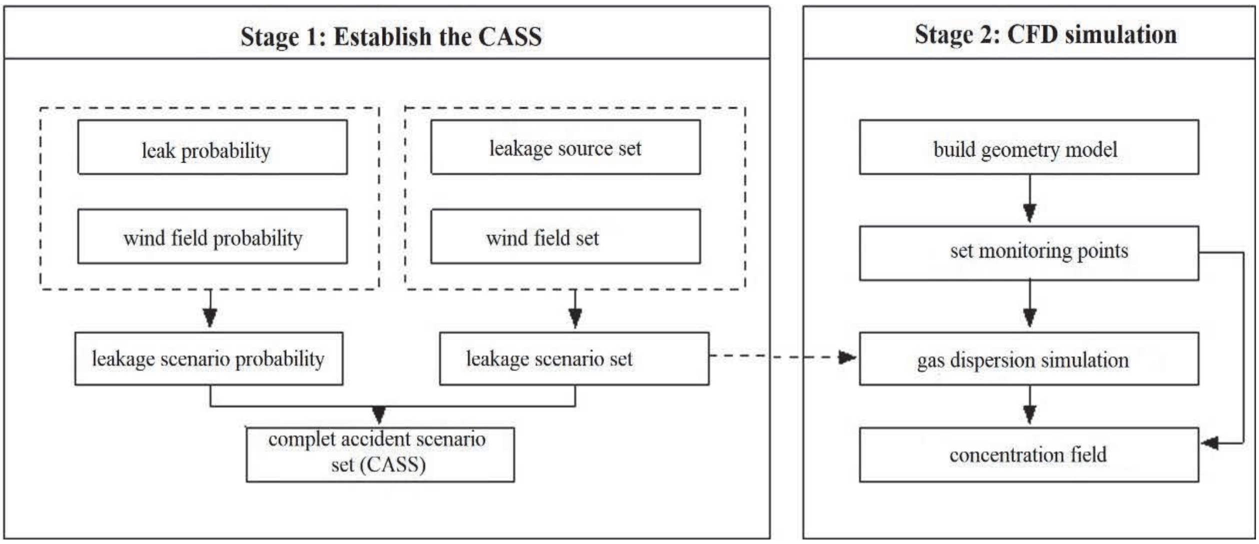


Fig. 2. The methodology of predicting leakage consequences by CFD

2.2.1 Establish the CASS

A former CFD simulation research has established the CASS to quantitatively represent the probability of leakage scenarios (Fu, 2017; Zhang, 2017). Wind field parameters according to local meteorological records and leakage sources based on the actual conditions of this factory are determined. Taking 8 different wind directions and 7 wind velocities in this area as parameters, the wind field set is established. The leakage source is identified by analyzing the liquid chlorine preparation system by experienced engineers, and four types of equipment: tank, liquefier, submerged pump, cylinder are determined.

Besides, four typical leakage apertures: small aperture, medium aperture, large aperture and catastrophic aperture are determined. The software LEAK 3.2, which uses a built-in failure database about chemical accidents in the world, is applied to predict the leakage probability of chlorine in different leakage sources with different leakage apertures (Fang et al., 2018).

By comparing the chlorine preparation system to similar facilities with available historical records in the database, the leakage probability can be calculated. Afterward, the leakage source set is built. According to the wind field set and leakage source set, the CASS built by 510 leakage scenarios is acquired. 88 leakage scenarios that account for over 90% of the total occurrence probability are screened out to reduce the computation costs.

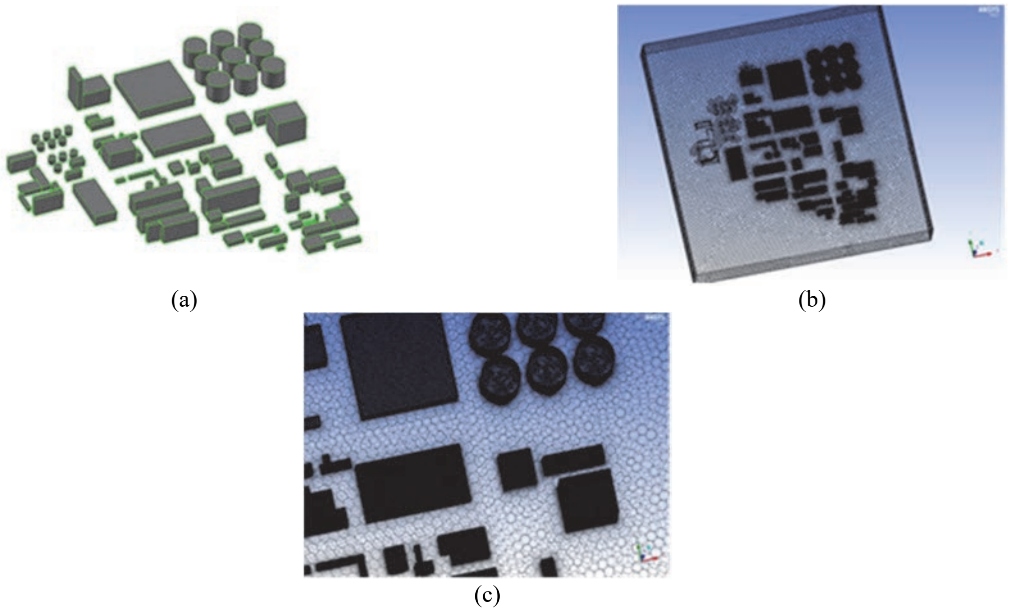
2.2.2. CFD simulation

According to the detailed dimensions of the facility, the three-dimensional geometric model of the simplified chemical plant is established and meshed by the CFD preprocessor GAMBIT 2.4.6. And the grid is converted into the polyhedral grid after importing into CFD commercial code, Ansys-Fluent 14.5. The geometry model and the mesh are presented in Fig. 3. According to the Chinese standard “Human dimensions of Chinese adults”, the mean shoulder height of Chinese male adults is 136.7 cm (CNSI, 1988). And Environmental Engineering Dictionary (Spellman, 2018) details the breathing zone is a hemisphere forward of the shoulders, centered on the mouth and nose, with a radius of 15.24 cm to 22.86 cm (6 to 9 inches). So 1.5 m above the ground is chosen as the height of monitor points to represent the actual height of human inhalation of chlorine. A total of 301 monitoring points is set up with a horizontal interval of 5 m to monitor the time-dependent chlorine concentration during the process of CFD solving, as shown in Fig. 4.

The concentration of chlorine can be recorded and exported as data files which contain important information for afterward calculations of toxic exposure doses. The simulation of chlorine leakage under 88 different leakage scenarios that screened out is implemented by Fluent.

The standard *k*-epsilon model is used for turbulent simulations. The Semi-Implicit Method for Pressure Linked Equations (SIMPLE) pressure-velocity coupling algorithm is applied to solve the pressure and velocity equations. The leakage duration time is 300 s with a time step of 2 s. The simulations are performed on a server with an Intel i7-4790 CPU (3.6 GHz and 32 GB RAM).

Chlorine concentration contours which are similar to those presented in Fig. 5 can be given through the CFD simulation of gas dispersion. By defining the concentration iso-surface of 10×10^{-6} mole fraction (10 ppm), the dispersion process of chlorine cloud is retrieved. The example shown in Fig. 5 is a medium aperture leakage of a tank in south wind, which illustrates the time sequence of chlorine concentration, the toxic gas cloud size and the affected area.



(a) (b)

(c)

Fig. 3. (a) the three-dimensional geometry model, (b) (c) mesh generated for the model

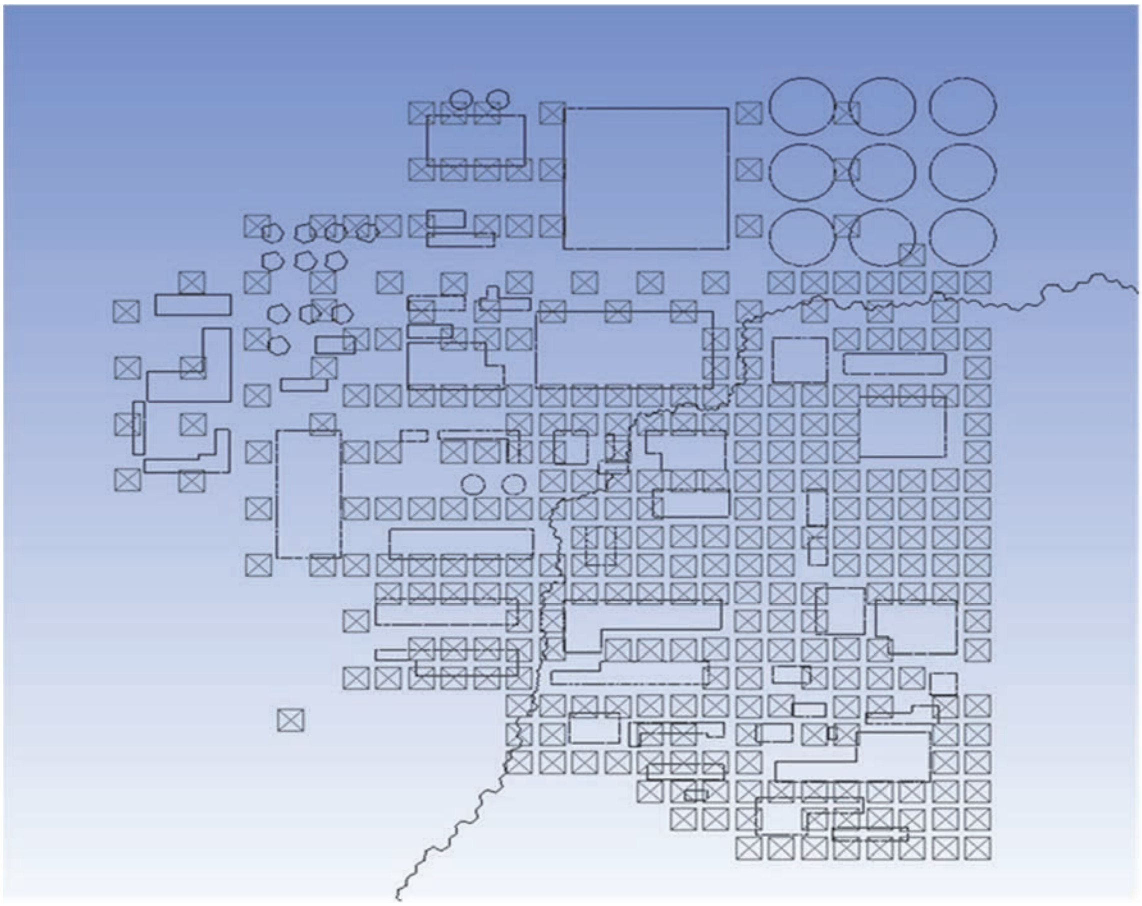
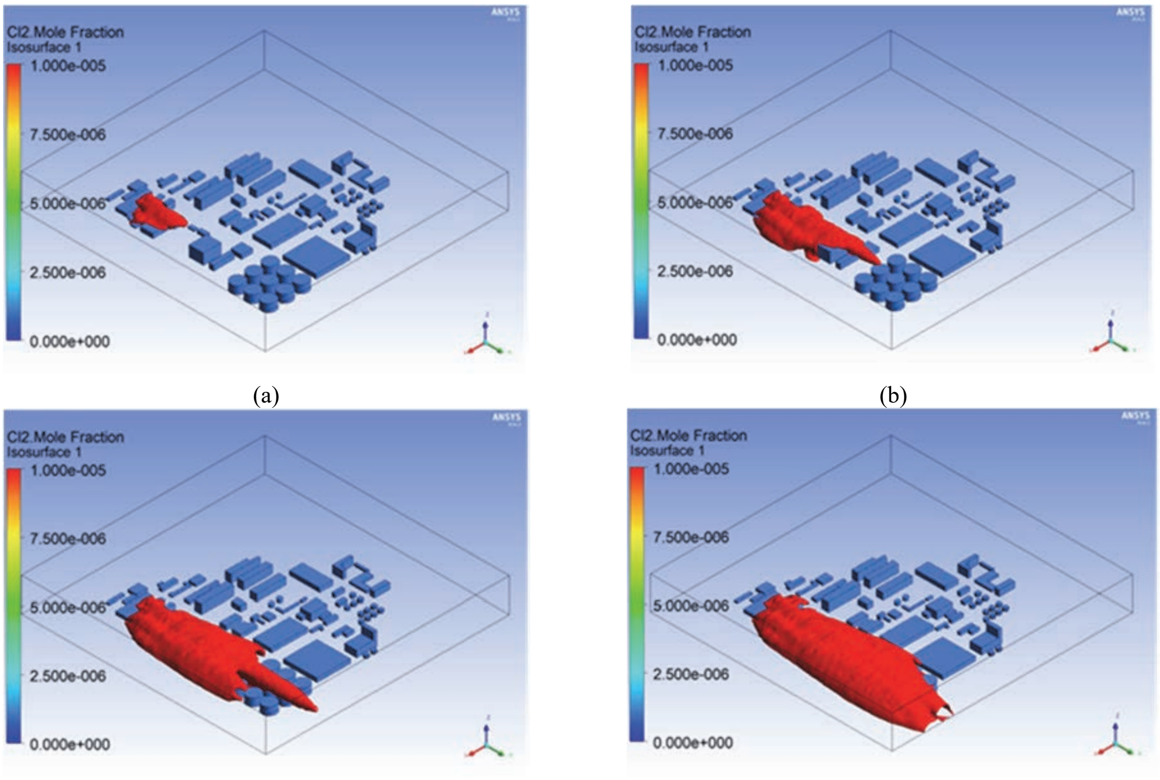


Fig. 4. The distribution map of monitoring points (the symbol '☒' represents the monitoring point)



(a) (b)

(c) (d)

Fig. 5. An example of chlorine dispersion simulation results when a tank leaks at a medium aperture, south wind: (a) in 60 seconds, (b) in 120 seconds, (c) in 180 seconds, (d) in 240 seconds

2.3 CIR modeling

2.3.1 CIR calculation

In this paper, we use the definition of individual risk (IR) proposed by Health and Safety Executive (HSE) (Franks and Maddison, 2006) to judge the exposure risk. IR is defined as the risk that a typical user of a development is exposed to a dangerous dose or worse of toxic substance, heat or blast overpressure (Health and Safety Executive, 1989).

In the evacuation network defined by Graph=(V, E), $V=\{v_1,v_2,...v_n\}$ is the set of nodes corresponding to the intersections and $E\subseteq V\times V$ is the set of arcs (v_i,v_j) corresponding to the roads. At the point (x,y), the time-dependent concentration of chlorine can be obtained from simulation. Based on the evacuation speed, and the distance of arc (v_i,v_j), the exposure dose D_{ij} when evacuating through arc (v_i,v_j) can be calculated by (Eq. 1).

$$D_{ij}=\int_{t_i}^{t_j} c_{ij}^{m}(x,y)\,dt \tag{1}$$

where m is the toxic concentration index which depends on the types of toxic gases.

And then, the exposure dose on route R, $D(R)$ can be illustrated by (Eq. 2).

$$D(R)=\sum\nolimits_{i=1}^{n}\sum\nolimits_{j=1}^{n} M_{ij}D_{ij} \tag{2}$$

M_{ij} is a decision variable, which will be mentioned in the next section. After calculating the exposure dose under a certain leakage scenario, *IR* under leakage scenario k on route R can be calculated by Eqs. (3-5).

$$P_r = A + B\ln D(R) \tag{3}$$

$$P = 50\left[1+\frac{P_r-5}{|P_r-5|}erf\left(\frac{|P_r-5|}{\sqrt{2}}\right)\right] \tag{4}$$

$$IR_k(R) = f\times P_k\times P \tag{5}$$

In (Eq. 3), P_r is the probit variable, A and B are constants depending on the types of toxic gases. (Eq. 4) is the “probit function (Georgiadou et al., 2010)” used to calculate the individual fatality probability P on route R, where *erf* is the error function. *IR* under leakage scenario k on route R can be calculated by (Eq. 5), which is a product of f, P_k and P. f is the exposure probability of employees to hazardous equipment per year.

Considering *IR* on route R under all leakage scenarios, the *CIR* can be formulated by (Eq. 6).

$$CIR(R)=\sum\nolimits_{k=1}^{I} IR_k(\mathrm{R}) \tag{6}$$

where I is the total number of leakage scenarios. In this paper, based on the actual conditions of this chemical plant, we set the evacuation speed v as 2.5 m/s (Arampatzis et al., 1999). Then the exposure time t can be calculated based on the travel speed and the length of the arc which is the distance between 2 nodes. The time-dependent chlorine concentration can be obtained from CFD simulation results. Assume that after the gas detector alarms, the response time of the personnel is 0.16 s (Thompson et al., 1992). For chlorine, A is -5.3, B is 0.5, m is 2.75. Provided that working hours per year are 2000 hours based on the Labour Contract Law of the People’s Republic of China (NPCSC, 2007), and according to the practice, the exposure time to hazardous equipment is 250 hours, then f is 0.125. P_k is the occurrence probability of leakage scenario k, which can be obtained from CASS. I is 88.

2.3.2 Modeling

In this paper, the objective is minimizing the *CIR* along a route. The linear programming formulation for evacuation route optimization is shown in Eqs. (7-10).

$$\min CIR(R) \tag{7}$$

s.t.

$$\sum\nolimits_{j=1,j\neq i}^{n} M_{ij}=0 \quad i=n \tag{8}$$

$$\sum_{j=1,j\neq i}^{n} M_{ij}-\sum_{j=1,j\neq i}^{n} M_{ji}=\begin{cases}1 & i=1\\ -1 & i=n\\ 0 & i\neq 1, i\neq n\end{cases} \tag{9}$$

$$M_{ij}\in\{0,1\} \qquad i,j=1,2,\cdots,n \tag{10}$$

Constraints (Eqs. 8-10) determine a complete route (Gai et al., 2017), where, M_{ij} is the decision variable in this model, constraint (Eq. 10) is the 0-1 integer constraint, if arc (v_i,v_j) is included in route R, $M_{ij}=1$; $M_{ij}=0$ means that arc (v_i,v_j) is not included in route R. Constraint (Eq. 9) limits that evacuees can’t run backward after reaching the destination node, and constraint (Eq. 8) ensures R is a route from the starting node to the destination node without break.

3. Results and discussion

3.1. Find all possible routes by the DFS algorithm

The DFS algorithm is a recursive algorithm that uses the idea of backtracking, involving exhaustive searches of all the nodes by going ahead, is possible, else by backtracking. And it is an example of the brute-force search or exhaustive search (Coppin, 2004). First, the node v_1 is visited. From v_1, any nearby node v_i can be visited. Then start from node v_i, and visit v_j, which has not been accessed before and is close by v_i. Continue this way until the destination node v_n is reached. Based on the evacuation network topology of this chemical plant, the DFS algorithm is used in MATLAB R2018a to define the evacuation route collection. The methodology is shown in Fig. 6, and the route collection is shown in Table 2.

According to Fig. 1, the starting point is v_1, and the destination node is v_{10}, 15 evacuation routes are determined based on the directed evacuation network topology, and every route is connected by nodes according to Table 2.

3.2. Solving the risk model by MATLAB

Based on the actual conditions of this chemical plant and the exhaustive search, two sets of codes are implemented in MATLAB. The first one is the data extraction process, which is used to extract the time-dependent concentration from CFD simulation results, and form MAT files. The other one applies two IF loops to solve the CIR model. In detail the methodology looks like the following:

- Step1: Input data including time-dependent concentration at 301 monitoring points under 88 leakage scenarios, the routes presented by arcs and the occurrence possibilities of leakage scenarios. Let $v_1 = v_i$.
- Step 2: Start from v_i, search arc (v_i, v_j), $i \neq j$ with $j = 1, 2, ...n$. If arc (v_i, v_j) is included in route R, go to step 3, else, continue search.
- Step 3: Retrieve the time-dependent concentration at arc (v_i, v_j), calculate the corresponding dose. If $v_j = v_n$, go to step 4. Otherwise, $v_j \neq v_n$, let $v_j = v_n$ and go back to step 2.
- Step 4: Calculate $\sum_{k=1}^{I} IR$ on route R considering all leakage scenarios.

CIR on every route is calculated by the MATLAB code. According to the assessment criteria of IR proposed by HSE, the routes can be classified as 3 types: broadly acceptable risk route (CIR less than 10^{-6} per year), non-acceptable risk route (CIR larger than 10^{-4} per year) and affordable risk route (CIR between 10^{-4} to 10^{-6} per year) (Franks and Maddison, 2006; Jonkman et al., 2003). The corresponding results are shown in Table 3.

From the results, with minimizing the *CIR* as the objective, it is obvious that route 10, 11, 12 have a higher risk than all other routes, thus they should be avoided when evacuating. The *CIR* of the other 12 evacuation routes are broadly acceptable according to the criteria of HSE and can be selected when liquid chlorine releases. The optimal routes among all evacuation routes are route 3 and 8. By analyzing all routes, it is found that these 3 routes of non-acceptable risk all include arc (v_1, v_6), while all the other routes don’t contain it. The arc (v_1, v_6) is firstly visited, the later arcs visited have little effect on the CIR. Though some routes like route 13 include point v_6, the risk is relatively low and acceptable. Thus, it can be given that evacuees will take more risks when they run through arc (v_1, v_6) and it should be avoided when evacuating.

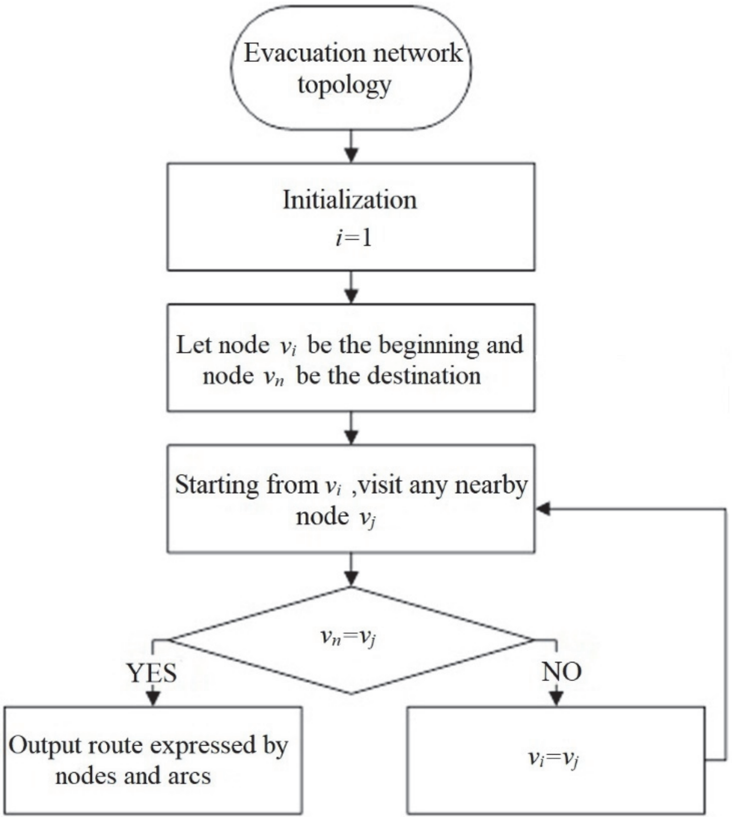


Fig. 6. The methodology of DFS algorithm

Table 2. The evacuation route collection defined by DFS

Route	***Nodes***
1	1→2→3→4→5→10
2	1→2→3→4→5→9→8→10
3	1→2→3→4→5→9→8→7→6→10
4	1→2→3→9→5→10
5	1→2→3→9→8→10
6	1→2→3→9→8→7→6→10
7	1→2→8→10
8	1→2→8→7→6→10
9	1→2→8→9→5→10
10	1→6→10
11	1→6→7→8→10
12	1→6→7→8→9→5→10
13	1→7→6→10
14	1→7→8→10
15	1→7→8→9→5→10

Table 3. *CIR* on each route

Risk level	***Route***	***Individual evacuation risk***	***Risk level***	***Route***	***Individual evacuation risk***
Broadly acceptable risk	1	2.41e-08		9	2.42e-08
	2	2.35e-08		13	2.06e-09
	3	4.63e-10		14	3.79e-08
	4	2.48e-08		15	3.79e-08
	5	2.41e-08	Non-acceptable risk	10	3.04e-02
	6	1.06e-09		11	3.04e-02
	7	2.42e-08		12	3.04e-02
	8	4.63e-10	Affordable risk	None	None

4. Conclusions

This paper proposes a methodology for evacuation route optimization when accidental toxic gas release occurs within chemical plants, which can be applied in most chemical plants. Former CFD simulations have constructed the CASS and finished the simulation of chlorine leakage under 88 leakage scenarios. The purpose of this study is to systematically determine the evacuation routes and put forward the method of building and solving the optimization model. Applying the time-dependent concentration of chlorine that extracted from CFD simulation results, the DDR model and the probit function, the CIR can be systematically presented. Using the DFS algorithm, which is an example of the exhaustive search, all possible evacuation routes can be determined from the accident area to the safe area. With minimizing the CIR as the objective, a MATLAB script based on the exhaustive search is proposed to solve the optimization model. According to the IR criteria defined by HSE, the routes with unaccepted CIR as well as routes with broadly acceptable CIR can be finally determined, which can provide guidance for practical evacuation in chemical plants.

The exhaustive search i.e. the DFS algorithm, is effective when the problem does not have a huge number of potential solutions, but it may bring huge computation costs when the problem reaches a combinational explosion.

In future works, we should switch to heuristic algorithms like Swarm Intelligence Algorithm to solve problems with numerous potential solutions. Besides, the optimization model proposed in this paper does not take individuals' behaviors into account. But in practice, individual's behaviors do affect their evacuation process. For example, evacuation may be slower than expected due to panic, which will ultimately increase the CIR.

Moreover, it is generally required that the evacuation should go toward the upwind direction, while it is possible that a planned route is in the downwind direction under some specific gas release scenarios. Under this circumstance, choosing four routes of lower CIR concerning four different wind directions can be more beneficial for evacuees when making evacuation decisions. We are planning on looking into these points in the future to make the evacuation route optimization method more practical.

One of the future efforts of this work lies in using the heuristic algorithms and exhaustive search to solve the evacuation route optimization respectively, and compare their computation speed and final results. Then verify the effectiveness of exhaustive search when the problem does not have a huge number of potential solutions as well as the effectiveness of heuristic algorithms when the problem reaches a combinational explosion. Another future effort focuses on the improvement of optimization models, we will take the panic coefficient into account to make the model more practical.

Acknowledgments

This work was supported by the fundamental research funds for the central universities (18CX05028A). In addition, we are grateful to the anonymous reviewers and the editor for their constructive comments and suggestions.

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