Numerical Study on the Leakage and Diffusion Characteristics of Low-Solubility and Low-Volatile Dangerous Chemicals from Ship in Inland Rivers

Shuifen Zhan[1, 2, 3], Mingchao Wang[2, *], Min Wang[5, *], Qianqian Shao[4], Zefang Zhang[3], Wenxin Jiang[2] and Xuemin Chen[1]

Abstract: Considering the accidents of ships for dangerous chemicals transportation in inland rivers, a numerical method for the simulation of the leakage and diffusion processes of dangerous chemicals in inland rivers is proposed in this paper. Geographic information, such as rivers and buildings in the model, is obtained through Google Earth and structures of rivers and buildings are described by Auto CAD. In addition, the Fluent is adopted to simulate the leakage and diffusion processes of the dangerous chemicals where the standard k-ε model is used to calculate the turbulent flow. Considering the interaction between chemicals and water, the VOF method is used to describe the leakage, drift and diffusion process of dangerous chemicals groups on the water surface. Taking a section of the Yangtze River as an example, the leakage and diffusion processes from a ship carrying 3,000 tons of low-solubility and low-volatile dangerous chemicals are studied, and the characteristics of leakage and diffusion are analyzed in detail. During the simulation, the area of the maximum group of leaked dangerous chemicals reaches up to about 1800 m^2, and the number reaches up to 45. Furthermore, the influence of density, viscosity, water velocity and leakage velocity on the leakage and diffusion processes is investigated in this paper.

Keywords: Inland rivers, low-solubility and low-volatile dangerous chemicals, leakage and diffusion, VOF.

1 Introduction

In recent years, waterway transportation of dangerous chemicals in China has been developing quickly and the transport amount in 2017 has exceeded 250 million tons according to statistics. With the increase of the transportation volume of dangerous

[1] Lanzhou Jiaotong University, Lanzhou, 730070, China.
[2] Tianjin Research Institute for Water Transport Engineering, M.O.T., Tianjin, 300456, China.
[3] Tianjin Dongfang Tairui Technology Co. Ltd., Tianjin, 300192, China.
[4] Guangdong University of Petrochemical Technology, Maoming, 525000, China.
[5] Beijing Computational Science Research Center, Beijing, 100193, China.
[*] Corresponding Authors: Ming Wang. E-mail: wangmin@csrc.ac.cn;
Mingchao Wang. Email: wangmingchao@tk-aq.com.
Received: 13 August 2019; Accepted: 28 November 2019.

chemicals, accidents of leakage caused by ships collision occur frequently. Once the low-solubility and low-volatile dangerous chemicals are leaked into inland rivers, it floats on the water surface, forming the groups of dangerous chemicals, causing fire, or even explosion and water pollution. Therefore, in order to reduce the influence of leakage and diffusion, prevent secondary accidents (mainly includes the combustion and explosion of the groups of the dangerous chemicals) and take immediate measures, it is of great significance to perform the research on the leakage and diffusion processes of low-solubility and low-volatile dangerous chemicals in inland rivers and predict the influence areas of leakage. Different types of leakage, different seasons and dangerous chemicals should be taken into consideration for investigation.

As one of the most powerful and useful methods, numerical simulation has been widely applied in many research fields, such as complex process simulation [Hong and Huan (2017); Zhang, Qian, Zhang et al. (2018)], accident simulation and others. In the accident of water transportation, the leakage of the dangerous chemicals in inland rivers has been studied with numerical simulation by many researchers and some useful results are obtained. The diffusion model was established by Kachiashvili et al. [Kachiashvili, Goreziani and Lazarov (2007); Chen, Jiang and Yin (2007)] respectively, and both of them studied the diffusion process and influencing factors of low-solubility dangerous chemicals using this model. Focusing on the leakage, drifting and diffusion characteristics of the massive pollutants in inland rivers, some researchers established the numerical model of the leakage and diffusion of dangerous chemicals using the software of Delft3D-FLOW, FLUENT, etc. [Guo and Cheng (2019); Lin (2018); Rui, Shen, Khalid et al. (2015)]. The variations of the diffusion area and the evolution of the concentration of dangerous chemicals were investigated in detail. For the leakage of the underwater pipeline, some researchers have established models for oil spilling, drifting and diffusing in the special situation of the inland river. Numerical model was solved and leakage characteristics were studied systematically [Gao (2013); Zhao, Wang and Zhang (2012); Kuang, Xing and Liu (2010); Song, Wei and Qian (2011)]. Furthermore, many researchers have discussed the diffusion process of the tidal river network and the estuary oil spill accident and the research results are mainly focused on marine oil spill accidents. Also there have been researches on numerical simulation of the leakage of dangerous chemicals such as Methanol and LNG [Li and Li (2012); Chen (2012); Liu and Sun (2009); Qu (2015); Cao, Lin and Sun (2015)]. The IWIND-LR was used to simulate the migration process of oil, and the concentration distribution at different intercept locations was obtained [Wang, Liu and Wang (2016); Liu (2017)] in order to deal with urgent oil spill in rivers and provide support for subsequent emergency treatment. Based on a two-dimensional average power flow mathematical model, an oil spill diffusion hydrodynamic model based on the Euler-Lagrange system tracking technology was established. The model was used to study the expansion, migration and weathering process of oil film after the oil spill in the Yangtze River estuary-Hangzhou Bay. However, the release and migration processes of the leaked oil were not discussed in detail, and the characteristics of the leaked oil groups were not mentioned [Song, Cheng and Liu (2013)]. In addition, a series of related experiments have been conducted to study the flow and diffusion process of dangerous chemicals in water tanks. The mathematical model was used to simulate the flow field of the curved water tank and the migration as well as diffusion process of dangerous chemicals [Duan and Nanda (2006); Chen, Jiang and Han (2008)].

In summary, although previous researchers have devoted many efforts on studying the leakage and diffusion characteristics of dangerous chemicals in inland rivers, there are some shortages. Firstly, previous researches mainly studied the leakage characteristics from underwater pipelines in marine and inland rivers, while few studies focused on the leakage and diffusion in inland rivers. Secondly, studies on the evolution of the groups of dangerous chemical after leakage such as the size, number and area were seldom reported. Thirdly, the influence of dangerous chemicals species, water velocity and leakage velocity on the leakage and diffusion processes is unclear. Thus general physical and mathematical models for the leakage and diffusion characteristics of low-solubility substances (diesel, heavy oil, etc.) and low-volatile substances (diesel, crude oil, etc.) are proposed in this paper. Taking a section of Yangtze River in Nanjing as an example, the leakage and diffusion characteristics are studied in detail, and the influences of density, viscosity, water velocity and leakage velocity on the leakage and diffusion processes are analyzed systematically.

2 Physical and mathematical models

2.1 Physical model

Due to collision in voyage in inland rivers, ships carrying dangerous chemicals may be wrecked and leakage of dangerous chemicals in the ship occurs. For low-solubility and low-volatile dangerous chemicals with density smaller than water, the chemicals floats on the water and groups of dangerous chemicals forms as flowing downstream.

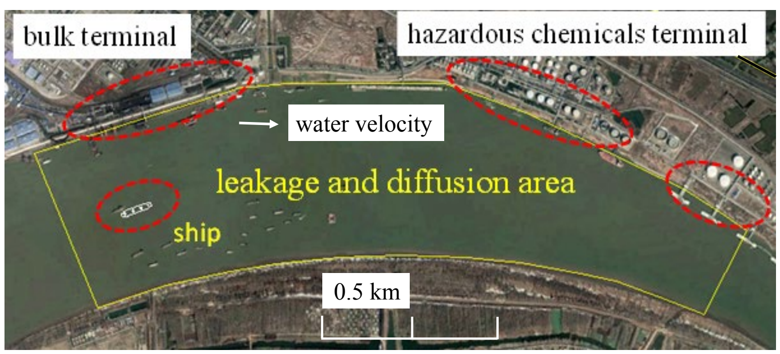


Figure 1: Physical model of the leakage and diffusion of dangerous chemicals from a ship in an inland river

Considering the leakage and diffusion of dangerous chemicals in inland vessels, this paper establishes a general physical model for leakage and diffusion of dangerous chemicals applicable to rivers. Taking into account the irregularities of the river boundary, maps (such as Google Earth, Baidu Maps, etc.) are used to obtain satellite maps of the river area. Graphics software (such as Auto CAD, SolidWorks, etc.) are employed to accurately depict rivers, ships and buildings, and obtain a complete two-dimensional physical model describing dangerous chemical leakage from ships and its diffusion in inland rivers, as shown in Fig. 1. The upstream of the river is a bulk cargo dock and the downstream is a liquid dangerous chemicals dock. The area enclosed by the solid yellow lines is the leakage area of dangerous chemicals, and the ship is located upstream of the area.

2.2 Mathematical model

The low-solubility and low-volatile dangerous chemicals float on the river surface after leakage and form a leaking zone and this process is a two-phase flow. VOF (volume of fluid) method is used to capture the leakage, drift and diffusion process of dangerous chemicals groups in this paper. In fact, the size of the transport ship is large and the Reynolds number is high, so the flow process is turbulent during the leakage. For example, for a 3,000-ton diesel ship, when the leakage port size is 1.0 m and the leakage velocity is 1.5 m/s, the Reynolds number is about 4.0×10^5. Based on this, the standard k-ε model is adopted to calculate the turbulent flow. Therefore, the governing equations of leakage and diffusion of dangerous chemicals in inland rivers are as follows [Malgarinosa, Nikolopoulos and Gavaise (2015)].

$$\frac{\partial \rho}{\partial t}+\nabla\cdot(\rho\mathbf{u})=0 \tag{1}$$

$$\frac{\partial(\rho\mathbf{u})}{\partial t}+\nabla\cdot(\rho\mathbf{u}\cdot\mathbf{u})=-\nabla p+\nabla(\mu_{eff}\nabla\mathbf{u})+\frac{\rho\sigma\kappa\nabla f}{0.5(\rho_w+\rho_{dc})} \tag{2}$$

$$\frac{\partial f}{\partial t}+\mathbf{u}\cdot\nabla f=\dot{m} \tag{3}$$

where, μ_{eff} is the effective viscosity, defined as $\mu_{eff}=\mu+\mu_t$, in which μ is the viscosity and μ_t is the turbulent viscosity. σ is the surface tension. κ is the interface curvature, and $\kappa=\nabla\cdot\mathbf{n}$ where $\mathbf{n}$ is the interface normal vector. f is the volume fraction of the water phase in the control volume. ρ_w and ρ_{dc} are the density of water and dangerous chemicals respectively, kg/m^3. $\dot{m}$ is leakage flow rate of dangerous chemicals, m/s.

During the leakage process of dangerous chemicals, the volume fraction of dangerous chemicals in the calculation area changes, resulting in the variation of fluid properties. Eq. (4) is used in this study.

$$\phi=f\phi_w+(1-f)\phi_{dc} \tag{4}$$

where, ϕ_w and ϕ_{dc} are the volume fraction of water and dangerous chemicals respectively. Considering the turbulent flow of water and dangerous chemicals in the calculation region, the calculation is performed using the standard k-ε equation. The kinetic energy k, the turbulent energy dissipation rate ε and the turbulent viscosity μ_t are calculated by Eqs. (5), (6) and (7), respectively.

$$\frac{\partial(\rho k)}{\partial t}+\nabla(\rho\mathbf{u}k)=\nabla\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\nabla k\right]+G_k\text{-}\rho\varepsilon \tag{5}$$

$$\frac{\partial(\rho\varepsilon)}{\partial t}+\nabla(\rho\mathbf{u}\varepsilon)=\nabla\left[\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\nabla\varepsilon\right]+c_1\frac{\varepsilon}{k}G_k\text{-}c_2\rho\frac{\varepsilon^2}{k} \tag{6}$$

$$\mu_t = \rho c_\mu \frac{k^2}{\varepsilon} \tag{7}$$

where, c_1, c_2, c_μ, σ_k, and σ_ε are constants, which are 1.44, 1.92, 0.09, 1.0, and 1.3 respectively. G_k is a kinetic energy generation term, and it can be calculated by Eq. (8).

$$G_k = \mu_t |\mathbf{S}|^2 \tag{8}$$

where, $|\mathbf{S}|$ is the modulus of the strain rate tensor, $|\mathbf{S}| = \sqrt{2S_{ij}S_{ij}}$.

2.3 Boundary conditions and initial conditions

2.3.1 Boundary conditions

As can be seen from Fig. 1, the boundary conditions of the calculation region include inland river boundary conditions and ship boundary conditions.

(1) Inland river boundary conditions,

left boundary, $u = u_w, v = 0,\ f = 0$

upper boundary, $u = u_w, v = 0, f = 0$

right boundary, $\dfrac{\partial u}{\partial n} = 0, \dfrac{\partial v}{\partial n} = 0, \dfrac{\partial f}{\partial n} = 0$

lower boundary, $u = 0, v = 0, f = 0$

(2) Ship boundary conditions,

leakage orifice, $u = u_{dc}, v = 0$, $f = 1.0$

other, $u = 0, v = 0, f = 0$

2.3.2 Initial conditions

Only the river flow in the calculation region and the flow process is stable at the initial moment before leakage. Simulation process begins when dangerous chemicals flow out from the orifice of the ship.

3 Numerical method and simulation cases

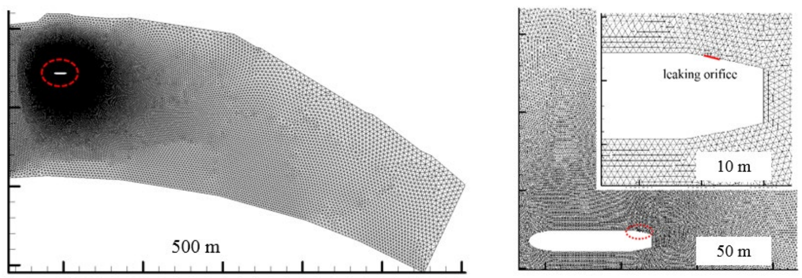
3.1 Numerical method

The pressure and velocity are coupled by SIMPLE algorithm. The convection term and the diffusion term are discretized using the second-order upwind scheme and central difference scheme respectively. Unsteady terms are discretized by full implicit scheme. The convergence criterion is that the residuals of the continuity equation and the momentum equations are less than 1.0×10^{-5} simultaneously in each time step.

3.2 Simulation cases

The Nanjing section of the Yangtze River is selected as the calculation area, as shown in Fig. 1. The calculation area is about 4.0 km in length and the width of the river is about

1.0 km. The ship which is loaded with dangerous chemicals is about 3000 tons and its length and width are 81.0 m and 13.6 m respectively. An orifice of about 1.0 m in diameter appeared at the stern of the ship due to collision. Setting the leakage time as 30 min with the consideration of the emergency response in Yangtze River, the leakage and diffusion characteristics are studied systematically.



(a) (b)

Figure 2: Grid generation: (a) global mesh; (b) dense mesh at the leakage region

The computational domain is meshed before calculation and the whole region is discretized using the triangle mesh, as shown in Fig. 2. Dense mesh is performed near the ship, especially at the orifice. In this paper, the grid size at the orifice is 0.05 m. Through comparison of the trial results for three groups of mesh and time step, ultimately the total grid number and time step selected in this research are 199615 and 0.1 s respectively.

To study the leakage, drift and diffusion process of dangerous chemicals in inland rivers, and to analyze the effect of density, viscosity, water velocity and leakage velocity, numerical cases for this study are shown in Table 1, among which case 2 is selected as the basic case.

Table 1: Simulation cases

case	density ρ kg/m^3	viscosity μ Pa·s	water velocity u_w m/s	leakage velocity u_l m/s
1	730	0.0033	0.5	1.5
2	830	0.0033	0.5	1.5
3	950	0.0033	0.5	1.5
4	830	0.033	0.5	1.5
5	830	0.33	0.5	1.5
6	830	0.0033	0.75	1.5
7	830	0.0033	1.0	1.5
8	830	0.0033	0.5	1.0
9	830	0.0033	0.5	2.0

It should be noted that the groups of dangerous chemicals enclosed by the concentration contour of 5% are counted and studied in this paper, and the area of the maximum group of dangerous chemicals is computed by Auto CAD. Furthermore, curves of the distribution of the leaked groups are fitted, by which the length and width of the leakage area are calculated directly.

4 Results and discussion

In this section, numerical simulation is performed and the characteristics of leakage and diffusion of low-solubility and low-volatile dangerous chemicals in inland rivers are studied. Before simulation, the model proposed in this research is validated using the results in literatures.

4.1 Model validation

The key point of the low-solubility and low-volatile dangerous chemicals leakage, drifting and diffusion in river is the interaction between two liquid materials, which is described by VOF model in this paper. The accuracy of the model is verified by comparing the calculation results of the water column collapse in the square cavity with the experimental data. The variations of the dimensionless distance in the horizontal direction with time are shown in Fig. 3. The variations of the liquid fraction distribution in the square cavity are shown in Fig. 4. From these two figures, it can be seen that the calculation results in this paper agree well with those in literatures [Martin and Moyce (1952); Sun (2009)].

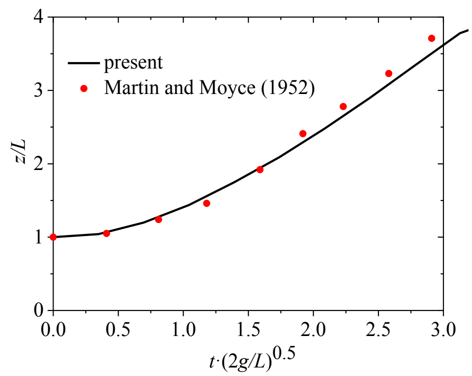
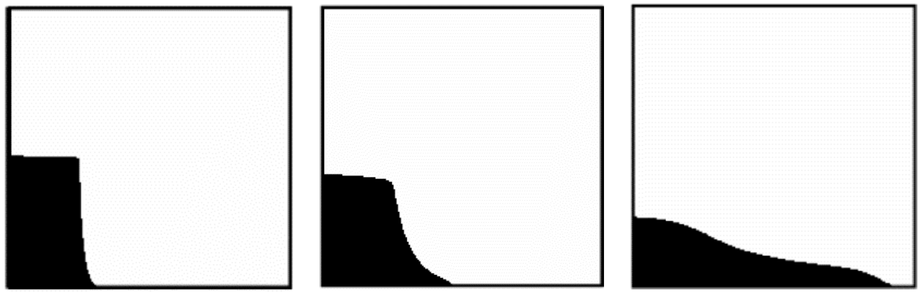


Figure 3: Variations of the dimensionless distance in horizontal direction of water with time

(i)

(ii) 

(a) (b) (c)

Figure 4: Comparison for the liquid fraction distribution in a square cavity of the present (i) results with those of Martin and Moyce (1952) (ii): (a) 0.06 s; (b) 0.12 s; (c) 0.24 s

4.2 Leakage and diffusion characteristics of dangerous chemicals

Accurate determination of the leakage and diffusion ranges of dangerous chemicals is of great significance for the containment, emergency response of accidents and the prevention of subsequent accidents that may happen. Therefore, the variation of the leakage area of dangerous chemicals with time is studied in this subsection. The leakage area is related closely to the properties of dangerous chemicals (density, viscosity), water velocity and leakage velocity. Therefore, the leakage, drift and diffusion processes are studied firstly, then the variations of the leakage range of dangerous chemicals with time are analyzed. The dangerous chemicals leakage and diffusion processes for case 2 in Tab. 1 are calculated in this subsection and the variations of the concentration for the dangerous chemicals in the inland river are shown in Fig. 5.

It can be seen from Fig. 5 that after leakage, the dangerous chemicals accumulated and are stretched at the stern of the ship under the impact of water, leading to the forming of elliptical groups gradually. At this moment, the groups have not yet detached from the ship as shown in Fig. 5(b). As the leakage process continues, the leaked dangerous chemicals begin to rotate in clockwise direction under the combined action of the leakage velocity and water velocity, and drift downstream of the river, as shown in Figs. 5(c) and 5(d). At this stage, the elliptical group of dangerous chemicals continues to rotate rapidly and gradually returns to a circular shape with a diameter of about 20 m until completely escapes from the orifice, as shown in Fig. 5(e). In this research, the groups of dangerous chemicals released directly from the orifice are named the primary groups. When the primary groups leave the orifice, some dangerous chemicals at the edges of the primary groups break away, forming droplets of dangerous chemicals around the primary groups, as shown in Fig. 5(e). Furthermore, during the leaking process, two phase groups form gradually due to the rotation and entrainment of water. Under the combination effect of inertia force, centrifugal force and viscous force, the rotating two phase groups destroys, water is released again and the irregular groups forms gradually, as shown in Figs. 5(f)-5(h). The primary groups and the surrounding droplets are split apart and merge again and again, causing a more and more complex process of leakage and diffusion. Dangerous chemicals continue to flow out from the orifice, then a series of groups form gradually in the downstream of the river, as shown in Figs. 5(e)-5(h), until the end of the leakage.

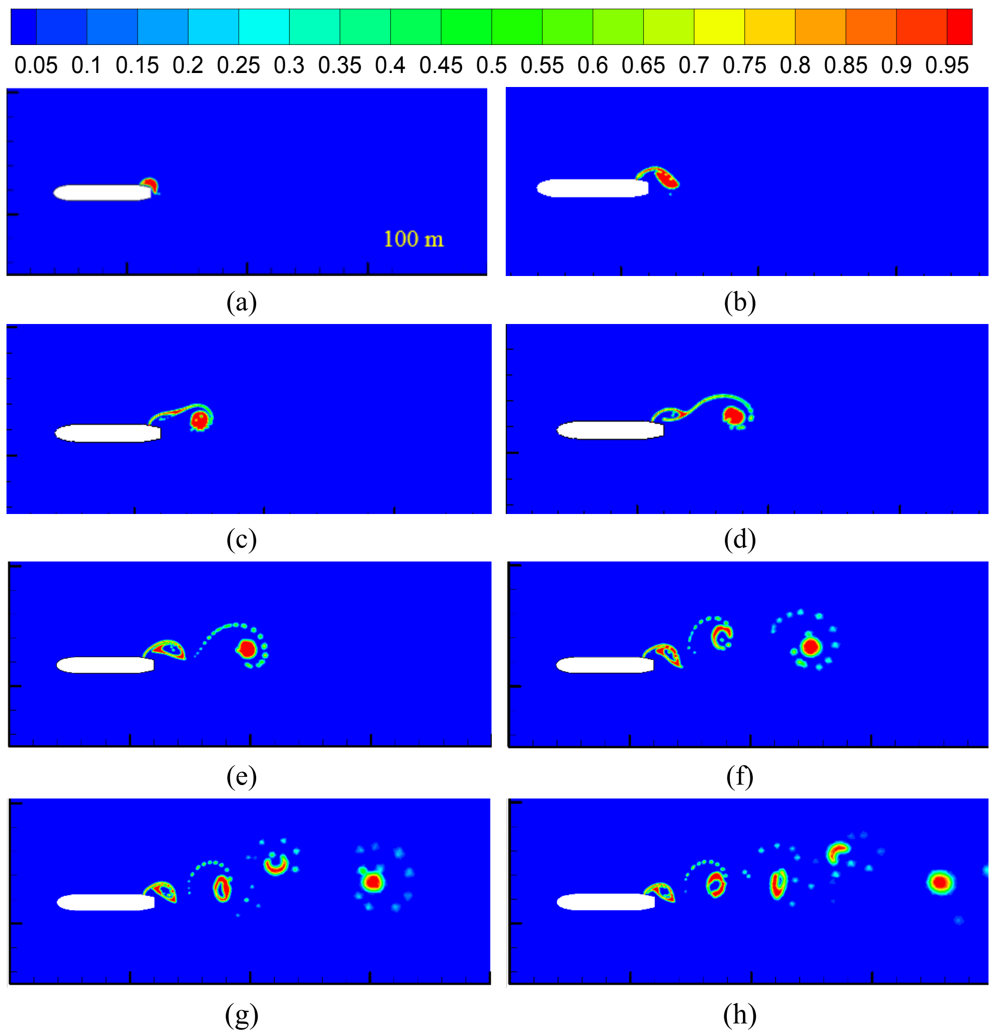
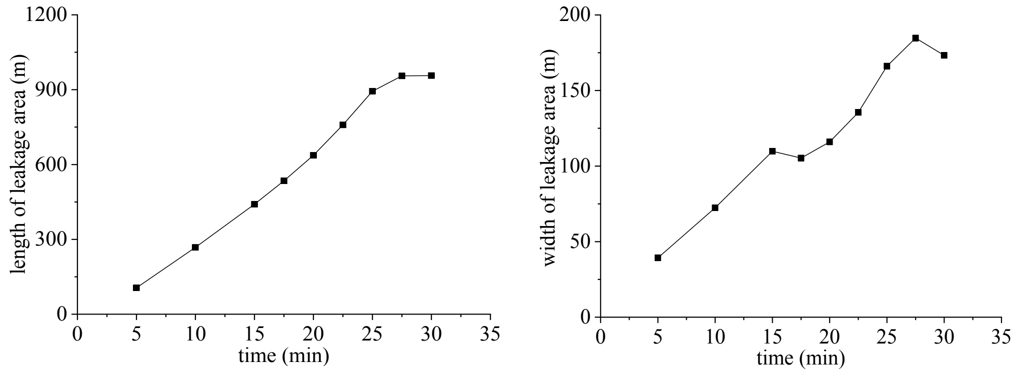


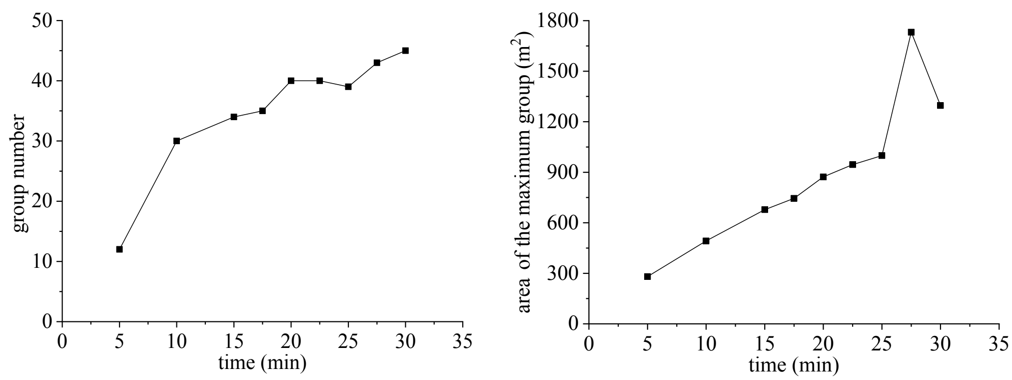
Figure 5: Evolution of the leakage and diffusion of dangerous chemicals: (a) 1 min; (b) 2 min; (c) 3 min; (d) 4 min; (e) 5 min; (f) 7 min; (g) 9 min; (h) 11 min

Determining the leakage range including the length and width of the leakage area accurately is critical for taking measures to control and dispose leaking dangerous chemicals. The variations of the leakage area for case 2 are shown in Fig. 6. It can be seen that the length and width of the leakage area gradually increase with an average growth rate of about 0.65 m/s and 0.1 m/s respectively. When the groups reach the bend of the river (about 900 m from the orifice), the increase rate of the length of leakage area slows down significantly under the coupled effects of groups mergence and viscous force between groups. The droplets are spun off from the primary groups as a result of the rotation of dangerous chemical groups during drifting downstream. Due to the flow of the water, the diffusion of the primary groups and droplets in the longitudinal direction is inhibited, and the growth of the width of the leakage area slows down. Furthermore, the groups and droplets are in a drifting and merging state during the leakage and diffusion processes, therefore, the growth of the width of leakage area fluctuates slightly, as shown in Fig. 6(b).



(a) (b)

Figure 6: Variations of the leakage area of the dangerous chemicals with time: (a) length of the leakage area; (b) width of the leakage area



(a) (b)

Figure 7: Evolution of the groups of leaked dangerous chemicals: (a) group number; (b) area of the maximum group

The number of groups and maximum group area can reflect the risk (combustion and explosion of the dangerous chemicals groups floating on the surface water) caused by the dangerous chemicals after leakage directly. In this paper, the groups of the dangerous chemicals refer to those groups enclosed by the concentration contour of 5%. Fig. 7 shows the variations of the number and maximum area of groups with time. From Fig. 7(a) it can be seen that the number of groups increases with time, showing a gradually decreasing increase rate. From the beginning to 25 min, the area of the maximum group grows with an approximately constant rate of around 34.42 m^2/min. After 25 min, the groups reach the bend of the river, the merging process of groups accelerates sharply and the area of the maximum group is nearly 1800 m^2 at 27.5 min.

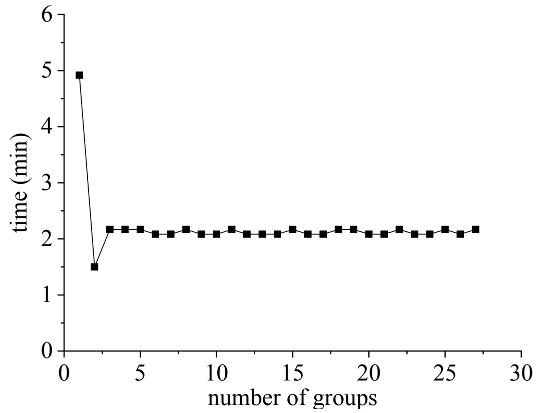


Figure 8: Cycle of the release of the dangerous chemicals

The release process from the orifice determines the total amount of dangerous chemicals leaked into the river, which should be considered for the emergency response. In this paper, the release characteristics are studied and analyzed, as shown in Fig. 8, which can be explained based on the above analysis. At the initial moment, due to the viscous force of dangerous chemicals as well as the interaction between dangerous chemicals and water, it costs about 5 min for the release of the first group, much longer than other groups, corresponding to Figs. 5(a)-5(e). From the third group, the release time of the groups is almost constant, with values around 2 min, which is also indicated by Figs. 5(e)-5(h).

4.3 Influence factors analysis

Physical properties of dangerous chemicals (such as density, viscosity), water velocity and leakage velocity have great influence on the leakage and diffusion processes. Therefore, the influence factors are studied and analyzed in this subsection.

4.3.1 Influence of density

To study the influence of the density of dangerous chemicals on the leakage and diffusion processes, the leakage, drift and diffusion processes are simulated numerically under the three groups of density as shown in Tab. 1, and the results are shown in Fig. 9. It can be seen from Fig. 9 that the variations in density has a slight effect on the length and width of the leakage area. The reason is that when dangerous chemicals leaks from the orifice, the groups of dangerous chemicals form and drift downstream with water. During this period, water velocity has greater impact on the leakage area, while the density of dangerous chemicals has a relatively weak influence on the leakage area, especially on the leakage length, as shown in Fig. 9(a).

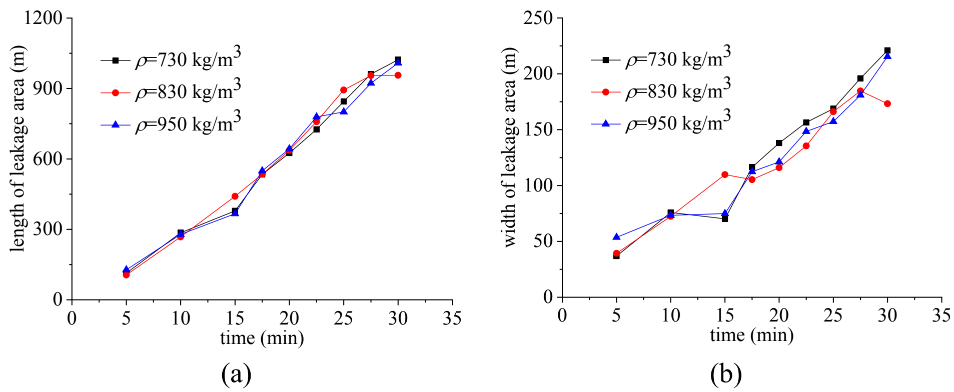


Figure 9: Influence of the density of dangerous chemicals on the leakage area of the dangerous chemicals: (a) length of the leakage area; (b) width of the leakage area

Fig. 10 shows the effect of density on the number of groups and the area of the maximum group. Overall speaking, larger density of dangerous chemicals leads to more groups and larger area of the maximum group. This is because that the increase of density results in the increase of the number of droplets which is spun off, then ultimately leads to the increase of the number of groups. For the area of maximum group, the increase of density has little effect on the leakage process from orifice. Also, density has little influence on the drift and rotation of groups. Based on these two reasons, the density has slight effect on the area growth of the maximum group at the initial stage of leakage. However, when the length of the leaking area exceeds 900 m, the groups of the dangerous chemicals reach the bend of the river. The drift process slows down and the merging process accelerates, so in this period, the area of the maximum group increases rapidly, as shown in Fig. 10(b).

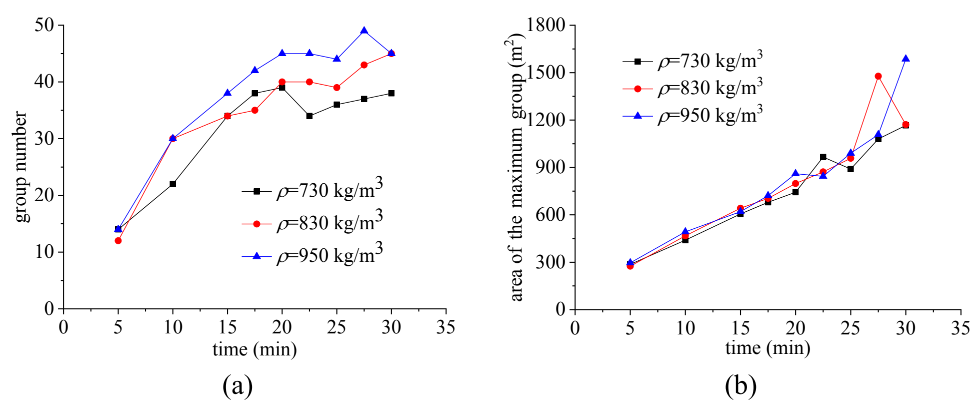


Figure 10: Influence of the density of dangerous chemicals on the total number and maximum area of the groups: (a) group number; (b) area of the maximum group

In general, the increase of density has little influence on the leakage area and the maximum group area, however, the increase of the density of dangerous chemicals has a certain influence on the number of group. Therefore, increasing the density can increase the risk of accident to some extent.

4.3.2 Influence of viscosity

Viscosity of the dangerous chemicals affects group formation and evolution. Therefore, the effect of viscosity of dangerous chemicals on the leakage and diffusion processes is studied systematically in this subsection.

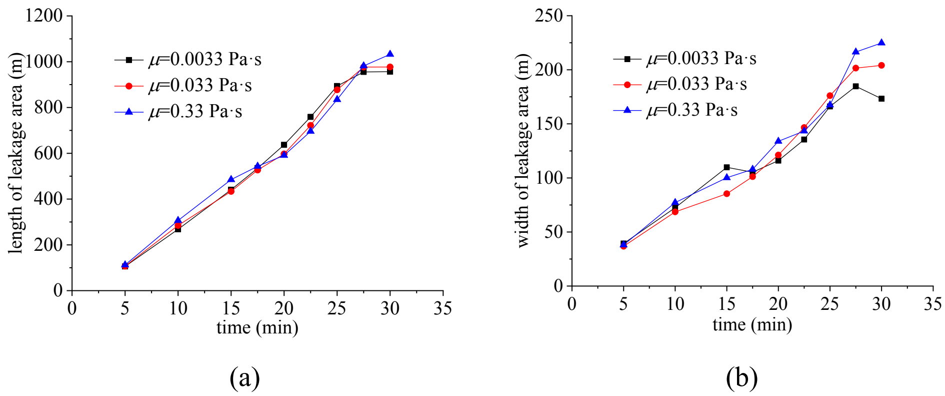


Figure 11: Influence of the viscosity of dangerous chemicals on the leakage area of the dangerous chemicals: (a) length of the leakage area; (b) width of the leakage area

Fig. 11 shows the effect of viscosity on the leakage area of dangerous chemicals. Compared with Fig. 9, it can be seen that the viscosity and density have similar effect on the leakage and diffusion processes of dangerous chemicals. Specifically, viscosity has less influence on the leakage area. The reason is that the length of the dangerous chemical leakage area is mainly affected by the water velocity and viscosity has slightly effect on the length of the leakage area. On the other hand, with the increase of viscosity, the viscous force between groups increases. Under the action of the centrifugal force and viscous force, the number of droplets decreases, which causes a slight decrease in the width of the leakage area at the initial moment, as shown in Fig. 11(b). When the groups reach the bend of the river, under the effect of the inertia force, centrifugal force and viscous force, the width of the leakage area increases again, as shown in Fig. 11(b).

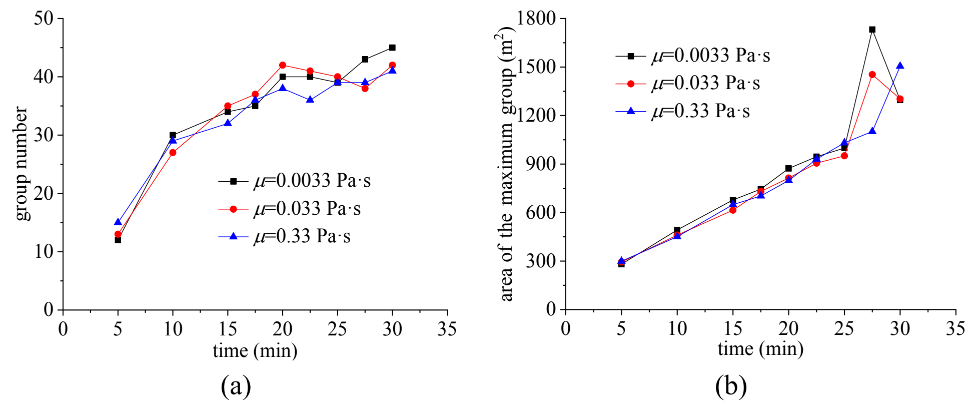


Figure 12: Influence of the viscosity of dangerous chemicals on the total number and maximum area of the groups: (a) group number; (b) area of the maximum group

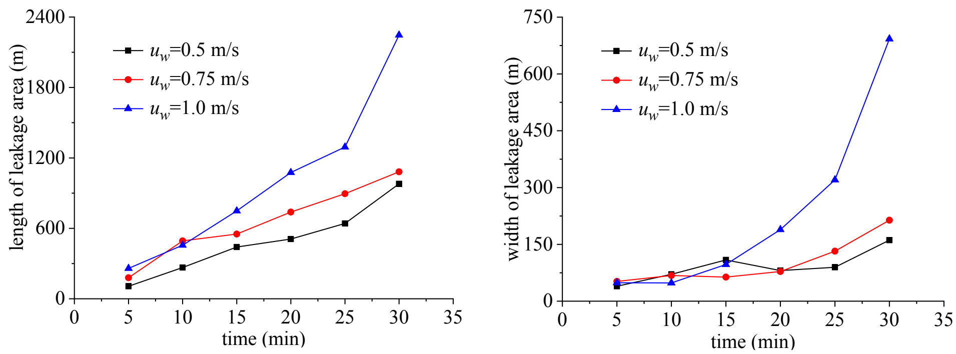
Fig. 12 shows the evolution of the group number and the maximum group area with time for three different viscosities of the dangerous chemicals. Increase of the chemicals' viscosity results in the increase of viscous force between groups and water. As the number of groups and the area of the maximum group are related with the centrifugal force and viscous force, a smaller number of groups as well as a smaller maximum group area are shown in Fig. 12 along with the increase in the viscosity. The influence of chemicals' viscosity on the number and maximum area of groups is similar with that of density. When the groups approach the bend of the river, the mergence process of groups accelerates and the maximum group area increases rapidly, as shown in Fig. 12(b).

In general, similar to density, viscosity of dangerous chemicals has slight effect on the leakage area of dangerous chemical, the number of dangerous chemicals, and the maximum group area.

4.3.3 Influence of water velocity

During dry and rainy seasons, the water velocity in river is quite different, which may lead to different leakage and diffusion processes of the dangerous chemicals. In this subsection, the leakage and diffusion processes of dangerous chemicals under three water velocities are studied and the results are shown in Figs. 13 and 14.

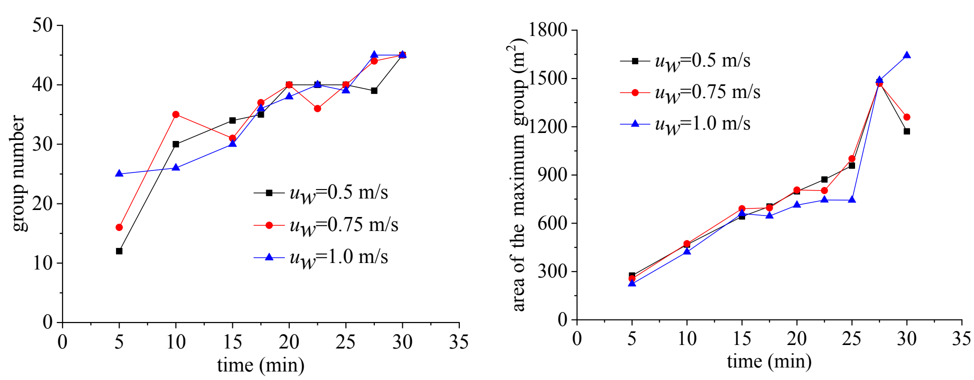
The effect of water velocity on the leakage area is shown in Fig. 13. It is indicated that both the length and width of the leakage area depend largely on the water viscosity of the river. Generally, there are larger length and width of the leakage area at larger water viscosity in the river. According to the analysis, the groups of dangerous chemicals drift downstream with water after being released from the orifice and the water velocity has a decisive influence on the length of dangerous chemical area. When the river channel is straight, the effect of water velocity on the length of the leakage area is approximately linear. While, when the river channel is curved, the increase of the water velocity leads to an increase in the centrifugal force. In addition, in the narrowed region of the river at the bend in Fig. 2, the influence of the water velocity on the length of the leakage area is gradually increased, as shown in Fig. 13(a). When the leakage time is less than 15 min, the rotation rate of the group increases, and the water velocity has less influence on the width of the leakage area. When the leakage time exceeds 15 min, the rotation rate of the group decreases. The diffusion process of the droplets accelerates under the impact of the water velocity and the width of the leakage area increases gradually, as shown in Fig. 13(b).



(a) (b)

Figure 13: Influence of the water velocity on the leakage area of the dangerous chemicals: (a) length of the leakage area; (b) width of the leakage area

Variations of the group number and area of the maximum group of dangerous chemicals under different water velocity are shown in Fig. 14. Before the merging of the primary groups, the number of group and the maximum group area rise with a constant rate, corresponding to the initial stage of leakage (leakage time is less than 10 min). After leakage of 15 min, the leaking groups reach the bend of the river. At this moment, the mergence accelerates, which results in the slow increase of the group number and the rapid increase of the maximum group area. When the leakage time is 30 min, the number of groups is about 45 and the maximum group area is over 1500 m^2.



(a) (b)

Figure 14: Influence of the water velocity on the total number and maximum area of the groups: (a) group number; (b) area of the maximum group

In general, the water velocity has an obvious influence on the leakage range, especially the length of the leakage range, while shows very small impact on the number of groups and the maximum group area. It is inferred that increasing water velocity leads to increasing risk of secondary accidents.

4.3.4 Influence of leakage velocity

The flow rate of the dangerous chemicals from the orifice directly determines the leakage process, which brings influence to the whole process of leakage, drift and diffusion in inland rivers. In this subsection, the leakage and diffusion processes of dangerous chemicals under three different leak velocities are simulated and the results are shown in Figs. 15 and 16.

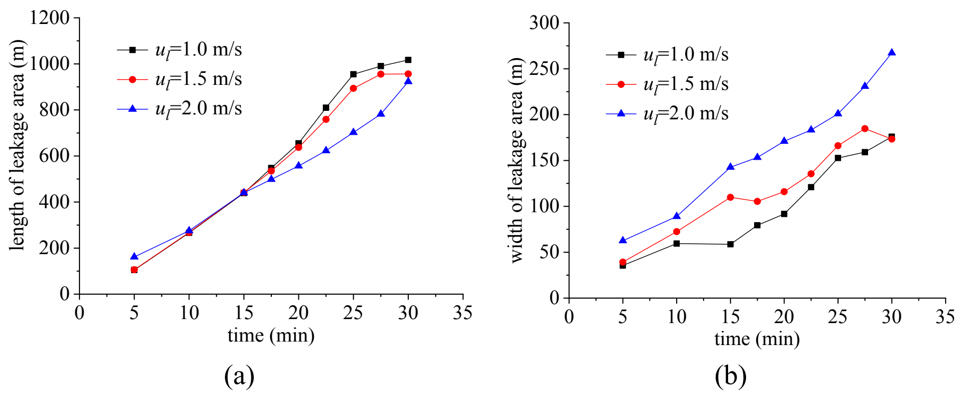
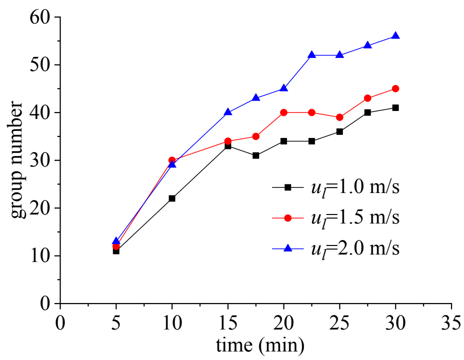
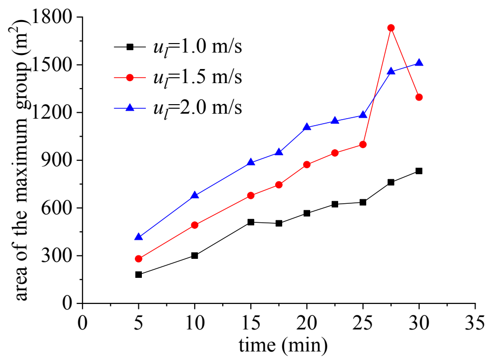


Figure 15: Influence of the leakage velocity of dangerous chemicals on the leakage area of the dangerous chemicals: (a) length of the leakage area; (b) width of the leakage area

As can be seen from Figs. 15 and 16, as the leakage velocity increases, the length of the leakage area decreases and the width of leakage area increases obviously. Increasing the leakage velocity results in an increase in both the number of groups and the maximum group area. The reason is that when the leakage velocity increases, the leakage amount of dangerous chemicals increases at the same time, which results in the increase of the leakage group volume and maximum group area, as shown in Fig. 16(b). For the case of this paper, when the leakage velocity increases by 0.5 m/s, the average increase of the maximum group area is about 150 m^2. Due to the viscous force of the groups, the interaction between the groups is enhanced and the length of the leakage region decreases. On the other hand, the groups rotate in the clockwise direction. The group with larger volume has a larger centrifugal force, and the number of spun-off droplets increases, which leads to the increase of the group number and the increases of the width of leakage area, as shown in Fig. 16(a).



(a)



(b)

Figure 16: Influence of the leakage velocity on the total number and maximum area of the groups: (a) group number; (b) area of the maximum group

In general, the leakage velocity has great influence on the leakage and diffusion processes of dangerous chemicals in inland rivers and the impact is mainly reflected in the width of the leakage area, the number of group and the maximum group area.

5 Conclusion

A general numerical method for simulating the leakage and diffusion of low-solubility and low-volatile dangerous chemicals in an inland river is proposed in this research. Taking the section of Yangtze River as an example, the leakage and diffusion characteristics are studied in detail and the influence factors are analyzed systematically. The following conclusions are obtained.

(1) The leaked dangerous chemicals form a series of groups with different sizes and shapes after flowing out from the orifice of the ship. During the subsequent diffusion process, the primary groups drift downstream of the river in a clockwise rotation, and lots of the droplets forms due to the spun off from the primary groups. With the increase of the leakage time, the area of the primary groups increases gradually and the maximum group area exceeds 900 m^2 by the leakage time of 25 min. In addition, when the groups are close to the bend of the river, the mergence process of groups accelerates, and the maximum group area is as large as approximately 1800 m^2, and the risk of secondary accidents (mainly includes the combustion and explosion of the groups of the dangerous chemicals) increases significantly.

(2) Compared with the density and viscosity of dangerous chemicals, water velocity and the leakage velocity of the dangerous chemicals show more obvious impact on the leakage and diffusion processes. The influence of water velocity on the leakage and diffusion processes is reflected mainly in the length of leakage area, while the influence of leakage velocity is reflected mainly in the width of the leakage area, the number of group and the area of the maximum group. In general, both water velocity and leakage velocity has great influence on the leakage and diffusion processes. Therefore, emergency responses on the leakage and diffusion of the dangerous chemicals in inland rivers should be focused on the situation of huge leakage during the flood season.

Acknowledgement: This research is supported by the special fund for the basic research business of the central public welfare research institutes (TKS160222, TKS160211), and the key technology projects of the transportation industry (TKS180403) and the Tianjin Science and Technology Project (the project) (17YFZCSF01250). This research is also supported by National Natural Science Foundation of China (No. U1930402).

Conflicts of Interest: The authors declare that they have no conflicts of interest to report regarding the present study.

References

Cao, J. M.; Lin, F.; Sun, L. (2015): Simulation of dangerous chemicals leakage accidents in rivers based on Fluent. *China Water Transport*, vol. 15, pp. 132-133.

Chen, L. P.; Jiang, J. C.; Yin, L. (2007): Numerical simulation water pollution diffusions for sudden dangerous chemical. *Journal of Hydrodynamics*, vol. 22, pp. 761-765.

Chen, S. Q. (2012): *Three-dimensional Numerical Simulation of the Influence of Accident-induced Oil Film on the Water Source in Huangpu River and Changjiang Estuary (Ph.D. Thesis)*. East China Normal University, China.

Gao, L. X. (2013): *Modeling and Simulation of Oil Spill Diffusion from Inland Ships (Ph. D. Thesis)*. Fudan University, China.

Guo, G. M.; Cheng, G. (2019): Mathematical modelling and application for simulation of water pollution accidents. *Process Safety and Environmental Protection*, vol. 127, pp. 189-196.

Hong, Y. Yeh.; Huan, J. Keh. (2017): Axisymmetric slow motion of a prolate particle in a circular capillary with slip surfaces. *Computer Modeling in Engineering & Sciences*, vol. 113, no. 3, pp. 361-385.

Kachiashvili, K.; Goreziani, D.; Lazarov, R.; Melikdzhanian, D. (2007): Modeling and simulation of pollutants transport in rivers. *Applied Mathematical Modeling*, vol. 31, pp. 1371-1396.

Kim, K. S.; Kim, M. H.; Jang, H.; Cho, H. C. (2018): Simulation of solid particle interactions including segregated lamination by using MPS method. *Computer Modeling in Engineering and Sciences*, vol. 116, pp. 11-29.

Kuang, C. P.; Xing, F.; Liu, S. G. (2010): Numerical simulation and analysis of emergency measures for water pollution accident in Huangpujiang river. *Yangtze River*, vol. 41, pp. 43-47.

Li, T.; Li, S. Y. (2012): Numerical simulation of fate of oil spill in tidal river-network. *Acta Scientiae Circumstantiate*, vol. 32, pp. 1424-1435.

Lin, L. (2018): Simulation of sudden benzene leakage water pollution events. *IOP Conference Series: Earth and Environmental Science*, 208.

Liu, W. F.; Sun, Y. L. (2009): Study and improvement of oil spill simulation methods. *Journal of East China Normal University (Natural Science)*, vol. 3, pp. 90-97.

Liu, X. W. (2017): *Simulation of Accidental River Oil Spill and Emergency Countermeasure Research Based on IWIND-LR (Ph.D. Thesis)*. North China Electric Power University, China.

Malgarinosa, I.; Nikolopoulos, N.; Gavaise, M. (2015): Coupling a local adaptive grid refinement technique with an interface sharpening scheme for the simulation of two-phase flow and free-surface flows using VOF methodology. *Journal of Computational Physics*, vol. 300, pp. 732-753.

Martin, J. C.; Moyce, W. J. (1952): An experimental study of the collapse of fluid columns on a rigid horizontal plane. *Philosophical Transactions of the Royal Society of London: Series A*, vol. 244, pp. 312-324.

Qu, C. L. (2015): Simulation of gas diffusion, fire and explosion on inland river LNG vessels. *Natural Gas Industry*, vol. 35, pp. 105-110.

Rui, Y. K.; Shen, D. T.; Khalid, S.; Yang, Z. G.; Wang, J. C. (2015): GIS-based emergency response system for sudden water pollution accidents. *Physics and Chemistry of the Earth, Parts A/B/C*, vol. 79-82, pp. 115-121.

Song, Z. K.; Cheng, H. Q.; Liu, C. X. (2013): Numerical simulation of oil spill (accident) and its influence on water source area in Chang Jiang estuary. *Resources and Environment in the Yangtze Basin*, vol. 22, pp. 1055-1063.

Sun, D. L. (2009): *Construction of Advanced Velocity-pressure Coupling Algorithms and Interface Capture Method (Ph.D. Thesis)*. Xi'an Jiao Tong University, China.

Wang, B.; Liu, X. W.; Wang, L. Z. (2016): Simulation of the accidental river oil spill and emergency response analysis based on IWIND-LR model. *Safety and Environmental Engineering*, vol. 23, pp. 148-153.

Song, Y. X.; Wei, Y. N.; Qian, H.; Fang, Y. (2011): Analysis of the groundwater and soil pollution by oil leakage. *Procedia Environmental Sciences*, vol. 11, pp. 939-944.

Zhang, J.; Qian, X. Q.; Zhang, H. X.; Liu, Z. C. (2018): Fluid-structure interaction simulation of aqueous outflow system in response to Juxtacanalicular meshwork permeability changes with a two-way coupled method. *Computer Modeling in Engineering & Sciences*, vol. 116, no. 2, pp. 301-314.

Zhao, Y. X.; Wang, Y. G.; Zhang, W. S. (2012): Two-dimensional numerical simulation model for oil spill in river. *Yangtze River*, vol. 43, pp. 81-84.