Peculiarities of hazardous chemical fire in high-rise R&D buildings based on numerical simulation

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Abstract. There are lots of chemical laboratories in high-rise R&D buildings. Large amounts of hazardous chemicals were stored in them. Once a fire breaks out in high-rise R&D buildings, its severity will be much greater than that of high-rise residential building fire. Inflammable chemicals, explosive chemicals, toxic chemicals are usually get involved in hazardous chemical fire. FDS software is usually used for numerical simulation of hazardous chemical fire. Then, the impact of hazardous chemicals fire in high-rise R&D buildings can be analyzed under different fire conditions. This paper collected the hazardous chemicals stocks of 69 companies in the R&D buildings and screened the storage data of hazardous chemicals. Typical hazardous chemicals were selected as fire simulation objects. The consequences of hazardous chemical fires can be analyzed by simulation results. The difference between hazardous chemical fire in R&D high-rise buildings and residential building fire can be found out. At the same time, relevant performance indexes will be proposed for the evacuation of high-rise R&D hazardous chemical fire.

1. Introduction
With the development of R&D enterprises, a large number of R&D enterprises have settled in high-rise buildings of chemical parks. A large amount of flammable and explosive hazardous chemicals will be stored and used in the production process of the enterprise [1] At present, most of the enterprises in the R&D buildings have different amounts of hazardous chemicals storage. This paper collects the storage and use of chemicals in 69 companies in a R&D center. The hazardous chemicals used by each company range from dozens of types to hundreds of types. Among them, hydrochloric acid, ethanol, methanol, tetrahydrofuran, petroleum ether and other hazardous chemicals have large storage capacity. Ethanol is a Class A fire hazard. The storage of hazardous chemicals is as follows. In the event of a fire, losses and casualties are immeasurable.

Enterprises in modern high-rise R&D buildings store and use hazardous chemicals in large quantities, the storage of a large amount of flammable and explosive hazardous chemicals has greatly increased the factors causing fires [2]. Most chemical reagents will not only be accompanied by the release of toxic and harmful gases when burning, but also the large amount of smoke released will
reduce the visibility inside the building and affect the evacuation of personnel. Therefore, it is very important to predict the diffusion path of smoke in high-rise buildings [3]. Compared with high-rise residential building fire, the difficulty of rescue of hazardous chemical fires not only depends on factors such as smoke, temperature and toxic gases [4]. More importantly, when a flammable liquid fires, other stored hazardous chemicals will quickly gasify, burn or even explode with the influence of thermal radiation. Due to the diversity of storage of hazardous chemicals, uncontrollable factors also increase in the event of a fire. If volatile and corrosive chemicals are stored on site, the injury to personnel will greatly increase when a hazardous chemical fire occurs.

Therefore, it is urgent to improve the safety of the laboratory of high-rise R&D building and the storage place of hazardous chemicals. In order to reduce the risk of laboratory accidents, it is indispensable to conduct fire accident simulation analysis on the laboratory of high-rise R&D enterprises. It is very important to master the internal temperature distribution, smoke diffusion, smoke visibility, toxic and harmful gas concentration in a R&D high-rise building when a hazardous chemical fire occurs [5]. Establishing a scientific and feasible emergency evacuation index for high-level R&D enterprises can effectively strengthen the enterprise's emergency response capabilities and minimize the casualty rate caused by accidents.

In recent years, the number of accidents in R&D laboratories has increased significantly. On December 26, 2018, a burning explosion occurred in the Laboratory of Municipal and Environmental Engineering at Beijing Jiaotong University, two doctors and one master died of it. On December 18, 2015, an explosion occurred in the chemistry department laboratory of Tsinghua University, a doctoral student died of it. On March 27, 2017, an explosion occurred in the reaction kettle of a laboratory in the West Building of Chemistry, Handan Campus of Fudan University, which caused an undergraduate who was doing experiments to be injured. Through the statistics of 28 laboratory accidents that occurred in recent years, there were 19 explosion accidents, 8 fire accidents, and 1 toxic substance leakage accident. These accidents caused many students and researchers to be injured or even died.

With the continuous development of Chinese petrochemical enterprises, high-rise R&D buildings will continue to increase. The use and storage of a certain volume of hazardous chemicals in high-rise R&D buildings will increase the probability and consequences of fire accidents in high-rise buildings. At present, many researches on the analysis of the fire safety hidden danger in the storage places are about dangerous chemical products, and most researchers have put forward the fire prevention countermeasures of the storage places of dangerous chemical products. In particularly, there are a large number of flammable liquids and inflammmable gases in the park. Once a fire occurs, the site is complex, sudden, changeable, and secondary combustion explosions, which will spread violently and produce a large amount of toxic gases, threatening the safety of rescue workers [6]. This will bring difficulty to fire rescue personnel rescue, because the building deformation collapse, easily caused by burning.

2. Literature review

2.1. Numerical simulation in hazardous chemical fire

The safety accidents of hazardous chemicals are mainly fire, explosion, poisoning and suffocation, etc. At present, the fire simulation is used for hazardous chemical pool fire. High-rise building and hazardous chemical warehouse is in the majority. However, there are few numerical simulations of indoor fires caused by hazardous chemicals in high-rise buildings. FDS software was used to conduct numerical simulation of the fire occurrence and development process of hazardous chemicals production workshop in real environment, which confirmed the feasibility of current laboratory fire simulation of hazardous chemicals [7]. FDS was used to simulate the fire in a hazardous chemicals warehouse, studied the fire growth process and smoke spread law, and analyzed the impact of high temperature burn, carbon monoxide.
poisoning, oxygen and asphyxia on casualties. If a hazardous chemical fire occurs in a high-rise building, it is not only the impact of burn and poisoning, but also involves evacuation [8].

Olewski T [9] pointed out that in the process of developing new technologies or synthesizing new substances, scientific research laboratories must involve more hazardous chemicals. Different hazardous chemicals have different properties, storage conditions and treatment methods, which leads to the tedious safety management and heavy workload of hazardous chemicals in laboratories.

Chang L et al established an evacuation model combining heuristic algorithm with network flow control for the multi exit evacuation problem and route capacity problem under the condition of smoke restriction in building fire [10].

Dineno et al. studied the common mode and spreading development characteristics of high-rise building fire, and simulated the fire scene by scientific means [11].

Kaufman emphasized the difference between hazardous chemicals laboratory and other workplaces, as well as the necessity of different safety requirements. During the use of R & D laboratory. It is necessary to ensure that laboratory staff understand the hazards of hazardous chemicals in their workplaces, and protect them from exposure beyond the allowable level [12].

2.2. Performance-based evacuation index design

At present, the building scheme designed according to the national fire protection technology is not applicable to all types of high-rise buildings [21]. Because of the high location of high-rise building fires, it will be more difficult to rescue and evacuate. R&D high-rise building fires are often accompanied by the generation of toxic or harmful gases and the leakage of flammable and explosive materials. Because of the specificity of hazardous chemical fire, it is necessary to carry out numerical simulation of hazardous chemical fire in a typical R&D building. It is particularly important to establish performance-based evacuation index which is different from high-rise residential building fire.

In the fire performance design of high-rise buildings, the state has issued some relatively broad index system. However, more detailed index system is needed for chemical fire in chemical laboratory in high-rise research and development building. Therefore, high-rise R&D buildings should not only meet the performance-based requirements stipulated in laws and regulations, but also be more targeted.

3. Methodology

A methodology is developed to study the difference between hazardous chemical fire and high-rise residential building fire by simulating hazardous chemical fires in a R&D building. The destructiveness of the hazardous chemical fire and the specificity of the evacuation index can be found out from the simulation results. Proportional modeling of the R&D building through FDS software. Then inspect the storage of hazardous chemicals in the R&D building and screen and summarize the inventory. The whole methodology is presented in six steps and shown in Fig. 2. Detailed descriptions of these steps are presented in the following subsections.
3.1. Data collection
As the chemical storage of each R&D building is different, different R&D buildings have different storage conditions for hazardous chemicals. The data are classified and summarized, and the collected data are processed according to the quantity and type. Then, the relatively large stockpiles of hazardous chemicals in the R&D center building were extracted as the ideal storage model. In the fire simulation, numerical analysis is carried out according to the ideal storage model. The difference of consequence and evacuation difficulty between hazardous chemical fire and high-rise residential building fire will be researched further.

3.2. Selection of performance indexes
The safe evacuation time of personnel under different fire conditions can be obtained through simulation. The simulation results are used to put forward relevant requirements for the performance indexes of high-rise R&D buildings.

Within the available evacuation time, if some people do not evacuate to a safe area, their safety will be threatened. That is, they are considered unable to evacuate safely. The evaluation indexes include temperature, thermal radiation, minimum oxygen content in the air, flue gas concentration, toxic gas, etc. [20].

The available evacuation time formula is as follows:

\[ \text{ASET} = \min\{T_a, T_b, T_c, T_d, T_e, T_f\} \]

Among above:

“\( T_a \)” denotes the critical time at which thermal radiation causes harm to the human body; “\( T_b \)” denotes the critical time for flue gas temperature to cause harm to human body; “\( T_c \)” denotes the critical time when visibility impedes human movement; “\( T_d \)” denotes the critical time when a poisonous gas causes harm to human body; “\( T_e \)” denotes the critical time for harmful combustion products to cause harm to human body; “\( T_f \)” denotes the critical time for other factors to cause harm to the human body; “ASET” denotes the available evacuation time.
4. Application of the methodology

Before the setting of the fire scene, this paper collected the hazardous chemicals storage of a total of 69 companies in this R&D building. Analyze and screen the inventory of hazardous chemicals in the R&D building based on usage and storage. The ratio of hazardous chemical stockpiles is as follows.

![Pie chart of hazardous chemicals inventory](image)

The situation of hazardous chemicals stored in each company is different. Therefore, a general model can be established for the storage of hazardous chemicals in the company based on statistical data. Hazardous chemicals with dosage greater than 2% were selected as model objects. The ideal storage model for hazardous chemicals is: hydrochloric acid, ethanol, petroleum ether, dichloromethane, ethyl acetate, nitrogen [compressed or liquefied], methanol, acetic anhydride, acetonitrile, n-butanol, etc. Therefore, the storage type of hazardous chemicals at the time of fire was determined as the above model.

In this paper, a 20-story high-rise building model was built based on a R&D building in a chemical park. Each floor is roughly similar in structure, with offices, laboratories, analysis rooms, lounge areas and public areas set up on each floor.

According to the ideal model of hazardous chemicals storage, it can be seen that ethanol storage ranks first. In addition, ethanol is A Class a fire substance. So the ethanol fire reaction is designed for this simulation. In the simulation calculation according to the actual situation of the hazardous chemicals laboratory. The air flow caused by the volume occupied by the human body and the position change of the personnel should be ignored. It is assumed that there is sufficient air to fully burn the ethanol during the combustion reaction, and the fire source is fixed and does not diffuse. Considering the worst result, the location of the fire source is set in the room closest to the stairs. The grid size of this model is 0.5×0.5×0.5. The location of the fire source is as follows.

The combustion reaction used in this simulation is the ethanol combustion reaction. The combustion heat of ethanol is 1366.8KJ/mol; the specific heat is 2470J/(kg·K); the enthalpy of vaporization is 42.42KJ/mol; and the boiling point is 351.65K. From figure.5, the release rate of ethanol combustion heat \(^7\) can be calculated as 1458.724kW/m\(^2\).

![Heat release rate calculation formula](image)
According to the classification of NFPA, the fire can be divided into four types according to the speed of development: slow, medium, fast and super fast. The division is based on the time required for the heat release rate of the fire source to reach 1055KW \cite{14}. The details are showed in the table below.

| Fire type   | slow | medium | fast | super fast |
|-------------|------|--------|------|------------|
| Time required to reach 1055KW(s) | 600  | 300    | 150  | 75         |
| b           | 0.002913 | 0.01172 | 0.04698 | 0.1878     |

Since the flash point of ethanol is 12\(^{\circ}\)C, it is a type of ultra-fast growth fire, and the fire development coefficient is taken as 0.1878. The relationship of fire heat release rate \(Q\) \cite{14} is as follows:

\[
Q = 0.1878t^2
\]  \hspace{1cm} (7)

In this simulation, R&D enterprises are distributed on each floor from the 2nd floor to the 20th floor, and the enterprise with the largest methanol reserves is on the 14th floor. Therefore, fire conditions are set on the 2nd and 14th floors in this simulation. This simulation is divided into four working conditions:

Fire condition I: The hazardous chemical fire occurred on the 14th floor, and the fire room is at location A in Fig.7.

Fire condition II: The high-rise residential building fire occurred on the 14th floor, and the fire room is at location A in Fig.7.

Fire condition III: The hazardous chemical fire occurred on the 2nd floor, and the fire room is at location A in Fig.7. This condition has twice the area of fire condition I.

Fire condition IV: The hazardous chemical fire occurred on the 2nd floor, and the fire room is at location B in Fig.7. This condition has twice the area of fire condition I.

The main purpose of fire condition I and fire condition II is to simulate the difference between hazardous chemical fire in high-rise buildings and residential building fire. Analysis of smoke diffusion law, visibility change law, temperature and thermal radiation change law, toxic and harmful gas concentration and other aspects of the difference. The main purpose of fire condition III and fire condition IV is to compare the fire development rules of different positions on the same floor. By simulating the fire development law of different positions on the same floor, the best place for storing hazardous chemicals is analyzed. So as to reduce the consequences of fire accidents. The main purpose of fire condition I and fire condition III is to compare the influence of fire area on fire consequences. By simulating the consequences of the fire, the amount of storage per floor or per room can be limited. So as to meet the entire research and development building evacuation performance.

According to the former data, ethanol combustion reaction was set, and gas visibility and temperature monitoring points were set at 1.6 meters away from the floor on the 2nd and 14th floors. On the one hand, the influence of hazardous chemical fire in high-rise R&D buildings and residential building fires on evacuation was compared in different floors and positions. On the other hand, the secondary effects of ethanol leakage on other hazardous chemicals in the burning room can be analyzed. Comprehensively considering the time of safe evacuation and fire development \cite{13}, the simulation time of this fire was set as 600s.
5. Results and discussion

In this paper, detailed data of simulation results are screened and summarized, and the analysis is as follows:

![Figure 5. Comparison of temperature between condition I and fire condition II](image1)

![Figure 6. Comparison of temperature between condition I and fire condition II](image2)

In the four small figures in Figure 5: $T(w)$ and $T(p)$ respectively represent the temperature of hazardous chemical fire and ordinary fire. $T(wL)$, $T(wM)$ and $T(wR)$ respectively represent the temperature of the stairwell near the fire source, the elevator area and the stairwell far from the fire source in the hazardous chemical fire. $T(pL)$, $T(pM)$ and $T(pR)$ respectively represent the temperature of the stairwell, elevator area and stairwell far from the fire source of ordinary fire. $T(14)$-$T(20)$ respectively represent the temperature of the stairwell on the side of the 14-20 floor close to the fire source in fire condition I(lower left) and fire condition II(lower right).

The broken line at the upper left of Figure 6 shows the temperature change above the fire source. It can be seen that the temperature above the simulated hazardous chemical fire is obviously higher than that of ordinary fire. The broken line on the upper right in Figure 6 shows a comparison of temperature changes between the stairwell and elevator area. It can be found that the temperature of hazardous chemical fire is higher than that of ordinary fire, and the rise rate is faster. The following two small figures in Figure 6 respectively represent the broken line diagram of the temperature of the stairwell on the 14-20 floor close to the fire source under fire working condition I and II. It can be found from these two figures that the temperature of fire condition I is significantly higher than that of fire condition II. That is to say, when a hazardous chemical fire occurs, the temperature of the stairwell is higher than that of an ordinary fire.

The time that human body can stand in the high temperature environment of fire is shown in the following table [15].
Table 2 The amount of time the body is exposed to high temperatures

| The flue gas temperature (℃) | Human endurance time                                      |
|------------------------------|-----------------------------------------------------------|
| 60                           | Bear for a short time                                      |
| 110                          | Irreversible losses will occur within 15 minutes           |
| 150                          | 5min                                                      |
| 180                          | Irreparable damage can be caused to human body within 1min |
| Over 200                     | Unable to endure                                           |

It can be known from the influence of different air temperature and humidity on human safety under high temperature environment [16]. When the heat radiation of building fire smoke reaches 60℃, it will harm human body and affect the evacuation process [17].

By analyzing the simulated data, we can get the time when each area reaches the dangerous temperature as follows:

| Monitoring Area (14th floor) | Stairwell close to fire | Stairwell away from fire | The elevator area | Different parts of the corridor |
|------------------------------|-------------------------|--------------------------|--------------------|---------------------------------|
| Time to reach 60℃/s          | 238                     | 515                      | 194                | 197, 175, 172, 283               |

It can be seen from the above table that some areas have reached the dangerous value within 3min after the fire occurred in the ignition layer.

The comparison of visibility and CO concentration in fire condition I and fire condition II is as follows:

Figure 7. Comparison of visibility between condition I and fire condition II

Figure 8. Comparison of Carbon monoxide concentration between condition I and fire condition II
In Figure 7, V(wL), V(wM) and V(wR) respectively represent the visibility of the stairwell on the side close to the fire source, the visibility in the elevator area, and the visibility on the side far from the fire source in fire condition I. V(pL), V(pM) and V(pR) respectively represent the visibility of the stairwell on the side close to the fire source, the visibility in the elevator area and the visibility on the side far from the fire source in the second fire condition. V(1) and V(2) respectively represent the broken line diagram of visibility in the corridor at the door of the room in fire condition I.

Figure 7 shows that the visibility of the simulated hazardous chemical fire has a small impact. After 300s of ordinary fire, the visibility in the elevator area and stairwell decreases to 5m in succession. Figure 8 is the numerical diagram of CO concentration in each area of the fire floor under fire condition I and II.

As can be seen from the left figure in Figure 8, CO concentration in most regions reaches the dangerous value of 500×10⁻⁶mol/mol. In normal building fire simulation, only one outlet of the burning room (CO(2)) has a CO concentration that reaches a dangerous value. According to the specific simulation values, the time when CO concentration reached the dangerous value in fire condition I were 172s, 496s, 482s and 301s. The hallway in the room where the fire started was the first to reach critical levels. Therefore, the personnel at the door of the fire room and the adjoining room should be evacuated quickly within 3 minutes. All personnel on the fire floor should be evacuated within 5 minutes.

By comparing the simulation results of fire condition III and fire condition IV, it can be found that: on the same floor, the difficulty of evacuation is reduced when the burning room is away from the stairwell and elevator area. By comparing fire working condition I and fire working condition III, it can be found that: when the area of fire source increases, the influence on the temperature, CO concentration and visibility of fire will increase correspondingly.

6. Conclusions

In this paper, FDS software is used to simulate the hazardous chemical fire in a R&D building. According to the comparison of fire values under four conditions, it can be seen that: When the fire room is close to the stairwell, the temperature in the elevator area reaches 60°C at 194s. The stairwell on the left side close to the fire source reached 60°C at 238s, and the stairwell on the right side far from the fire source reached 60°C at 515s. The rest of the corridor reaches 60°C as soon as 172s. Therefore, in the hazardous chemical fire of the building, the best evacuation time of the elevator should be controlled within 194s, and the evacuation time from the stairs should be within 238s, or the evacuation from the stairwell far from the fire source should be within 515s. Comparing with the hazardous chemical fire and the ordinary fire, the hazardous chemical fire is reached in a shorter time under different aspects such as the hazardous value of temperature, thermal radiation and CO concentration. The available evacuation time is also shorter in the hazardous chemical fire. When the types and stocks of hazardous chemicals stored on site exceed the minimum effective time for rescue, restrictions on the storage of enterprise hazardous chemicals in the R&D building should be considered. As the type and stock of storage increase, the risk of fire and the consequences of fire will increase accordingly.

To sum up, in the event of a hazardous chemical fire in the R&D building, the rescue time should be shortened considering the storage situation of the chemical products comprehensively. In addition, the uncontrollable factors of inflammable and explosive dangerous chemicals make the evacuation time of hazardous chemical fire far less than that of ordinary civil buildings. Therefore, the evacuation plan should be formulated according to the actual storage situation of hazardous chemicals instead of the ordinary fire evacuation index as the rescue reference to reduce fire casualties.

7. Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.
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References
[1] Shi Xianzhao, Ma Chenxin, Zhou Ning, Wu Dongwei, Yuan Xiongjun, Liu Xuanya, Huang Weiqiu. (2017) Present Situation and Countermeasures of Safety Management of Dangerous Chemicals Storage [J]. Industrial Safety and Environmental Protection, 43(07):55-57.
[2] Wu Bin. (2018) Risk Analysis of Fire Explosion in Chemical Laboratory[J]. Chemical Engineering Design Communications, 044(012):171.
[3] Ahn C S, Bang B H, Kim M W, et al. (2019) Theoretical, numerical, and experimental investigation of smoke dynamics in high-rise buildings[J]. International Journal of Heat and Mass Transfer, 135(JUN.):604-613.
[4] Liu Xiao, Cai Zhiyong, Ma Shengjie, et al. (2019) Numerical Simulation of High-rise Building Fire Based on FDS [J]. Value Engineering, (31).
[5] Zhang Wenkai, Xu Lei, Wang Mengzhu. (2019) Analysis of the Office Building Fire Risk based on Fire Dynamics Simulator [J]. Journal of Dalian Minzu University, 021(003):P.272-279.
[6] Liu Aili, Liu Tiaotiao. (2018) Analysis on the Safety Management of Laboratory hazardous chemicals [J]. Science and Technology Innovation Herald, 15(17):190-191.
[7] Han Zhizhong. (2018) Numerical simulation of fire smoke distribution based on combustion heat calculation model [J]. China Adhesives, 27(12):49-54+64.
[8] Wang Jun. (2016) Numerical simulation of fire risk for a hazardous chemicals warehouse based on FDS [J]. Fire Service (Electronic Version), No.8(04):34-36.
[9] Olewski T, Snakard M. (2017) Challenges in Applying Process safety management at university laboratories[J]. Journal of Loss Prevention in the Process Industries,209-214.
[10] Liu C, Mao Z, Fu Z. (2016) Emergency Evacuation Model and Algorithm in the Building with Several Exits[J]. Procedia Engineering, 135:12-18.
[11] Philip J.DiNeno,Dougal Drysdale,Craig L.Beyler etc. (2002) The SFPE Handbook of Fire Protection Engineering[M].Bethesda:The National Fire Protection Association
[12] Kaufman, James A (2002) Occupational exposure to hazardous chemicals in laboratories: Understanding the OSHA laboratory standard[J]. Journal of Chemical Education, 69(11):911.
[13] Wang Yige, Xie Fei, Song wenhua,et al. (2012) FDS Simulation of the Whole-area Pool Fire in Dichloropropane Tank Area [J]. Acta Scientiarum Naturalium Universitatis Nankaiensis, 045(004):18-25,29.
[14] Yuan Hui,Dai Changqing. (2014) Numerical Simulation Research on Combustion Characteristics of High-rise Building Fire [J]. Journal of Anhui Jianzhu University, 000(006):77-81.
[15] Wang Shuai. (2015) Research on fire smoke spreading and personnel safety evacuation in high-rise building [D]. Hebei University of Engineering.
[16] Liu Yang. (2012) Study of Numerical Simulation and Safe Evacuation for Building Fire Based on FDS [D]. Liaoning University of Engineering and Technology..
[17] Hay, Adrian. (1996) Positive Pressure Ventilation A Study of Overseas Experience, Research Report Number 8/96, Home Office Fire R&D Group.
[18] Su Yong. (2018) Simulation study on the Influence of High-rise Building Structure and Stair Type On Evacuation Time [D].
[19] Wang Yabin. (2014) On the application of performance-based design in fire protection design of super high-rise buildings. [J] Jiangxi building materials. (02):36-36.