

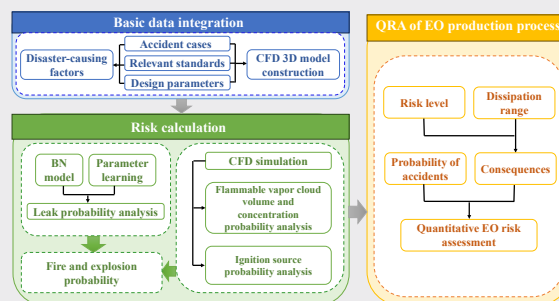
Quantitative risk assessment of EO leakage integrating KG, BN, and CFD simulation

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ABSTRACT: Ethylene oxide (EO), a crucial derivative of ethylene, involves high temperature and pressure as well as flammable, explosive, and toxic materials. This complexity predisposes its production to severe industrial accidents. To systematically identify the risk factors that may lead to EO accidents, this study conducted an integrated analysis by leveraging a knowledge graph (KG), a Bayesian network (BN), and computational fluid dynamics (CFD) simulation. First, the key risk factor nodes leading to leakage were identified by using KG. Subsequently, a BN was constructed, which enabled the clarification of typical EO leakage scenarios. Then, for the identified typical leakage scenarios, a CFD geometric model was developed. This model was employed to simulate the dispersion patterns following an EO leak under different conditions. Finally, by integrating the results from the BN and CFD analyses, the working conditions with the highest risk level were identified. The results indicated that leakage caused by chemical corrosion or physical erosion of reactors or pipelines presented the highest quantified risk value. This scenario exerts a significant impact on the safe production of EO, necessitating prioritized and focused inspection. Through the integrated KG–BN–CFD methodology, this study has effectively elucidated the disaster-causing mechanisms and evolution patterns of EO leakage accidents. It thereby provides a theoretical foundation and practical guidance for the precise identification of risks, the formulation of targeted prevention and control measures, and the enhancement of inherent safety levels in EO production facilities.

KEYWORDS: ethylene oxide (EO); leakage quantitative risk assessment; computational fluid dynamics (CFD); Bayesian network (BN)



1 Introduction

Ethylene oxide (EO) serves as a key feedstock for producing polyether surfactants and polyether polyols. It ranks as the third most important ethylene derivative, following only polyethylene and polyvinyl chloride. The EO production process comprises multiple interconnected units, each housing various high-temperature and high-pressure equipment. The complex on-site operating environment contains numerous flammable, explosive, toxic, and hazardous gases (Bubbico et al., 1998; Wang et al., 2013). These conditions make the system highly prone to leaks, which can trigger serious safety incidents resulting in significant casualties and substantial property damage. For instance, in 2022, a pipeline rupture in the EO purification column area at a petrochemical enterprise in Shanghai triggered EO leakage, which subsequently led to an explosion. This incident resulted in one fatality and one injury. In a 2015 incident at an enterprise in Nanjing, spontaneous polymerization occurred within an EO purification tower. This led to the blockage of instrument impulse

lines. Improper handling by operators then caused EO leakage, which subsequently induced an explosion inside the tower, resulting in one minor injury. Therefore, identifying the risk factors present in the EO production process and clarifying its key causative elements are of great significance for implementing targeted management and control in EO production.

In recent years, researchers have conducted extensive studies on the safety issues inherent in the EO production process. Wang et al. (2013) employed HAZOP to analyze safety issues in an EO/EG plant. Their results indicated that an abnormally high cooling water temperature was the primary factor leading to accidents. Khan and Haddara (2004) conducted a risk analysis of an EO production facility. Their study found that ethylene pipelines posed the highest risk. Li et al. (2016) applied the pool fire evaluation method to conduct a quantitative assessment of a pool fire scenario involving an EO storage tank. Their calculations indicated that personnel must evacuate to a minimum distance of 67.35 m from the tank area to avoid injury from thermal radiation. Zhong et al. (2014) employed FLUENT software to

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simulate the dynamic dispersion of EO. Their simulation results revealed a positive correlation between the leakage rate and the affected area, an inverse correlation between wind speed and the affected area, and a negligible influence of ground roughness. Liu et al. (2017) performed hazard analysis and identification of major hazard sources for the EO storage tank area in a chemical plant. The findings demonstrated that excessively rapid temperature increase, equipment rupture, and operational errors were identified as the key factors contributing to the accidents. The aforementioned studies indicate that accidents in EO production involve multiple contributing factors, which exhibit interconnections and correlations. However, research that accounts for the interactions among these different factors to assess the risk of accidents occurring during the EO production process is scarce.

Presently, some researchers have undertaken preliminary investigations into the interrelationships among multiple factors within the production process. Zhang et al. (2025) assessed the spatiotemporal evolution of risks associated with flammable liquid transport in waterways using a Bayesian network. Their results demonstrated that addressing the inherent hazards of the flammable liquid itself, double-walled containers, and sealing mechanisms can significantly minimize the possibility of liquid leakage. Wang et al. (2025) conducted a comprehensive risk assessment for ocean-going vessels using a modified dynamic Bayesian network model. Their study revealed that human behavior is a critical factor influencing the safety of such vessels. Hosseini et al. (2020) employed fault tree analysis (FTA) and event tree analysis (ETA) to conduct a safety assessment of fire risk in a natural gas processing plant. Their evaluation results indicated that the plant's risk level was categorized as "medium". Luo et al. (2018) developed an integrated risk assessment methodology by combining a modified fishbone diagram with a risk matrix model. This approach can quantify both accident consequences and their possibility of occurrence. Marhavilas et al. (2019) integrated HAZOP, DEMATEL, and AHP to conduct a safety assessment for the chemical processing industry. Their research demonstrated that this integrated methodology effectively identifies critical points and determines risk priorities. The reviewed literature reveals that BN is capable of determining

the possibility of accident occurrence and identifying key elements and causative pathways and has been widely adopted for risk assessment in chemical operations. However, current Bayesian network analyses applied to chemical operations predominantly rely on subjective expert judgment to estimate the risk magnitude of causative factors. Consequently, they lack the capability to quantify the actual consequences resulting from specific factors.

This study synthesizes EO production accident investigation reports and relevant literature, analyzes the EO production process, and summarizes the evolution patterns and causative factors of EO accidents. Subsequently, KG is utilized to establish a corresponding indicator system. Utilizing the BN model, the key causative factors of EO leakage accidents and the interrelationships among different factors were analyzed. This led to the identification of the most critical causative elements and typical leakage scenarios contributing to accidents. Combined with CFD simulation, the dispersion process of EO following a leak under various pressure and temperature conditions was modeled. This enabled a clear determination of the formation envelope and concentration distribution pattern of the resulting toxic vapor cloud. Finally, an integrated risk assessment of the EO production process was conducted by CFD and BN analyses. This integrated approach also enabled the prediction of potential accident consequences.

2 Methods and process introduction

2.1 Introduction of the EO production process

The EO production process comprises three primary units: EO reaction unit, CO₂ removal and EO recovery unit, and light component removal & EO purification unit. A simplified flowchart of the EO production process is shown in Fig. 1.

This section provides a demonstration of the hazard identification process using the representative part as an example, along with a systematic approach to identifying risk factors. Within the EO production process, the EO reaction unit exhibits higher inherent operational hazards compared to other processing units. Within the EO reaction unit, the oxidation reactor is designated as the central processing equipment. Ethylene, oxygen, and recycling gas are premixed, preheated, and fed into an

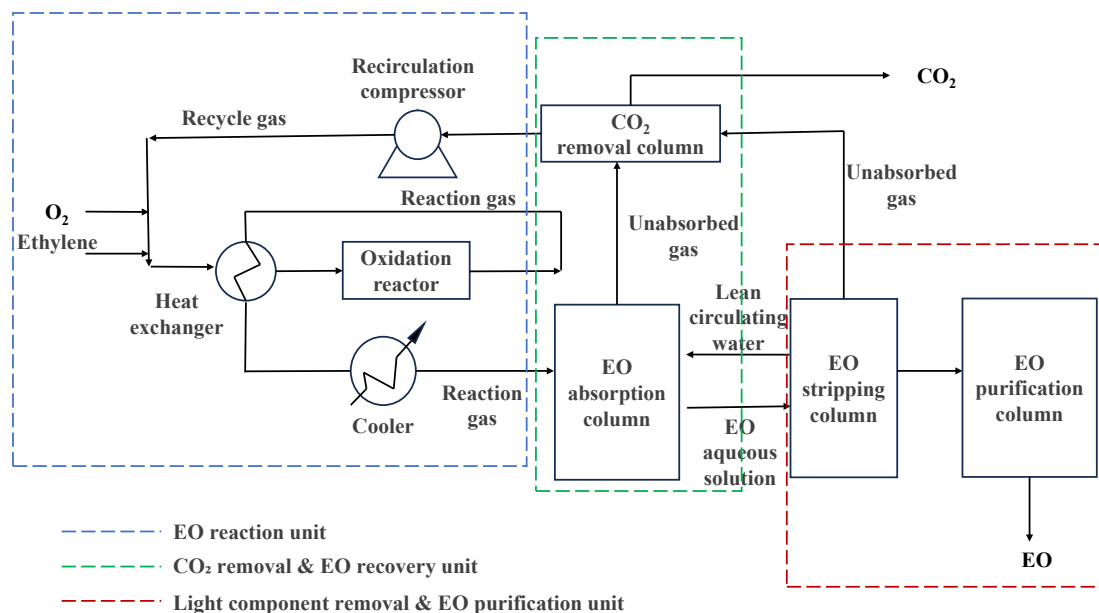


Fig. 1 Simplified flowchart of the EO production process.

oxidation reactor. Under the action of a silver-based catalyst, these reactants undergo conversion to EO. The resultant reaction gases are subsequently cooled through a heat exchanger before being transferred to the CO₂ removal and EO recovery unit. This process operates under elevated temperature (255 °C) and high-pressure (3 MPa) conditions, which can trigger fire incidents, explosions, or toxic exposure events. A schematic diagram of the oxidation reactor is shown in Fig. 2.

2.2 Knowledge graph (KG)

A KG is a data structure that employs structured knowledge representation to model concepts, entities, events, and their interrelationships (Wang et al., 2023). It consists of knowledge entities (nodes) and the relationships between them, which are represented as various types of edges. The construction process of a KG typically involves steps such as entity extraction, relation extraction, and knowledge storage. Logically, its architecture can be divided into two tiers: the schema layer and the data layer. The schema layer primarily establishes a logical structural framework for the knowledge by building an ontology, which defines the representation format for the data layer. The data layer stores factual data. Following knowledge extraction, the relevant data undergo processes such as data integration, entity linking, and ontology construction across both the data and schema layers, ultimately leading to the formation of the complete KG.

2.3 Bayesian network (BN)

BN represents a class of probabilistic graphical models that encode conditional dependencies among random variables via directed acyclic graphs, thereby explicitly capturing causal relationships between variables (Fu et al., 2024; Pearl, 1985). A BN is formally structured as a directed acyclic graph comprising nodes, directed edges, and conditional probability tables. The nodes represent a set of random variables modeled by the BN, while the directed edges encode causal dependencies between these variables. Each node's conditional probability tables quantify the probabilistic

strength of these causal relationships through explicitly defined conditional distributions. A simple BN is shown in Fig. 3.

BNs are based on probabilistic knowledge for probabilistic reasoning. Through the logical relationships between nodes, uncertainty reasoning within the system is completed. Posterior probability can be obtained based on the prior probability using the Bayes formula, where X represents target variables and E denotes observed evidence.

Based on the basic principles of the BN model briefly introduced above, it is possible to conduct forward risk prediction and diagnostic reasoning for the analyzed system:

(1) Predictive inference of accident initiation probability

The goal is to be able to reason and calculate based on the causes of the accident to predict the probability of the outcome. The joint probability of a set of variables $X = (X_1, X_2, \dots, X_3)$ can be expressed as shown in Formula (1):

$$P(X) = \prod_{i=1}^n P(X_i | \pi(X_i)) \quad (1)$$

(2) Reverse reasoning accident cause diagnosis

Given that the result event has already occurred, we can infer the probability of the corresponding cause event that could have triggered it. Based on the magnitude of this probability, we can diagnose the main factors that caused the result event (accident).

When $P(X_i)$ changes, to identify the possible causes for the change in the child node X_i (the parent nodes $X_{i1}, X_{i2}, \dots, X_{im}$), the posterior probability $\pi(X_i)$ after the change in the child node X_i caused by the parent node X_{ij} can be expressed by Formula (2):

$$P(X_{ij} | X_i) = \frac{P(X_i | X_{ij}) P(X_{ij})}{P(X_i)} = \frac{P(X_i, X_{ij})}{P(X_i)} \quad (2)$$

In industrial production processes, BN is capable of identifying key elements contributing to failures in complex systems. They enhance the capability for quantitative analysis of uncertainties and improve the foresight of risk early warning, thereby enabling targeted control and management.

2.4 Computational fluid dynamics (CFD)

CFD constitutes a numerical simulation methodology grounded in the conservation laws of mass, momentum, and energy (Fu et al., 2016; Jiang et al., 2021). Fundamentally, it quantitatively characterizes fluid flow, heat transfer, and chemical reaction processes by solving the Navier-Stokes equations. A CFD model integrates three essential components: governing equations defining the physical behavior of fluids, geometric models delineating the spatial topology of the computational domain, and boundary conditions prescribing external constraints at domain

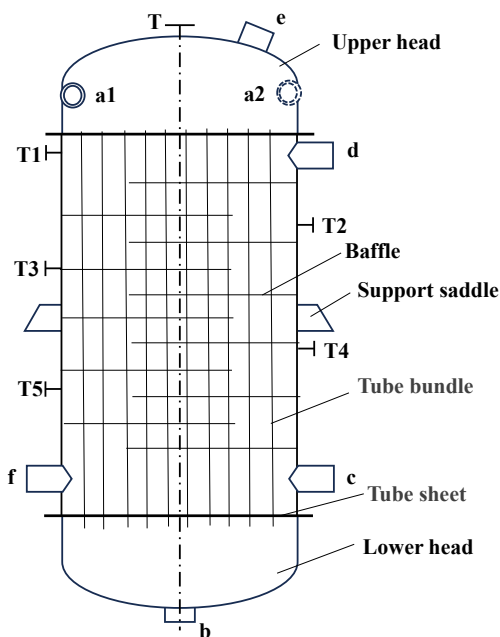


Fig. 2 Schematic diagram of the oxidation reactor. a1 and a2 are the gas inlet, b is the gas outlet, c is the feed liquid inlet, d is the feed liquid outlet, e is the explosion-proof opening, f is the feed liquid discharge opening, T1–T5 are the temperature measurement openings for the feed liquid, and T is the temperature measurement opening for the catalyst bed layer.

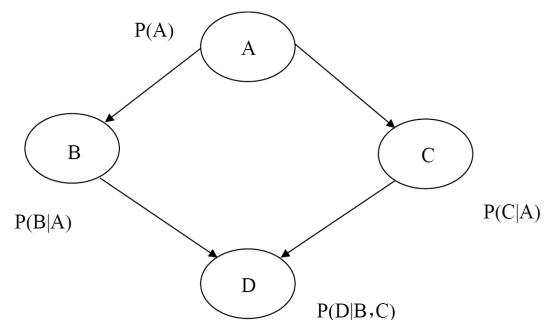


Fig. 3 BN example diagram. A is the parent node, with the prior probability being $P(A)$; B, C, and D are child nodes, with the conditional probabilities being $P(B|A)$, $P(C|A)$, and $P(D|B,C)$, respectively; B and C are also the parent nodes of D.

interfaces. Collectively, these elements establish a complete mathematical representation of fluid dynamics phenomena.

As a specialized discipline within fluid dynamics, CFD employs numerical algorithms to solve nonlinear problems associated with fluid flows. CFD finds extensive application in industrial practice, notably for combustion modeling (Hua et al., 2005). It is further validated as an appropriate methodology for simulating vapor dispersion and explosion dynamics. Advancements in computational technology enable high-performance computing resources to execute three-dimensional simulations (Harlow, 2004). This approach enables the prediction of industrial accident impact areas, reduces subjective biases in the risk assessment process, and enhances the accuracy of quantitative risk assessment.

This study established a geometric model based on the 6-18 Shanghai petrochemical fire accident. The constructed EO production platform is shown in Fig. 4.

During mesh generation, grid refinement is implemented at fluid-solid interfaces proximal to leakage sources to enhance resolution accuracy. A pressure-based solver is selected for this simulation, employing a transient calculation model with gravitational effects incorporated. Turbulent flow dynamics are resolved using the realizable k - ϵ model. This study involves the leakage of EO in the air and uses the component transport model. The boundary conditions are shown in Table 1.

To facilitate the simulation calculation, the EO production platform model is simplified, and the following assumptions are made:

- (1) The EO leakage remains in a continuous leakage state, and the leakage rate remains unchanged during the leakage process.
- (2) The EO mixture is composed of EO and oxygen.
- (3) It is assumed that leakage occurs in an environment without wind.

Computational accuracy is directly governed by mesh quality during numerical simulation. Systematic refinement studies are conducted to evaluate solution convergence, establishing an optimal grid resolution that satisfies both precision requirements and computational efficiency. The number of grids set was 37,774, 47,217, 54,390, and 78,178, respectively. Finally, the gas concentration changes 5 m ahead of the EO leakage outlet Inlet 1 were calculated, as shown in Fig. 5.

By comparing the gas concentrations at the same location, it was found that the maximum deviation of grid number 37,774 compared to 78,178 was 28%, and the maximum deviation of grid number 54,390 compared to 78,178 was 2.7%. When the number of grids is greater than 54,390, the obtained results are less affected by the number of grids and are relatively accurate. Considering both accuracy and efficiency, the number of grids used in this calculation is 54,390.

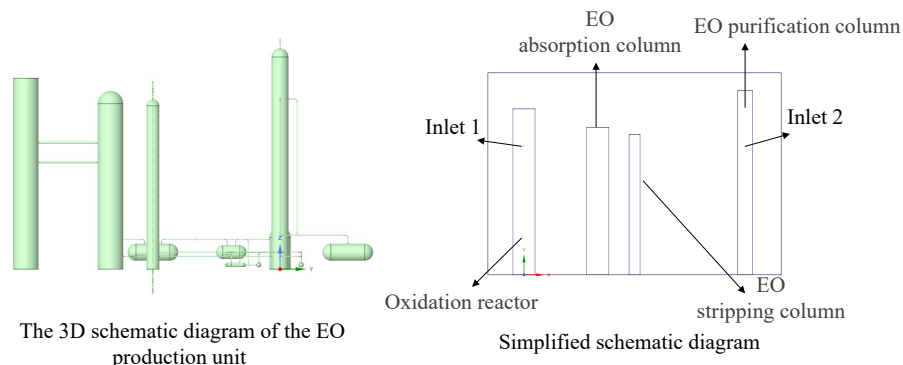


Fig. 4 Model of the EO production platform.

2.5 Research framework

To enhance objectivity and reliability in EO production safety research, a methodology integrating BN and CFD is established, with the detailed research framework illustrated in Fig. 6.

Initially, fundamental data integration is performed to identify latent hazards that induce unsafe conditions in EO production. Concurrently, critical process equipment parameters are acquired. Subsequently, a BN model is constructed. The probability of leakage accident occurrence is determined by parameter learning algorithms. Concurrently, CFD simulation is employed to quantify the spatial distribution and concentration thresholds of flammable vapor clouds following leakage incidents. Combined with probabilistic ignition analysis, the probability of fire and explosion scenarios is determined. Finally, quantitative risk assessment for EO production processes is obtained by integrating risk classification, impact zone delineation, and accident probability.

3 Results and discussion

3.1 Risk identification

The establishment of an indicator system for the causative factors of EO leakage accidents is fundamental to conducting risk assessment. In this study, KG was utilized to construct a dedicated KG for EO leakage accidents. This graph clarifies the causes of accidents and their interrelationships and incorporates a database of 360 recorded EO leakage incidents. Based on relevant studies (Bao, 2023; Dai, 2013) and historical accident statistics, this research focused on individual process units as the primary subjects of analysis. The causative factors associated with these units were first identified and then systematically collated and categorized. This process was further integrated with the statistics derived from the EO leakage accident KG. From the perspective of the entire operative workflow, an indicator system for the causative factors of EO leakage accidents was subsequently constructed. The specific KG is shown in Fig. 7.

By analyzing objective data, including historical accident case reports, relevant literature, and legal regulations, the graph determined the key nodes and their relationship networks. These key disaster nodes and paths that led to leakage were classified into 3 intermediate nodes and 10 root nodes and are listed in Table 2. Specific nodes are shown in Table 2.

3.2 BN analysis of the EO production process

3.2.1 Construction of the BN model for the EO production process

The risk structure model for EO leakage accidents is constructed utilizing GeNIe software. The random variables represented by

each node were added to the software interface. The relationships between nodes were determined based on the KG and relevant accident investigation reports and then connected sequentially with arrows to construct the topological structure of the BN. Finally, the parameter learning module of the GeNIe software was used to analyze the data, and the prior probabilities and conditional probabilities of each node were obtained. As illustrated in Fig. 8.

As evidenced in Fig. 8, node N exhibits the highest occurrence probability among the ten root nodes at 32%. This is primarily due to the complex operating environment of EO production, where systems often function under high-pressure or vacuum conditions. Such conditions subject the equipment to sustained significant stress over prolonged periods, thereby accelerating component aging. Secondly, node M exhibits a significantly elevated probability of occurrence at 30%. This is mainly because the flow rate of materials within the system is influenced by multiple factors. Variables such as abnormal material ratios and pipe scaling can lead to changes in the flow rate.

Table 1 Boundary condition setting parameters

Boundary name	Boundary type
Inlet 1	Velocity-inlet
Inlet 2	Velocity-inlet
Outlet	Pressure-outlet

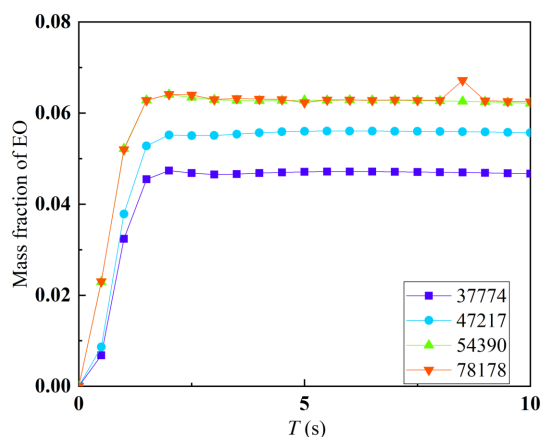


Fig. 5 Grid independent analysis.

3.2.2 Posterior probability analysis

Posterior probability denotes the probability of event A occurring given new evidence B. This probability metric provides a more accurate representation of an event's actual occurrence probability (Bai et al., 2023). With the probability of node A fixed at 100%, posterior probabilities of contributing factors are computed through diagnostic inference, as visualized in Fig. 9.

As shown in Fig. 9, when the probability of a leakage accident in the EO production process is set to 100%, the occurrence probabilities of all key nodes increase accordingly. Among them, node D exhibits the highest posterior probability at 75%, making it the primary causative factor for leakage. This is primarily due to the potential formation of acidic byproducts within the reaction system. When combined with moisture, these byproducts create a corrosive environment that can induce pitting corrosion or stress corrosion cracking at equipment weld seams or stress concentration zones.

3.2.3 Sensitivity analysis

With node A designated as the target variable, sensitivity analysis of the BN model for EO production processes is conducted using the dedicated module within GeNIe software, as detailed in Fig. 10.

As illustrated in Fig. 10, node D, corresponding to chemical corrosion or physical erosion, exhibits the highest sensitivity with a value of 0.116. It is therefore identified as a critical factor contributing to the occurrence of EO leakage accidents. The next most significant is node K, which is associated with pressure. This finding is consistent with the results of the posterior probability analysis.

3.3 CFD simulation of EO leakage

In this study, in addition to calculating the probability of leakage accidents during EO production, we also accounted for the volume and dispersion of the resulting toxic vapor cloud, which is closely linked to casualties in such incidents.

3.3.1 Establishment of EO leakage and diffusion model

Based on the constructed KG, we summarize the accident development path. The results show that there are three risk factors directly linked to the top event: high-temperature burn-through of the reactor or pipeline, high-pressure rupture reactor

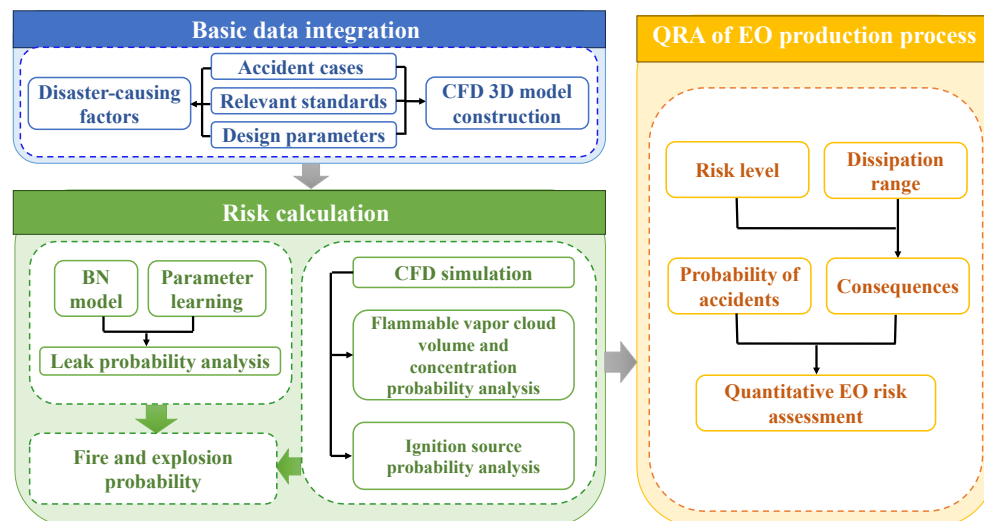


Fig. 6 Research framework.

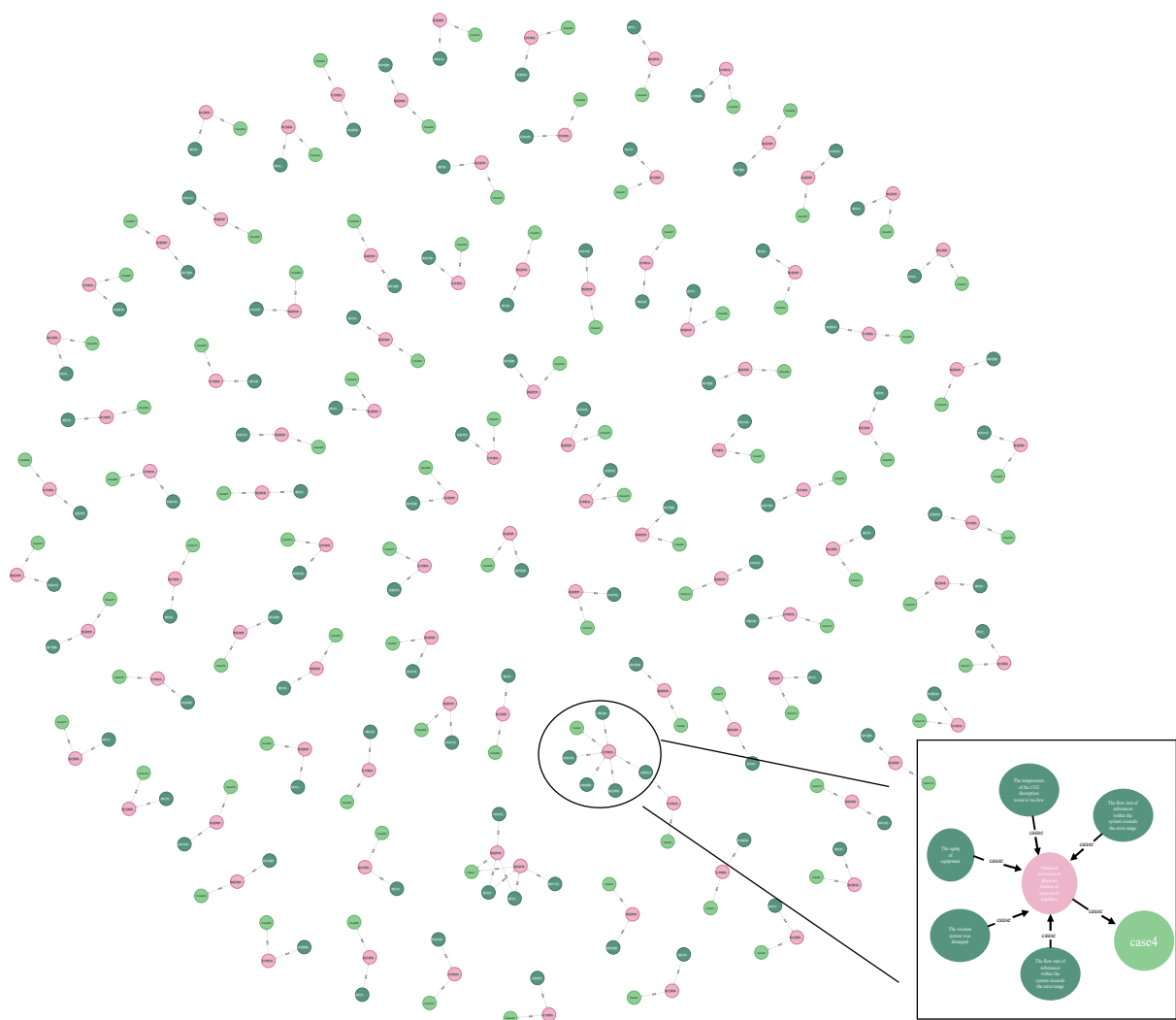


Fig. 7 The initial KG of the EO leakage accidents.

Table 2 BN node

ID	Meaning
A	EO leakage occurred
B	High-temperature burn-through of the reactor or pipeline
C	High-pressure rupture reactor or pipeline
D	Chemical corrosion or physical erosion of reactors or pipelines
E	Abnormal boiler temperature
F	Cooling water supply failure
G	The feed ratio and feed rate are beyond the error range.
H	Catalyst failure
I	Circulating gas compressor blockage
J	Failure to regularly clean impurities within the system
K	The vacuum system was damaged (specifically referring to the negative pressure part of the production system)
L	The temperature of the CO ₂ desorption tower is too low
M	The flow rate of substances within the system exceeds the error range
N	The aging of equipment

or pipeline, and chemical corrosion or physical erosion of reactors or pipelines. To systematically convert these factors identified by KG into CFD modeling scenarios, we adopted the following screening strategy: “chemical corrosion or physical erosion” factor is simulated with leakage occurring under normal operating conditions to reflect the progressive degradation process of the

material; for “overheating burn-through” and “high-pressure rupture”, different high-temperature and high-pressure conditions are applied to characterize the corresponding failure mechanisms. The oxidation reactor and EO purification column are selected as representative leakage-containment equipment in this investigation. The normal operating values of the equipment,

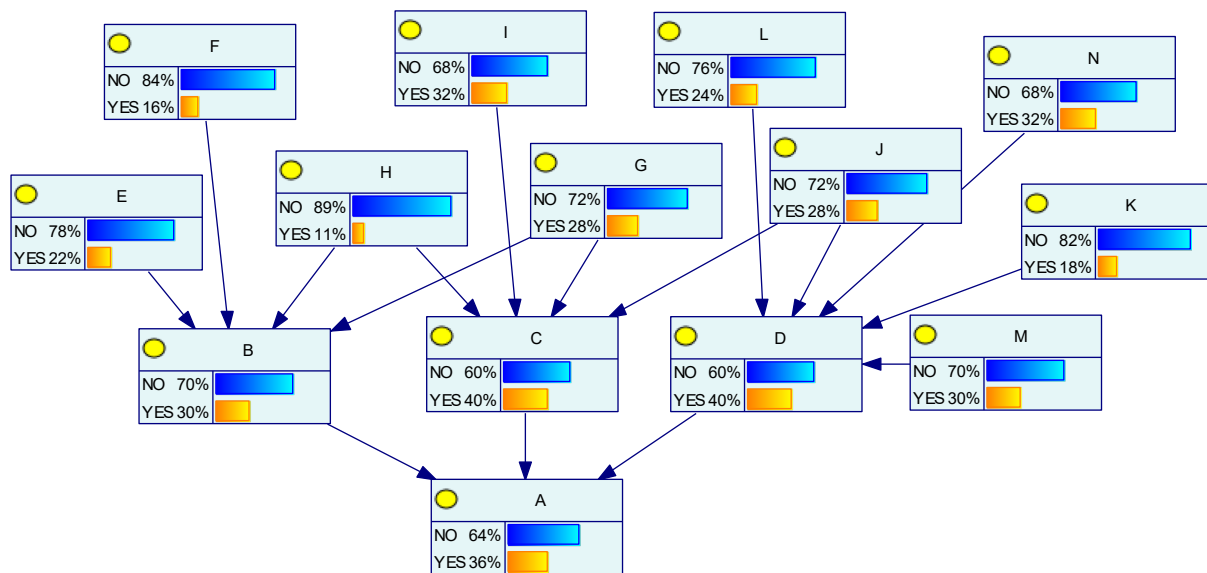


Fig. 8 BN for safety assessment in the EO production process.

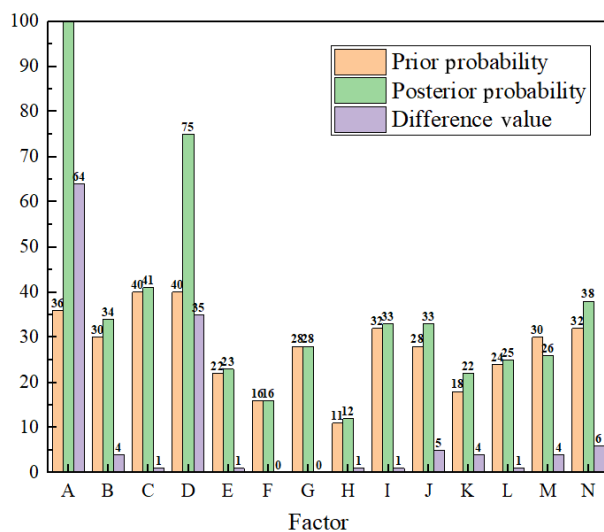


Fig. 9 The BN after the A node status is set to 100%.

alarm values, and critical numbers are combined. 10 different cases are set up. The leakage that occurs under normal parameters corresponds to “chemical corrosion or physical erosion of reactors or pipelines”. The specific working conditions scenarios are shown in Table 3.

3.3.2 Discussion and analysis of numerical simulation results

(1) The influence of pressure on the diffusion of EO leakage

The affected area formed by EO dispersion after 300 s under different pressure conditions was compared. A cross-section through the leakage orifice was created to analyze the dispersion characteristics of EO. The resultant visualization from this cross-sectional analysis is presented in Fig. 11.

As shown in Fig. 11, the asymmetric distribution of the molar concentration reflects a two-stage diffusion process. This is mainly because in the early stage, the leaked EO is in a liquid state under high temperature and high pressure, and after release, it rapidly vaporizes. The dense heavy gas cloud formed has a higher density than the surrounding air, so it tends to sink toward the ground. In the later stage, as the cloud mixes with the surrounding air and heats up, its density decreases, and the buoyancy effect causes it to rise upward. This transition from heavy gas diffusion to buoyancy-

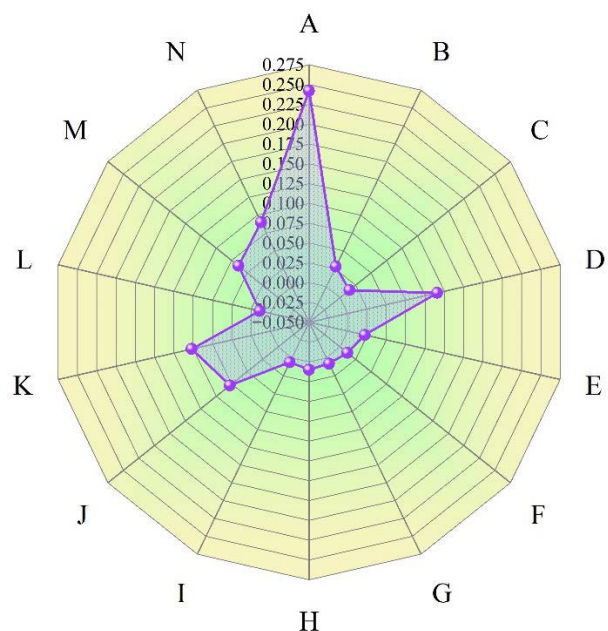


Fig. 10 Sensitivity radar chart.

Table 3 Setting of operating conditions

Case	Leak point	Pressure (MPa)	Temp. (K)
1	Inlet 1	2.00	500
2	Inlet 1	2.25	500
3	Inlet 1	2.50	500
4	Inlet 1	2.00	550
5	Inlet 1	2.00	600
6	Inlet 2	0.40	320
7	Inlet 2	0.60	320
8	Inlet 2	0.80	320
9	Inlet 2	0.40	360
10	Inlet 2	0.40	400

driven movement results in the observed asymmetry phenomenon.

The dispersion range of EO in air under different pressure conditions gradually expands as the pressure increases,

accompanied by a rise in molar concentration. This is primarily because elevated pressure leads to a higher initial molar concentration of EO at the leakage point, thereby establishing a steeper concentration gradient between the leak source and the ambient environment. According to Fick's law of diffusion, a stronger concentration gradient provides a greater initial driving force for dispersion, thereby promoting the migration of EO molecules over longer distances. However, as the dispersion range expands, the migration path of EO molecules through the air lengthens. Under the continuous influence of air resistance, their dispersion velocity gradually decreases. These findings are consistent with descriptions in the relevant literature (Zhang and Mu, 2013).

(2) The influence of temperature on the diffusion of EO leakage

The influence range formed by the diffusion of EO over 300 s under different temperature conditions was compared. A cross-sectional treatment was carried out at the location of the leakage hole, and the diffusion characteristics of EO were analyzed. The resulting graph from the cross-section is shown in Fig. 12.

As shown in Fig. 12, under varying temperature conditions, the dispersion range of EO in air gradually decreases as the temperature rises. Concurrently, the gas leakage rate also declines with increasing temperature. This is primarily because, under constant pressure, an increase in the tank temperature causes thermal expansion of the gas, thereby reducing its density. This

reduction in density diminishes both the leakage mass flow rate and the initial driving force for dispersion. Consequently, this leads to a contraction of the observable dispersion range. In this scenario, the enhancing effect of temperature on molecular velocity is overshadowed.

In addition, the thermal buoyancy effect is worthy of attention. As the temperature rises, the temperature difference between the leaked gas and the ambient air increases, and the resulting buoyancy effect also strengthens accordingly. This upward buoyancy will cause the leaked gas to rise, thereby affecting the distribution pattern of the diffusion cloud. In low-temperature conditions, the gas density is relatively high, and the diffusion range is narrower and tends to be closer to the ground. However, in high-temperature conditions, the thermal buoyancy drive causes some gases to migrate upward, and the mole concentration distribution shows a more obvious upward trend in the vertical direction.

3.4 Quantitative risk assessment for EO leakage accidents

Risk is typically defined as the combination of the possibility and severity of consequences (Society for Risk Analysis, 2018). In this study, the risk of EO leakage is expressed by Eq. (3), where P_{leak} represents the leakage probability calculated by the BN in Section 3.2. The severity index S corresponds to the concentration range of EO that causes human toxicity (Ministry of Industry and

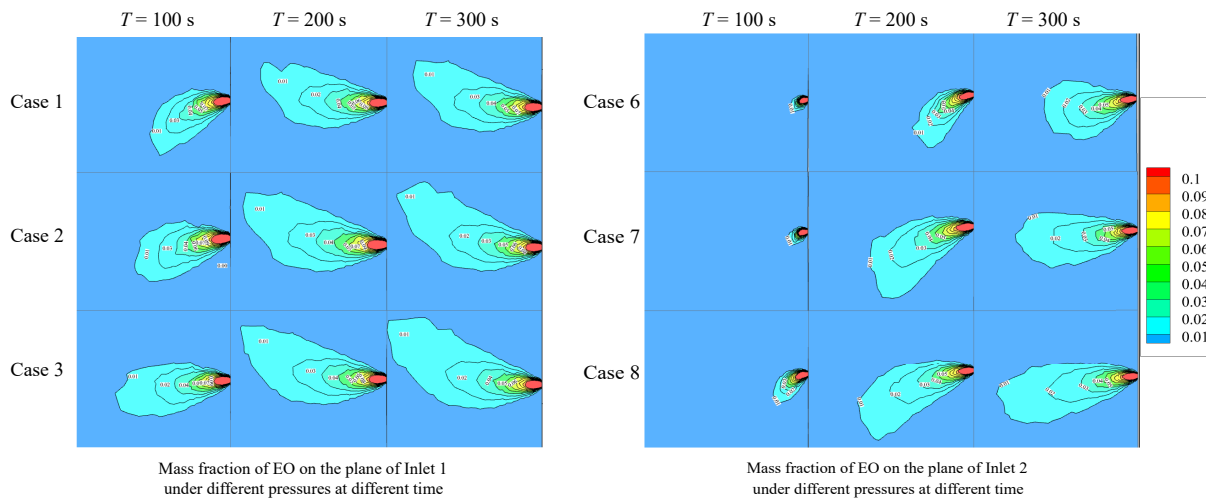


Fig. 11 Cloud diagram of the mole concentration distribution of EO leakage under different pressures.

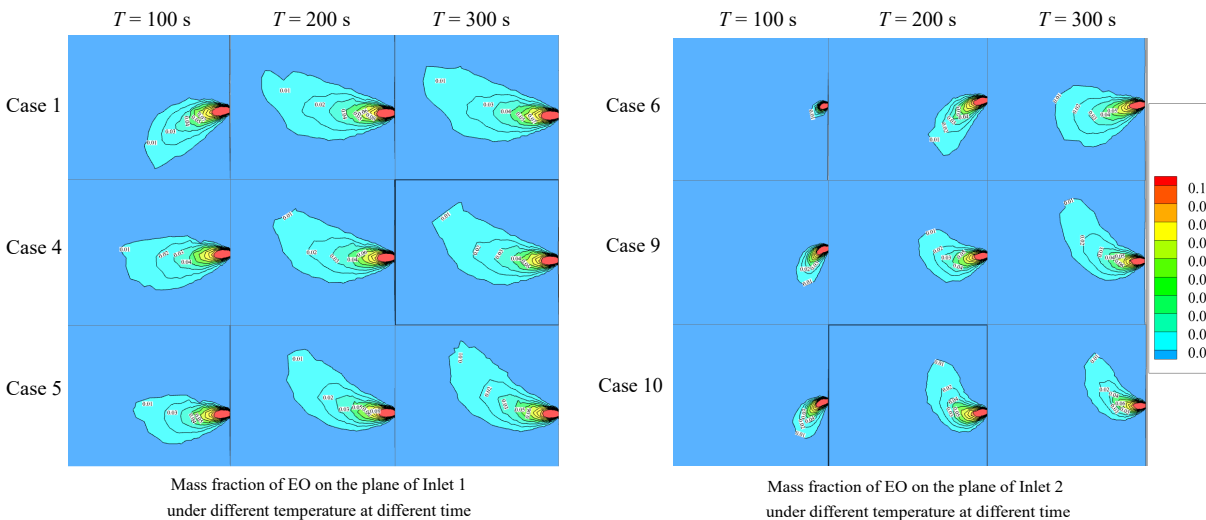


Fig. 12 Cloud diagram showing the distribution of mole concentrations of EO leakage at different temperatures.

Information Technology of the People's Republic of China, 2023), quantified based on the extent of vapor cloud dispersion simulated via CFD (Wu and Jing, 2024).

Specifically, BN analysis is used to determine the prior probability of accident scenarios based on available evidence, with these probabilities directly serving as occurrence frequencies in risk quantification. Additionally, CFD simulations are conducted for representative leakage scenarios to quantify the consequences by calculating the gas leak extent. Finally, an integrated quantification is performed using the standard risk equation (risk = probability × consequence) to determine the final risk level.

$$R = PS \quad (3)$$

After calculation, the value of risk R is shown in Table 4.

This is attributed to both a higher probability of leakage occurrence in Case 1 and a larger dispersion range capable of causing human intoxication in this scenario. Under the combined influence of high accident likelihood and severe consequences, this scenario is prone to resulting in casualty events. Therefore, it is essential to prioritize and allocate greater attention to high-temperature and high-pressure equipment during routine maintenance and inspection to prevent potential accidents.

It should be noted that in this study, the determination of P_{leak} only considered the individual effects of pressure, temperature and corrosion on the pipe wall. In actual scenarios, the three influencing factors interact with each other. Therefore, the value of P_{leak} should be greater than the value obtained in this study. In particular, the probability of corrosion leakage is significantly higher than that of the other two factors, which may result in the calculated risk values in Cases 2–5 and 7–10 being lower than the actual risk values.

4 Conclusions

As an important derivative of ethylene, the safe production of EO has raised concerns. To identify the risk factors existing in the production process of EO and clarify the key causal factors in the production process, this paper presents a quantitative risk assessment method for epoxy ethane leakage accidents based on BN and CFD. It systematically integrates the probability of gas leakage, the dispersion range of the gas, and the consequences of poisoning accidents. The main conclusions of this article are as follows.

(1) According to the BN analysis, the posterior probabilities and sensitivities of corrosion and erosion were the highest, and they were the key factors leading to the occurrence of EO leakage accidents. This phenomenon primarily stems from acidic byproducts generated within the EO production reaction system,

which establishes corrosive microenvironments predisposing equipment to pitting corrosion and stress corrosion cracking. At the same time, when the reaction gas and liquid flow at high speed in the pipeline, it will cause mechanical wear and make the pipe wall thinner.

(2) The CFD simulation analysis reveals that when leakage occurs, the diffusion range of the gas expands as the pressure increases and decreases as the temperature rises. This phenomenon primarily originates from elevated pressure imparting higher initial velocity to leaking gas, while thermal expansion at increased temperature reduces gas density, consequently diminishing both mass leakage flux and initial diffusive driving force.

(3) The risk calculation results indicate that Case 1 presents the highest risk value, at 10.5, which would have a substantial impact on the safe production of EO. During routine maintenance and repair, more effort should be devoted to conducting thorough inspections to ensure that accidents do not occur.

Due to the limitations of computing resources and storage space, this study did not simulate all possible scenarios. Based on this, more detailed optimization analysis is needed (for different protective facilities, leakage equipment and operating conditions). The accuracy of BN can be enhanced by combining methods such as machine learning.

CRedit author statement

Yujie Wang: Data curation, methodology, supervision, investigation, resources, visualization, writing – original draft. Huaying Cui: Formal analysis, investigation, writing – original draft. Kong Xin: Visualization, writing – review & editing. Jinlong Zhao: Conceptualization, supervision, funding acquisition, visualization.

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.

Data availability

Data will be made available on request.

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Table 4 EO leakage risk

Case	P	S	R
1	0.75	14.00	10.500
2	0.44	15.00	6.600
3	0.44	15.50	6.820
4	0.34	12.50	4.250
5	0.34	11.00	3.740
6	0.75	9.00	6.750
7	0.44	11.50	5.060
8	0.44	12.50	5.500
9	0.34	8.75	2.975
10	0.34	7.00	2.380

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