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BI-IEnKF coupling model for effective source term estimation of natural gas leakage in urban utility tunnels

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ABSTRACT

As an effective way to facilitate the increasing demand for reliable infrastructure, energy supply and sustainable urban development, underground utility tunnels have been developed rapidly in recent years. Due to the widespread distribution of utility tunnels, the safe operation of natural gas pipelines accommodated in utility tunnels has caused great concern considering fire, explosion, and other coupling consequences induced by the gas pipeline leakage. However, the limited information on leakage source terms in accidental leakage scenarios could preclude timely consequence assessment and effective emergency response. In this study, a BI-IEnKF coupling source term estimation (STE) model is developed, with the combination of gas dispersion model, Bayesian inference (BI) and iterative ensemble Kalman filter (IEnKF) method, to achieve the effective source term estimation (including leakage location and leakage rate) and gas concentration distribution prediction. The newly developed model is first evaluated by the twin experiment with good reliability and accuracy. Furthermore, three contributing factors affecting the performance of the developed BI-IEnKF coupling STE model were investigated to assist parameter selection for practical use. Additionally, the novel application of mobile sensors serving as an alternative for fixed sensors is explored, and an application framework is sequentially given to guide the deployment of the developed coupling model in utility tunnels. The results show that the developed model has great performance in accuracy, efficiency and robustness, as well as the potential to be applied in actual utility tunnel scenarios. This study can provide technical supports for safety control and emergency response in the case of natural gas pipeline leakage accidents in utility tunnels. Also, it could be helpful to reasonable references for gas lekage monitoring system design.

1. Introduction

With the rapid development of urbanization, utility tunnel, as an effective way to address the pressing requirement of reliable infrastructure, energy supply, and higher environmental protection, has been utilized widely in the past few decades (Broere, 2016; Wang et al., 2018; Yin et al., 2020; Apak et al., 2022). Natural gas pipeline characterized by widespread distribution is more vulnerable to accidental, natural, and intentional threats (Chen et al., 2021; Vairo et al., 2021; Wang et al., 2021). Once the inevitable accidental leakage cannot be well treated with reasonable emergency response by decision-makers, it can constitute a major contributor to the escalation of leakage into fire/explosions (Zhang et al., 2020; Tang et al., 2020; Deng et al., 2022). And thus the accommodation of the natural gas pipeline in utility tunnels has caused a wide concern considering the potential consequence induced by the unexpected leakage accident (Yang et al., 2021; Cheng et al., 2022). Therefore, it is necessary to pay sufficient attention to the leakage accident of the natural gas pipeline from the emergency response point of view, which has a pivotal role in the safe operation of urban underground utility tunnels.

In the early years, there have been some studies regarding gas leakage and dispersion in utility tunnel scenarios by employing numerical simulation methods and experimental analysis. Tan et al. (2017) employed Ansys Fluent to analyze the dispersion behaviors of leaking gases and the effect of mechanical ventilation was also considered. The results showed that mechanical ventilation plays a significant role in leaking gas mixing and dilution. Lu et al. (2018) took the actual Yanyingshan tunnel as a research subject and investigated the effect of

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multi-factors (e.g. leakage location, leakage direction, the shape of leakage hole) on the gas leakage and dispersion processes. It was indicated that the pipeline operating pressure has a more adverse influence on the leakage consequence. Liu et al. (2019) studied the influence of temperature and humidity on the leaking gas dispersion characteristics and a relatively apparent gas dispersion promotion phenomenon was found. Wang et al. (2020) conducted a scenarios analysis considering the effect of leakage size, pipeline pressure, and mechanical ventilation on gas dispersion through the two-dimensional numerical analysis. Zhang and Lan (2020) developed a large-scale experimental mockup for the numerical model validation purpose and the optimization of ventilation speeds and sizes of ventilation vents in the utility tunnels was also discussed. Zhang et al. (2021) explored the possibility of the water–gas integrated compartment in utility tunnels from the perspective of energy-saving oriented. It is revealed that the present emergency response treatment can be applied to the novel water–gas compartment safely. Zhou et al. (2021, 2022) have built a utility tunnel experimental apparatus to simulate the gas leakage and dispersion in the underground utility tunnel using alternative safe gas with CO_2. And the adopted numerical model was validated by the experimental data. Moreover, the layout scheme of gas sensors in the utility tunnel networks was optimized as well. Bu et al. (2021) proposed a methane invasion distance (MID) equation for describing the gas leakage process in the utility tunnel, which is beneficial to the optimized gas sensor layout. In conclusion, most of the aforementioned studies usually employed a forward numerical model (i.e., e.g. Computational Fluid Dynamics model) to handle the process of gas release and dispersion, which needs to prescribe initial parameters (e.g., leakage source term and wind conditions). It can be used to reproduce the scenarios after the occurrence of accidents and provide some reasonable reference for later accident planning. However, when an unexpected natural gas leakage accident occurs in utility tunnels, the unknown source term and unstable wind conditions can cause varying degrees of errors, which inevitably deviates the simulation results from real situations. Therefore, the aforementioned issues make the timely and reasonable emergency response difficult when coping with the unclear or unknown source term (i.e., leakage location and leakage rate) scenarios in utility tunnels.

As a widely used method to realize the source term estimation and physical field correction by assimilating observation data into the gas dispersion model, the reliability and practicability of the data assimilation (DA) method have been validated in different scenarios, such as atmospheric conditions (Zhang et al., 2015; Wang et al., 2017; Wu et al., 2021), river pollution (Zhang and Huang, 2017; Wang et al., 2019), and urban environment (Xue et al., 2018; Jia and Kikumoto, 2021). The natural gas compartment of utility tunnels can serve as a potential scenario for the application of the DA method since the gas sensors are required to be accommodated inside the natural gas compartment according to GB50838-2015 *Technical Specification for Urban utility Tunnel Engineering* (CPS, 2015), which facilities the data collection and utilization. There have been some studies using the DA method to achieve the gas dispersion prediction under the unknown source term in utility tunnels. Yuan et al. (2019) and Cai et al. (2022) developed a one/three-dimensional CFD-ensemble Kalman filter (EnKF)based model respectively for the gas concentration prediction and the leakage rate estimation, but this model could not deal with the inversion of the leakage location. Wu et al. (2020) proposed a source term estimation model based on the Bayesian inference method, which was capable of both the leakage rate and leakage location inversion. However, the proposed Bayesian inference-based model can not realize a gas concentration distribution prediction. These abovementioned studies mainly employed one specific DA method and focused on one objective (i.e., only source term estimation or gas concentration prediction). They have difficulties in achieving release source term estimation and the leaking gas concentration prediction simultaneously. Therefore, coupling prediction of source term and gas concentration distribution is still a very challenging task aiming for both emergency response and consequence assessment. Moreover, the utilization of mobile sensors has great prospects in terms of both the DA model improvement and gas sensor system design but has not been investigated in utility tunnel scenarios.

In this paper, a BI-IEnKF coupling STE model is developed with the combination of the gas dispersion model, Bayesian inference, and the iterative ensemble Kalman filter method, which can help to realize the source term (both leakage location and leakage rate) estimation and gas concentration prediction. Firstly, the effectiveness of the developed model is validated by a widely used twin experiment. Furthermore, the parameter sensitivity analysis is conducted to evaluate the performance of the developed model further in the context of different ensemble sizes, prior distribution, and time intervals of available observation data. Moreover, the novel application of mobile sensors in utility tunnels and its enhancement for the developed model is demonstrated. Finally, an application framework of the BI-IEnKF coupling STE model is proposed. This study contributes to providing technical support for source term estimation and gas concentration prediction of the commonly used gas transportation facilities in process industries, such as utility tunnels and chemical plants equipped with gas sensors.

2. Methodology

In this study, the developed BI-IEnKF coupling STE model consists of a forward gas dispersion model and a novel coupling DA model. This section is organized as follows: Firstly, the adopted gas dispersion model is defined to ensure that the main gas leakage and dispersion characteristics in utility tunnels can be well captured; Secondly, the Bayesian inference method and iterative ensemble Kalman filter method are introduced respectively. With the combination of two DA methods, a newly coupling DA model is developed. In the developed coupling DA model, the computational burden stemming from the sampling section of the BI method can be reduced significantly. Meanwhile, the drawback of the IEnKF method in possibility and uncertainty analysis will also be complemented. Finally, the combination of the gas dispersion model and the newly developed coupling DA model is elaborated.

2.1. Gas dispersion model

The natural gas compartment of utility tunnels is constructed as a long and narrow structure, which means that the ratio of the cross-section and length of utility tunnels is very small (Liu et al., 2022). Moreover, when an accidental gas leakage happens, the leaking gas will be mixed within the cross-section rapidly and transported along with the length direction of the utility tunnel under the effect of mechanical ventilation. Therefore, the one-dimensional gas advection–diffusion equation is selected as the gas dispersion model (i.e. the forward model) because of the special structure and gas dispersion characteristics (Yuan et al., 2019; Wu et al., 2020). This gas dispersion model can propagate the leaking gas as time marches by presetting the initial source term parameters. This simplification can reduce computational consumption to a large extent and satisfy the emergency demand for rapid prediction of gas leakage and dispersion. As a result, it can help to construct the fast source term estimation model. The adopted advection–diffusion equation is presented as follows:

$$\frac{\partial \rho c}{\partial t}+\frac{\partial (\rho u c)}{\partial x}=\frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right)+S \tag{1}$$

Where

c represents the volume fraction of natural gas,

ρ is the gas density,

u is the gas velocity corresponding to the x-direction,

D is the gas diffusion coefficient and S is the leakage source term.

2.2. Data assimilation method

2.2.1. Bayesian inference method

The Bayesian inference method is derived based on the framework of the Bayes theorem. The Bayesian inference method is used to obtain the posterior probability of interest parameters, the calculation of the posterior distribution is given as follows:

$$P(\alpha|\beta) = \frac{P(\alpha)P(\beta|\alpha)}{P(\beta)} \tag{2}$$

Where

α is the unknown parameter matrix of the gas leakage source term (i.e., the. leakage location and leakage rate),

β is the observation data matrix obtained from the gas sensors,

$P(\alpha)$ represents the prior distribution that can help to predefine the range of the source term parameters, and $P(\beta)$ is a normalization factor,

$P(\beta|\alpha)$ and $P(\alpha|\beta)$ denote the likelihood function and the posterior distribution respectively.

Generally, the direct calculation of $P(\beta)$ needs to solve a complex multidimensional integral. In this study, the IEnKF method is chosen to simplify the calculation of the posterior probability presented in Eq. (2). Meanwhile, the predictive deterioration problem can be avoided to a large extent by the iteration calculation involved in the IEnKF method (Sousa and Gorlé, 2019).

2.2.2. Iterative ensemble Kalman filter method

The iterative ensemble Kalman filter method is developed to address the crux in solving the strongly non-linear inversion problem. The specific procedure of the IEnKF method can be found in the study proposed by Iglesias (Iglesias et al., 2013). In this study, only some key steps are presented.

Taking an inversion problem for the calculation of u as an example:

$$y = G(u) + \eta \tag{3}$$

Where.

$G : X \rightarrow Y$ is the forward response operator, which can map the unknown parameter u to observation space,

X and Y are hilbert spaces (i.e., the state spaces of the leakage source term and ga s concentration respectively in this study),

η represents the noise following distribution with 0 mean and Γ variance,

$y \in Y$ is observation data.

To solve the inversion problem mentioned above, the artificial dynamics model (Gas dispersion model in this study) based on state augmentation is defined as follows:

$$z_{n+1} = \Xi(z_n) \tag{4}$$

$$y_{n+1} = Hz_{n+1} + \eta_{n+1} \tag{5}$$

The mapping rule Ξ: $Z \rightarrow Z$ is achieved by constructing a state-space $Z = X \times Y$, and the corresponding equation is presented below:

$$\Xi(z) = \begin{pmatrix} u \\ G(u) \end{pmatrix}, z = \begin{pmatrix} u \\ p \end{pmatrix} \in Z \tag{6}$$

Where $H : Z \rightarrow Y$ is the projection operator and $H = (0, I)$. $\{\eta_n\}_{n \in Z^+}$ is a random variable sequence with independent distribution, and η_1 $N(0, \Gamma)$.

Moreover, a prior set $\left\{z_n^{(j)}\right\}_{j=1}^{J}$ is constructed for finding the true unknown parameter by blending the artificial dynamics model and available observation data. The unknown parameter u can be obtained by:

$$u_n \equiv \frac{1}{J}\sum_{j=1}^{J} u_n^{(j+1)} = \frac{1}{J}\sum_{j=1}^{J} H^{\perp} z_n^{(j)} \tag{7}$$

Where $H^{\perp} : Z \rightarrow X$ is a mapping operator and $H^{\perp} = (I, 0)$.

The solving process of the standard EnKF method has been involved in many studies (Zhang et al., 2015; Zhang and Huang, 2017; Sousa and Gorlé, 2019). Similar to the conventional EnKF method, every iteration of the IEnKF method involves two steps (i.e., the forecast step and the analysis step). The specific solving procedure of the IEnKF method is listed as follows:

(i) Forecast step

$$\hat{z}_{n+1}^{(j)} = \Xi\left(z_n^{(j)}\right) \tag{8}$$

$$\overline{z}_{n+1} = \frac{1}{J}\sum_{j=1}^{J} \hat{z}_{n+1}^{(j)} \tag{9}$$

$$C_{n+1} = \frac{1}{J}\sum_{j=1}^{J} \hat{z}_{n+1}^{(j)}\left(\hat{z}_{n+1}^{(j)}\right)^T - \overline{z}_{n+1}\left(\overline{z}_{n+1}\right)^T \tag{10}$$

Where Eq. (8), Eq. (9), and Eq. (10) are used to calculate the results of model prediction $\hat{z}_{n+1}^{(j)}$, the ensemble means $\overline{z}_{n+1}$, and covariance respectively C_{n+1}.

(ii) Analysis step

$$K_{n+1} = C_{n+1}H^*\left(HC_{n+1}H^* + \Gamma\right)^{-1} \tag{11}$$

$$z_{n+1}^{(j)} = I\hat{z}_{n+1}^{(j)} + \beta K_{n+1}\left(y_{n+1}^{(j)} - H\hat{z}_{n+1}^{(j)}\right) \tag{12}$$

$$y_{n+1}^{(j)} = y + \eta_{n+1}^{(j)} \tag{13}$$

Where Eq. (11), Eq. (12), and Eq. (13) are used to calculate the Kalman gain K_{n+1}, the posterior results $z_{n+1}^{(j)}$, and observation data with a perturbation noise $y_{n+1}^{(j)}$. β is a damping coefficient to alleviate the inbreeding problem, which can be set ranging from 0 to 1.

Finally, the optimal state of the unknown parameters is obtained by the average of state matrix:

$$u_{n+1} \equiv \frac{1}{J}\sum_{j=1}^{J} H^{\perp} z_{n+1}^{(j)} = \frac{1}{J}\sum_{j=1}^{J} u_{n+1}^{(j)} \tag{14}$$

2.3. BI-IEnKF coupling STE model

With the combination of the gas dispersion model and coupling DA method mentioned above, the specific procedure of the BI-IEnKF coupling STE model is shown in Fig. 1. Firstly, the BI module provides a prior ensemble sampled from the initial-guess prior distribution for the gas dispersion model calculation. The results calculated by the gas dispersion model are used to construct the state matrix of the IEnKF module, which consists of gas concentration distribution, leakage location, and leakage rate. When the available observation data is obtained, the state matrix can be revised by the IEnKF model. Finally, the calculated posterior distribution of the source term parameters and revised gas concentration distribution can be utilized for the next iteration or serve as reasonable outcomes according to the predefined/ideal iteration (Sousa and Gorlé, 2019).

3. Model configurations

The developed BI-IEnKF coupling STE model needs to integrate the observation data into the gas dispersion model for the source term estimation and gas concentration prediction. Fig. 2 presents the whole process of the validation and evaluation of the developed BI-IEnKF coupling model. Firstly, the rhoReactingBuoyantFoam solver in the OpenFOAM platform is selected as a good candidate to serve as the observation data generator. This solver has been widely validated in the buoyant gas dispersion scenario, e.g., methane and carbon dioxide (Fiates et al., 2016; Fiates and Savio, 2016; Wu et al., 2021). Meanwhile,

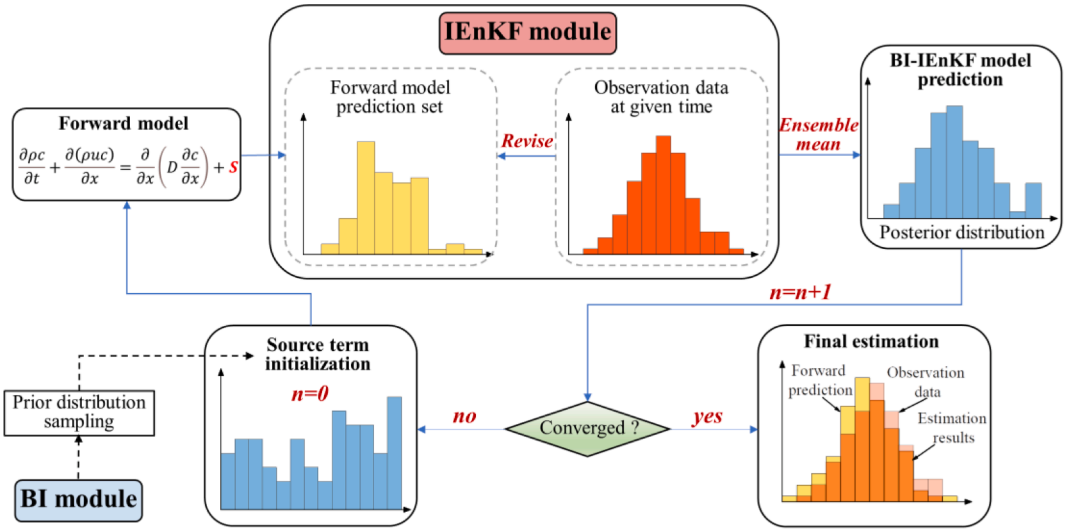

Fig. 1. Schematic of the BI-IEnKF coupling STE model.

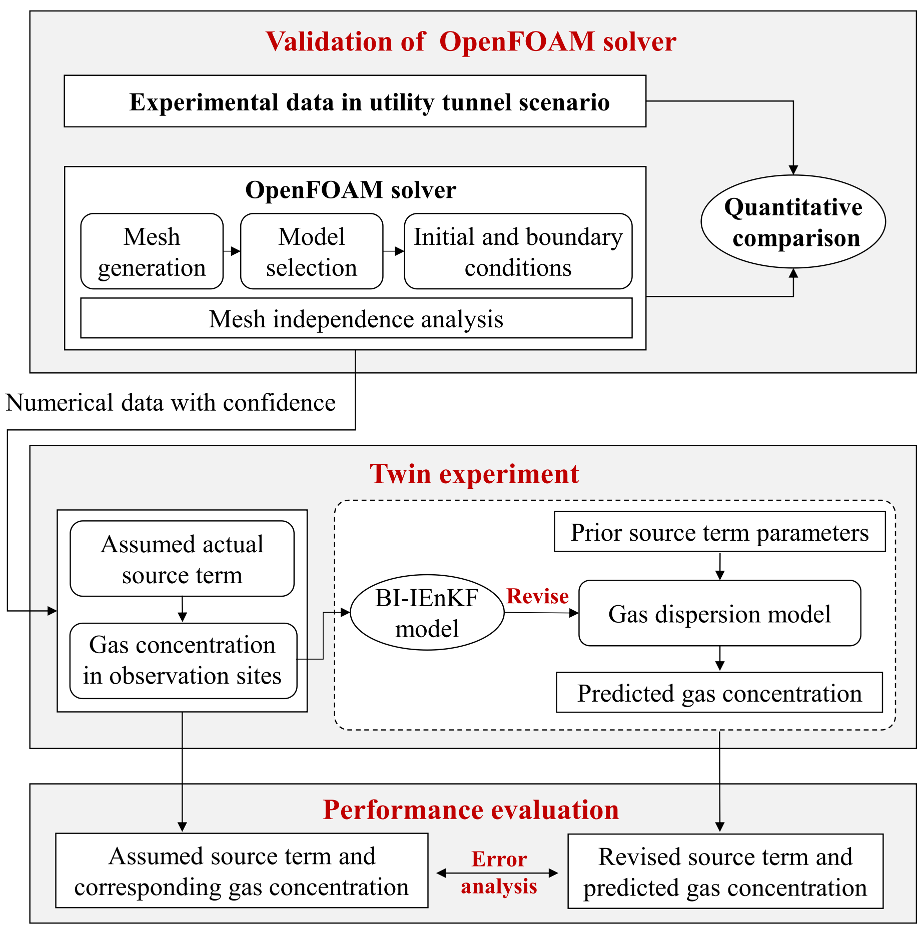

Fig. 2. Validation and evaluation of the developed BI-IEnKF coupling model.

the validation of the rhoReactingBuoyantFoam solver has been achieved in our previous studies, where the experimental data obtained from a gas release scenario in a confined utility tunnel system was used. And a maximum relative error less than 5% could be seen, which indicates a good agreement between simulation results and experimental data (Cai et al., 2022). Therefore, the data generated from the rhoReactingBuoyantFoam solver have its rationality in the validation of the developed BI-IEnKF coupling model by using the twin experiment (Zhang et al., 2014; Yuan et al., 2019; Wu et al., 2020); In the twin experiment, the prior source term parameters, which simulate the uncertainty and deviation from the actual source term parameters in real gas leakage situation, will be initialized into the gas dispersion model. Then, the generated data from the validated rhoReactingBuoyantFoam solver are assumed as actual data. It will be integrated into the gas dispersion model by the BI-IEnKF coupling model to minimize the predictive error derived from the aforementioned uncertainty and deviation; Finally, the performance of the developed BI-IEnKF coupling model can be evaluated by the relative error between assumed actual parameters and predicted parameters by BI-IEnKF coupling model. In the following subsections, the specific configuration parameters of the developed model are presented.

3.1. Configurations of OpenFOAM simulation

The computational domain is created by referring to the requirement of GB50838-2015 *Technical Specification for Urban utility Tunnel Engineering* (CPS, 2015), and it has a dimension of 200 m × 2 m × 2.25 m. The specific layout of the computational domain and corresponding boundary conditions is presented in Fig. 3. Moreover, the detailed parameters used in the simulation are listed in Table 1.

By referring to GB50838-2015 Technical Specification for Urban utility Tunnel Engineering (CPS, 2015), the adopted boundary conditions and the determination of the specific value are shown as follows:

(i) Inlet: the velocity at the ventilation vent is calculated by Eq. (15) (Wang et al., 2020; Zhang et al., 2020):

$$v = \frac{N \times V}{3600 \times F} \tag{15}$$

Where

N is the air change rate,

F is the area of the ventilation vent,

V is the volume of the natural gas compartment.

(ii) Leakage hole: The leakage rate can be obtained through the Eq. (16) (Wang et al., 2020; Zhang et al., 2020):

$$Q_m = CAP_a\sqrt{\frac{kM}{RT}\left(\frac{2}{k+1}\right)^{\frac{k+1}{k-1}}} \tag{16}$$

Where

C is the release coefficient and the value of C range from 0.9 to 0.98,

A is the area of the leakage hole,

P_a is the pressure of the natural gas pipeline and is assumed to be 0.2 Mpa,

k is the isentropic index and equal to 1.29,

M is the molar mass and the value is set as 16 g/mol,

R is the molar gas constant and the value is set as 8.314472 J/(mol·K),

T is the temperature and the value is set as 293 K.

(iii) Outlet: A pressure-outlet boundary condition is utilized at the Outlet and the pressure is set as atmospheric pressure.

(iv) Walls: All the walls involved in the computational domain are set as no-slip conditions.

Besides, the SST turbulence model is chosen to account for the process of turbulent diffusion.

Since the leaked gas can be rapidly mixed within the cross-section of the natural gas compartment. The average gas concentrations within the cross-sections are used as observation data at the observation sites (ten observation sites in this study). Also, a perturbation noise is involved in the observation data to represent the observation errors in the real situation.

Table 1
Configuration parameters of OpenFOAM simulation.

Parameters	Value
Length (m)	200
Wide (m)	2
Height (m)	2.25
Area of ventilation vent (m^2)	1
Velocity of Inlet (m/s)	1.54
Location of leakage hole (m)	(20, 0.75,0.6)
Diameter of leakage hole (mm)	60
Leakage rate (m/s)	100
Diameter of the natural gas pipeline (mm)	300
Total simulation time (s)	145

3.2. Configurations of the BI-IEnKF coupling STE model

The determination of configuration parameters in the BI-IEnKF coupling STE model can affect the performance of assimilation to a certain degree. In this study, the time interval of available observation data is set as 5 s, which means that the observation data will be assimilated into the gas dispersion model every 5 s. The interval of observation sensors is 20 m (i.e., 10 observation sensors in total). The actual leakage rate and location are assumed as 0.5654 m^3/s and 20 m respectively, which serve as the initial condition of OpenFOAM simulation to generate synthetic observation data (Yuan et al., 2019). These configuration parameters were employed for representing an assumed real situation (using initial parameters without uncertainty). Meanwhile, the prior distributions of the leakage location (m) and leakage rate (m^3/s) follow the uniform distribution $U(0,100)$ and $U(0,1)$ respectively. It represents an accidental leakage without information about the actual source term. Therefore, the performance of the BI-IEnKF coupling STE model can be evaluated by the difference between the actual source term parameters and the source term parameters

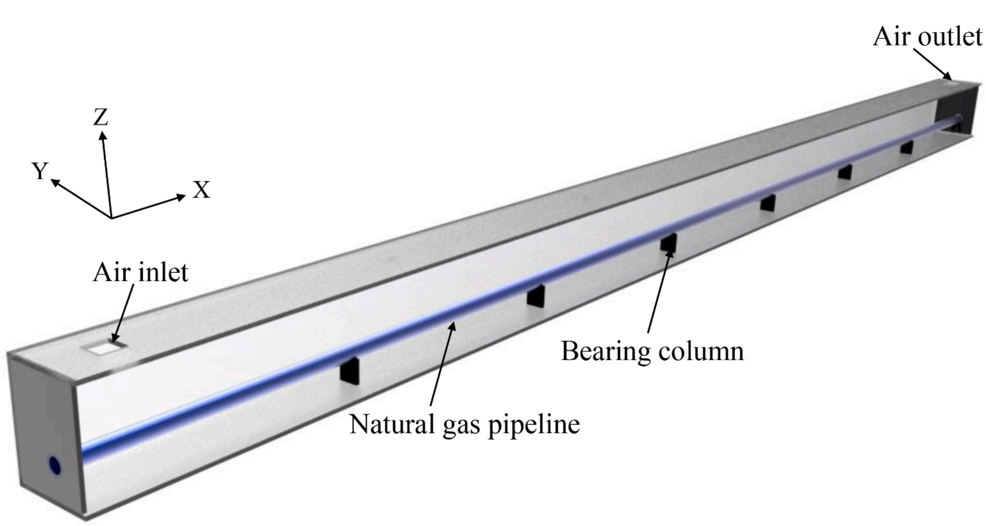

Fig. 3. Computational domain of the natural gas compartment in utility tunnels.

predicted by the developed model, namely, the twin experiment (Zhang et al., 2014; Yuan et al., 2019). The specific configuration parameters related to the developed model are presented in Table 2.

4. Results and discussion

4.1. Evaluation of the BI-IEnKF coupling STE model

As mentioned in Section 3.2, the accuracy of the developed model is evaluated by comparing the model predictions with the actual source term parameters (leakage location and leakage rate). Moreover, the correction effect of the gas concentration distribution under an initial-guess source term is also involved in the model evaluation. Besides, the skill scores are adopted to evaluate the performance of the developed model further (Ma et al., 2018).

The posterior distributions of the source term parameters and the gas concentration distribution revised by the developed model are presented in Fig. 4 and Fig. 5. As shown in Fig. 4, the blue columns are the posterior distributions of the source term and the red lines represent the Gaussian fitting curve of the source term. Meanwhile, the prior probability distributions of the source term are contained in the form of a small chart and the red line denotes the predefined actual value of the source term parameters. It can be seen that the posterior probability peaks of the leakage location and the leakage rate are 20.2125 m and 0.5593 m^3/s respectively. The relative errors between the actual source term (leakage location and leakage rate) and model prediction are 0.9% and 1%, which demonstrates a good agreement with the actual source term. As can be seen from Fig. 5, the gas concentration distributions are closer to the actual gas concentration distribution with the increase of the model iteration number. A reliable result is achieved when the model iteration number is 5 and the average relative error is less than 1%. Therefore, the developed BI-IEnKF coupling STE model can realize the reasonable source term estimation and gas concentration prediction at the same time.

The skill scores are used to evaluate the performance of the developed model quantitatively, and the definition of the related equations are presented below:

$$S_i = \left| \frac{m_{eva,i} - m_{true,i}}{m_{true,i}} \right| \tag{17}$$

$$S_l = \sqrt{\sum_{k=x,y,z} S_k^2} \tag{18}$$

$$S_{ave} = \frac{S_l + S_Q}{2} \tag{19}$$

$$S_{t,ave} = \left| \frac{t_{ave}}{2t_{max}} \right| \tag{20}$$

$$S_{r,ave} = \left| \frac{r_{ave}}{2r_{max}} \right| \tag{21}$$

Where

S_i is the relative error of the source term parameters,

5 i Represents the specific source term parameters (i.e., leakage location S and leakage rate Q),

$m_{eva,i}$ and $m_{true,i}$ are the model predictions and actual value of the source term parameters,

S_l denotes skill score of the location,

S_k is the skill score at a specific coordinate,

$S_{t,ave}$ and $S_{r,ave}$ are skill scores of the computational time and robustness,

t_{ave} and t_{max} are the average computational time of 10 calculations and max computational time,

r_{ave} and r_{max} are the average relative error of 10 calculations and max relative error.

According to the abovementioned equations, the total skill score can be calculated as follows:

$$S_{sum} = S_l + S_{ave} + S_{t,ave} + S_{r,ave} \tag{22}$$

The calculated skill scores are summarized in Table 3. Generally, the lower skill scores (ranging from 0 to 1) represent a greater performance of the developed model (Ma et al., 2013). As shown in Table 3, all the skill scores are at a low level. The score of the leakage location and leakage rate are both 0.009, which indicates that the developed model can achieve a good source term estimation. The score of the computational time and robustness are 0.15 and 0.1 respectively, which demonstrates the low computation cost and high robustness of the developed model.

Table 2
Configuration parameters of the BI-IEnKF coupling STE model.

Parameters	Value
Ensemble size	60
Number of observation sensors	10
Time interval of available observation data (s)	5
Interval of observation sensors (m)	20
Max iteration of the developed model	10
Damping coefficient	0.01

4.2. Sensitivity analysis of model parameters

There are still some uncertainties in the determination of model parameters when coping with a specific scenario. In this section, three contributing factors (i.e., the ensemble sizes, the prior distributions, and the time intervals of available observation data) affecting the performance of the developed model are investigated to analyze the effect of these three factors. It can serve as an effective reference for the performance improvement of the developed model in actual application scenarios in terms of accuracy, efficiency, robustness, and cost-effectiveness.

4.2.1. Effect of the ensemble sizes

As a key factor influencing the performance of the developed model, a reasonable selection of the ensemble size can balance the model's accuracy and efficiency (Wang et al., 2019). In this section, the ensemble sizes of 10, 30, 60, 90, and 120 are compared for the appropriate determination of the ensemble size. The variance of the estimation results for the source term parameters and gas concentration distribution when employing different ensemble sizes are shown in Fig. 6 and Fig. 7. Fig. 6 indicates that there is a gradual fall error of the estimation results with the increase of the ensemble size and the accuracy of both leakage location and leakage rate are improved. When the ensemble size is 60, an accurate estimation result can be obtained. As the stepwise increase of the ensemble sizes from 60 to 120, the increased computational time achieved a slight accuracy improvement, which can also be observed in Fig. 7. Therefore, the ensemble size of 60 can be considered an ideal candidate for both computational accuracy and efficiency.

4.2.2. Effect of the prior distributions

The prior distribution represents the available information about the source term parameters when an unexpected leakage occurs in the natural gas compartment of the utility tunnel. Generally, the prior distribution of the source term can be predefined by empirical determination. Taking a 200 m natural gas compartment as an example, the physical boundary ranges from 0 to 200 m and the range of leakage rate can be determined by the theoretical formula estimation. In this section, two prior distributions largely derived from the actual source term parameters are used to investigate the influence of the prior distribution on the source term estimation. As shown in Table 4, Case 1 and Case 2

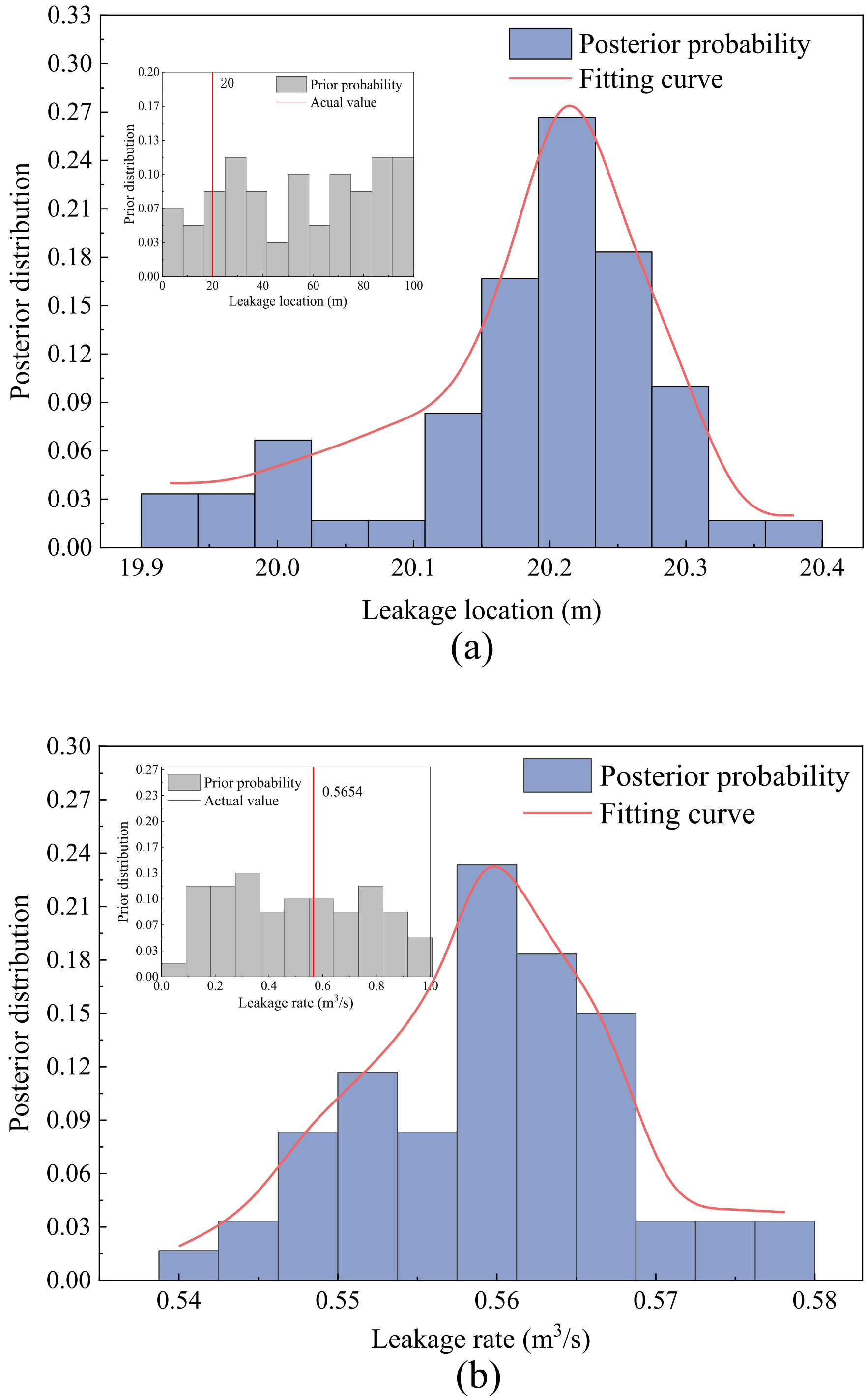

Fig. 4. The posterior distributions of the source term, (a) leakage location, and (b) leakage rate.

represent two rough prior distributions, the average values of the prior distributions of these two cases are much larger and smaller than the actual value respectively. However, the estimation results predicted by the developed model show good agreement with the actual value of the source term parameters, which demonstrates the robustness and practicability of the developed model when handling an uncertain scenario with a rough prior distribution.

4.2.3. Effect of the time intervals of available observation data

Gas sensors accommodated in the natural gas compartment of the utility tunnel can provide continuous data measurement. However, intensive data collection will pose a huge burden for data storage and transmission, which can cause an increased cost. In this section, three different time intervals of available observation data (i.e., 5 s, 10 s, 15 s) are compared for the optimization of the developed model with the consideration of accuracy and cost-effectiveness. Table 5 presents the comparison of the actual value and estimation results with different time intervals. It can be seen that the errors between the actual value and estimation results become smaller with the decrease of the time interval. Besides, the root mean square error is adopted to evaluate the developed model by Eq. (23).

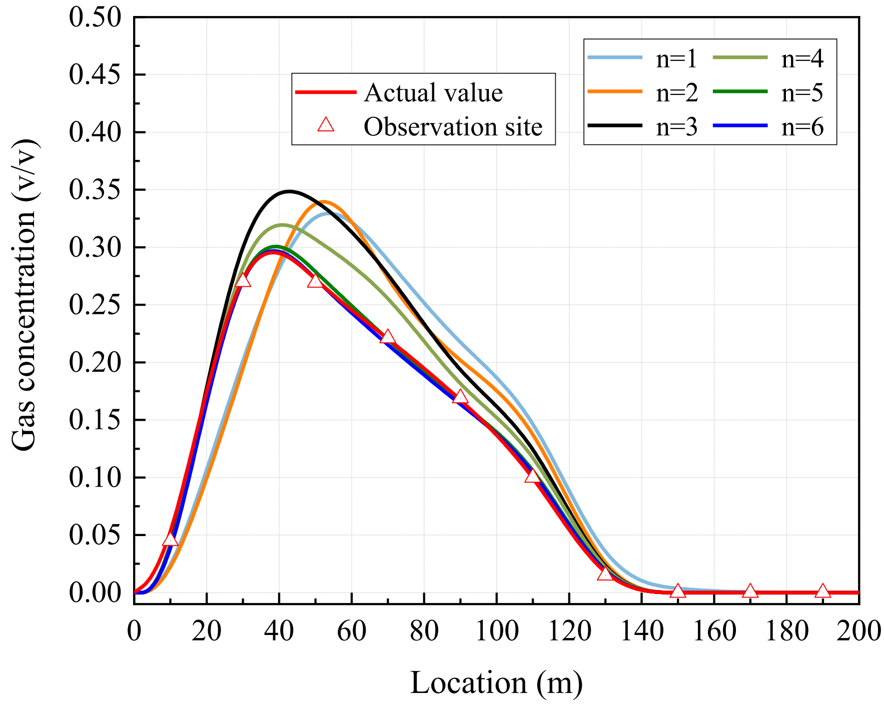

Fig. 5. Gas concentration distributions with different model iteration numbers.

Table 3
Skill scores of the BI-IEnKF coupling STE model.

Performance evaluation parameters		Value
The score of the source term	S_S	0.009
	S_Q	0.009
The score of the location	S_l	0.009
Average score	S_{ave}	0.009
The score of the computational time	$S_{t,ave}$	0.15
The score of the robustness	$S_{r,ave}$	0.1
Total skill score	S_{sum}	0.287

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(X_t - X_s)} \tag{23}$$

Where N is the ensemble size, X_t and X_s are the actual value and estimation results of the source term respectively.

The root mean square error of source term parameters can be reduced to a low level rapidly when employing a small time interval, which can be observed in Fig. 8. This is because the small time interval provides more available observation data and thus accelerates the process of assimilation. Moreover, Fig. 9 shows the estimation results of the gas concentration distribution with different time intervals. When the

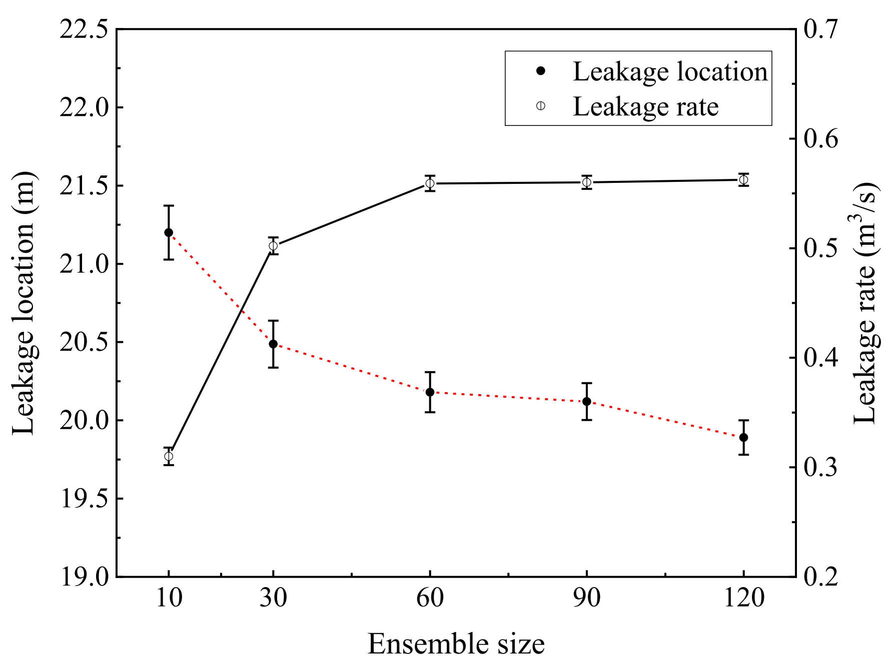

Fig. 6. Results of the source term parameters with different ensemble sizes.

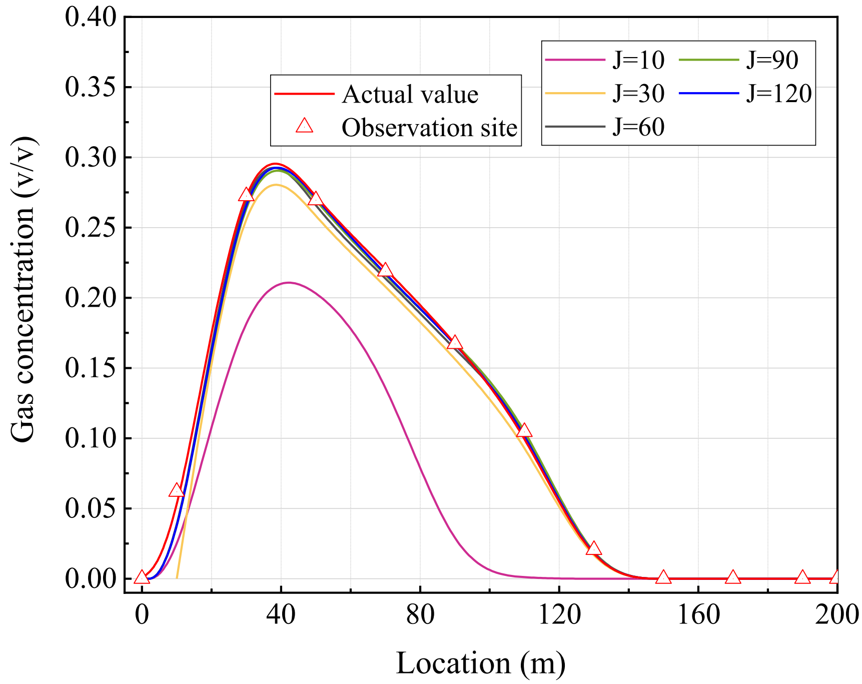

Fig. 7. Results of the gas concentration distribution with different ensemble sizes.

Table 4
Results of the source term parameters with different prior distributions.

	Source term parameters	prior distribution	Actual value	Average of the prior distribution	Estimation results
Case 1	Leakage location (m)	$U(0, 200)$	20	121.8	20.2
	Leakage rate (m^3/s)	$U(0, 10)$	0.5654	5.04	0.5666
Case 2	Leakage location (m)	$U(0, 5)$	20	4.56	20.24
	Leakage rate (m^3/s)	$U(0, 0.1)$	0.5654	0.059	0.5565

Table 5
Results of the source term parameters with different time intervals of available observation data.

Time intervals of observation data	Source term parameters	Actual value	Estimation results	Relative errors
5 s	Leakage location (m)	20	20.18	0.009
	Leakage rate (m^3/s)	0.5654	0.5598	0.009
10 s	Leakage location (m)	20	19.69	0.015
	Leakage rate (m^3/s)	0.5654	0.5457	0.034
15 s	Leakage location (m)	20	20.56	0.028
	Leakage rate (m^3/s)	0.5654	0.5125	0.093

time interval is set as 5 s, the gas concentration distribution can be well predicted. Therefore, the time interval of 5 s can achieve reasonable and satisfactory estimation considering both source term estimation and gas concentration prediction.

4.3. Dynamic sensors analysis

The layout of gas sensors is of significance for the performance of the DA method, which has been investigated and verified in the utility tunnel scenarios (Yuan et al., 2019; Wu et al., 2020). However, due to the long and narrow structure of the gas compartment in utility tunnels, the leaked gas needs a relatively long time to be detected by the majority of sensors. At the initial stage of leakage, this situation usually causes invalid monitoring of some sensors, which are located far from the leakage location. Mobile sensors can adjust the specific layout according to the leaked gas concentration automatically. Therefore, it can provide more leakage-related information compared with conventional gas sensors, which is helpful to achieve a better performance of the developed model and save monitoring equipment investment to a certain extent (Hutchinson et al., 2017). In this section, two basic rules of mobile sensors are assumed: (i) the natural gas compartment is divided into two parts (i.e., search zone 1 and search zone 2), mobile sensors are stationary and start to approach the leakage location when anyone gas sensors are triggered; (ii) The moving speed of the gas sensor is 1 m/s, and the collected data will be provided to the developed model for data assimilation every 5 s. Fig. 10 presents the moving path of mobile sensors in two search zones when an accidental leakage occurs. Moreover, the mobile sensors in each zone will monitor the leaked gas in the corresponding zone periodically. In this study, the total calculation time is set as 145 s and the specific locations of mobile sensors within 40 s are exemplified in Table 6.

Fig. 11 shows the posterior distributions of the source term predicted by using 8 mobile sensors. The estimation results of the leakage location and leakage rate are 19.96 m and 0.5464 m^3/s. And the relative errors between the actual value and the estimation results are 0.7% and 0.65%, which achieve a better prediction compared to the estimation results by using 10 fixed sensors in Section 3.1. This is because the gas sensors installed in the natural gas compartment can be fully utilized by continuous movement and thus provide more available spatiotemporal information. The comparison of estimation results by using the mobile sensor and the fixed sensor is presented in Fig. 12. It can be seen that the estimation result by using the mobile sensor has a good agreement with both actual value and fixed sensor prediction. Therefore, the mobile

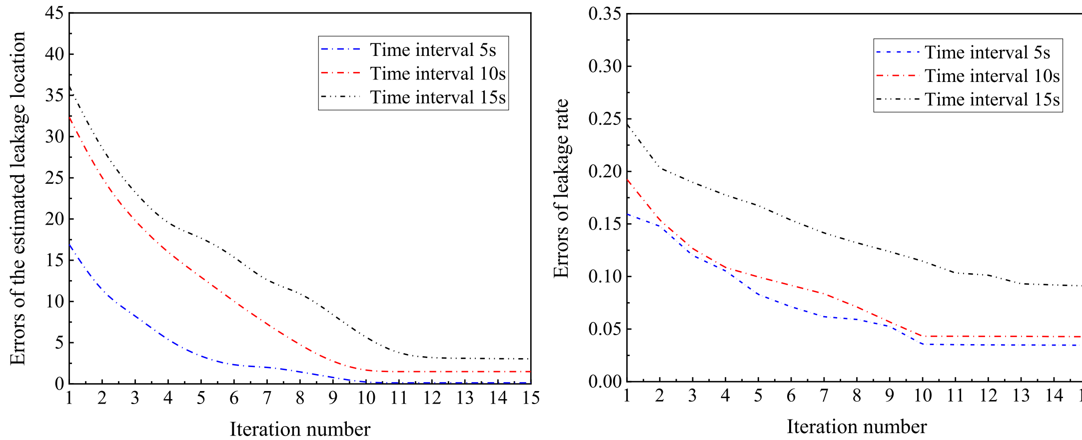

Fig. 8. Root mean square error of source term parameters with different time intervals.

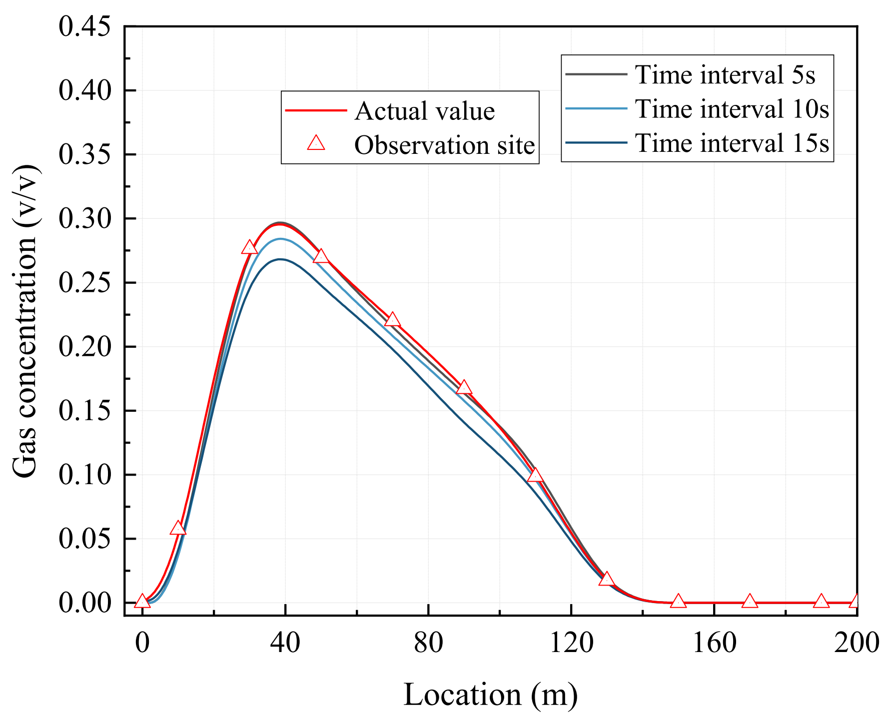

Fig. 9. Results of the gas concentration distribution with different time intervals.

sensor can be used as an alternative tool for the conventional sensor considering the benefits of predictive accuracy, flexibility, and economy.

4.4. Model application and limitations

4.4.1. Application framework

The BI-IEnKF coupling STE model shows great advantages in the aspect of accuracy, efficiency, and robustness, which has been demonstrated above. And the utilization of mobile sensors is also practical and promising. Therefore, a reliable framework for the application of the developed model is proposed in this section. Such a framework can serve as a useful guide to support the deployment of the developed BI-IEnKF coupling STE model in utility tunnels. As a result, it could be helpful to facilitate emergency response treatment in accidental leakage scenarios and provide a reasonable reference for monitoring system design. Finally, this framework is expected to be a basis for an early warning system in utility tunnels.

Fig. 13 presents an application framework of the developed BI-IEnKF coupling STE model in utility tunnels, which consists of four main modules (i.e., sensor layer, model layer, decision layer, and response layer). For the purpose of providing more flexible and effective data acquisition, mobile sensors could be installed in the utility tunnel as a feasible alternative to conventional fixed sensors. As shown in Fig. 13, the adopted mobile sensors system connects gas sensors to the ceiling of the utility tunnel by guide rails, which allows each mobile sensor to have a wide span of movement. Once an accidental leakage accident occurs, the mobile sensor system will be triggered and available data can be assimilated into the BI-IEnKF coupling STE model. Then, the rapid source term estimation and corresponding gas concentration distribution can be achieved automatically. Furthermore, the crucial information conducive to decision-making will be visualized and the sequent emergency response treatment can be implemented more informed. In addition to being beneficial to the data collection of the developed model, the mobile sensor system could reduce the number of used sensors and sensor false alarm rates. It could help to enhance the efficiency,

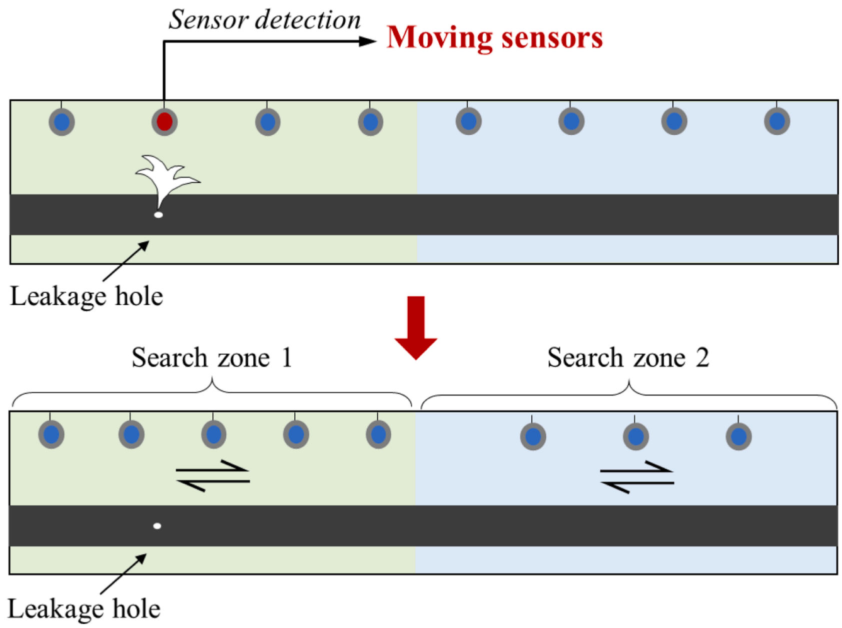

Fig. 10. Moving path schematic of mobile sensors in two search zones.

Table 6
Specific locations of gas sensors within 40 s.

	Sensor index	Time (s) 5	10	15	20	25	30	35	40
Search zone 1	1	5 m	10 m	15 m	20 m	15 m	10 m	5 m	0 m
	2	25 m	30 m	35 m	40 m	35 m	30 m	25 m	20 m
	3	45 m	50 m	55 m	60 m	55 m	50 m	45 m	40 m
	4	65 m	70 m	75 m	80 m	75 m	70 m	65 m	60 m
	5	85 m	90 m	95 m	100 m	95 m	90 m	85 m	80 m
Search zone 2	6	105 m	110 m	115 m	120 m	115 m	110 m	105 m	100 m
	7	135 m	140 m	145 m	150 m	145 m	140 m	135 m	130 m
	8	165 m	170 m	175 m	180 m	175 m	170 m	165 m	160 m

reliability, and maybe cost-benefit of the monitoring system in utility tunnels.

4.4.2. Limitation and outlook

In this study, the one-dimensional gas advection–diffusion equation was employed as the forward model in the BI-IEnKF coupling model. The used forward model can capture the main characteristics associated with the gas leakage and dispersion process in the underground tunnel considering the long and narrow structure. Therefore, it can be integrated with data assimilation methods (i.e., BI-IEnKF coupling algorithm in this study) to achieve the source estimation and gas concentration prediction. When it comes to application in outdoor areas, although the developed framework is applicable, an appropriate forward model able to describe the gas leakage and dispersion process in outdoor areas should be selected first, such as the two/three-dimensional CFD model. Then, the developed BI-IEnKF coupling model can be extended to outdoor area scenarios like chemical parks. However, the integration of a two/three-dimensional CFD model will cause a huge computational burden. The estimation efficiency of the BI-IEnKF coupling model cannot be guaranteed. Therefore, high-performance computing (HPC) and machine learning (ML) techniques have great potential to facilitate the BI-IEnKF model for application in more complex scenarios, which is also expected to be a basis for an early warning system.

Due to the unavailability of sufficient experimental data, we first validated the CFD model (i.e., rhoReactingBuoyantFoam solver in the OpenFOAM platform). Then, the data generated from the rhoReactingBuoyantFoam solver was used to validate the BI-IEnKF coupling model by the twin experiment. In fact, the gas leakage experiment using CH4 can rarely be allowed in the laboratory because of the potential fire and explosion risk. In further, the utility tunnel experiments can be conducted by using alternative safety gases such as CO2 and neon, which can provide more available data for various model validation.

5. Conclusion

In this paper, a BI-IEnKF coupling STE model with the combination of gas dispersion model, Bayesian inference, and iterative ensemble Kalman filter method was developed to achieve the source term estimation (leakage location and leakage rate) and gas concentration prediction when an accidental leakage occurs in utility tunnels. Also, its practical use was explored by sensitivity analysis of model parameters and mobile sensors application. The main conclusions are summarized as follows:

(a) The BI-IEnKF coupling STE model was applied in natural gas leakage scenarios of the utility tunnel and the skill scores were used to evaluate the performance of the developed model. The results show that the deviation between the predefined actual value and model prediction is less than 1% and the developed model has an optimistic performance in accuracy, efficiency, and robustness.

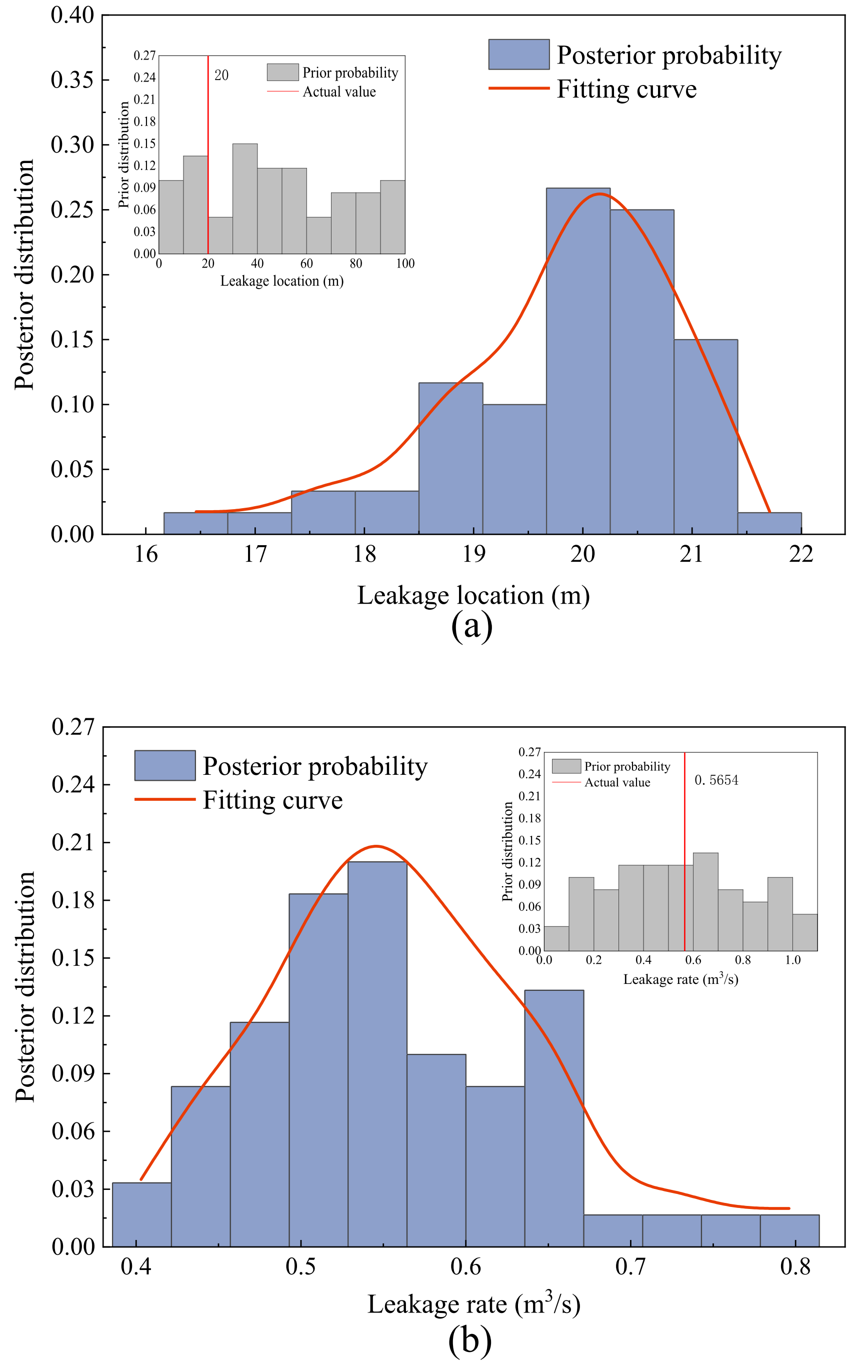

Fig. 11. Posterior distributions of the source term parameters, (a) leakage location, (b) leakage rate.

(b) The sensitivity analysis was conducted in the context of different ensemble sizes, prior distributions of the source term, and time intervals of available observation data. The results show that the developed model has good robustness characterized by not being sensitive to prior distributions. And the appropriate prediction can be obtained when the ensemble size and time interval are set as 60 and 5 s in the specific utility tunnel scenarios. It can provide some reasonable reference for the parameter adjustment of the developed model and its practical use.

(c) The model prediction results obtained by using 8 mobile sensors and 10 fixed sensors were discussed. The results show that comparable results can be realized by using the mobile sensor with a relative error less than 5%, which indicates that the mobile sensor can be used as an alternative monitoring scheme for the conventional sensor considering the benefits of model accuracy and flexibility. Meanwhile, it was found that mobile sensors have a good prospect in utility tunnels. And the corresponding application framework by combing the developed model and mobile sensors in utility tunnels is proposed, which helps to guide the application of the BI-IEnKF coupling STE model.

CRediT authorship contribution statement

Jiansong Wu: Conceptualization, Methodology, Writing – original draft, Resources, Supervision. **Jitao Cai:** Data curation, Writing – original draft. **Zhe Liu:** Software, Visualization. **Shuaiqi Yuan:** Writing – review & editing. **Yiping Bai:** Formal analysis. **Rui Zhou:** Formal

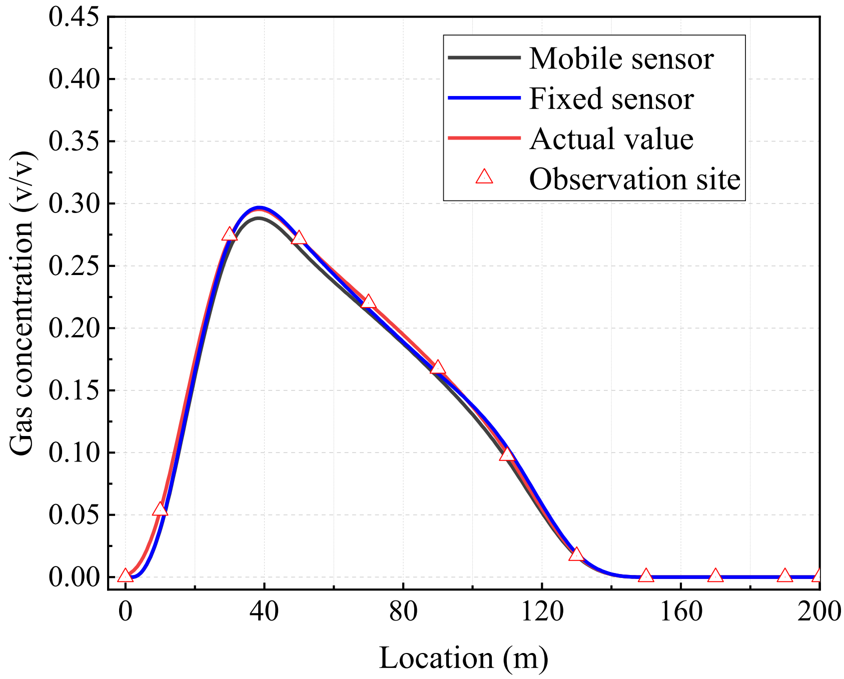

Fig. 12. Results of the gas concentration distribution with different gas sensors.

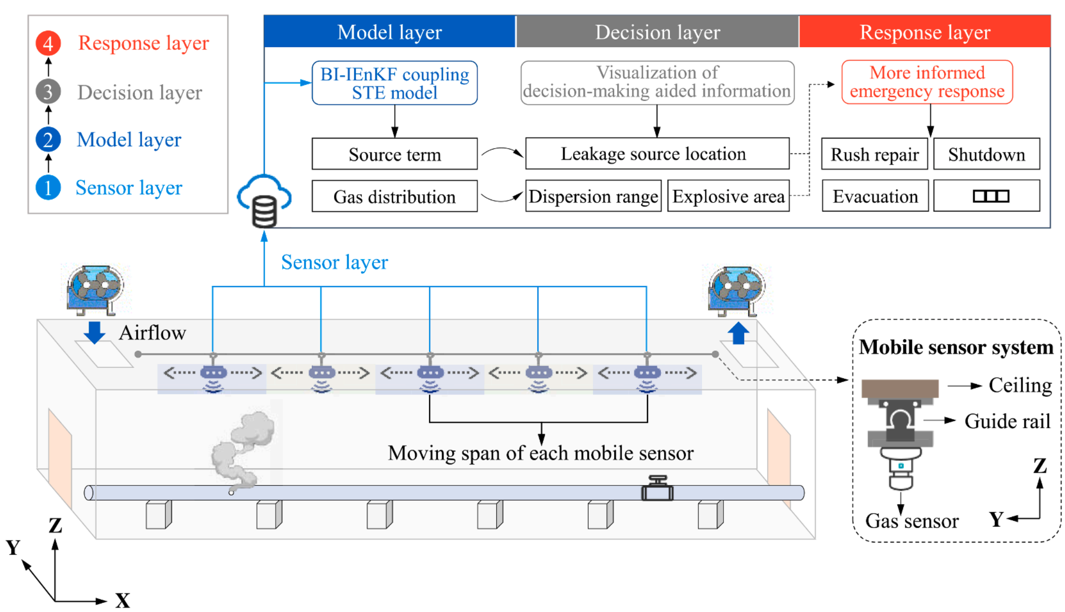

Fig. 13. Application Framework of the BI-IEnKF coupling STE model.

analysis, Writing – review & editing.

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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