Identification of source information for sudden hazardous chemical leakage accidents in surface water on the basis of particle swarm optimisation, differential evolution and Metropolis–Hastings sampling

Haidong Yang (✉ yanghaidong@fzu.edu.cn)
  Fuzhou University School of Economics and Management   https://orcid.org/0000-0002-6734-249X
Jinjin Li
  Fuzhou University School of Economics and Management
Biyu Liu
  Fuzhou University School of Economics and Management
Luying Chen
  Fuzhou University School of Economics and Management

Identification of source information for sudden hazardous chemical leakage accidents in surface water on the basis of particle swarm optimisation, differential evolution and Metropolis–Hastings sampling

Haidong Yang[a, b], Jinjin Li[a], Biyu Liu[a, b*], Luying Chen[a]

(a. *School of Economics and Management*, *Fuzhou University*, *Fuzhou 350116*, *China*;

b. *Department of Business Administration*, *Technology and Social Sciences*, *Luleå University of Technology*, *Luleå*, *97187*, *Sweden*)

Abstract: A quick and accurate identification of source information on sudden hazardous chemical leakage accident is crucial for early accident warning and emergency response. This study firstly regards source identification problem of sudden hazardous chemical leakage accidents as an inverse problem and constructs a source identification model based on the Bayesian framework. Secondly, a new identification method is designed on the basis of particle swarm optimisation (PSO), differential evolution (DE) and the Metropolis–Hastings (M-H) sampling method. Lastly, the designed method, i.e. PSO-DE-MH, is verified by an outdoor experiment analyses in a section of the South–North Water Transfer Project. Results show that the number of iterations, the average absolute error, the average relative error and the average standard deviations of the identification results obtained by PSO-DE-MH are less than those of PSO-DE and DE-MH. Moreover, the relative error and the sampling relative error of the identification results under five different measurement errors (MEs) (σ = 0.01, 0.05, 0.1, 0.15, 0.2) are less than 9.5% and 0.2%, respectively. The designed method is effective even when the standard deviation of the ME increases to 0.2. Therefore, the designed method can effectively and accurately obtain the source information of sudden hazardous chemical leakage accidents. This study provides a new idea and method to solve the difficult problems of emergency management.

Keywords: Emergency identification; Bayesian inference; Particle swarm optimisation; Differential evolutionary; Sudden hazardous chemical leakage accident

1 Introduction

With the implementation of the 'One Belt, One Road' strategy and the acceleration of urban construction, the production, storage, transportation and utilisation of hazardous chemicals in China have also increased (Zhao et al., 2018; Sun et al., 2019). However, the production, storage, transportation and utilisation of hazardous chemicals easily trigger the sudden hazardous chemical leakage accidents (SHCLAs) in surface water (Zhang et al., 2018; Yoo and Choi, 2019). According to the China Ecological Environment Bulletin in 2019, an average of 84 sudden environmental

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pollution accidents every four working days was directly dispatched or disposed by the Ministry of Ecological Environment, including many SHCLAs, such as the leakage of sodium cyanide in Yiyang County, Jiangxi Province and the leakage of cadmium in the Beijiang River, Guangdong Province. Many heavy SHCLAs have occurred in China since 2010. For example, in July 2010, an SHCLA was caused by chemical leakage in the Songhuajiang River, Jilin Province; in June 2011, a phenol leakage accident occurred in Xinanjiang, Zhejiang Province; in January 2012, a cadmium leakage accident occurred in the Longjiang River, Guangxi Province; in January 2013, an aniline leakage accident happened in the ZhuoZhang River, Shanxi Province; in May 2014, a waste lye leakage accident occurred in Jingjiang, Jiangsu Province; in November 2015, water pollution in the Jialing River was caused by tailing leakage in Longnan City, Gansu Province (Wang et al., 2015); in March 2016, a chemical leakage to irrigation sources in Chizhou, Anhui Province and a diesel oil leakage accident in Hanzhong, Shanxi Province occurred; in May 2017, a thallium leakage accident occurred in the Jialing River, Sichuan Province; in August 2018, a waste lye leakage accident happened in Nanyang City, Henan Province; in May 2019, water pollution outbreak occurred in the Beiluo River, Shanxi Province. These accidents have a series of uncertainties, such as leakage time, leakage position, leakage intensity, damage degree and influence range, which usually damage the water ecological environment and threaten human health, even affecting social stability (Yu et al., 2015; Andrle and Badia, 2015; Wang et al., 2019; Lei et al., 2019). Many hazardous chemicals, such as organic matter, heavy metals and bacteria, are difficult to detect with the naked eye before causing harm (Wu et al., 2020). Once an SHCLA occurs, emergency decision-makers only grasp the law of hazardous chemical's migration and diffusion in water at the first time and then issue an accurate warning level and formulate appropriate emergency response measures (Yang et al., 2018; Lei et al., 2019). Amongst them, the historical reconstruction process of SHCLA is the key to reflect the migration and diffusion law of hazardous chemicals in water and track the responsible persons (Liu and Wang, 2020). Therefore, the ability to identify the leakage source information of SHCLA quickly and accurately plays an important role in the process of formulating emergency disposal and rescue measures.

At present, many scholars study the source information identification problem of sudden water pollution accidents (SWPAs) from the perspective of an inverse problem (Yang et al., 2016; Ashyralyev and Emharab, 2018). According to the mathematical characteristics of the existing emergency identification methods, which can be divided into four types, namely, the analytical, regularisation, deterministic and stochastic methods (Yang et al., 2016; Wang et al., 2016; Liu and Wang, 2020).

The analytical method is a method to obtain identification results by using the speed of

hazardous chemical diffusion and the concentration of the source of hazardous chemical leakage (Alapati and Kabala, 2000). For example, Skaggs and Kabala (1995) studied the reconstructed problem of a single point source release process at some observation point by using the quasireversibility method and found that this reconstructed problem can be changed into a well-posed problem. Although this method has high computational efficiency, its accuracy is relatively poor (Wu et al., 2020).

The regularisation method is a classical inverse method that obtains a numerical or analytic solution by converting ill-posed problems into a well-posed problem (Jana and Nair, 2020; Ma et al., 2017). For example, Skaggs and Kabala (1994) explored the release process of a pollutant base on a one-dimensional homogeneous steady flow by using the Tikhonov regularisation method. Wei et al. (2010) designed a new method based on optimal perturbation regularisation to identify the fractional diffusion equation of multipoint SWPAs. Hamdi and Adel (2007) studied the two-dimensional source identification problem of SWPAs by using the classical least square regularisation method. This method is used to solve the emergency identification problem, but it sacrifices the precision of the partial solution.

The deterministic method based on optimisation is a method to obtain the identification results of pollution sources by minimising the differences between simulated and observed values (Guan et al., 2006; Ayvaz and Tamer, 2016; Huang et al., 2018). For example, Parolin et al. (2015) studied the source identification problem of SWPAs using the Luus–Jaakola algorithm, the particle collision algorithm, ant colony optimisation and the golden section method, and the effectiveness of these methods were verified by a case study on the Macae estuary on the southeast coast of Brazil. Zhang and Xin (2017) studied the source identification problem of single- and multipoint source SWPAs on the basis of the genetic algorithm (GA). Jing et al. (2018) studied the source identification problem of SWPAs that occur in rivers by using an improved GA. Sun et al. (2019) studied the emergency identification problem of SWPAs that occur in rivers on the basis of the variable decoupling method and GA. Pan et al. (2020) studied the emergency identification problem of SWPAs that occur in groundwater, including the intensity and the permeability coefficient, by using a simulation–optimisation method. The source identification problem of SWPAs is an ill-posed problem; however, if a small error in observation value or identification model exists, the identification result can be obtained with a larger error by using the deterministic method (Hazart et al., 2014).

Multivariate nonlinear regression and the associated maximum likelihood method are two stochastic methods firstly used to identify the source information of SWPAs, whereas statistical induction, minimum relative entropy and the probability method are the three most commonly

1   used stochastic methods at present (Jing et al., 2020; Wu et al., 2020). Statistical induction can

2   analyse the uncertainty of emergency identification problems, but it needs substantial

3   measurement data. Minimum relative entropy is a method that can analyse the uncertainty of the

4   source identification problem of SWPAs and change the problem into a new problem, which can

5   be solved by a priori distribution. The inverse probability density method based on adjoint

6   equation is one of the most popular stochastic methods based on probability theory. For example,

7   Skiba and Parra-Guevara (2017) considered various factors related with oil spill, and proposed a

8   bioremediation strategy for an oil-polluted marine ecosystem based on adjoint equation approach.

9   Hu et al. (2019) used this method to identify the source identification problem of SWPAs and

10 analysed computational divergence during the process of emergency identification. Ghane et al.

11 (2016) and Jing et al. (2020) studied the inverse problem of the intensity of SHCLAs that occur in

12 rivers by using the inverse probability density method based on an adjoint equation and verified

13 the effectiveness of the method. Emergency identification problems are relatively difficult to

14 identify under high-dimensional unsteady flow, and the stability of the method requires further

15 study. The Bayesian inference method is another stochastic method based on probability theory,

16 and it transforms emergency identification problems into the posterior estimation of unknown

17 parameters on the basis of Bayesian inference and Markov chain Monte Carlo sampling technique

18 (Bayesian-MCMC) (Han et al., 2014; Yang et al., 2016; Yu et al., 2020; Zhang et al., 2020). For

19 example, Jiang et al. (2017) studied the source identification problem of SWPAs that occur in

20 rivers on the basis of Bayesian theory and the tracer experiment. Guo et al. (2016) studied the

21 source identification problem of SWPAs that occur at the South-to-North Water Diversion project

22 by using Bayesian-MCMC. The identification results obtained by Bayesian-MCMC have strong

23 randomness and avoid the decision risk caused by 'optimal' parameter distortion; however, its

24 calculation increase exponentially with the increase in parameters.

25   Considering the urgency of dealing with SWPA, some scholars have designed coupling methods

26 based on the optimisation and stochastic methods (Chen et al., 2007; Wang et al., 2016; Yang et al.,

27 2016; Cao and Yun, 2017; Wu et al., 2020). Two types of coupling methods exist: one is based on

28 different optimisation methods, whereas the other is based on the stochastic method and one

29 optimisation method. For example, Cao and Yun (2017) studied single-point source identification

30 problem and multipoint source identification problem by coupling particle swarm optimisation

31 (PSO) and differential evolution (DE) and verified the accuracy of this designed method through

32 several examples. Wang et al. (2018) analyzed the advantage and disadvantage of fuzzy adaptive

33 Kalman filter and weighted recursive least squares algorithm, developed an inverse analysis

34 method for the real-time monitoring of pollutant diffusion. Yang et al. (2016) studied the

multipoint source identification of SWPA by coupling DE and the Metropolis–Hastings (M-H) sampling method and verified the effectiveness and accuracy of the designed method by conducting outdoor experiments. Wu et al. (2020) explored the identification problem of SWPAs in rivers or lakes and designed a new identification method based on an adaptive Metropolis sampling method and DE and verified the accuracy of this designed method by conducting a case study. Although the first type of coupling method has better searching ability than the deterministic method, it cannot deal with uncertainties during the process of source identification; the other type of coupling method has the same ability to deal with uncertainties as the stochastic method, but its searching ability needs to be strengthened. As typical SWPAs, SHCLAs have general characteristics similar to sudden accidents but also have the characteristics of sprawl, transformation and coupling (Chen et al., 2007; Wang et al., 2016). Therefore, in consideration of resource limitations and the urgency of emergency response, designing a faster and more accurate emergency identification method is necessary.

Based on the above analysis and the characteristics of different methods, this study designs a new identification method on the basis of the M-H sampling method, PSO and DE. In this method, a set of possible solutions is firstly found from the solution space by PSO, and then the most likely solution set, which is close to the true value, is found from a set of possible solutions by DE; the identification results are finally obtained by M-H sampling from the most likely solution set. The new approach not only uses the search ability of PSO and the propagation thought of DE to improve the accuracy and search speed in the posterior space but also uses the sample point update strategy to reduce the uncertainty in the process of emergency identification problem. To verify the effectiveness and accuracy of the new method, this study takes outdoor experiment as a case study and comparatively analyses the identification results by using the new method, PSO-DE and DE-MH. The calculation results show that the new method effectively improves calculation efficiency, thus meeting the needs of emergency management.

This paper is organised as follows: Section 2 describes the source identification problem of SHCLAs and constructs the emergency identification model. Section 3 designs a new coupling method on the basis of the searching ability of DE and PSO under the Bayesian inference framework. Section 4 presents the process and results of a case study. Section 5 provides the conclusions.

2 Problem description and model formulation

The unknown parameters of hazardous chemical leakage sources (e.g. positions, intensity and time) can be identified through observation and prediction values (Jun et al., 2007), where prediction values can be obtained on the basis of the laws of the pollutants' migration and diffusion and the available pollutants' concentration distribution information. Therefore, in this

1   section, the leakage source identification problem of SHCLA is first described, and then the laws

2   of hazardous chemical migration and diffusion in water is discussed, an emergency identification

3   model of SHCLA is finally is established.

4   **2.1 Description of source identification problem**

5   With the rapid development of economy and society, the transportation and utilisation of

6   hazardous chemicals are increasing, thus greatly increasing the occurrence probability of SHCLAs.

7   We take an SHCLA that occurs in a river or a canal as an example; if we consider a section with a

8   length of L and width of B, then the geometric shape of the section does not change much. S

9   represents the leakage source information of hazardous chemicals (e.g. intensity, position and

10   leakage time), as shown in Figure 1. The section has m observation points, and $q_j(t)$ is used to

11   represent the concentration distribution function of water quality index obtained from the jth
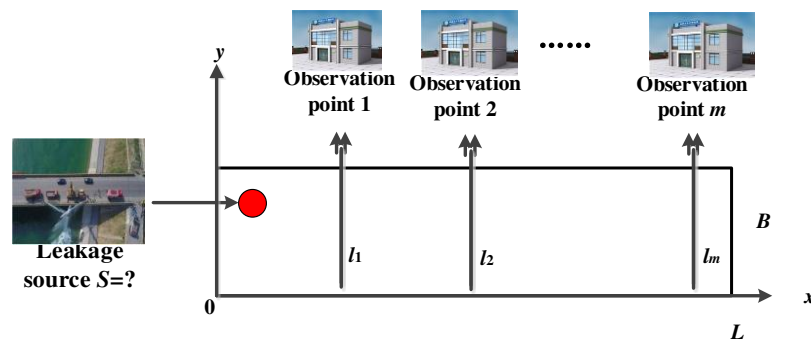
12   observation point at time t.

13
14   **Fig. 1.** Schematic of the emergency identification of SHCLA
15

16   Figure 1 shows that once the observation values from the jth (j=1, 2, ..., m) observation point

17   suddenly appears abnormal, that is, once SHCLA occurs, emergency decision-makers urgently

18   need to identify leakage source information S and then formulate emergency response measures to

19   ensure the safety of water quality downstream. In other words, the source identification problem

20   of SHCLA is how to obtain the source information S by the observation values $q_j(t)$ quickly and

21   accurately.

22   **2.2 Emergency identification model**

23   Two-dimensional convection–diffusion equations are widely used in water quality models and

24   are commonly used to simulate the migration and diffusion of hazardous chemicals in water after

25   SHCLA occurs.

1

$$\begin{cases} \dfrac{\partial C(x,y,t)}{\partial t} + u_x \dfrac{\partial C(x,y,t)}{\partial x} + u_y \dfrac{\partial C(x,y,t)}{\partial y} = \\[2mm] D_x \dfrac{\partial^2 C(x,y,t)}{\partial x^2} + D_y \dfrac{\partial^2 C(x,y,t)}{\partial y^2} - K(t)C(x,y,t) + S \\[2mm] C(x,y,0) = g(x,y), x \in [0,L], y \in [0,B] \\[2mm] C(0,0,t) = 0, \dfrac{\partial C(L,y,t)}{\partial x} = 0, \dfrac{\partial C(x,B,t)}{\partial y} = 0, t \in [0,T] \end{cases} \quad , \quad (1)$$

2 where $C(x, y, t)$ is the concentration of hazardous chemicals in position (x, y) at t moment (g/L); u_x,

3 u_y represent the longitudinal and transverse velocity of water flow (m/s), respectively; D_x, D_y are

4 the longitudinal dispersion and transverse diffusion coefficients (m^2/s), respectively; $K(t)$ is the

5 degradation function of hazardous chemicals.

6 However, the diffusion of hazardous chemicals in the water body is restricted by boundary and

7 reflection due to the constraint of shore and bottom. Assume that the initial conditions are $C=C_0|_{x=0}$

8 and $C=C_0|_{t=\infty}$. If the bilateral reflection on both sides of the water body is considered and the

9 leakage position of SHCLA is taken as the origin point, then the solution of Equation (1) is shown

10 as Equation (2).

11
$$C(x,y,t) = C_1(x,y,t) + C_2(x,y,t) + C_3(x,y,t) + C_h, \quad (2)$$

12
$$C_1(x,y,t) = \frac{M}{4\pi h \sqrt{D_x D_y} t} \exp[-kt - \frac{(x-u_x t)^2}{4D_x t} - \frac{(y-u_y t)^2}{4D_y t}], \quad (3)$$

13
$$C_2(x,y,t) = \sum_{n=1}^{\infty} \frac{M}{4\pi h \sqrt{D_x D_y} t} \exp[-kt - \frac{(x-u_x t)^2}{4D_x t} - \frac{(2nb+y-u_y t)^2}{4D_y t}], \quad (4)$$

14
$$C_3(x,y,t) = \sum_{n=1}^{\infty} \frac{M}{4\pi h \sqrt{D_x D_y} t} \exp[-kt - \frac{(x-u_x t)^2}{4D_x t} - \frac{(2bB-2nb-y-u_y t)^2}{4D_y t}], \quad (5)$$

15 where M is the leakage intensity of hazardous chemicals, g; b is the distance between the leakage

16 point and the shore, m; B and h are respectively the width and average depth of the water body, m;

17 n is the number of reflections across the boundary; x and y are respectively the longitudinal

18 distance and transverse distance from the predicted point to the leakage position, m; $C_1(x, y, t)$ is

19 the concentration increment generated by the leakage source of hazardous chemicals at point (x, y);

20 $C_2(x, y, t)$ is the concentration increment generated by reflection near the shore at the point (x, y);

21 $C_3(x, y, t)$ is the concentration increment generated by reflection from the far shore at the point $(x,$

22 $y)$; C_h is the background concentration of water.

23 SHCLAs have many leakage modes, and one of which is instantaneous nonshore leakage mode

24 (e.g., the leakage accident occurs when a vehicle carrying hazardous chemicals is driving on the

25 bridge due to traffic accidents, machine malfunction or other reasons). If the background

1 concentration of the water body is ignored, then the concentration of hazardous chemicals at the

2 downstream point (x, y) can be expressed as Equation (6).

3
$$C(x,y,t) = \frac{M}{4\pi h\sqrt{D_x D_y}\,t}\exp(-Kt - \frac{(x-u_x t)^2}{4D_x t})[\exp(-\frac{(y-u_y t)^2}{4D_y t}) + \exp(-\frac{(2b+y-u_y t)^2}{4D_y t})] \quad (6)$$

4   If the hazardous chemical leakage mode is an instantaneous shore leakage, then the

5 concentration of the hazardous chemical at the downstream point (x, y) can be expressed as

6 Equation (7).

7
$$C(x,y,t) = \frac{M}{2\pi h\sqrt{D_x D_y}\,t}\exp(-Kt - \frac{(x-u_x t)^2}{4D_x t} - \frac{(y-u_y t)^2}{4D_y t}) \quad (7)$$

8   If an SHCLA has $q(q \geqslant 1)$ leakage sources and $k\,(k \geqslant 1)$ observation points, $d=\{d_1, d_2,\ldots, d_k\}$,

9 $g=\{g_1, g_2,\ldots, g_k\}$ and $h=\{h_1, h_2,\ldots, h_k\}$ respectively denote the set of observation value, prediction

10 and true values of the observation points, then there exist measurement errors (MEs) and

11 prediction errors (PEs). Given the characteristics of symmetry, unimodality, boundedness and

12 offsetting, the ME and PE are usually assumed to obey the normal Gauss distribution (Guo et al.,

13 2009; Kastner et al., 2013). Therefore, the probability density of ME and PE at the ith observation

14 point are respectively expressed as Equation (8).

15
$$\begin{cases} f(d_i \mid h_i, S) \propto \dfrac{1}{(2\pi\sigma_{d,i})^{1/2}}\exp[-\dfrac{(d_i - h_i)^2}{2\sigma_{d,i}^2}] \\ f(h_i \mid g_i, S) \propto \dfrac{1}{(2\pi\sigma_{g,i})^{1/2}}\exp[-\dfrac{(h_i - g_i)^2}{2\sigma_{g,i}^2}] \end{cases} , \quad (8)$$

16   where $\sigma_{d,i}$ and $\sigma_{g,i}$ are respectively the standard deviations of the ME and PE at the ith

17 observation point.

18   Given that $k\,(k \geqslant 1)$ observation points are independent of each other, then the likelihood

19 function can be described as Equation (9) (Carrera and Neuman, 1986a; Aster et al., 2005).

20
$$L(d \mid S) = \prod_{i=1}^{k} f(d_i \mid S) = \prod_{i=1}^{k} \int_{g_i} f(d_i \mid h_i, S) f(h_i \mid g_i, S)\,dg_i$$
$$\propto \frac{1}{(2\pi)^{k/2}\prod_{i=1}^{k}(\sigma_{g,i}^2 + \sigma_{d,i}^2)^{1/2}}\exp[-\sum_{i=1}^{k}\frac{(C_i(x,y,t) - C_i(x,y,t\mid S))^2}{2(\sigma_{g,i}^2 + \sigma_{d,i}^2)}], \quad (9)$$

21 where $C_i(x, y, t) = g_i$, $C_i(x, y, t \mid S) = d_i$, in which d is the observation vector with length k.

22   The maximum likelihood estimator (MLE) is a method that can be used to estimate parameters

23 by using given observation values. Its principle is to find a parameter vector, which maximises the

24 probability of observation values (Zeunert and Günter, 2020). To improve the evaluation and

25 convergence of parameters, the MLE is usually determined by minimising the negative

1   log-likelihood function (MNLL) (Carrera and Neuman, 1986b). Therefore, the emergency

2   identification model of SHCLA should be expressed as Equation (10).

3

$$MNLL = \arg\min_{S}[-2\ln L(d \mid S)] \propto \min \sum_{i=1}^{k} [\ln(\sigma_{f,i}^2 + \sigma_{d,i}^2) + \frac{(C_i(x,y,t) - C_{obs}^i)}{(\sigma_{f,i}^2 + \sigma_{d,i}^2)}] \quad (10)$$

4   If we substitute Equation (6) or Equation (7) into Equation (10), then the source information S

5   can be identified or estimated by using the M-H sampling method. However, some limitations,

6   such as large amount of computations and low sampling efficiency, exist when the M-H sampling

7   method is used to solve the leakage source identification problem of SHCLA. To obtain a more

8   accurate source information of SHCLA, the M-H sampling method needs to adjust the Markov

9   chain to reach the convergence domain through a vast number of calculations, and this

10   requirement reduces the identification efficiency and then affects the emergency effect of SHCLA.

11   A vast number of calculations outside the convergence domain can be avoided if we can improve

12   the efficiency of M-H sampling. Given that DE and PSO have strong global and local searching

13   ability respectively, a new identification method that combines PSO, DE and M-H sampling is

14   designed to identify the source of SHCLA in this study.

15 **3 Emergency identification method**

16   This new identification method is designed by combining PSO, DE and M-H sampling on the

17   basis of Bayesian inference. To explain the proposed identification method, we firstly discuss the

18   procedure of PSO, DE and M-H sampling, then explore the searching mechanism and operation

19   process of the new method, and finally discuss the index to diagnose the convergence of the new

20   method.

21 **3.1 Particle swarm optimisation**

22   PSO, which was proposed in 1995, is an evolutionary algorithm based on the behaviour of birds

23   (Eberhart and Kennedy, 1995a). The basic idea of PSO is to find the optimal solution through the

24   cooperation and information sharing amongst individuals in the population (Eberhart and Kennedy,

25   1995b). In contrast to other evolution algorithms, PSO is easy to implement with few evolution

26   parameters (Gupta et al., 2016; Jain et al., 2018). In PSO, it firstly initialises a group of random

27   particles, where each particle has its position and velocity (Tang et al., 2007; Hou and Jiang, 2017).

28   Then, the optimal solution is found by updating the iteration. In each iteration, the updated

29   velocity of each particle is determined mainly by p_{best} and g_{best}, where p_{best} denotes the best

30   solution found so far by a particle in the position, and g_{best} indicates the best value found so far by

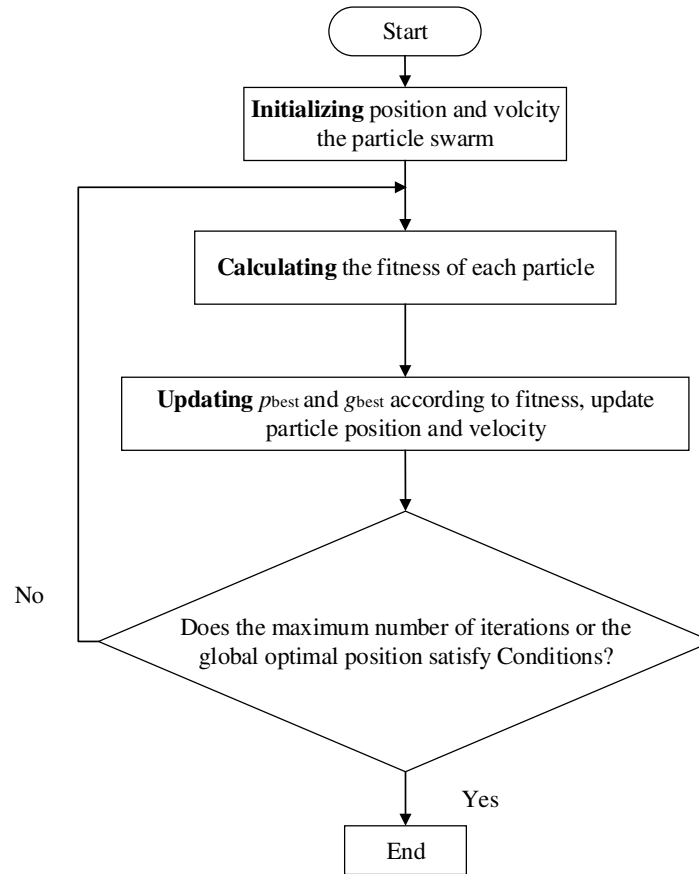31   all the particles in the population. Figure 2 shows the procedure of PSO.

Fig. 2. Procedure of PSO

The convergence speed of PSO is fast and easy to realise and thus has shown its unique advantages in solving and applying various problems. However, it easily stagnates, and the convergence accuracy is low in the process of convergence.

3.2 Differential evolution

DE is a population-based evolutionary algorithm that searches solutions randomly over a continuous space through real vector coding (Storn and Price, 1997). The core idea of DE is to obtain the mutation operator by the difference of the multiple pairs of vectors selected arbitrarily in the population (Ali and Törn, 2004). Figure 3 illustrates the procedure of DE.

DE has fast convergence rate and strong robustness and thus can be used to solve optimisation problems over continuous spaces (Bergey and Ragsdale 2005; Rönkkönen et al. 2005; Qin et al. 2009).
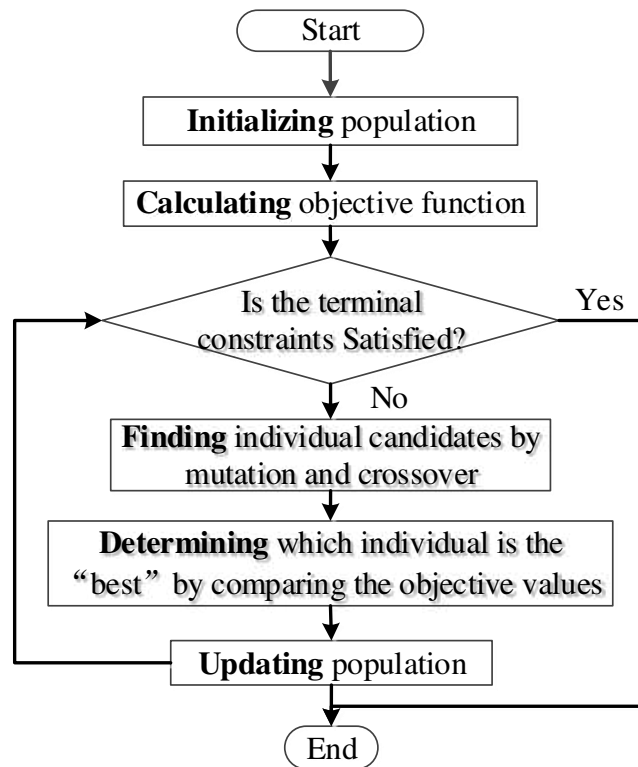
Fig. 3. Procedure of DE

Given the advantage of greedy optimisation, DE has improved optimisation performance, but it greatly reduces the ability of the population to resist the local extremum attraction. As a result, DE is more suitable for accelerating convergence in the later state of the algorithm.

3.3 Metropolis–Hastings sampling method

M-H sampling is a method to estimate unknown parameters by constructing a Markov chain (Raje and Krishnan 2012). To make the method ergodic in solution space, however, new samples are usually generated on the basis of a proposal distribution (Brooks and Roberts, 1998). But the proposal distribution should satisfy the following three conditions: (a) its probability density function is a constant, (b) it can be calculated, and (c) it can generate random numbers. Figure 4 illustrates the procedure of M-H sampling method.
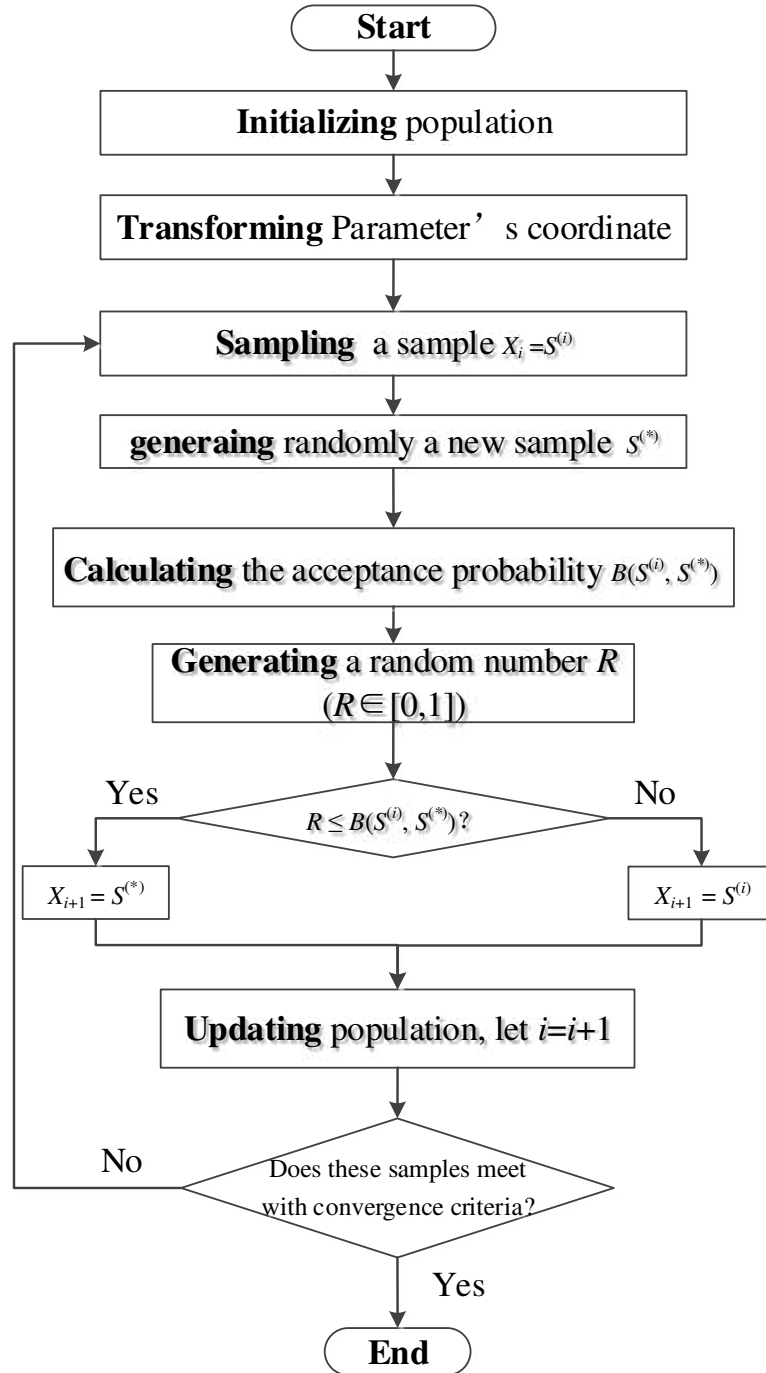
Start

↓

Initializing population

↓

Transforming Parameter's coordinate

↓

Sampling a sample $X_i = S^{(i)}$

↓

generaing randomly a new sample $S^{(*)}$

↓

Calculating the acceptance probability $B(S^{(i)}, S^{(*)})$

↓

Generating a random number R ($R \in [0,1]$)

↓

$R \leq B(S^{(i)}, S^{(*)})$?

Yes → $X_{i+1} = S^{(*)}$

No → $X_{i+1} = S^{(i)}$

↓

Updating population, let $i=i+1$

↓

Does these samples meet with convergence criteria?

No → (back to Sampling)

Yes → **End**

1

2   **Fig. 4.** Procedure of M-H sampling method

3

4   However, the sampling efficiency of M-H sampling is not high because the acceptance rate of

5   the constructed Markov chain during the transfer process may be small; thus, the Markov chain

6   easily stands during the sampling process and refuses to jump large numbers.

7   **3.4 PSO-DE-MH**

8   Numerous uncertainties exist in the source identification problem of SHCLA, leading to the

9   poor efficiency or low accuracy of the identification results obtained by the existing emergency

1   identification methods. Therefore, to improve the efficiency and accuracy of identification results,

2   a new method is proposed in this section by combining PSO, DE with M-H on the basis of

3   different searching mechanisms.

4   For M-H, the calculating efficiency and accuracy of the identification results largely depend on

5   the convergence rate of the Markov chain. However, the convergence rate of the Markov chain is

6   slow because M-H needs to use less unknown parameters for prior information to obtain the exact

7   target region, especially for complex or high-dimensional models.

8   PSO and DE exactly improve the convergence rate of the Markov chain constructed by M-H.

9   For example, the new testing parameters are examined by updating the position and velocity of

10   particles based on the movement rule of PSO, or they are determined by mutation and

11   cross-operation based on the propagation idea of DE. To consider the uncertainties of source

12   identification problem fully and ensure that the parameter space is searched efficiently, we firstly

13   search the possible solutions that are close to true values on the basis of PSO, and then the

14   possible solutions closer to the true values are obtained by an improved mutation formula based on

15   the propagation idea of DE. Therefore, the new testing parameters $X_{pbest}^{(*)}$ are generated in

16   accordance with Equation (11).

17
$$X_{pbest}^{(*)} = X_{i,pbest}(r_1) + E \times (X_{i,pbest}(r_2) - X_{i,pbest}(r_3)) + \varepsilon , \qquad (11)$$

18   where $X_{i,best}$ is the ith generation population consisting of the individual optimal Y_{best} of all

19   particles generated by PSO; r_1, r_2, r_3 are   mutually different integers in the ith generation

20   population; E is a scaling factor of the difference vector and is a positive real number; ε is the

21   given disturbance that reflects the uncertainties existing in the identification problem.

22   In Equation (11), scaling factor E and disturbance ε are the tuning parameters. Scaling factor E

23   has a great influence on identification solutions. A small E value converges prematurely and falls

24   into local optimum, whereas a large E value easily slows down the search speed and skips global

25   optimal solutions (Vitaliy, 2006). In addition, if the value of ε is too large, then it reduces the

26   accuracy of identification solutions (Roberts and Rosenthal, 2004). An interaction exists between

27   E and ε. When we choose a large value of E and ignore ε, the search process becomes random;

28   when the chosen ε is too large, it cannot reflect the influence of E on the sampling method.

29   Therefore, neither E nor ε should be set too large or too small. Regarding the proposed problem in

30   this study, we choose E as a constant value in [0, 2] and set ε to 1%–20% of the range of prior

31   distribution (Storn and Price, 1997; Roberts and Rosenthal, 2004). Moreover, the size of NP

32   affects the searching efficiency. Generally, to maintain the balance between variety of convergence

33   rate and population, the size of NP should be set to [10, 50], where $NP \in [10,35]$ is suitable for

34   low-dimensional problems and $NP \in (35,50]$ for high-dimensional problems (Mohamed and Sabry,

1 2012). Figure 5 shows the process of generating new testing parameters with three dimensions by

2 PSO and DE. $X^{(i)}(j)$ in Figure 5 represents the individuals in the jth population with the ith
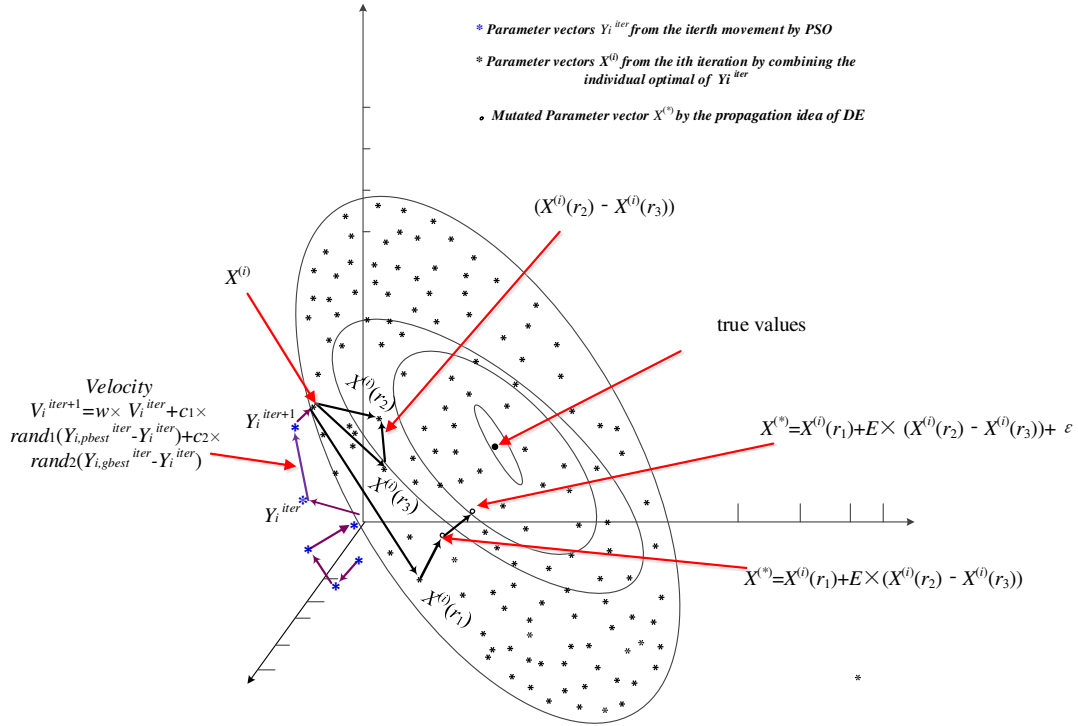
3 iteration, $j \in [1, NP]$.

4

5 **Fig. 5.** Process of generating new testing parameters $X^{(*)}$ with three dimensions by PSO and DE

6

7 PSO-DE-MH is an integrated method based on PSO, DE and M-H. In other words, we firstly

8 find the approximate location of the optimal solution by PSO, and then the optimal solution is

9 found by using the propagation idea of DE and the sampling idea of M-H. To coordinate the global

10 and local search capability, the new method adopts a nonlinear change strategy, including inertial

11 weight, learning factor and scaling factor. The detailed procedure of the new method to solve this

12 considered problem is as follows:

13   (i) Initialising the particle swarm

14   In accordance with the number of variables S, the population size (NP), the maximum number

15 of particle swarm movement $iter_{max}$ and the maximum sampling times I_{max} are determined,

16 initialling velocity V_i^{iter} ($i=1,2,\cdots, I_{max}$; $iter=1, 2, \ldots, iter_{max}$) and position Y_i^{iter} ($i=1,2,\cdots,I_{max}$; $iter=1,$

17 $2, \ldots, iter_{max}$).

18   (ii) Calculating the inertial weight

19   Inertial weight w is a key parameter that affects the performance of the algorithm. To make the

20 particle swarm have good global and local search ability at the initial and later stages of iteration,

respectively, a dynamic inertial weight is adopted, as shown in Equation (12).

$$w_{iter} = w_{\min} - (w_{\max} - w_{\min})(\frac{iter - iter_{\max}}{iter_{\max}})^3, iter \in [1, iter_{\max}] , \qquad (12)$$

where $iter$ is the number of particle swarm movement, w_{max} is the maximum value of inertial weight, w_{min} is the minimum value of inertial weight. Generally, $w_{max} = 0.9$, and $w_{min} = 0.4$.

(iii) Calculating the time-varying learning factor

The learning factors c_1 and c_2 affect the individual optimal and global optimum of each particle, respectively. Venter and Sobieszczanski-Sobieski (2004) donated c_1 as self-confidence and c_2 as swarm-confidence. The smaller learning factor limits the movement of the particle, whereas the larger learning factor causes the particle to be divergent. A time-varying learning factor is adopted in the designed method, as shown in Equation (13).

$$\begin{cases} c_1 = c_{11} - c_{12} \times (\dfrac{2 \cdot iter - iter_{\max}}{iter_{\max}})^3 \\ c_2 = c_{21} - c_{22} \times (\dfrac{2 \cdot iter - iter_{\max}}{iter_{\max}})^3 \end{cases} , \qquad (13)$$

where c_{11}, c_{12}, c_{21} and c_{22} are constants. Generally, $c_{11} = c_{12} = 1.5$, and $c_{21} = c_{22} = 0.5$.

(iv) Calculating and updating the fitness, position and movement speed of the particle swarm

$$\begin{cases} V_i^{iter+1} = w \cdot V_i^{iter} + c_1 \times rand_1(Y_{pbest}^{iter} - Y_i^{iter}) + c_2 \times rand_1(Y_{gbest}^{iter} - Y_i^{iter}) \\ Y_i^{iter+1} = Y_i^{iter} + V_i^{iter+1} \end{cases} , \qquad (14)$$

where $Y_{i,pbest}^{iter}$ is the individual optimum of the particle swarm after $iter$ movement, and $Y_{i,gbest}^{iter}$ is the optimal value of $Y_{i,pbest}^{iter}$.

(v) Repeating steps (ii)–(iv) until $iter = iter_{\max}$ or $Y_{i,gbest}^{iter}$ satisfies the minimum limit

(vi) Combining the individual optimal $Y_{i,pbest}^{iter}$ ($iter = 1, 2, …, iter_{\max}$) to form the ith iteration population $X^{(i)}$ and calculating the concentration of hazardous chemical and conditional probability density of $X^{(i)}$

(vii) Selecting randomly three different particles from a new particle swarm and then performing mutation in accordance with Equation (15) to obtain a new test parameter $X^{(*)}$

$$X^{(*)} = X^{(i)}(r_1) + E \cdot \left(X^{(i)}(r_2) - X^{(i)}(r_3) \right) + \varepsilon , \qquad (15)$$

where E is a scaling factor; r_1, r_2 and r_3 are respective mutually different integers in the ith generation population.

(viii) Obtaining the accept probability $A(X^{(*)}(r_1), X^{(*)})$ at which the Markov chain moves from $p(X^{(*)}(r_1))$ to $p(X^{(*)})$ by Equation (16)

1

$$A(X^{(i)}(r_1), X^{(*)}) = \min\{1, \frac{p(X^{(*)})}{p(X^{(i)}(r_1))}\}$$

(16)

2   (ix) Generating a random number R ($R \in [0,1]$) that follows a uniform distribution

3   If $R < A(X^{(*)}(r_1), X^{(*)})$, then the testing parameters are accepted, and $X^{(i)} = X^{(*)}$;

4   otherwise, $X^{(i)} = X^{(*)}(r_1)$.

5   (x) Repeating steps (i)–(ix) until the predetermined iterations are completed

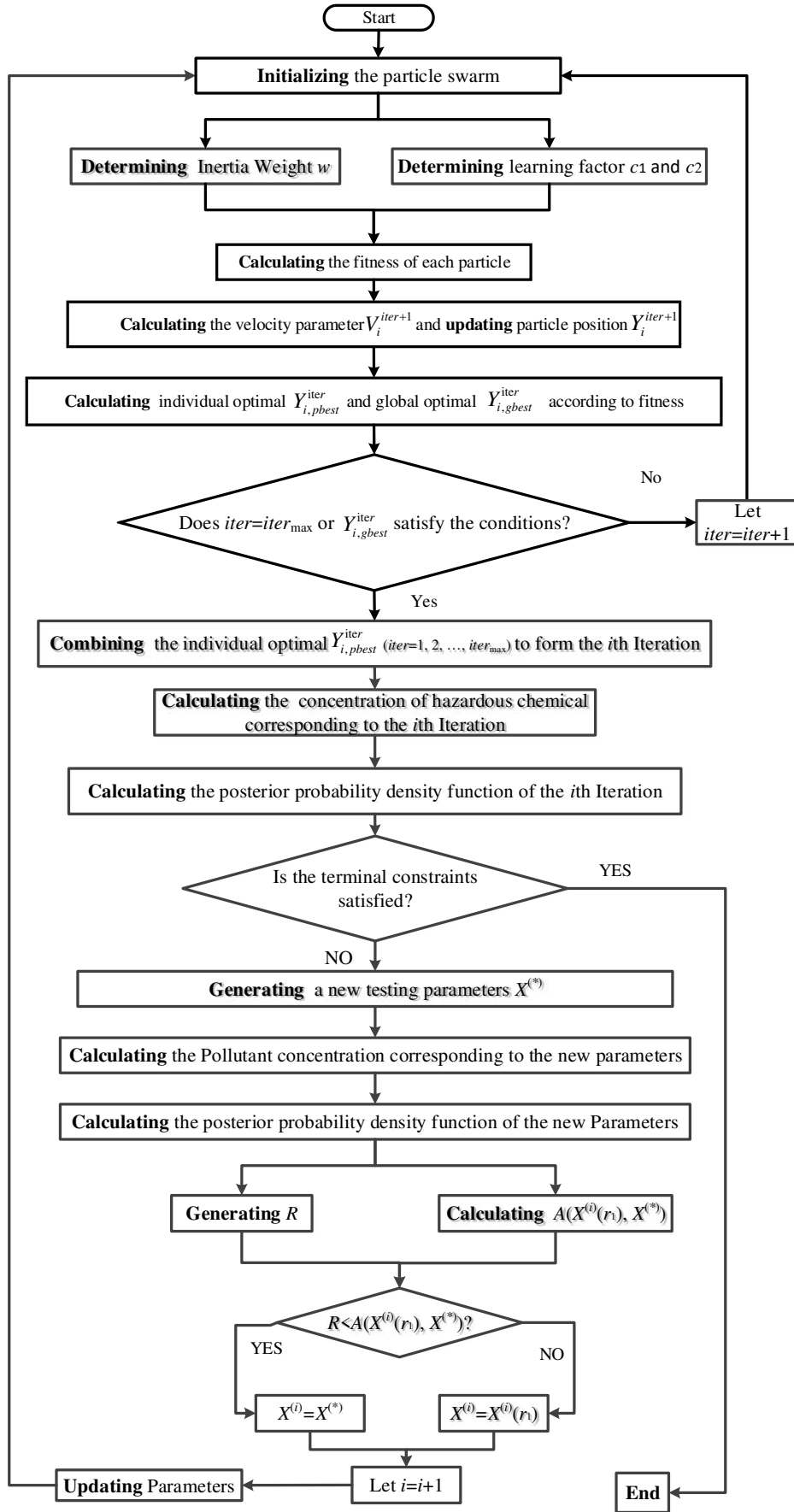6   Figure 6 shows the detailed operation process of PSO-DE-MH.

Start

Initializing the particle swarm

Determining Inertia Weight w **Determining** learning factor c_1 and c_2

Calculating the fitness of each particle

Calculating the velocity parameter V_i^{iter+1} and **updating** particle position Y_i^{iter+1}

Calculating individual optimal $Y_{i,pbest}^{iter}$ and global optimal $Y_{i,gbest}^{iter}$ according to fitness

Does $iter=iter_{max}$ or $Y_{i,gbest}^{iter}$ satisfy the conditions?

No → Let $iter=iter+1$

Yes ↓

Combining the individual optimal $Y_{i,pbest}^{iter}$ ($iter=1, 2, ..., iter_{max}$) to form the ith Iteration

Calculating the concentration of hazardous chemical corresponding to the ith Iteration

Calculating the posterior probability density function of the ith Iteration

Is the terminal constraints satisfied?

YES → End

NO ↓

Generating a new testing parameters $X^{(*)}$

Calculating the Pollutant concentration corresponding to the new parameters

Calculating the posterior probability density function of the new Parameters

Generating R **Calculating** $A(X^{(i)}(r_1), X^{(*)})$

$R<A(X^{(i)}(r_1), X^{(*)})$?

YES → $X^{(i)}=X^{(*)}$ NO → $X^{(i)}=X^{(i)}(r_1)$

Let $i=i+1$

Updating Parameters

End

1

2   **Fig.** 6. Operation process of the PSO-DE-MH method

3.5 Convergence diagnostic method

Scale Reduction Score (SRS) is a method to judge the convergence of an algorithm by calculating a quantitative diagnostic indicator (Gelman and Rubin, 1992). The proceeds of the method as follows:

(i) Initializing the number of sampling sequences k and is the number of iterations within each sequence n

(ii) Calculating the average variances of all the sampling sequences H by Equation (17)

$$H = \frac{n}{(k-1)} \sum_{i=1}^{k} (\sum_{j=1}^{n} x_{ij} - \frac{1}{k} \sum_{i=1}^{k} \sum_{j=1}^{n} x_{ij})^2 , \tag{17}$$

where x_{ij} is the jth sample value of the ith sampling sequence.

(iii) Calculating the average value of the k within-sequence variances W by Equation (18)

$$W = \frac{1}{k} \sum_{i=1}^{k} (\frac{1}{n-1} \sum_{j=1}^{n} (x_{ij} - \frac{1}{n} \sum_{j=1}^{n} x_{ij})^2) \tag{18}$$

(iv) Calculating an index called scale reduction score (SRS) by using Equation (19)

$$\sqrt{SRS} = \sqrt{\frac{n-1}{n} + \frac{k+1}{nk} \frac{H}{W}} \tag{19}$$

(v) If $\sqrt{SRS} \approx 1$, then the generated samples converge to the posterior distribution of the unknown parameters which need to be identified. Otherwise, the generated samples do not converge to the posterior distribution.

4 Results and discussion

4.1 Outdoor experiment analyses

As we all know, China is a country with extremely uneven water resources. In order to balance water resources, China has been building the South–North Water Transfer Project (SNWTP) since 2002, which is divided into East Route Project (ERP), Middle Route Project (MRP) and West Route Project (WRP), as shown in Figure 7(a). The starting point of MRP is the Danjiangkou Reservoir in Hubei Province, its water supply area comprises the Henan province, Hebei province, Beijing city and Tianjin city (Yang, et al., 2020). The total distance of MRP is 1276 km, which including many hydraulic structures, such as over 1300 bridges, 88 diversion sluice gates, 53 exist sluice gates, 26 aqueducts, and so on. Moreover, MRP is constructed in the form of three-dimensional cross arrangement, along which there are 1640 cross buildings, such as river channel crossing, left bank drainage, canal crossing, railway crossing and highway crossing. It is worth noting that, according to the survey of china south-to-North water diversion group, more than 600 pollution sources along the MRP, which can easily prone to the occurrence of SHCLA.

1   To verify the proposed method, we choose 3km canal section as the experimental object, which

2   along the direction of DongyangGe to the bridge of Baiyun in Baoding city, Hebei province, and

3   take DongyangGe sluice gate as observation point D, as shown as Figure 7(b). During the

4   experiment, we use sucrose as tracer, the system and pollutant characteristics shown in Table 1.

5   The first time the studied section was discovered to be polluted is set as 10:00 am, and the

6   measurement is conducted every 10 min thereafter until 2:00 pm. The concentration distribution of

7   hazardous chemicals at observation point D, as shown in Figure 8.

8

9   **Fig.7.**Sketch of the South-North Water Transfer Project (a) and experimental canal section (b)

10

11   **Table 1** Parametrization of the experimental canal section.

Parameter	Description	Value
System- and pollutant-dependent model parameters		
h	Canal depth	3.5m
W	Canal width	40m
D_x	Dispersion coefficient in x-direction	1225 ㎡/min
D_y	Dispersion coefficient in y-direction	36 ㎡/min
u_x	Flow velocity in x-direction	21.6m/min
u_y	Flow velocity in y-direction	0.12m/min
K	Decay rate	1/14400
Hazardous chemical source parameters		
m	Intensity	10^6g/ m³
x_0	x-coordinate of source location	5000m
y_0	y-coordinate of source location	21m
t_0	Leakage time	120min

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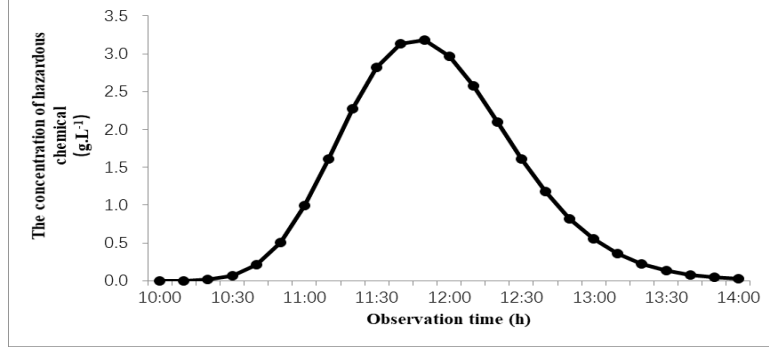
Fig. 8. Sequence values of pollutant concentration at observation point D

Figure 8 shows that the sequence value of pollutant concentration at observation point D are approximately normally distributed, and the highest value is approximately 3.1777 g/m³, occurring at approximately 11:50 am.

**4.2 Analysis of emergency identification results**

In accordance with the characteristics of SHCLA and the prior information of the leakage source, all unknown parameters are uniformly distributed and independent of each other. Then, the posterior probability density function of the unknown parameters can be expressed as Equation (20).

$$\sigma_\alpha(m,x_0,y_0,t_0) = \begin{cases} \lambda \exp\{\sum_{i=1}^{25}[-\dfrac{\left(C_i\left(m,x_0,y_0,t_0\right)-d_i\right)^2}{2(\sigma_{g,i}^2+\sigma_{d,i}^2)}]\} & \begin{matrix} 0.\,4\times10^6 < m < 1.6\times10^6, \\ 0 < x_0 < 10^4, 0 < y_0 < 40, 0 < t_0 < 200 \end{matrix} \\ 0 & else \end{cases} \quad (20)$$

where d_i is the observation value, λ is the proportionality constant, $\sigma_{d,i}$ and $\sigma_{g,i}$ are respectively the standard deviations of ME and PE.

To simplify the calculations, only ME is considered in this section and is assumed to follow a Gaussian distribution with $\sigma_{d,i} = 0.01$. Moreover, we set the parameters E, NP and ε as stated in the rule in Section 3.4. After repeated computation, we set $E = 0.1$, $NP = 10$, $\varepsilon_m = 0.01$, $w_{max} = 0.9$, $w_{min} = 0.4$, $c_{11} = c_{12} = 1.5$, $c_{21} = c_{22} = 0.5$, $iter_{max} = 3000$ and $I_{max} = 10,000$. In accordance with the operation process of PSO-DE-MH, the Frequency distribution and the iterative curve of pollution sources, such as the intensity m, position (x_0, y_0) and leakage time t_0, are illustrated in Figures 9-11, respectively. The comparison of identification results and truth values is shown in Table 2. At the same time, according to Equations (18)–(20), we calculate the scale reduction scores of the unknown parameters with $k = 4$ and $n = 10000$. Calculating result shows $\sqrt{SRS} = 1.033$, that is, the proposed method (i.e. PSO-DE-MH) has convergence.
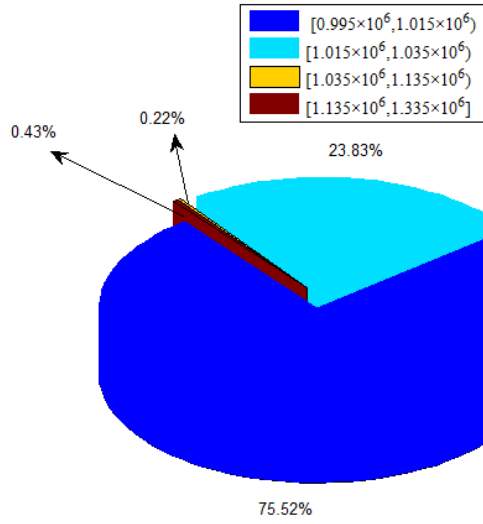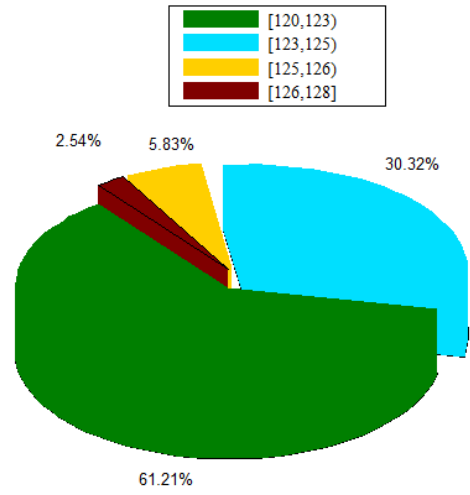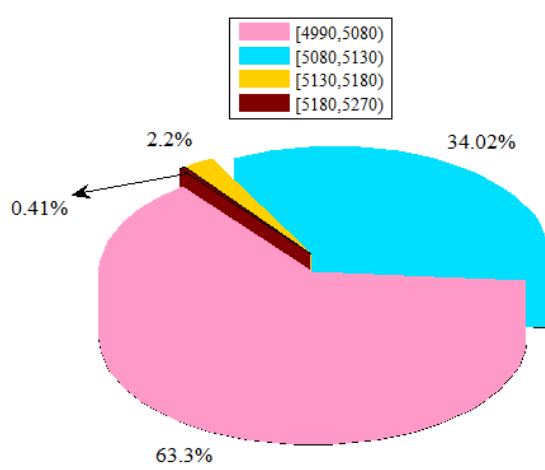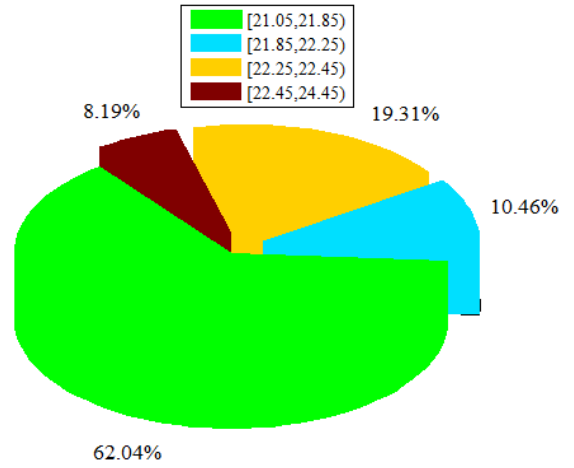
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2   Fig.9. the Frequency distribution of Intensity (a) and Leakage time (b) based on PSO-DE-MH

3

4

5   **Fig.10.** the Frequency distribution of *x*-coordinate of source location (a) and *y*-coordinate of

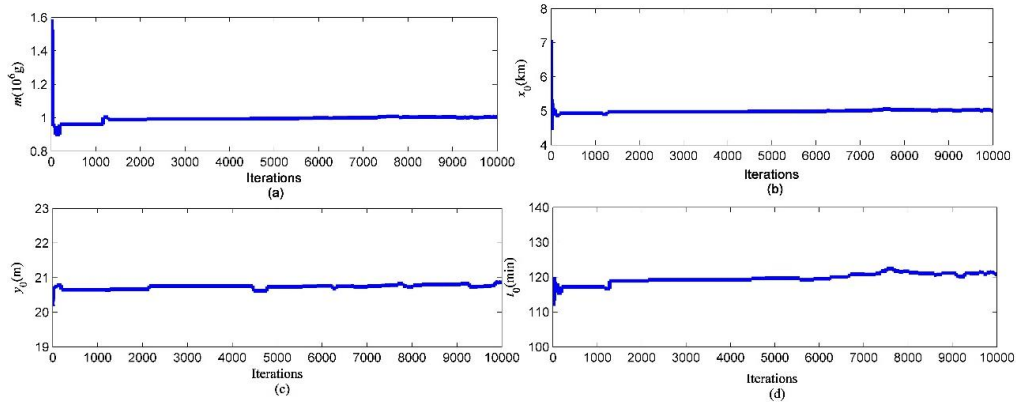6   source location (b) based on PSO-DE-MH

7

8

9   **Fig.11.** Iterative curve of unknown parameters based on PSO-DE-MH

Table 2 Comparison between identification results based on PSO-DE-MH and the true values

Parameters	Intensity m	Position (x_0, y_0)	Leakage time t_0
Identification result	0.994×10^6 g/m³	(4992.8m, 20.7381m)	119.6473min
Absolute error	6×10^3 g/m³	(7.2m, 0.2619m)	0.3527min
Relative error (%)	0.6%	(0.144%, 1.25%)	0.29%
Sampling standard deviation	0.0244	(0.0611,0.0546)	1.3551

As shown in Figure 9(a), the generated samples of source intensity m are almost fall in [0.995$\times$ 10^6, 1.035$\times 10^6$). Among them, 75.52% of the generated samples are fall in [0.995$\times 10^6$, 1.015$\times$ 10^6). Figure 9(b) shows that the generated samples of leakage time t_0 are almost fall in [120,125). Among them, 61.21% of the generated samples are fall in [120, 123). According to Figure 10, the generated samples of Leakage position (x_0, y_0) are almost respectively fall in [4990,5130) and [21.05,22.45). Among them, over 60 percent of generated samples are respectively fall in the [4990, 5080) and [21.05, 21.85). According to Figure 11, the identification results approach the truth values of the parameters after approximately 300 iterations, and the constructed Markov chain has the characteristics of stable and piecewise smooth. As shown in Table 2, if we adopt PSO-DE-MH to solve the identification problem of hazard chemical leakage source, then the relative error and the sampling standard deviation of unknown parameters are less than 1.3% and 1.4, respectively.

Therefore, the identification results with the proposed method are close to the true values, and the generated samples also converge to the posterior distribution.

4.3 Comparative analysis with PSO-DE and DE-MH

To verify the effect of PSO-DE-MH, DE-MH and PSO-DE are used in this study to solve this emergency identification problem of SHCLA simultaneously. The iterative curve of the unknown parameters is shown in Figures 12 and 13, respectively. We perform the following operations for the above three methods: (i) The identification results were analysed after eliminating the unstable results, as shown in Table 3. (ii) The calculation errors of the unknown parameters were extracted at intervals, as shown in Figure 14.
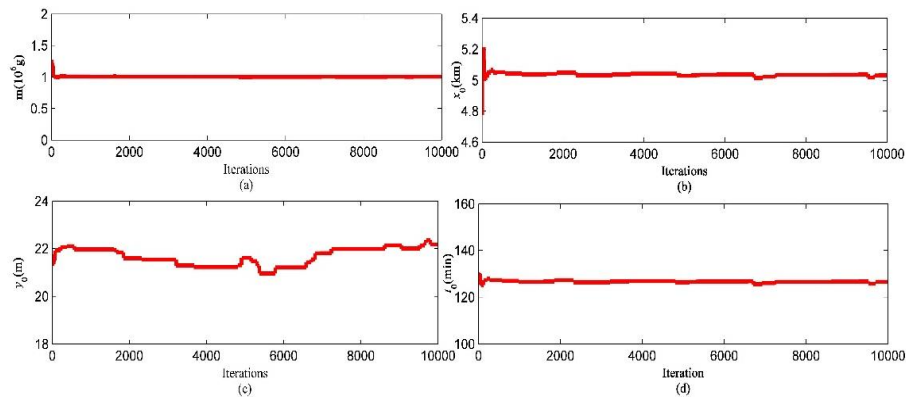

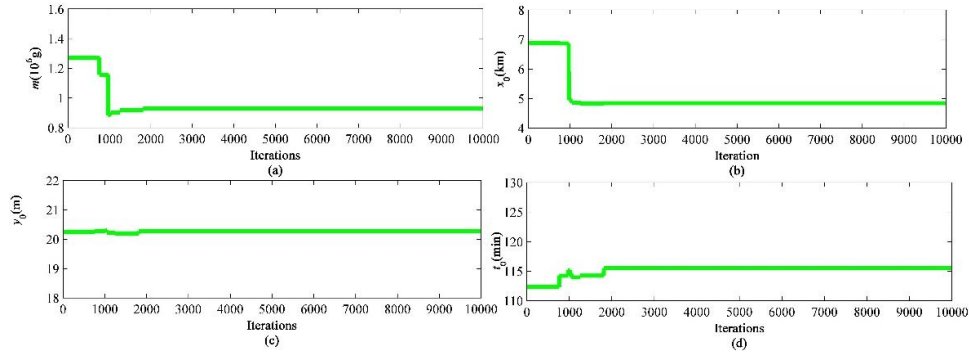**Fig. 12.** Iterative curve of unknown parameters based on DE-MH

Fig. 13. Iterative curve of unknown parameters based on PSO-DE

Table 3 Comparison between the true values and identification results based on PSO-DE and DE-MH

Parameters	Intensity m (g/m³)		Position (x_0,y_0) (m)		Leakage time t_0 (min)	
	PSO-DE	DE-MH	PSO-DE	DE-MH	PSO-DE	DE-MH
Identification result	928900	1010300	(4907.5, 20.39)	(5066.2, 21.75)	113.77	123
Absolute error	71100	10300	(92.5, 0.61)	(66.2, 0.75)	6.23	3
Relative error (%)	7.11	1.03	(1.85, 2.89)	(1.32, 3.59)	5.19	2.5
Sampling standard deviation	0.08	0.02	(0.58, 0.81)	(0.03, 0.48)	1.76	1.45
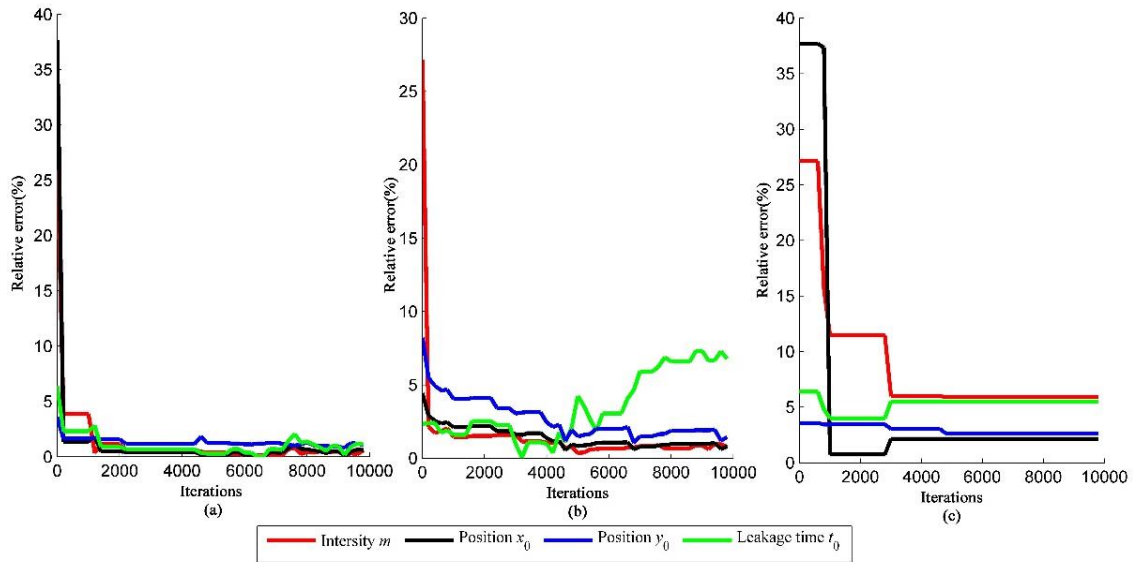
Fig. 14. Relative error analysis of inversion results based on PSO-DE-MH (a), DE-MH (b) and PSO-DE (c)

Table 4 Calculation error comparison amongst PSO-DE-MH, DE-MH and PSO-DE

Error	Intensity m			Position (x_0, y_0)			Leakage time t_0		
	①	②	③	①	②	③	①	②	③
Maximum (%)	27.17	27.17	27.16	(37.7, 3.58)	(4.44, 7.31)	(37.7, 3.58)	6.39	8.22	6.39
Minimum (%)	0.04	0.35	5.93	(0.01, 0.81)	(0.55, 0.05)	(0.74, 2.64)	0.03	1.05	4.00
Mean (%)	1.35	1.58	8.94	(1.28, 1.30)	(1.44, 3.51)	(5.41, 2.97)	1.04	2.72	5.27

2   Note: ①PSO-DE-MH; ②DE-MH; ③PSO-DE

3

4   Figures 11–14 and Tables 2–4 show that compared with DE-MH and PSO-DE, PSO-DE-MH has

5   the following advantages:

6   (i) The identification results quickly stabilise after the start of iteration. The identification results

7   are stable after 300 iterations, which are 200 and 1700 iterations less than that of PSO-DE and

8   DE-MH, respectively.

9   (ii) The maximum probability of sampling is close to the true values. The leakage intensity m,

10   positions (x_0, y_0) and time t_0 of hazardous chemicals are most likely at 0.9×10^6–1.1×10^6 g,

11   4.5–5.5 km, 20.5–21.5 m and 118–122 min.

12   (iii) The identification results have high computational accuracy. The relative error, sample

13   standard deviation and mean error of the unknown parameters are less than 1.3%, 1.4 and 1.5%,

14   respectively. The leakage intensity m is less than 1%, 0.03 and 1.4%; the leakage position x_0 are

15   less than 0.2%, 0.07 and 1.3%; the leakage position y_0 are less than 1.3%, 0.06 and 1.4%; and

16   those of the leakage time are less than 0.3%, 1.4 and 1.1%, respectively.

17   (iv) The sampling obtained by PSO-DE-MH are closest to the true values, followed by DE-MH

18   and PSO-DE. The average relative error, average standard deviation and average mean error of the

19   leakage source information which include intensity, position and leakage time by the proposed

20   method are 0.57%, 0.3738 and 1.24%, respectively, which are less than the results obtained by

21   DE-MH (2.11%, 0.4955, 5.65%) and PSO-DE (3.2%, 0.8059, 2.31%).

22   **4.4 Analysis of ME impact on identification results**

23   For SHCLA, the effectiveness of the identification method largely depends on the constructed

24   likelihood function, which is directly related to the distribution of ME. Therefore, the effects of

25   ME on the identification results must be discussed (Lu et al., 2019). The identification results are

26   obtained with limited sampling; thus, the sampling relative error (SRE) can be used to measure the

27   effects of ME on the identification method (Cao et al., 2015) and can be expressed as Equation

28   (21).

1 $$SRE = \sigma / (V \cdot \sqrt{n_1}) \times 100\% , \qquad (21)$$

2 where σ is the standard deviation of ME, V is the true value, and n_1 is the number of sampling.

3 To analyse the effects of ME on the identification results, we choose five different standard

4 deviations of ME (0.01, 0.05, 0.1, 0.15 and 0.2) to discuss the effects on the identification results.

5 The mean and standard deviation of the leakage intensity m, leakage positions (x_0, y_0) and leakage

6 time t_0 under the five different standard deviations of ME are calculated respectively by

7 PSO-DE-MH, as shown in Table 5. The relative error and SRE with five different standard

8 deviations of ME are also calculated on the basis of the proposed method, as shown as Figure 15

9 and Figure 16.

10 **Table 5** Statistics of pollution sources with five different standard deviations of ME

| Statistics	Mean			Standard deviation		
σ	Intensity m (10^6 g/m³)	Position (x_0, y_0) (m)	Leakage time t_0 (min)	Intensity	Position (x_0, y_0)	Leakage time t_0
0.01	0.994	(4992.8, 20.7381)	119.6473	0.0244	(0.0611, 0.0546)	1.3551
0.05	1.012	(5043.5, 20.5816)	121.2372	0.0278	(0.0899, 0.1344)	3.3088
0.10	1.0218	(5063.1, 20.4840)	122.1162	0.0350	(0.1395, 0.2255)	5.8676
0.15	1.0749	(5084.1, 21.6775)	123.0903	0.0394	(0.1964, 0.5917)	8.3764
0.2	1.0926	(5098.5, 21.9888)	124.5197	0.0499	(0.2956, 0.4181)	13.1481

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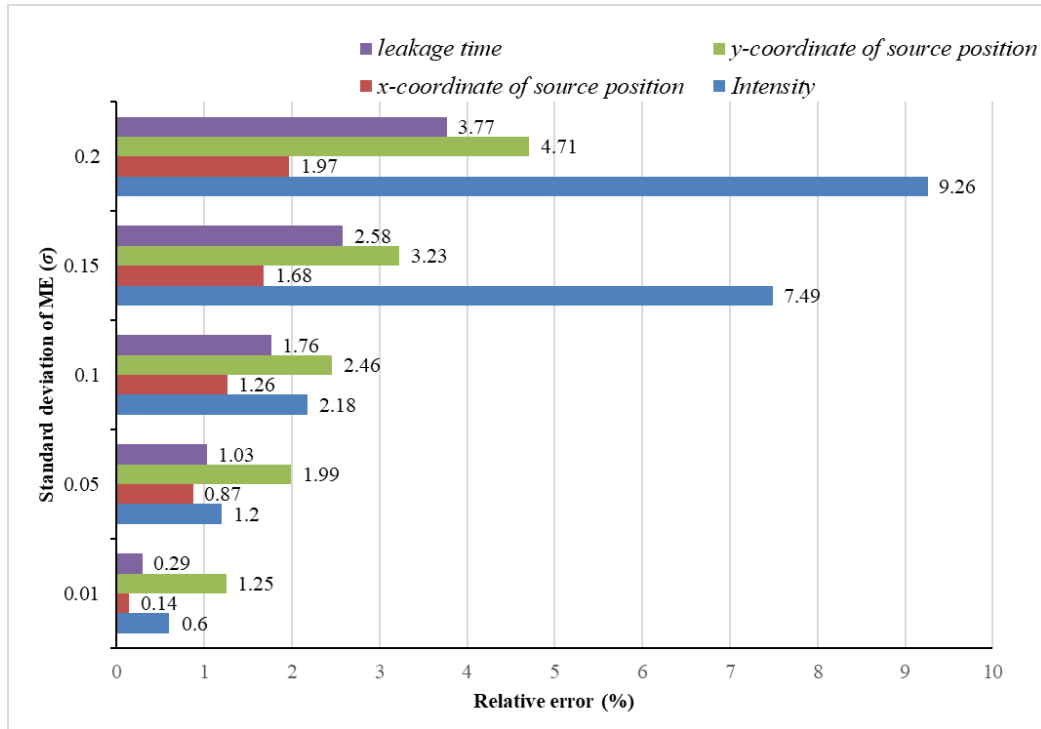
13 **Fig.15.** Variation diagram of the relative errors with different of MEs
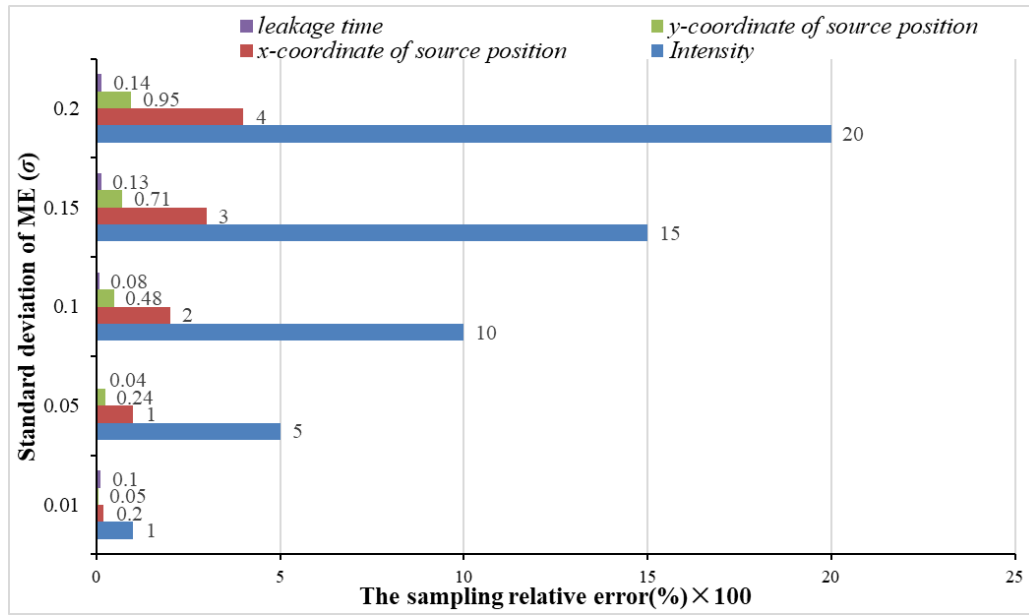
14

Fig.16. Variation diagram of the sampling relative errors with different of MEs

As shown in Table 5, Figure 15 and Figure 16, the standard deviation, relative error and SRE of the identification results with five different standard deviations of ME are less than 14, 10% and 2%, respectively. Figure 15 shows that the relative errors of unknown parameters increase with the standard deviations of ME. When the standard deviation of ME is greater than 0.1, the effects on the leakage intensity m and leakage position x_0 are maximum and minimum, respectively. Moreover, the relative errors of identification results are greater than 1%. The reason is that when $\sigma \geq 0.1$, ME has a significant effect on the information of leakage source through the accept probability of the proposed method. If ME is larger, then the accept probability is close to 1, which leads to the samples being far away from the true values. When $\sigma < 0.1$, the effects on the leakage positions y_0 and x_0 are maximum and minimum, respectively. Moreover, the relative errors of the identification results are less than 2.5%. The reason is that when $\sigma < 0.1$, ME mainly affects the accuracy of the identification results by the proposal distribution interval. If the range of proposal distribution of unknown parameters is small, then the identification results are affected by ME. Figure 16 shows that SRE also increases with the increase of the standard deviation of ME, the increasing speed of SRE is in turn leakage intensity, leakage position and leakage time. Because ME is an important factor affecting the sampling effectiveness of the proposed method by the accept probability.

Although ME is an important factor that affects the accuracy of identification results, PSO-DE-MH remains effective even when the standard deviations of ME increase to 0.2.

5 Conclusion

For SHCLA in the surface water, emergency rescue depends on the accuracy and effectiveness of

the identification of leakage sources. Therefore, it is the premise and foundation to build and design a scientific and reasonable emergency identification model and method to deal with this kind of accidents effectively. In this study, the emergency identification model is built on the basis of laws of pollutants and diffusion and Bayesian inference, and a new method called PSO-DE-MH is designed by integrating the advantages of PSO, DE and MH-MCMC. The proposed method is tested with an outdoor experiment in a section of SNWTP. The results show that the proposed method can effectively improve the calculation efficiency and identify the accuracy of source information for SHCLA. These results can be used for identifying the source information and establishing emergency response measures. The specific conclusions are as follows:

(i) The emergency identification model is proposed from the perspective of the probability statistic and provides a new method with strong search ability that avoids the decision risk caused by 'optimal' parameter distortion. However, there are some shortcoming in the constructed model, such as the failure to accurately capture the characteristics of water quality changes and the failure to fully describe the mechanism of pollutant migration and transformation in water bodies. In any case, these shortcomings do not prevent the application of this model to the identification of various source information. The results show that the proposed method can replace the original model with the identification model based on Bayesian inference in the study of the source identification of SHCLA. The reliability of this method is greatly affected by sample size, structural parameters and other factors.

(ii) In contrast to the M-H sampling method under the Bayesian framework, PSO and DE are used in this study to ensure that the samples can be quickly sampled around the true values. Hence, PSO-DH-MH does not need to have high approximation accuracy in the entire research area and only needs to have high accuracy in important areas, especially near the true values. This approach not only reduces the calculation cost but also improves the accuracy of inversion.

(iii) New samples generated by the proposed method can improve the accuracy of the identification model. During this process, the ranges of variables to be identified are controlled by the proposal distribution, and the search space of the identification problem solution is gradually reduced by the search ability of PSO and the propagation thought of DE, thus decreasing the selecting cost of new samples and improving convergence.

(iv) One great advantage of PSO-DE-MH is its low computational cost. This study shows that the identification results obtained by the proposed method quickly stabilise after the start of iteration. The more accurate the prior information of the leakage source is, the higher the effectiveness of the sampling by PSO-DE-MH is.

(v) Another great advantage of PSO-DE-MH is high accuracy. The uncertainty of information of

leakage sources increases with the increase in ME. This study shows that the average relative error and the average mean error of the leakage source information by PSO-DE-MH are 0.57% and 1.24% when the standard deviation ME is 1%. Even if the standard deviation of ME is increased to 20%, PSO-DE-MH can still accurately identify the leakage source's information.

In conclusion, compared with the existing models and methods, the proposed identification model and method have better noise immunity and thus can be used to solve the leakage source identification problem of SHCLAs. Considering the increasing complexity of water environments and the diversity of observation data, how to construct a more practical emergency identification model based on complex hydrodynamic water quality models and diversity data must be the focus of further research.

Ethics approval and consent to participate

Not applicable

Consent for Publication

Not applicable

Availability of data and material

All data generated or analysed during this study are included in this article.

Competing Interests

The authors declare that they have no competing interests.

Authors Contributions

All authors contributed to the study conception and design. Material preparation was performed by Haidong Yang and Biyu Liu. Data collection and analysis were performed by Jinjin Li and Luying Chen. Software design and test were performed by Haidong Yang and Jinjin Li. The first draft of the manuscript was written by Haidong Yang and all authors commented on previous versions of the manuscript. All authors read and approved the final manuscript.

Reference

Aster RC, Borchers B, Thurber C (2005) Parameter Estimation and Inverse Problems (International Geophysics). *Academic Press*. ISBN 0120656043. URL http:/www.ees.nmt.edu/outside/courses/GEOP529_book. html

Alapati S, Kabala ZJ (2000) Recovering the release history of a groundwater contaminant using a non-linear least-squares method. *Hydrological Processes*, 14(6), 1003 – 1016. http:/doi.org/10.1002/(SICI)1099-1085(20000430)14:6<1003::AID-HYP981>3.0.CO;2-W

Ali MM, Törn A (2004) Population set-based global optimization algorithms: some modifications and numerical studies. *Computers & Operations Research,* 31(10), 1703-1725. http:/doi.org/10.1016/S0305-0548(03)00116-3

Andrle M, EI Badia A (2015) On an inverse source problem for the heat equation application to a pollution detection problem, ii. *Inverse Problems in Science & Engineering*, 23(3), 389-412. http:/doi.org/10.1515/jiip.2002.10.6.585

Ashyralyev A, Emharab F (2018) Source identification problems for hyperbolic differential and difference equations. *Journal of Inverse and Ill-Posed Problems,* 27(3), 301-315. http:/doi.org/10.1515/jiip-2018-0020

Ayvaz, Tamer M (2016) A hybrid simulation–optimization approach for solving the areal groundwater pollution source identification problems. *Journal of Hydrology,* 538, 161-176. http:/doi.org/10.1016/j.jhydrol.2016.04.008

Bergey PK, Ragsdale C (2005) Modified differential evolution: a greedy random strategy for genetic recombination. *Omega*, 33(3), 255–265. http:/doi.org/10.1016/j.omega.2004.04.009

Brooks SP, Roberts GO (1998) Assessing convergence of Markov chain Monte Carlo algorithms. *Statistic & Computing*, 8(4), 319–335. http:/doi.org/10.1103/PhysRevE.72.016715

Cao HG, Yun WG (2017) Research of the abrupt waters pollution source based on optimization algorithm of PSO-DE. *China Environmental Science*, 37(10), 3807-3812.

Cao R, José A, Vilar, JM, et al (2015) Sampling Error Estimation in Stratified Surveys. *Open Journal of Statistics*, 3(3), 200-212. http:/doi.org/10.4236/ojs.2013.33023

Carrera J, Neuman SP (1986) Estimation of aquifer parameters under transient and steady state conditions: 1. maximum likelihood method incorporating prior information. *Water Resources Research,* 22(2), 199-210. http:/doi.org/10.1029/WR022i002p00199

Carrera J, Neuman SP (1986) Estimation of aquifer parameters under transient and steady state conditions: 2. uniqueness, stability, and solution algorithms. *Water Resources Research,* 22(2), 211-227. http:/doi.org/10.1029/WR022i002p00211

Chen LP, Jiang JC, Yin L (2007) Numerical simulation water pollution diffusions for sudden hazardous chemical. *Journal of Hydrodynamics (Ser. A),* 22(6), 761-765. http:/doi.org/10.1007/s10483-007-0101-x

Datta B, Chakrabarty D, Dhar A (2011) Identification of unknown groundwater pollution sources using classical optimization with linked simulation. *Journal of Hydro-environment Research*, 5(1), 25–36. http:/doi.org/10.1016/j.jher.2010.08.004

Eberhart RC, Kennedy J (1995a) A new optimizer using particle swarm theory. *Proceedings of the Sixth International Symposium on Micro Machine and Human Science*, *IEEE*, 39-43.

Eberhart RC, Kennedy J (1995b) Particle swarm optimization. *Proceedings of the IEEE conference on Neural Network*, *IEEE*, 1942-1948.

Gelman A, Rubin DB (1992) Inference from iterative simulation using multiple sequences. *Statistical Science*, 7(4), 457–472. http:/doi.org/10.2307/2246093

Ghane A, Mazaheri M, Jamal MVS (2016) Location and release time identification of pollution point source in river networks based on the Backward Probability Method. *Journal of Environmental Management*, 180, 164-171．http:/doi.org/10.1016/j.jenvman.2016.05.015

Guan J, Aral M, Maslia M, Grayman W (2006) Identification of contaminant sources in water distribution systems using simulation-optimization method: case study. *Journal of Water Resources Planning & Management,* 132(4), 252-262. http:/doi.org/10.1061/(ASCE)0733-9496(2006)132:4(252)

Guo S, Yang R, Weng W (2009) Source inversion of toxic gas dispersion in urban areas based on the MCMC method. *Journal of Tsinghua University* (*natural science edition*), 49(5), 629–634.

Guo ZW, Zhang C, Li, Y, et a1 (2016) Source identification of sudden contamination based on the parameter uncertainty analysis. *Journal of Hydro Informatics*, 18(6), 919-927．http:/doi.org/10.2166/hydro.2016.002

Gupta S, Singh RK, Sharan SN (2016) An approach to implement PSO to optimize outage probability of coded cooperative communication with multiple relays. *Alexandria Engineering Journal*, 55(3), 2805-2810. http:/doi.org/10.1016/j.aej.2016.07.018

Hamdi, Adel (2007) Identification of point sources in two-dimensional advection-diffusion-reaction equation: application to pollution sources in a river stationary case. *Inverse Problems in Science & Engineering,* 15(8), 855-870. http:/doi.org/10.1080/17415970601162198

Han JC, Huang GH, Zhang H, Li Z, Li YP (2014) Bayesian uncertainty analysis in hydrological modeling associated with watershed subdivision level: a case study of slurp model applied to the xiangxi river watershed, China. *Stochastic Environmental Research and Risk Assessment, 28*(4), 973-989. http:/doi.org/10.1007/s00477-013-0792-0

Hazart A, Giovannelli JF, Dubost S, Chatellier L (2014) Inverse transport problem of estimating point-like source using a Bayesian parametric method with MCMC. *Signal Processing*, 96, 346-361．http:/doi.org/10.1016/j.sigpro.2013.08.013

Hou J, Jiang B (2017) Predictions and estimations under a group of linear models with random coefficients. *Communication in Statistics- Simulation and Computation,* 47(1-2), 510-525. http:/doi.org/10.1080/03610918.2017.1283704

Hu Y, Zhang WJ, Ren HT, et a1 (2019) Adjoint method for source term inversion in reverse process of pollutant convection diffusion．*Advances in Science and Technology of Water Resources*，39(2), 7-11.

Huang LX, Wang LC, Zhang YY, Xing LT, Hao QC, Xiao Y, Zhu HH (2018) Identification of groundwater pollution sources by a SCE-UA algorithm-based simulation/optimization model. *Water,* 10(2), 193. http:/doi.org/doi: 10.3390/w10020193.

Jain NK, Nangia U, Jain J (2018) A Review of Particle Swarm Optimization. *Journal of the Institution of Engineers*, 99(4), 1-5. http:/doi.org/10.1007/s40031-018-0323-y

Jiang JP, Dong FJ, Liu RT (2017) Applicability of Bayesian inference approach for pollution source identification of river chemical spills: a tracer experiment based analysis of algorithmic parameters, impacts and comparison with Frequentist approaches. *China Environmental Science*, 37(10), 3813-3825.

Jing L, Kong J, Wang Q, Yao Y (2018) An improved contaminant source identification method for sudden water pollution accident in coaster estuaries. *Journal of Coastal Research,* 85, 946-950. http:/doi.org/10.2112/SI85-190.1

Jing P, Yang Z, Zhou W, Huai W, Lu X (2020) Inverse estimation of finite-duration source release mass in river pollution accidents based on adjoint equation method. *Environmental science and Pollution Research,* 27(13), 14679-14689. http:/doi.org/10.1007/s11356-020-07841-1

Jana A, Nair MT (2020) A truncated spectral regularization method for a source identification problem. *Journal of Analysis*, 28, 279-293. http:/doi.org/10.1007/s41478-018-0080-y

Jun K, Kang J, Lee K (2007) Simultaneous estimation of model parameters and diffuse pollution sources for river

water quality modeling. *Water Science and Technology*, 56(1), 155–162. http:/doi.org/10.2166/wst.2007.447

Kastner CA, Braumann A, Man PLW, Mosbach S, Brownbridge GPE, Akroyd J, et al (2013) Bayesian parameter estimation for a jet-milling model using metropolis-hastings and wang-landau sampling. *Chemical Engineering Sicence,* 89, 244-257. http:/doi.org/10.1016/j.ces.2012.11.027

Lei Y, Zhou X, Xie, L (2019) Emergency monitoring and disposal decision support system for sudden pollution accidents based on multimedia information system. *Multimedia Tools and Applications*, 78(8), 11047-11071. http:/doi.org/10.1007/s11042-018-6665-2

Liu X D, Wang, J (2020) Advances in methods for identifying surface water pollution sources. *Advances in Water Science*, 31(2), 302-311.

Lu ZR, Zhou J, Wang L (2019) On choice and effect of weight matrix for response sensitivity-based damage identification with measurement and model errors. *Mechanical Systems & Signal Processing*, 114, 1-24. http:/doi.org/10.1016/j.ymssp.2018.05.007

Ma D, Tan W, Zhang Z, Hu J (2017) Parameter identification for continuous point emission source based on tikhonov regularization method coupled with particle swarm optimization algorithm. *Journal of Hazardous Materials,* 325, 239-250. http:/doi.org/10.1016/j.jhazmat.2016.11.071

Mohamed AW, Sabry HZ (2012) Constrained optimization based on modified differential evolution algorithm. *Information Sciences*, 194, 171-208. http:/doi.org/10.1016/j.ins.2012.01.008

Pan ZD, Lu WX, Fan Y (2020) Identification of groundwater pollution source traceability based on simulation-optimization method. *Chinese Journal of Environmental Science*, 40(4), 1698-1705.

Parolin RDS, Silva N, Antônio J, Rodrigues, PPGW, Llanes Santiago O (2015) Estimation of a contaminant source in an estuary with an inverse problem approach. *Applied Mathematics & Computation*, 260, 331-341. http:/doi.org/10.1016/j.amc.2015.03.054

Qin AK, Huang VL, Suganthan, PN (2009) Differential evolution algorithm with strategy adaptation for global numerical optimization. *IEEE Transactions on Evolutionary Computation,* 13(2), 398-417. http:/doi.org/10.1109/TEVC.2008.927706

Raje D, Krishnan R (2012) Bayesian parameter uncertainty modeling in a macroscale hydrologic model and its impact on Indian river basin hydrology under climate change. *Water Resources Research,* 48(8), 2838-2844. http:/doi.org/10.1029/2011WR011123

Roberts GO, Rosenthal JS (2004) General state space Markov Chains and MCMC algorithms. *Probability Surveys,* 1(1), 20-71. http:/doi.org/10.1214/154957804100000024

Rönkkönen J, Kukkonen S, Price KV (2005) Real-parameter optimization with differential evolution. *IEEE Congress on Evolutionary Computation,* 1, 506 - 513. http:/doi.org/10.1109/CEC.2005.1554725

Singh RM, Datta B (2006) Identification of groundwater pollution sources using GA-based linked simulation optimization model. *Journal of Hydrologic Engineering,* 11(2), 1216-1227. http:/doi.org/10.1061/(ASCE)1084-0699(2006)11:2(101)

Skaggs TH, Kabala ZJ (1995) Recovering the history of a groundwater contaminant plume: method of quasi-reversibility. *Water Resources Research,* 31(11), 2669-2673. http:/doi.org/10.1029/95wr02383

Skaggs TH, Kabala ZJ (1994) Recovering the release history of a groundwater contaminant. *Water Resources Research*, 30(1), 71-79. http:/doi.org/10.1029/93WR02656

Skiba YN, Parra-Guevara D (2017) Application of adjoint approach to oil spill problems. *Environmental Modeling & Assessment, 22*(4), 379-395. http:/doi.org/10.1007/s10666-016-9540-4

Storn R, Price K(1997) Differential evolution–a simple and efficient heuristic for global optimization over continuous spaces. *Journal of Global Optimization*, 11(4), 341–359. http:/doi.org/10.1023/A:1008202821328

Sun J, Zhang WS, Jing L, Han X, Wang Q, Kong J (2019) Estuarine pollutant tracing method based on

evolutionary algorithm and water quality model. *Science, Technology and Engineering*, 19(14), 384-391.

Tang Y, Guan X (2007) Parameter estimation for time-delay chaotic system by particle swarm optimization. *Chaos Solitons & Fractals,* 40(3), 1391-1398. http:/doi.org/10.1016/j.chaos.2007.09.055

Venter G, & Sobieszczanski-Sobieski J (2004) Multidisciplinary optimization of a transport aircraft wing using particle swarm optimization. *Structural and Multidisciplinary Optimization*, 26(1), 121-131. http:/doi.org/10.1007/s00158-003-0318-3.

Vitaliy F (2006) Differential evolution in search of solutions. *Springer*, New York. http:/doi.org/10.1007/978-0-387-36896-2.

Wang J, Shih Y, Wang PY, Yu YH, Huang CP (2019) Hazardous wastes treatment technologies. *Water Environment Research,* 91(5), 1177-1198. http:/doi.org/10.1002/wer.1213.

Wang J, Zhao S, Li X, Cai F, Zhang L. (2016). Comparison of three methods for assessing damage of water resource in sudden water pollution accident. *Environmental Science & Technology*, 39(03), 200-204.

Wang Y, Zhang W, Engel BA, Peng H, Theller L, Shi Y, et al (2015) A fast mobile early warning system for water quality emergency risk in ungauged river basins. *Environmental Modelling & Software*, 73, 76-89. http:/doi.org/10.1016/j.envsoft.2015.08.003

Wei H, Chen W, Sun H, Li X (2010) A coupled method for inverse source problem of spatial fractional anomalous diffusion equations. *Inverse Problems in Science & Engineering,* 18(7), 945-956. http:/doi.org/10.1080/17415977.2010.492515

Wu W, Ren J, Zhou X, Wang J, Guo M (2020) Identification of source information for sudden water pollution incidents in rivers and lakes based on variable-fidelity surrogate-dream optimization. *Environmental Modelling & Software*, 104811. http:/doi.org/10.1016/j.envsoft.2020.104811

Yang HD, Liu BY, Huang JH (2018) Forecast model parameters calibration method for sudden water pollution accidents based on improved Bayesian-Markov chain Monte Carlo. *Control and Decision*, 33(4), 679-686. http:/doi.org/10.13195/j.kzyjc.2017.0213

Yang HD, Shao DG, Liu BY, et a1 (2016) Multi-point source identification of sudden water pollution accidents in surface waters based on differential evolution and Metropolis-Hastings-Markov Chain Monte Carlo．*Stochastic Environmental Research and Risk Assessment*, 30(2), 507-522．http:/doi.org/10.1007/s00477-015-1191-5

Yang YL, Lei XH, Long Y, Tian Y, Zhang YH, Yao Y, Hou XS, Shi MS., Wang PW, Zhang CL, Wang H, Quan J (2020) A novel comprehensive risk assessment method for sudden water accidents in the middle route of the south–north water transfer project (china). *Science of the Total Environment, 698*, 134167-. https://doi.org/10.1016/j.scitotenv.2019.134167.

Wang XD, Zhang DQ, Chen LY (2018) Real-time monitoring of pollutant diffusion states and source using fuzzy adaptive kalman filter. *Water, Air, & Soil Pollution*, 229: 238. https://doi.org/10.1007/s11270-018-3885-z

Yoo B, Choi SD (2019) Emergency evacuation plan for hazardous chemicals leakage accidents using GIS-based risk analysis techniques in South Korea. *International Journal of Environmental Research and Public Health,* 16(11), 1948. http:/doi.org/10.3390/ijerph16111948

Yu HL, Wu YZ, Cheung SY (2020) A data assimilation approach for groundwater parameter estimation under Bayesian maximum entropy framework. *Stochastic Environmental Research and Risk Assessment*, 34(2), 709-721. http:/doi.org/10.1007/s00477-020-01795-z

Yu LA, Li L, Wu JQ, et al (2015) Emergency policy exploration for network public opinion crisis in water pollution accident by hazardous chemicals leakage based on systematic dynamics. *Systems Engineering- Theory & Practice*, 35(10), 2687-2697. http:/doi.org/CNKI:SUN:XTLL.0.2015-10-029

Zeunert S, Günter M (2020) Influence of the spatial and temporal monitoring design on the identification of an instantaneous pollutant release in a river. *Advances in Water Resources*, 146, 103788.

https://doi.org/10.1016/j.advwatres.2020.103788

Zhang SP, Xin XK (2017) Pollutant source identification model for water pollution incidents in small straight rivers based on genetic algorithm. *Applied Water Science*, 7(4), 1955-63. https://doi.org/10.1007/s13201-015-0374-z

Zhang GX, Yang RH, Meng XF (2018) Construction of the emergency decision system for hazardous chemicals leakage based on "scenario-response" model. *Environmental Protection of Chemical Industry*. 38(5), 609-614.

Zhao L, Qian Y, Hu QM, Jiang R, Li M, Wang X (2018) An analysis of hazardous chemical accidents in china between 2006 and 2017. *Sustainability,* 10(8), 1-18. https://doi.org/10.3390/su10082935

Zhang S, Qiang J, Liu H, Li Y (2020) Optimization design of groundwater pollution monitoring scheme and inverse identification of pollution source parameters using bayes' theorem. *Water, Air, & Soil Pollution,* 231(1), 1-17. https://doi.org/10.1007/s11270-019-4369-5
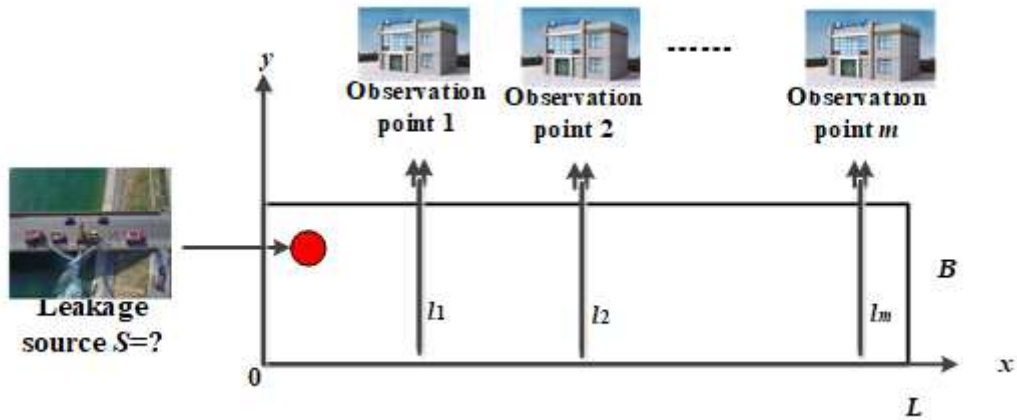
Figures

Figure 1

Schematic of the emergency identification of SHCLA
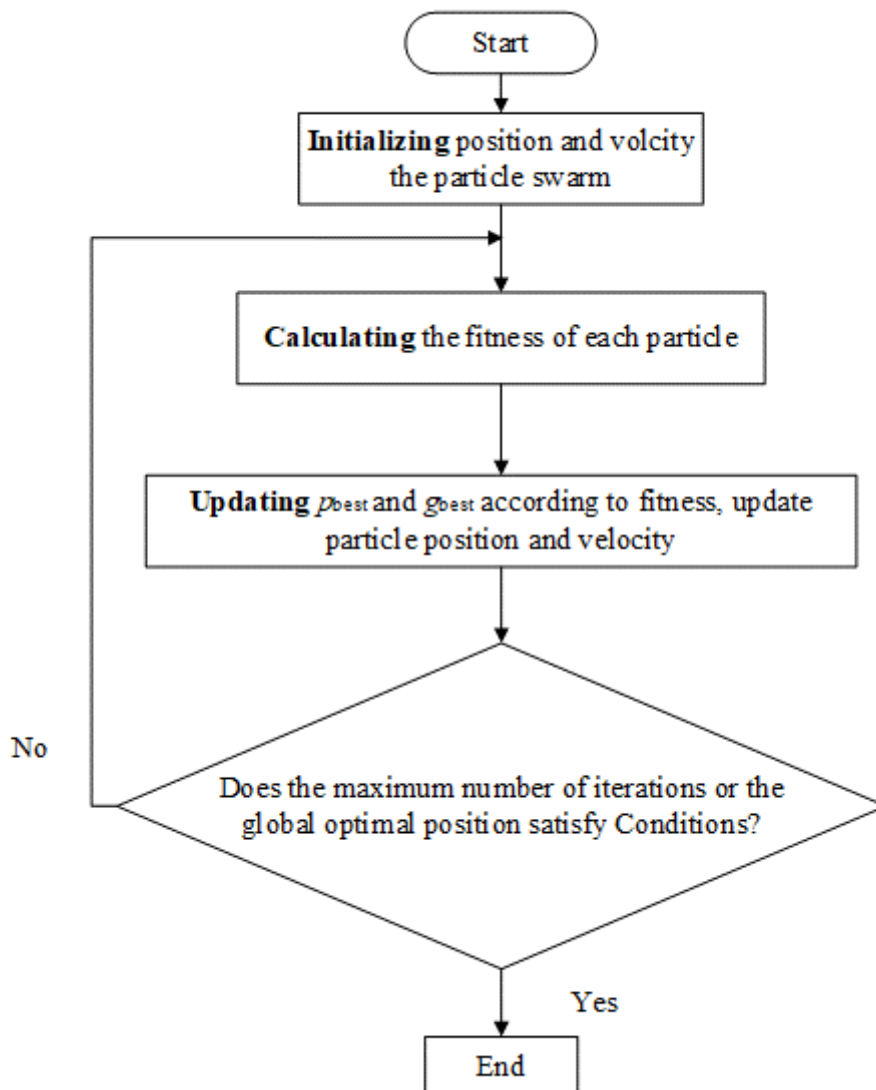
Figure 2

Procedure of PSO

Start

Initializing population

Calculating objective function

Is the terminal constraints Satisfied?   Yes

No

Finding individual candidates by mutation and crossover

Determining which individual is the "best" by comparing the objective values

Updating population

End

Figure 3

Procedure of DE

```
                    ┌─────────┐
                    │  Start  │
                    └────┬────┘
                         ▼
        ┌────────────────────────────────────┐
        │      Initializing population        │
        └────────────────┬───────────────────┘
                         ▼
        ┌────────────────────────────────────┐
        │  Transforming Parameter's coordinate │
        └────────────────┬───────────────────┘
                         ▼
        ┌────────────────────────────────────┐
  ┌────►│     Sampling a sample Xᵢ=S⁽ⁱ⁾        │
  │     └────────────────┬───────────────────┘
  │                      ▼
  │     ┌────────────────────────────────────┐
  │     │ generaing randomly a new sample S⁽*⁾ │
  │     └────────────────┬───────────────────┘
  │                      ▼
  │     ┌────────────────────────────────────────┐
  │     │ Calculating the acceptance probability   │
  │     │            B(S⁽ⁱ⁾, S⁽*⁾)                  │
  │     └────────────────┬───────────────────────┘
  │                      ▼
```

$$R \leq B(S^{(i)}, S^{(*)})?$$

$$X_{i+1} = S^{(*)}$$

$$X_{i+1} = S^{(i)}$$

Updating population, let $i = i+1$

Does these samples meet with convergence criteria?

Figure 4

Procedure of M-H sampling method

Figure 5

Process of generating new testing parameters X(*) with three dimensions by PSO and DE
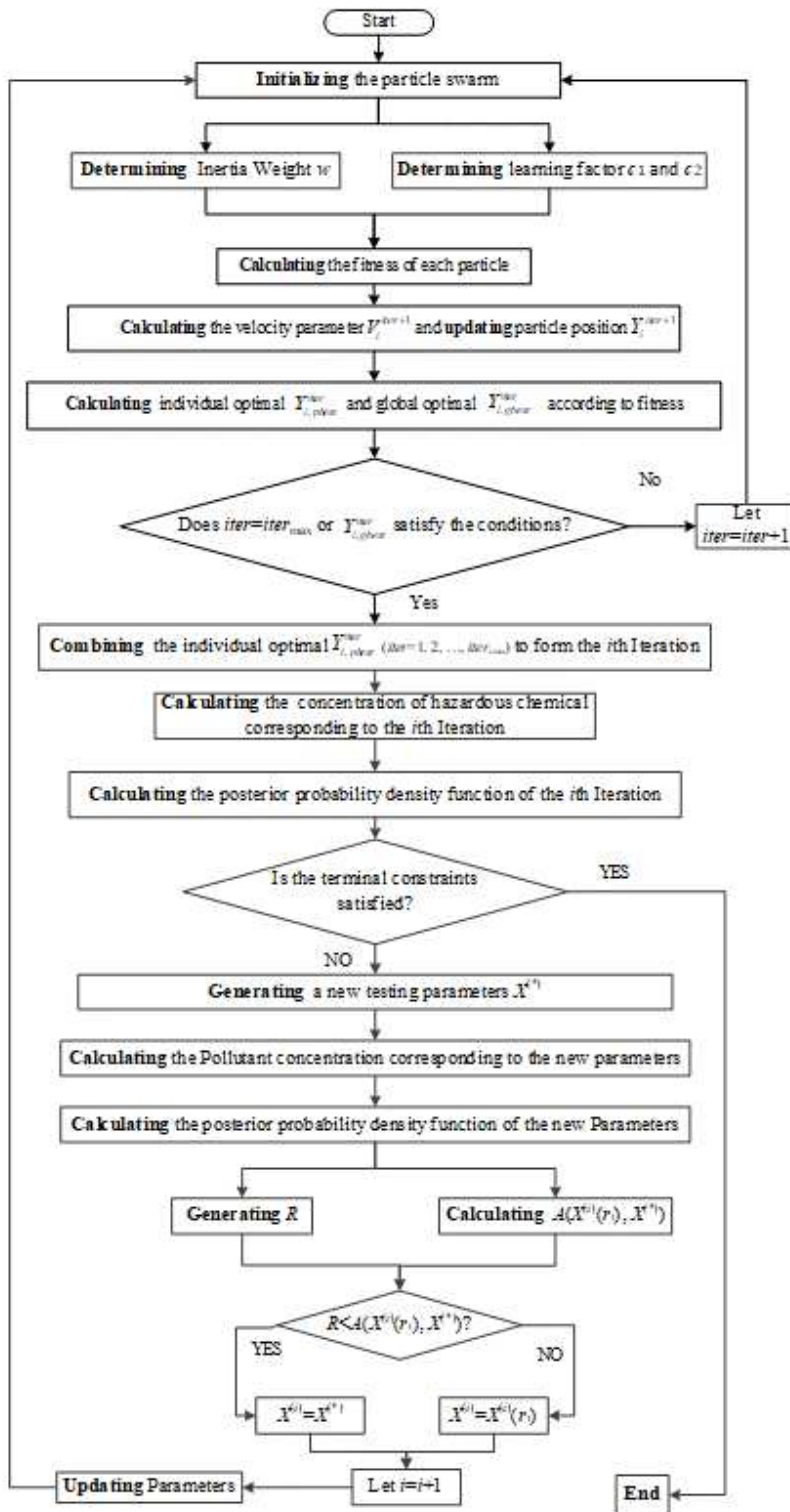
Figure 6

Operation process of the PSO-DE-MH method

Figure 7

Sketch of the South-North Water Transfer Project (a) and experimental canal section (b). Note: The designations employed and the presentation of the material on this map do not imply the expression of any opinion whatsoever on the part of Research Square concerning the legal status of any country, territory, city or area or of its authorities, or concerning the delimitation of its frontiers or boundaries. This map has been provided by the authors.
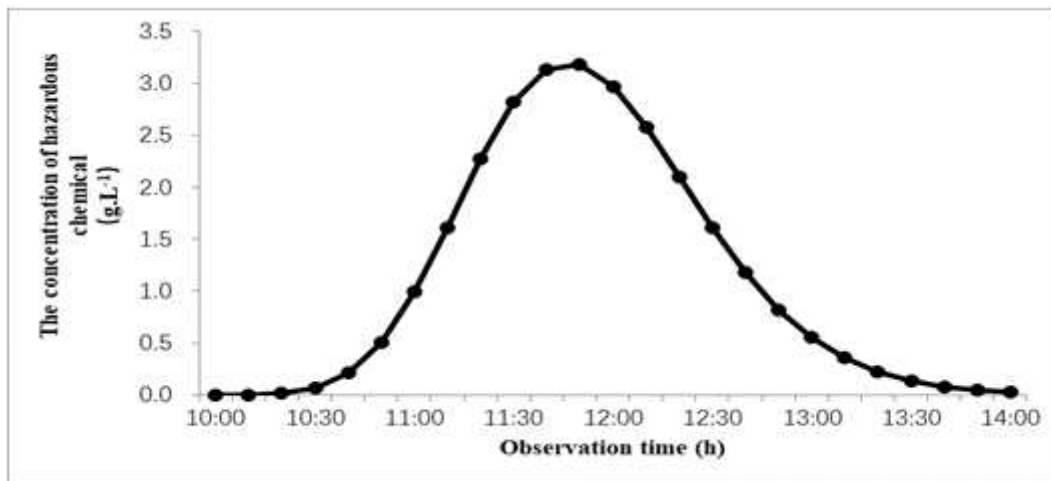
Figure 8

Sequence values of pollutant concentration at observation point D

(a) Intensity (*m*)
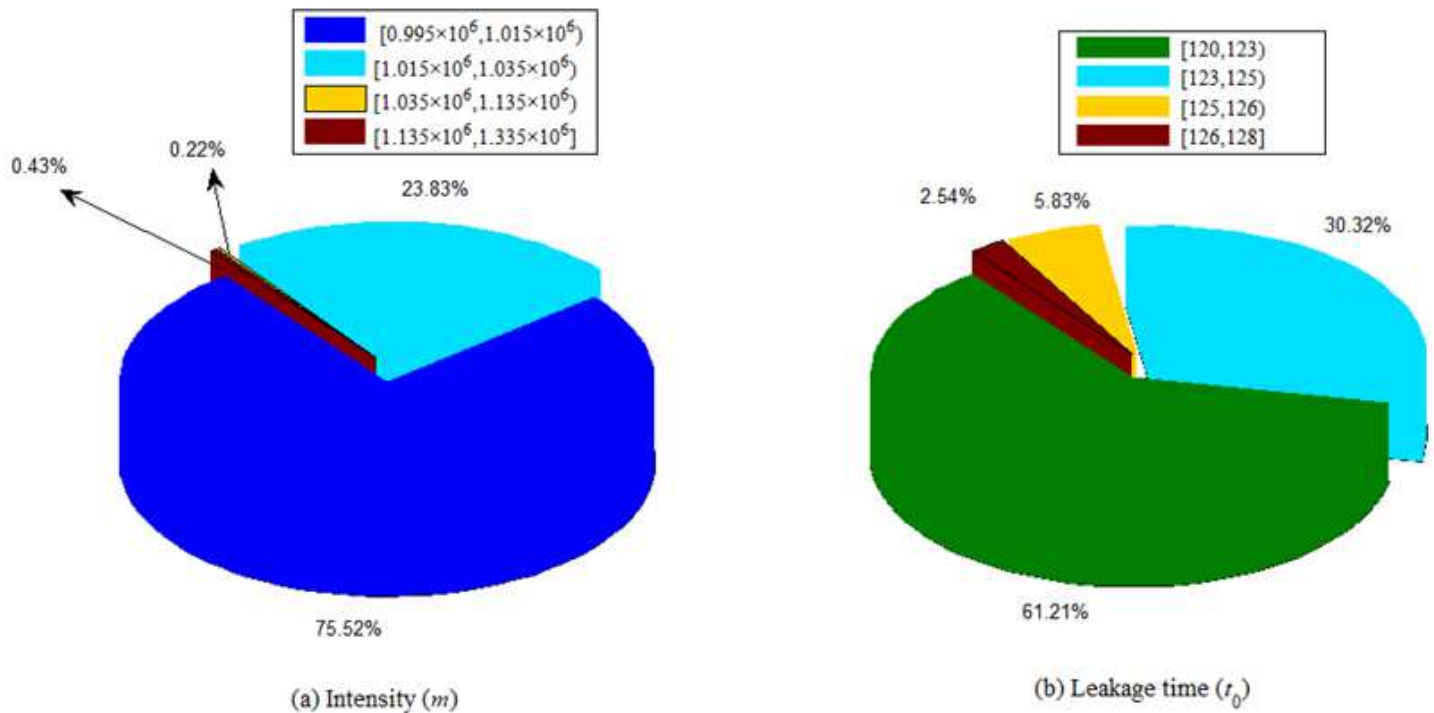
(b) Leakage time (t_0)

Figure 9

The Frequency distribution of Intensity (a) and Leakage time (b) based on PSO-DE-MH

(a) Leakage position (x_0)

(b) Leakage position (y_0)
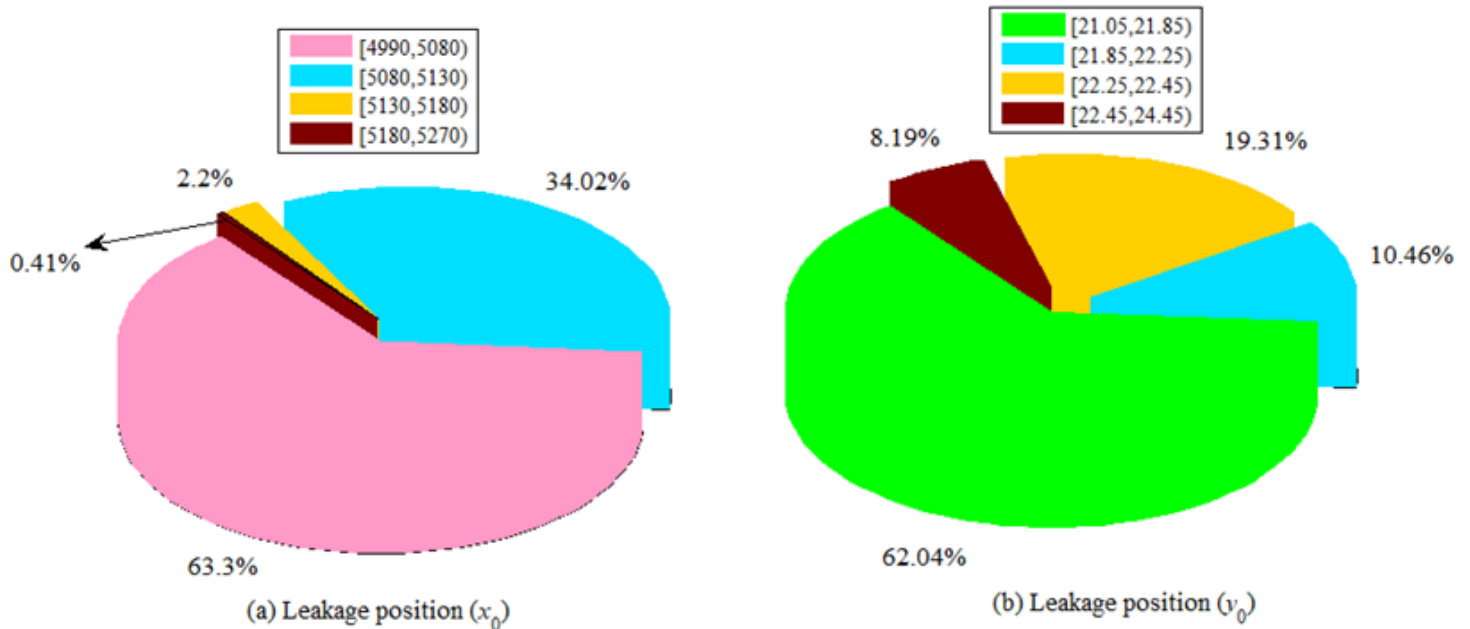
Figure 10

The Frequency distribution of x-coordinate of source location (a) and y-coordinate of source location (b) based on PSO-DE-MH
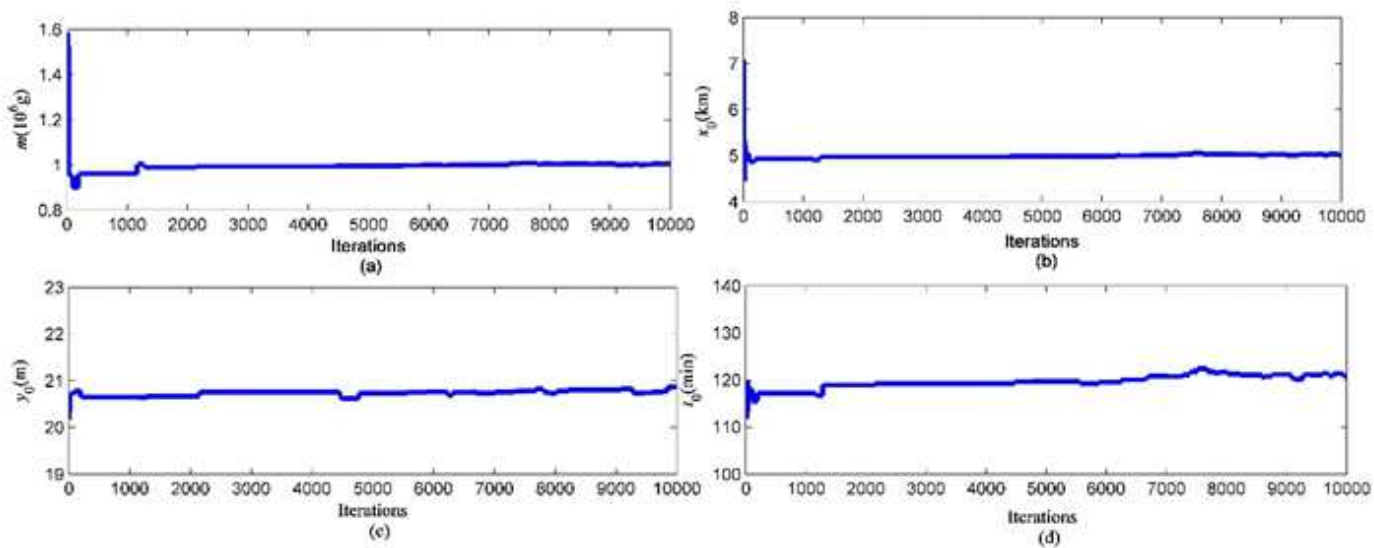
Figure 11

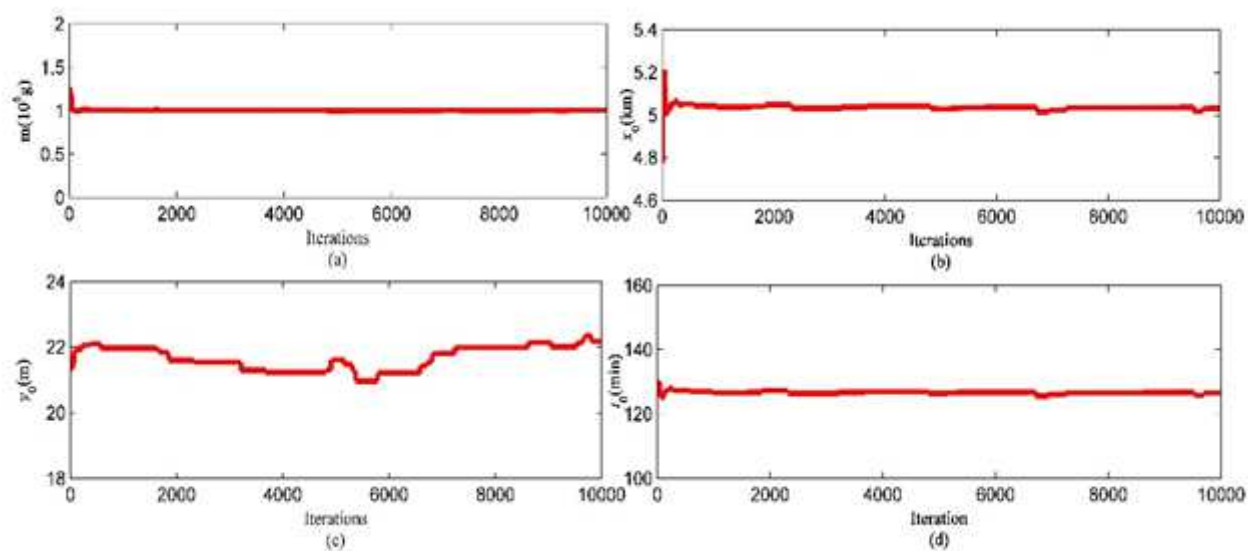Iterative curve of unknown parameters based on PSO-DE-MH
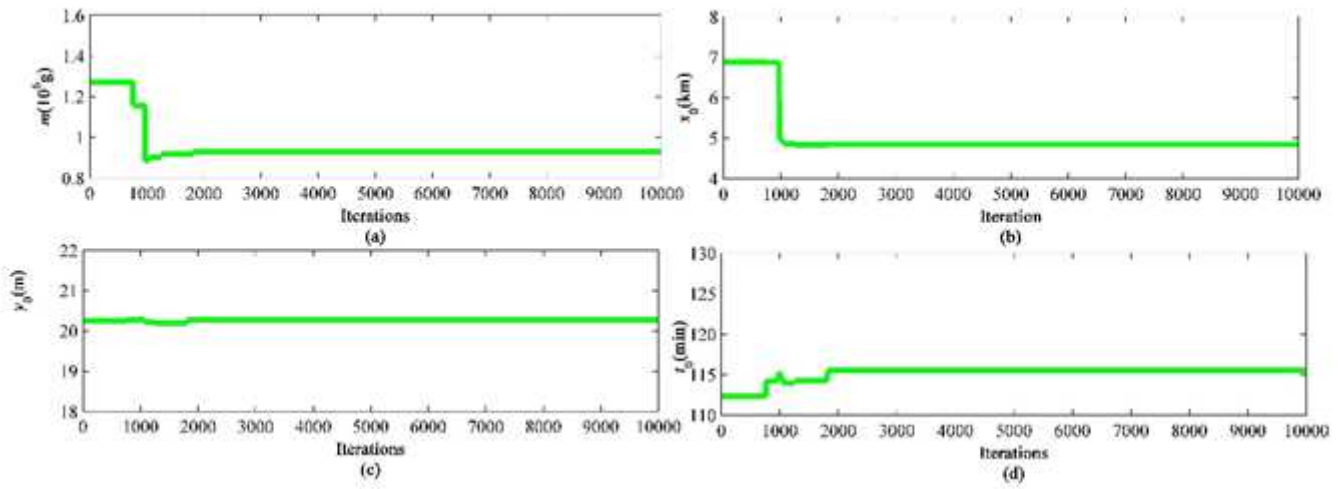

Figure 12

Iterative curve of unknown parameters based on DE-MH

Figure 13

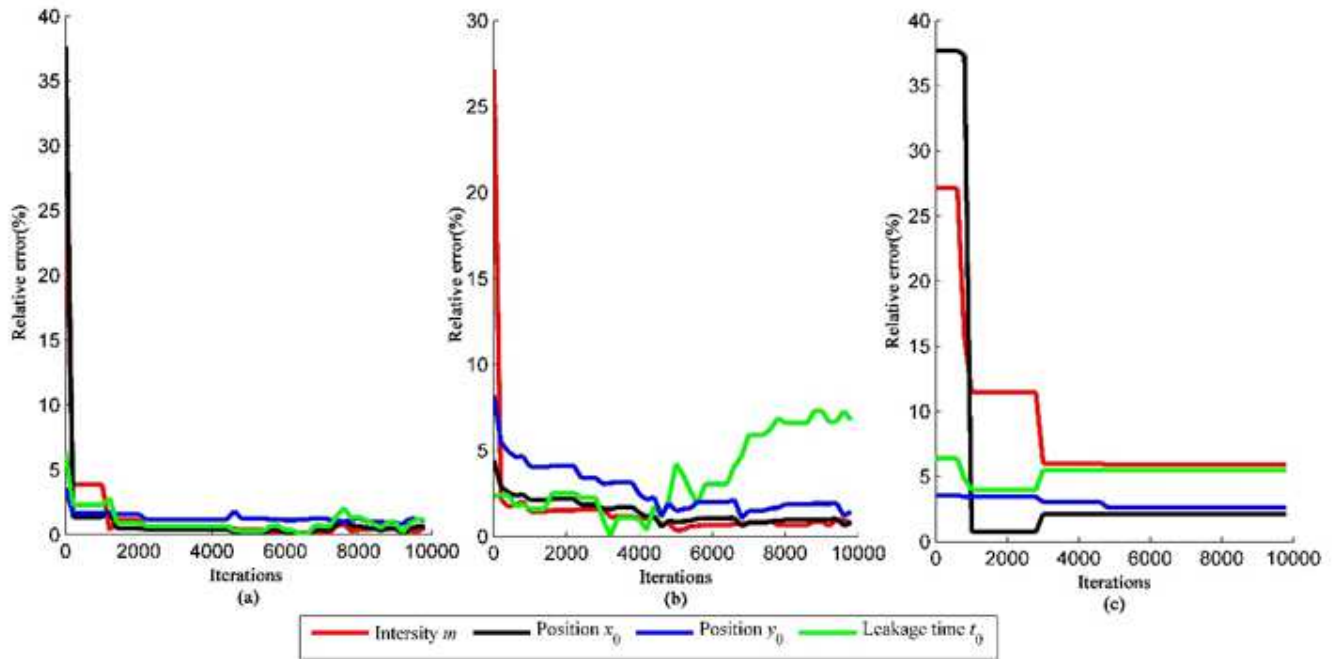Iterative curve of unknown parameters based on PSO-DE

Figure 14

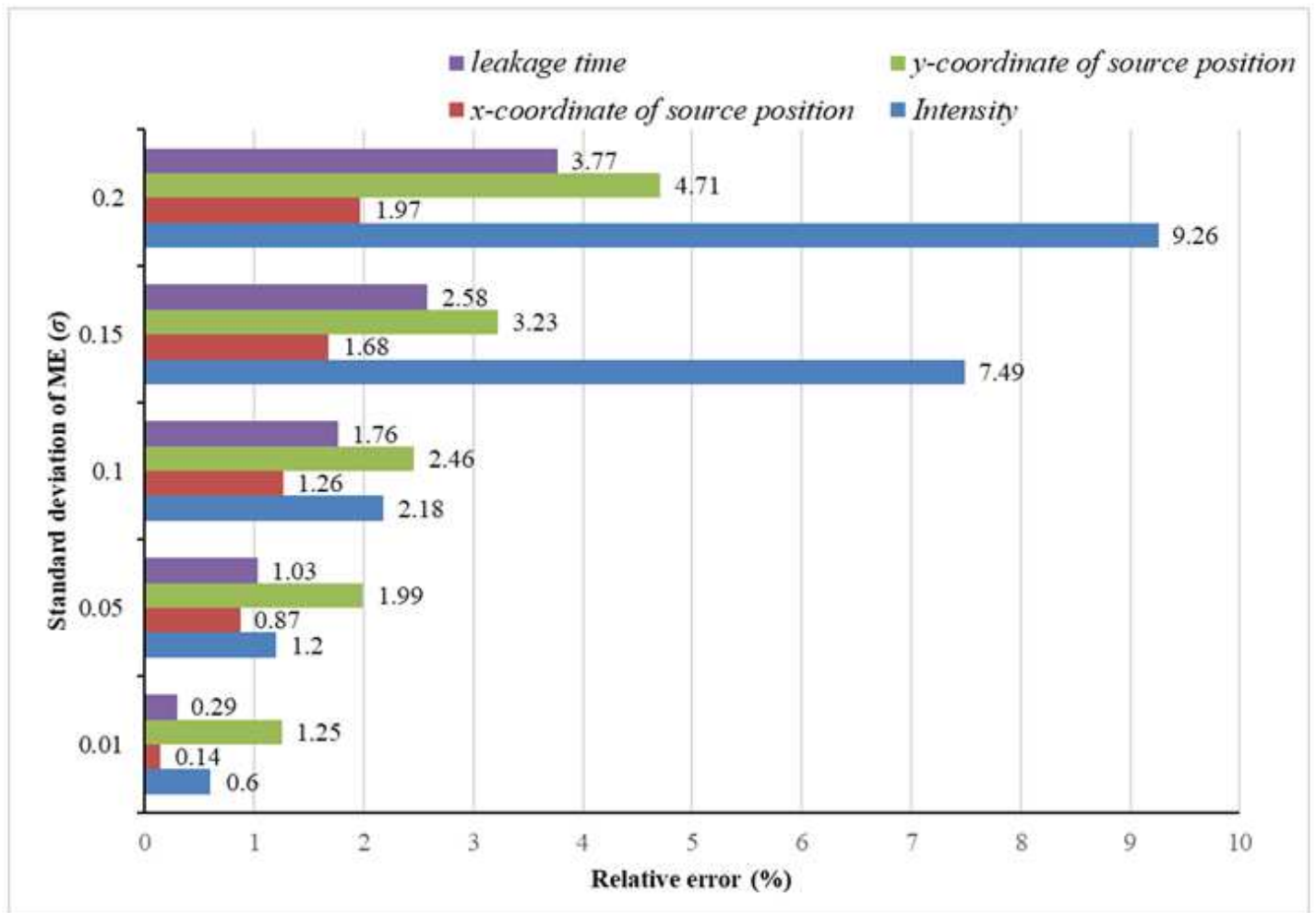Relative error analysis of inversion results based on PSO-DE-MH (a), DE-MH (b) and PSO-DE (c)

Figure 15

Variation diagram of the relative errors with different of MEs
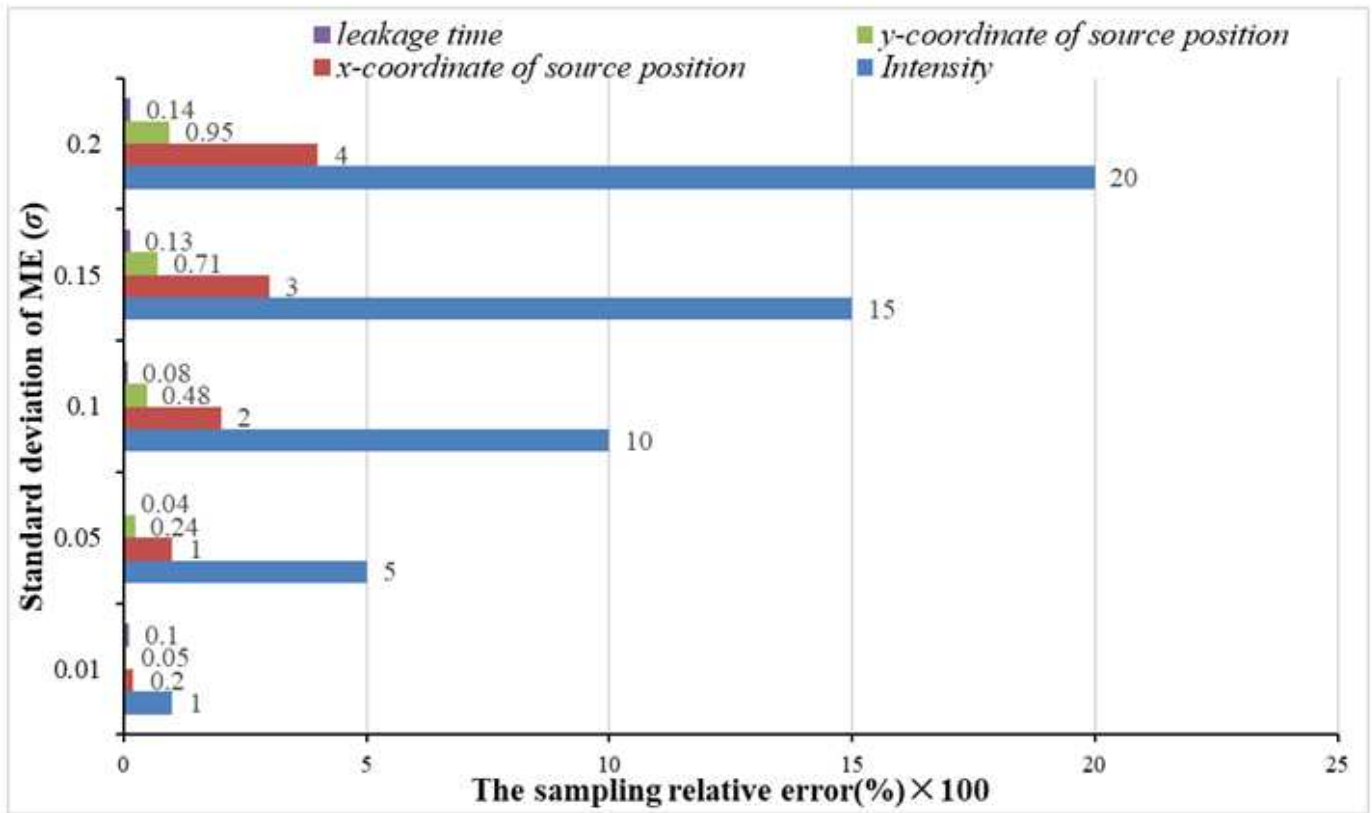
Figure 16

Variation diagram of the sampling relative errors with different of MEs