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Back-calculation of the strength and location of hazardous materials releases using the pattern search method

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ABSTRACT

Predicting quickly and accurately the strength and location of hazardous materials releases becomes a critical problem in emergency rescue. A technique that coupled the concentrations observed in the downwind direction of the source with a dispersion model was presented to back-calculate the strength and location of the release source by using the pattern search method. The technique was described as an optimization problem with an objective function constructed from a sum of squared errors between the observed concentrations and the calculated concentrations. The utility of the pattern search method was illustrated by testing the simulation data with practical data. The advantages of the method were demonstrated by a comparison with a gradient-based algorithm and an intelligent optimization algorithm. The computations indicate that this method can achieve optimal solutions in a relatively shorter time, hence more efficiently meeting the needs of emergency rescue.

1. Introduction

Accurate and timely evaluations of the strength and location of the pollutant sources play an important role in emergency responses involving hazardous materials, particularly when toxic gases are released. Prediction of the strength and location of the pollutant source is vital when determining suitable emergency evacuation areas and safety distance.

There is no difficulty to predict the concentration level of pollutants for a known release source by using a dispersion model. When the source is unknown, however, the source strength and location has to be identified by the use of the contaminant concentrations observed at fixed places. This type of identification, referred to as the inverse method, deduces the model parameters from the experimental data. It is widely used in the area of natural sciences and engineering technology [1,2]. Several previous investigations are devoted to this issue, which have coupled the observed concentrations with the dispersion model [3–14]. The investigations can be divided into two primary categories: one is based on statistical theory, and the other on optimization theory, as is shown in Table 1. The methods based on statistical theory, such as the Bayesian inference, are used to obtain the source strength and location [3,4]. With a set of observations and prior assumptions of the model parameters, the posterior probability of the parameters is obtained by the Bayesian inference. Subsequently, the Markov Chain Monte Carlo (MCMC) sampling is employed to obtain the estimation of the parameters. Since thousands of iterations are needed during the process of sampling, the methods based on statistical theory are rather time-consuming. The methods based on optimization theory minimize the objective function directly by comparing the observed concentrations and the calculated concentrations. In order to obtain the optimal solution, several different optimization algorithms have been employed. Gilbert and Khajehnajafi [5] constructed a SAFER System in their patented “Estimation of Toxic Substance Release”, where the objective function was determined by root-finding methods such as dichotomy and Newton’s iterative method. Elbern et al. [6], and Yumimoto and Uno [7] used the four-dimensional variational assimilation to characterize the source, and the parameters were dynamically adjusted by introducing the variable of time into the inversion process. The gradient-based method [8] was also used to optimize the objective function. All the optimization methods mentioned above are summed up as the indirect method where the calculations of the objective functions and its derivatives are required, which means that the calculations are difficult to attain when the objective function is complicated. In such cases, the direct search methods, such as simulated annealing [9,10] and genetic algorithm [11–14], are suitable for obtaining the optimal solution because the gradient information is not required. While these methods optimize the objective function successively until a given tolerance is reached, evaluations of objective functions costs too much time per iteration and therefore become a weakness in emergency rescues.

In the present research, the source inversion model was constructed by combining the observed concentrations with a dis-

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Table 1
Major source inversion methods.

Theoretical foundations	Representation methods		Principles	Characteristics and limitations	Representative achievements
Statistical theory	Bayesian inference		Assuming that the sampling results are in accordance with the priori distribution of the parameters, the observed concentrations are combined with Bayesian inference to deduce the posterior probability of the parameters. Then the sampling methods are used to obtain the estimation of the parameters	A priori distribution of the parameters is presupposed	Senocak et al. [3] and Yee [4]
Optimization theory	Indirect search methods	Four-dimensional variational assimilation	An air quality model is used to inversely locate the pollutant sources. The initial value of the model variables is assumed. The outputs are as close as possible to the corresponding observations in time and space through the continuous adjustment of the objective function	The introduction of time variables makes the model parameters dynamically adjusted, but the derivatives of the objective function are calculated	Elbern et al. [6] and Yumimoto and Uno [7]
		Gradient-based methods	Directly minimizing the objective function to obtain the optimal solution, the descent direction of the objective function is determined by the gradient of the objective function	The first-order or second-order derivative of the objective function is required, and the result depends on the initial value	Li and Niu [8]
	Direct search methods	Simulated annealing algorithm	Setting the initial value of the parameters and generating new values of parameters by random disturbances, the corresponding objective functional values are compared. The new values are accepted as the initial point of the next simulation with a certain probability. After iterative adjustment, the global optimal solution is achieved	Without calculating the derivative of the objective function, the simulated annealing algorithm uses the transfer probability to avoid local optimum	Thomson et al. [9] and Newman et al. [10]
		Genetic algorithm	The initial population of the parameters is randomly generated, and the individuals of the population are gradually optimized through a series of operations of selection, crossover, and mutation with a certain degree of probability	Genetic algorithm encodes with the parameters, it deals with the population other than the parameter itself	Haupt [11], Haupt et al. [12], Allen et al. [13] and Haupt et al. [14]

persion model in such a way that optimizes the sum of the squared errors between the observed concentrations and the calculated concentrations via the pattern search method. The results shown in this work were programmed by MATLAB.

2. Modeling and solution via the pattern search method

Many dispersion models have been developed to describe the dispersion of pollutants. In this research, a Gaussian puff model was applied to generate the calculated concentrations. The source inversion problem was modeled by minimizing the objective function, which was constructed from a sum of squared errors between the observed concentrations and the calculated concentrations. The pattern search method was then applied to adjust the objective function until a given tolerance has been achieved, and the value for obtaining the minimum of the objective function was regarded as the optimal solution. The source strength was treated as an unknown parameter and evaluated through an inversion model, which is described in Sections 2.1 and 2.2. The strength, location, and release time were all considered as unknown parameters, as described in Section 2.3.

2.1. Modeling

The inversion model was constructed by incorporating the observed concentrations with the dispersion model. In order to demonstrate the utility of the pattern search method in solving the inversion model, a Gaussian puff model was employed to simulate the instantaneous release of toxic gas. The formulation is given as

$$C(x,y,t)=\frac{2Q}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z}\exp\left(-\frac{1}{2}\left(\frac{(x-ut)^2}{\sigma_x^2}+\frac{y^2}{\sigma_y^2}\right)\right) \tag{1}$$

where $C(x, y, t)$ is the concentration in the location of (x, y) at time t, (x, y) is the Cartesian coordinate in the downwind direction from the source, Q is the strength of the release source, t is the time after the release, u is the wind speed, and σ_x, σ_y, and σ_z are the dispersion coefficients in the x, y, z direction respectively.

The above formulation was constructed with the release source located in the origin of the Cartesian coordinate system, and the positive direction of the x-axis was the same as the wind direction. Let C^i_{cal} and C^i_{obs} be the calculated concentration and the observed concentration at the fixed observation point i, the purpose being to minimize the objective function, which is in the form of

$$\min_Q f(Q)=\sum_{i=1}^{N}(C^i_{obs}-C^i_{cal})^2 \tag{2}$$

where N is the total number of the observation points. Since C^i_{cal} is calculated by Eq. (1), the final objective function can be written as

$$\min_Q f(Q)=\sum_{i=1}^{N}\left(C^i_{obs}-\frac{2Q}{(2\pi)^{3/2}\sigma_{x_i}\sigma_{y_i}\sigma_{z_i}}\exp\right. \times\left.\left(-\frac{1}{2}\left(\frac{(x_i-ut)^2}{\sigma_{x_i}^2}+\frac{y_i^2}{\sigma_{y_i}^2}\right)\right)\right)^2 \tag{3}$$

where the variables are the same as defined above, with the subscript i showing that the variables are defined in the observation point i.

In this formulation, the source strength Q was iteratively adjusted in order to optimize the fitness of the observed concentrations and the calculated concentrations until the optimal solution was obtained. Therefore, the source inversion problem was transformed into an optimization problem (see Eq. (3)). As described in the following sections, the pattern search method was used to back-calculate the source strength by gradually adjusting the objective function (3).

2.2. The pattern search method for solving the inversion model

The pattern search method optimizes the objective function without calculating any derivatives. It calculates the objective function value directly in the process of optimization, which includes two basic steps: the axis direction move (or axis exploration) and the pattern move. This method is based on a pattern e, which in this work is established according to the exploration of the neighborhood of the current point. Its form is

$$\mathbf{e}=\underbrace{\begin{bmatrix}1 & \cdots & 0\\ \vdots & \ddots & \vdots\\ 0 & \cdots & 1\end{bmatrix}}_{n}$$

where n is the number of unknown parameters. A trial step is defined by $\delta\mathbf{e}^i$, where δ is a constant that determines the length of the search step, and $\mathbf{e}^i$ is the ith column in $\mathbf{e}$. The trail point in the pattern is given by $y^{(k)}+\delta\mathbf{e}^i$, with $y^{(k)}$ being the current best solution. $y^{(k)}+\delta\mathbf{e}^i$ is then examined to see whether it is a better solution.

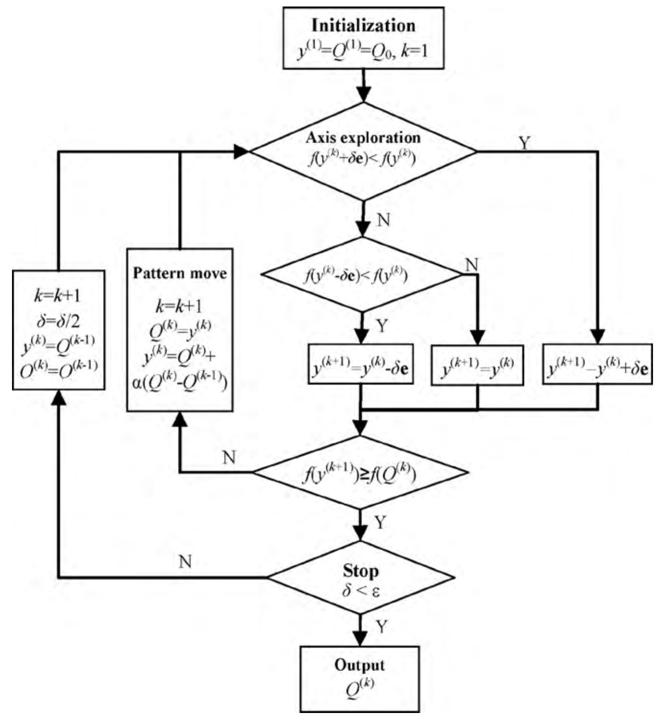

Fig. 1. Flowchart of the pattern search method in back-calculating the source strength.

The source strength Q was treated as an unknown parameter. The process of the pattern search method in back-calculating the strength Q is shown in Fig. 1.

Fig. 1 summarizes the process of the pattern search method in solving the inversion model. Starting from a given point Q_0, a sequence of points that may or may not approach the optimal point is computed. The axis exploration is started from the current point, which may be the initial starting point set by the user or rather calculated from the previous step of this method. By adding or subtracting the current point to a trail step $\delta\mathbf{e}_1$, the objective function values in these new points ($f(y^{(k)}+\delta\mathbf{e}_1)$ or $f(y^{(k)}-\delta\mathbf{e}_1)$) are compared with the value of the current point ($f(y^{(k)})$) so as to determine whether an improvement has been achieved. The pattern move is conducted after the improvement of the current point.

If there is no improvement for the explorations in all directions, the exploration is conducted with a reduced step size until a given tolerance (e.g. 1e−10) for the method to terminate has achieved. The pseudo code of the algorithm is shown in Appendix.

2.2.1. Solving the model via the pattern search method with different meshes

The feasibility of the pattern search method in back-calculating the source strength was tested with simulation data. It was carried out under these assumptions: (i) for the instantaneous release, the source strength $Q = 5 \times 10^6$ g, (ii) When the atmospheric stability class is F, (iii) the average wind speed is assumed to be 2 m/s. In a scope of 1 km by 1 km, the concentrations are discreted by Eq. (1) on five different meshes, including 2×2, 4×4, 8×8, 10×10, and 20×20.

For these five different meshes, the release source was fixed at the origin of the coordinate and the receptors were fixed in the grid points. For instance, Fig. 2a shows the 4×4 mesh, where 20 receptors (with symbol 'o') are used to detect the pollutants and to supply the concentration observations.

Table 2 shows the optimization results by the pattern search method with different meshes. For the 4×4 or much finer meshes,

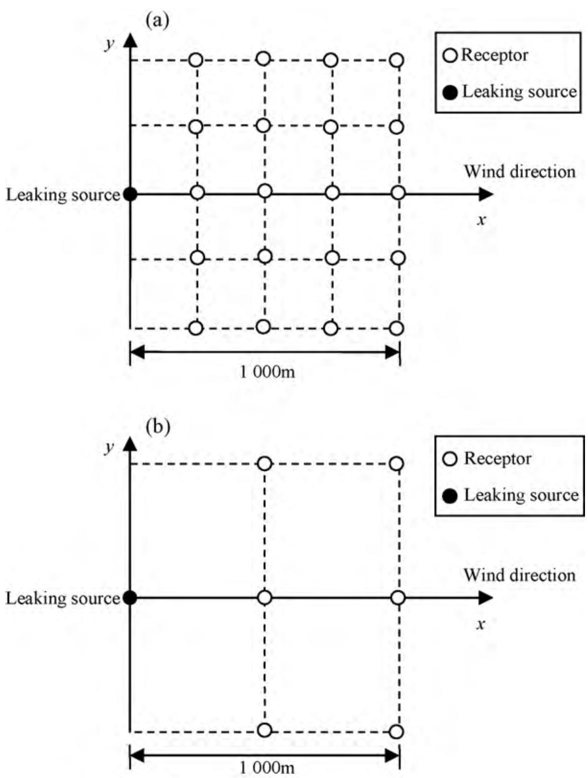

Fig. 2. (a) The setup for the 4 × 4 mesh of receptors. (b) The setup for the 2 × 2 mesh of receptors.

the identification of the source strength is successful, but it failed for the case of the 2 × 2 mesh. Since there are only 6 receptors in total to detect the pollutants (see Fig. 2b), and the concentration of the pollutant decreases with the increasing distance, the threshold value of the sensor can not be attained, so the concentrations below the threshold value are not be observed. Therefore, the available concentrations observed in the 2 × 2 mesh are limited, which leads to the failure to identify the proper solution.

Table 2
Comparison of the results with different meshes.

Grids	Separation distance (m)	Q_{opt} (g)	Iterations	Computational time (s)
2 × 2	500	1×10^6	34	0.121734
4 × 4	250	5×10^6	139	0.513487
8 × 8	125	5×10^6	139	1.762208
10 × 10	100	5×10^6	139	2.744549
20 × 20	50	5×10^6	139	15.807123

The superiority of the algorithm in characterizing the source strength was demonstrated. However, it still depended on the observation of the concentrations, i.e. the locations and the number of receptors. Therefore, this method could only be used when there were enough receptors to supply the observations.

2.2.2. Solving the model via the pattern search method with different acceleration factors

As is shown in Fig. 1, a sequence of points was constructed during the process of the algorithm, and the new point was calculated by the equation: $y^{(k+1)} = Q^{(k+1)} + \alpha(Q^{(k+1)} - Q^{(k)})$, where $Q^{(k)}$ is the current value, $Q^{(k+1)}$ is the point after the exploration, and α is the acceleration factor. Therefore, it was found that different acceleration factors affected the calculation efficiency. Fig. 3 shows that the number of iterations for the method to terminate varies with different acceleration factors. Although it is able to obtain the optimal solution, it requires different iterations as well as different consuming time to terminate. Hence, a carefully selected acceleration factor improves the efficiency of the method.

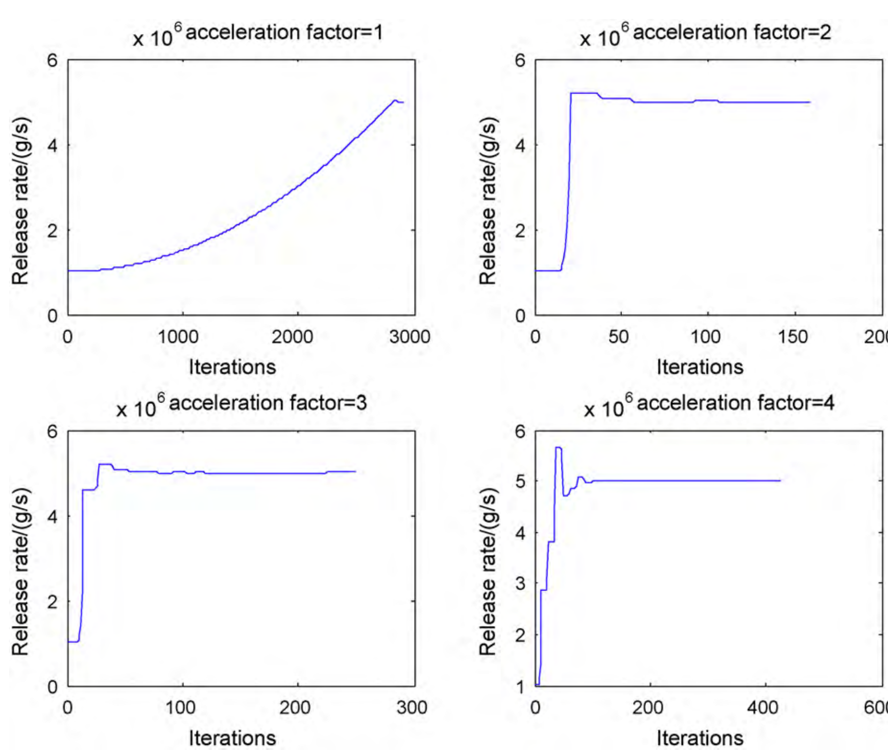

Fig. 3. Search results with different acceleration factors.

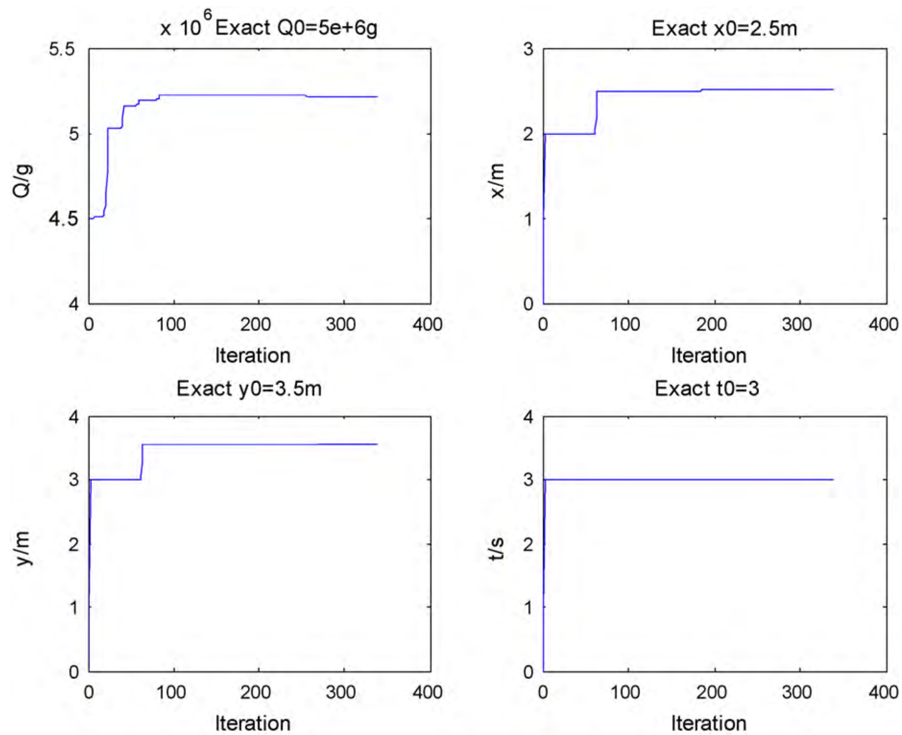

Fig. 4. Search results of thesource strength, location, and release time.

2.3. *Extension of the inversion model—characterizing the source with multiple parameters*

The results given above demonstrated the feasibility of the pattern search method in the back-calculation of the source strength. In this section, the method is extended to study the multiple parameters, which includes the unknown parameters of the source strength Q, location (x, y) and the initial release time t. In order to verify the applicability of the pattern search method in solving the multiple parameters, the location of the pollutant source was assumed to be (x_0, y_0) and was set as the origin of the new coordinate system. For the observation point (x, y) in the downwind direction, the transformation of the coordinate is

$$\begin{cases} x' = x - x_0 \\ y' = y - y_0 \end{cases} \tag{4}$$

Thus the concentration in any observation point can be expressed as

$$C(x, y, t)\Big|_{(Q, x_0, y_0, t_0)} = \frac{2Q}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z} \exp\left(-\frac{1}{2}\left(\frac{((x-x_0)-u(t-t_0))^2}{\sigma_x^2} + \frac{(y-y_0)^2}{\sigma_y^2}\right)\right) \tag{5}$$

Therefore, the objective function is

$$\min f(Q, x_0, y_0, t_0) = \sum_{i=1}^{N}\left\{C_{obs}^{i} - \frac{2Q}{(2\pi)^{3/2}\sigma_{x_i}\sigma_{y_i}\sigma_{z_i}} \exp\left(-\frac{1}{2}\left(\frac{((x_i-x_0)-u(t-t_0))^2}{\sigma_{x_i}^2} + \frac{(y_i-y_0)^2}{\sigma_{y_i}^2}\right)\right)\right\}^2 \tag{6}$$

Fig. 4 illustrates the search results when $Q_0 = 5 \times 10^6$ g, $x_0 = 2.5$ m, $y_0 = 3.5$ m, $t_0 = 3$ s.

This shows that the algorithm is capable of searching for the optimal solution with multiple parameters (see Table 3). Thus the pattern search method can also be extended to the study of multiple parameters.

3. Testing with practical data

The demonstrations shown above are based on instantaneous release; however, not all releases are instantaneous. In this section, the technique is tested for the continuous release by using practical data obtained from an experiment conducted in Hebei, China, before the 2008 Beijing Olympic Games.

3.1. *Continuous release*

For the continuous release, the Gaussian plume model was employed. The relevant formulation is

$$C(x, y, z, H_e) = \frac{Q'}{2\pi u\sigma_y\sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right)\left\{\exp\left(-\frac{(z-H_e)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+H_e)^2}{2\sigma_z^2}\right)\right\} \tag{7}$$

where $C(x, y, z, H_e)$ is the concentration at the location (x, y, z), H_e is the effective height of the source, Q' is the release rate, and the remaining variables are the same as defined in Section 2.1. There-

Table 3
Comparison of the search results with multiple parameters.

Parameter	Exact solution	Approximate solution	Relative error (%)
Q_0	5×10^6 g	5 209 919.320766 g	4.1984
x_0	2.5 m	2.503405 m	0.1362
y_0	3.5 m	3.558077 m	1.6593
t_0	3 s	3.001690 s	0.0563

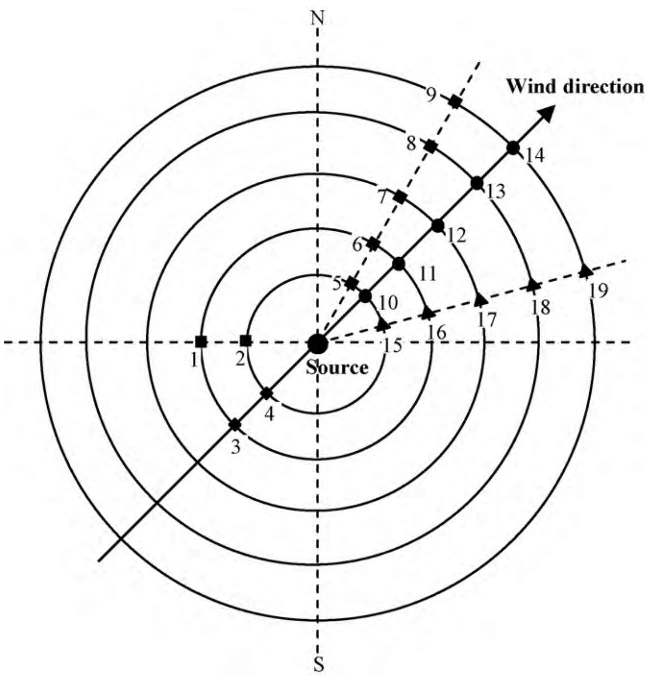

Fig. 5. Distribution of the sensors.

fore, the objective function is given as

$$\min_{Q'} f(Q') = \sum_{i=1}^{N} \left\{ C_{obs}^{i} - \frac{Q'}{2\pi u \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \times \left[\exp\left(-\frac{(z-H_e)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+H_e)^2}{2\sigma_z^2}\right) \right] \right\}^2 \quad (8)$$

3.2. Testing with practical data

In order to guarantee safety during the Beijing 2008 Olympic Games, particularly in the case of terrorist attacks involving toxic gas, certain experiments were conducted by the Chinese government, details are described below.

Fig. 5 shows the distribution of the observation points in the testing field. Ammonia (NH_3) was continuously released at 80 g/s, with the release rate being controlled by a valve. The wind was blowing to the northeast with an average speed of 6 m/s. Taken the release source as the original point, the radii of the circles were 100 m, 200 m, 500 m, 1000 m, and 2000 m. There were 19 testing points to detect the concentrations with sensors (such as CYBER sensors provided by Nano Environmental Technology (N.E.T. srl) of Italy, and the AreaRAE detector provided by RAE Systems of the U.S.), and each point detected the concentrations at two different heights of 1 m and 2 m above ground level.

The concentrations were observed ten minutes after the release, and the observations are shown in Table 4. Being that the experiment was conducted in the open field, the actual observations were somewhat decreased.

Following this, the pattern search method was applied to the test. According to the concentrations observed, the output of the method is 79.9485 g/s (shown in Fig. 6), which is almost equal to the experimental value. Therefore, the pattern search method can efficiently inverse the source even in practical cases.

Table 4
Effective observations in the testing points.

Effective points (z = 1 m)	Concentration (ppm)	Effective points (z = 2 m)	Concentration (ppm)
5	0.32	6	1.52
6	1.34	7	5.75
7	6.46	8	2.38
9	0.76	9	0.46
10	0.17	10	0.23
11	452.08	11	494.79
12	1996.54	12	2004.35
13	1073.62	13	1084.19
14	430.34	14	427.21
17	0.04	16	0.01
18	0.01	17	0.03

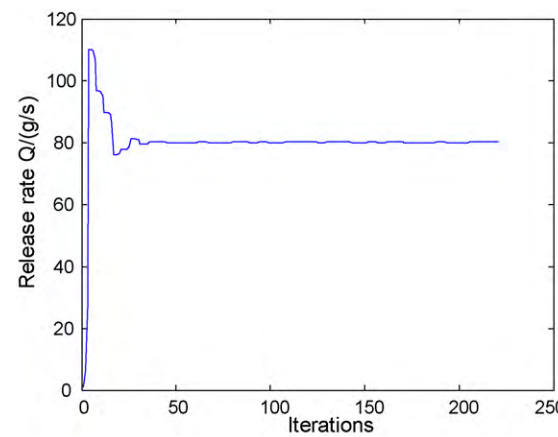

Fig. 6. Search results of the release rate.

4. Analysis and comparison

4.1. Analysis of the method

As a direct optimization method, the pattern search method depends on initial values. Compared with cases where initial values differ greatly from the true value, it appears to take less time to determine the optimal solution when the initial value is closer to the true value. The results are shown in Fig. 7.

For the testing of an unknown parameter, different initial values can provide solutions along with different iterations to terminate the method. In the case of multiple parameters, the method may

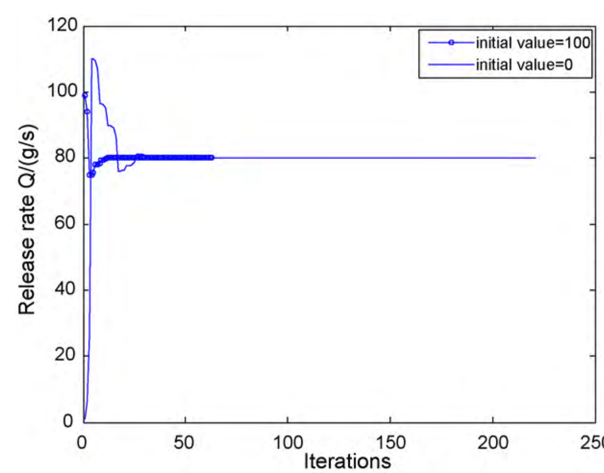

Fig. 7. Search results with different initial values.

Table 5
Comparison of different methods.

	Pattern search method	Gradient-based methods	Intelligent optimization algorithms (e.g. GA)
Initial value dependence (Y or N)	Y (users set)	Y (users set)	N (randomly generated)
Calculation of the derivatives of the objection function	N	Y	N
Amount of calculations	Small	Large	Quite large
Iterations	Depends on initial value	Small	The more iterations, the better accuracy
Computational complexity	Simple	Complex	Complex

approach a local optimal solution if the initial value is incorrectly chosen.

Furthermore, it is important to establish a termination criterion for the method. There may be some criteria for the pattern search method to terminate. These criteria are as follows:

- The step size is less than a given tolerance.
- The distance between the grid points, which are obtained in two consecutive successful iterations, is less than a given tolerance.
- The difference between the objective function values of the grid points, which are obtained in two consecutive successful iterations, is less than a given tolerance.
- The maximum number of the calculations of objective functions reaches a given value.
- The maximum number of the iterations reaches a given value.

Once one of the criteria is satisfied, the optimization process terminates with obtaining an optimal solution. The first criterion (step size) is generally used for this research. With the decrease of the termination step size, the accuracy of the solution is improved correspondingly; the computational time, however, is longer.

4.2. Comparison with other methods

In order to show the advantages and disadvantages of the pattern search method, it is compared with other methods, including the gradient-based methods and intelligent optimization algorithms. The differences are shown in Table 5.

From Table 5 one can see that the utilization of the pattern search method is comparatively effective given that no derivative information is required and only direct function evaluations are needed. In contrast, the gradient-based method requires the calculations of derivatives of the objective functions, which is difficult to program, particularly in the case of multiple parameters (see Section 2.3); therefore, the application of the gradient-based method is limited. Concerning Genetic algorithm (GA), its advantage is global optimization; however, it requires a large number of function evaluations per iteration, which result in the expenditure of much computational time.

In future research, it is suggested that a hybrid of GA and the pattern search method be used for the source inversion, thus the combination of the global optimization of the GA and the local search capability of the pattern search method will be more efficient to obtain the optimal solution.

5. Conclusions

In order to determine the strength and location of the release source, an inversion model is constructed based on the concentrations observed in the downwind direction of the release source and a dispersion model. The advantages of the pattern search method in solving this inversion model have been demonstrated. The calculation efficiency can be improved by adjusting the acceleration factor. Since the calculations of objective functions are only involved with the pattern search method, the approach is easily extended to the study with multiple parameters. The pattern search method is easier to implement than the gradient-based methods when the computational complexity is concerned, and it requires fewer functional evaluations than Genetic algorithm to obtain the optimal solution. Accordingly, the pattern search method can provide timely and accurately the vital information needed for emergency response and rescue.

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Appendix A. Pseudo code of the algorithm

Let y be an array to store the points obtained by the algorithm, $f(\cdot)$ is the objective function.

```
INITIALIZATION: y(1) = Q(1) = Q0, k = 1
IF Step size δ ≥ given tolerance THEN
  DO: Axis exploration
    IF f(y(k) + δe) < f(y(k)) THEN y(k + 1) = y(k) + δe
    ELSE IF f(y(k) − δe) < f(y(k)) THEN y(k + 1) = y(k) − δe
      ELSE y(k + 1) = y(k)
      END IF
    END IF
IF f(y(k + 1)) ≥ f(Q(k)) THEN
    DO: Pattern move
    k = k + 1
    δ = δ/2
    y(k) = Q(k-1)
    Q(k) = Q(k-1)
ELSE
    k = k + 1
    Q(k) = y(k)
    y(k) = Q(k) + α(Q(k) − Q(k − 1))
  END IF
ELSE
  Terminate, optimal solution ← Q(k)
END IF
```

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