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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