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Hybrid algorithm of minimum relative entropy-particle swarm optimization with adjustment parameters for gas source term identification in atmosphere

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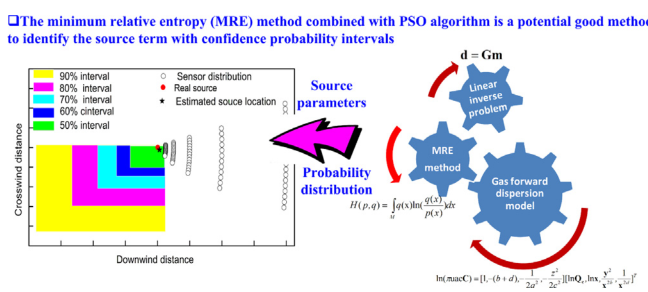
HIGHLIGHTS

- Improved MRE-PSO hybrid method was proposed to identify the source term.
- The method with adaptive parameter performs better than original method.
- The method can identify the source parameters with some confidence intervals.
- The method depends on prior input bounds and expected values slightly.
- The addition of error model improves the estimation performance.

GRAPHICAL ABSTRACT



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ABSTRACT

In order to identify the source term of gas emission in atmosphere, an improved hybrid algorithm combined with the minimum relative entropy (MRE) and particle swarm optimization (PSO) method was presented. Not only are the estimated source parameters obtained, but also the confidence intervals at some probability levels. If only the source strength was required to be determined, the problem can be viewed as a linear inverse problem directly, which can be solved by original MRE method successfully. When both source strength and location are unknown, the common gas dispersion model should be transformed to be a linear system. Although the transformed linear model has some differences from that in original MRE method, satisfied estimation results were still obtained by adding iteratively adaptive adjustment parameters in the MRE-PSO method. The dependence of the MRE-PSO method on prior information such as lower and upper bound, prior expected values and noises were also discussed. The results showed that the confidence intervals and estimated parameters are influenced little by the prior bounds and expected values, but the errors affect the estimation results greatly. The simulation and experiment verification results showed that the MRE-PSO method is able to identify the source parameters with satisfied results. Finally, the error model was probed and then it was added in the MRE-PSO method. The addition of error model improves the performance of the identification method. Therefore, the MRE-PSO method with adjustment parameters proposed in this paper is a potential good method to resolve inverse problem in atmosphere environment.

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1. Introduction

Source parameters, including source location, strength (mass emission rate), and emission characters etc., are required to be estimated urgently when some dangerous gases release to the atmosphere. For example, in carbon capture and storage (CCS) project, CO_2 gases storage underground may escape from the sequestration sites to the atmosphere (Yu et al., 2011; Ma et al., 2013a). There have been many methods to be applied for source identification. Besides direct way by portable instruments or widely distributed sensors, indirect method by computation algorithms coupled with measurement results is another effective tool to determine the gas emissions source parameters (Platt and Deriggi, 2010, 2012). Optimization method has been proved to be a feasible way to identify the gas emission source parameters (Haupt, 2005; Khlaifi et al., 2009; Long et al., 2010; Addepalli et al., 2011; Ma et al., 2013b). However, the reasonability of the estimation result is still doubtful due to the errors existed in the real operation. Yet, stochastic approximation method (Cannon and Yin, 1988; Heemink and Segers, 2002; Blau et al., 2008; Hazarta et al., 2014) based on inferences theory is a suitable option, which can obtain more reasonable probability distribution results under certain confidence levels.

Chow et al. (2008) reconstructed the source character by a combination of Bayesian inference and Markov chain Monte Carlo (MCMC) methods. Keats et al. (2006, 2007), Rao (2007) and Yee (2008) have addressed this problem by using the adjoint advection–diffusion equation in conjunction with MCMC methods to perform the computations efficiently. Their test cases demonstrate the feasibility of this method for practical applications in environmental emergency management. Although adjoint approach avoids solving the forward advection–diffusion equation for every required combination of source parameters, solving the adjoint advection–diffusion equation requires approximately the same computation time as the forward, which is also a time cost process, especially for a wider computational area. Therefore, a less expensive probability algorithm for source identification is necessary. The minimum relative entropy (MRE) method could meet this requirement to obtain an estimated result with higher efficiency at certain probability level.

The MRE is a method based on probability theory, which was first introduced by Kullback (1959) as a statistical method. Then the MRE approach was originally developed by Shore (1981) to inverse problem. Ulrych et al. (1990) applied the MRE philosophy to a one dimension inverse problem where the problem is underdetermined, and then they showed that the MRE is a general method of tackling linear underdetermined inverse problems. Woodbury and Ulrych (1996, 1998) used the MRE formalism to solve the general linear inverse problem, and they extended the MRE approach to solve the case of bounded problems and prior constraints. Neupauer (1999), Neupauer et al. (2000) compared the effectiveness of two inverse methods, Tikhonov regularization and the MRE to reconstruct the release history and showed that the MRE inversion reproduces the source history more effectively than Tikhonov regularization. Neupauer and Borchers (2001) also presented a MATLAB implementation of the MRE method for the linear inversion problem.

The gas emission source determination is a typical nonlinear inverse problem, which is difficult to be solved by the MRE method directly. Thus it will be transformed to be a linear form first, then the source parameters are identified by the MRE method combined with particle swarm optimization (PSO) algorithm.

2. The theory of minimum relative entropy

In the MRE method, the unknown model parameters ($\mathbf{m}$) are viewed as random variables. The solution of the inverse problem is obtained from the multivariate probability density function (PDF) of $\mathbf{m}$ (Woodbury and Ulrych, 1993, 1996, 1998). Let $\mathbf{x}$ be a state of a system, which has a set of possible states. $q^*(\mathbf{x})$ is its multivariate PDF. Let $q^*(\mathbf{x}) \geq 0$ denote a possible PDF, given by

$$\int q^*(\mathbf{x})\mathrm{d}\mathbf{x} = 1 \tag{1}$$

Suppose a priori estimation of $q^*(\mathbf{x})$ is $p(\mathbf{x})$. The goal of the MRE is to obtain a reasonable estimation of $q^*(\mathbf{x})$ based on the prior information provided. The solution is to minimize the entropy of $q(\mathbf{x})$ relative to $p(\mathbf{x})$, as shown as

$$H(p,q) = \int_M q(x)\ln[q(x)/p(x)]\mathrm{d}x \tag{2}$$

For a linear inverse problem, the problem can be expressed by Eq. (3)

$$\mathbf{d} = \mathbf{G}m \tag{3}$$

where $\mathbf{d}$ is a discrete set of known data, $\mathbf{G}$ is the known transfer functions and $\mathbf{m}$ is the vector of unknown "true" model parameters. A reasonable estimated $\widehat{\mathbf{m}}$ of $\mathbf{m}$, which satisfies the above equation, is the final goal.

Woodbury and Ulrych (1993, 1996) derived a prior distribution for linear model in hydrogeologic applications, which has the form

$$p(\mathbf{m}) = \prod_{i=1}^{M} \frac{\beta_i \exp(-\beta_i m_i)}{\exp(-\beta_i L_i) - \exp(-\beta_i U_i)} \tag{4}$$

where [L_i, U_i] is the lower and upper bound of m_i and β_i is the Lagrange multiplier, which is determined by the definition of Eq. (5).

$$\int_{\mathbf{m}} \mathbf{m}p(\mathbf{m})\mathrm{d}\mathbf{m} = \mathbf{s} \tag{5}$$

where $\mathbf{s}$ is the prior expected value constraints. By integrating Eq. (5), Eq. (6) is obtained to evaluate β_i (Neupauer and Borchers, 2001).

$$\frac{-(\beta_i U_i + 1)\exp(-\beta_i U_i) + (\beta_i L_i + 1)\exp(-\beta_i L_i)}{\beta_i[\exp(-\beta_i L_i) - \exp(-\beta_i U_i)]} = s_i \tag{6}$$

In order to obtain the posterior distribution, the entropy of $q(\mathbf{m})$ relative to $p(\mathbf{m})$, as shown with Eq. (2), is minimized subject to the expected value constraints in Eqs. (1)–(6). Finally, the posterior estimation of the PDF $q^*(\mathbf{x})$ is obtained (Woodbury and Ulrych, 1993, 1996) as

$$q(\mathbf{m}) = \prod_{i=1}^{M} \frac{a_{mi} \exp(-a_{mi} m_i)}{\exp(-a_{mi} L_i) - \exp(a_{mi} U_i)} \tag{7}$$

where $a_{mi} = \beta_i + \sum_{j=1}^{N} g_{ji}\lambda_j$. The posterior mean solution should fit the data within a specified tolerance, such as

$$\|\mathbf{d} - \mathbf{G}\widehat{m}\|^2 \leq \xi^2 \varepsilon^2 \tag{8}$$

where ξ is a parameter that depends on the assumed error model and ε is the measurement error. Therefore, λ_j should satisfy the nonlinear system of Eq. (9) when $F(\boldsymbol{\lambda}) = 0$.