Journal of Hazardous Materials 325 (2017) 239–250

Contents lists available at ScienceDirect

Journal of Hazardous Materials

journal homepage: www.elsevier.com/locate/jhazmat

Parameter identification for continuous point emission source based on Tikhonov regularization method coupled with particle swarm optimization algorithm

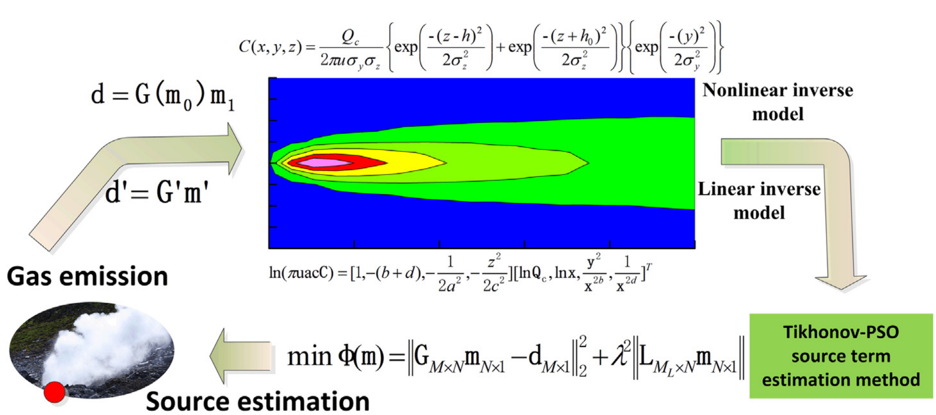
Denglong Ma[a,c], Wei Tan[a], Zaoxiao Zhang[b,c,*], Jun Hu[d]

[a] School of Food Equipment Engineering and Science, Xi'an Jiaotong University, No.28 Xianning West Road, Xi'an 710049, PR China
[b] State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University, No.28 Xianning West Road, Xi'an 710049, PR China
[c] School of Chemical Engineering and Technology, Xi'an Jiaotong University, No.28 Xianning West Road, Xi'an 710049, PR China
[d] School of Chemical Engineering, Northwest University, No.229 Taibai North Road, Xi'an 710069, PR China

HIGHLIGHTS

- Tikhonov-PSO regularization method was proposed to estimate the hazardous gas source term.
- The method can estimate the source term without previous information.
- The method can identify the source parameters with reasonable confidence intervals.
- The linear method with converted model performs better than nonlinear method.
- High order regularization obtains more reasonable result than zero-order form.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 25 June 2016
Received in revised form 25 November 2016
Accepted 26 November 2016
Available online 2 December 2016

Keywords:
Contaminant emission
Inverse problem
Source estimation
Stochastic method

ABSTRACT

In order to identify the parameters of hazardous gas emission source in atmosphere with less previous information and reliable probability estimation, a hybrid algorithm coupling Tikhonov regularization with particle swarm optimization (PSO) was proposed. When the source location is known, the source strength can be estimated successfully by common Tikhonov regularization method, but it is invalid when the information about both source strength and location is absent. Therefore, a hybrid method combining linear Tikhonov regularization and PSO algorithm was designed. With this method, the nonlinear inverse dispersion model was transformed to a linear form under some assumptions, and the source parameters including source strength and location were identified simultaneously by linear Tikhonov-PSO regularization method. The regularization parameters were selected by L-curve method. The estimation results with different regularization matrixes showed that the confidence interval with high-order regularization matrix is narrower than that with zero-order regularization matrix. But the estimation results of different source parameters are close to each other with different regularization matrixes. A nonlinear Tikhonov-PSO hybrid regularization was also designed with primary nonlinear dispersion model to estimate the source parameters. The comparison results of simulation and experiment case showed that the linear Tikhonov–PSO method with transformed linear inverse model has higher computation efficiency than nonlinear Tikhonov-PSO method. The confidence intervals from linear Tikhonov-PSO are more reasonable

* Corresponding author at: State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University, No.28 Xianning West Road, Xi'an 710049, PR China.
E-mail addresses: zhangzx@mail.xjtu.edu.cn, zaoxiaoz@hotmail.com (Z. Zhang).

http://dx.doi.org/10.1016/j.jhazmat.2016.11.071
0304-3894/

than that from nonlinear method. The estimation results from linear Tikhonov-PSO method are similar to that from single PSO algorithm, and a reasonable confidence interval with some probability levels can be additionally given by Tikhonov-PSO method. Therefore, the presented linear Tikhonov-PSO regularization method is a good potential method for hazardous emission source parameters identification.

1. Introduction

It is not unusual that there is accidental release of hazardous gases from industrial or other fields. Gas emissions may spring from emergence explosions, sudden failure of storage tanks, reservoir and so on. For example, in carbon capture and storage (CCS) project, CO_2 gases storage underground may escape from the sequestration sites to the atmosphere. Hence, estimation of hazardous gas source parameters including source strength, source location and other source characters is vitally important when the accident occurs [1]. It is an inverse problem associated with forward atmospheric dispersion problem, which is a typically ill-posed and nonlinear problem [2,3]. In order to resolve this inverse problem, many methods have been developed. Direct solution with inverse dispersion equations suffers from its own ill-posed problem. Therefore it is difficult to obtain a satisfying result. Optimization methods have been used to identify the source terms successfully [4–9]. Nevertheless, uncertainty of estimation results is not considered with the optimization methods, but it does exist in the real world. The stochastic approximation method solves the problem with a probability density function [10,11], which is different from the optimization methods to obtain a possible solution by matching the estimation data with measurement within a reasonable tolerance. Bayesian inferences theory is often adopted in the stochastic approximation method and a probability distribution result at certain confidence levels can be obtained. Keats et al. [12], Guo et al. [13] and Schauberger et al. [14] identified the characters of source area by Bayesian estimationand Markov Chain Monte Carlo (MCMC) methods. Ma et al. [15] applied the minimum relative entropy (MRE) method, which based on probability theory, to identify the source parameters with the form of probability. Zhang et al. proposed a method with Kalman filter for source estimation in nuclear accidents [16,17]. However, the above stochastic approximation methods like MCMC often consume more computation time than optimization methods. Additionally, a lot of prior information such as measurement errors, parameter bounds and expected inputs should be determined previously in Bayesian estimation and MRE methods, but they are hard to be known in the real condition. Therefore, a method without prior error input and with reasonable uncertain intervals output should be considered.

Regularization method is a classical inverse method based on the least squares solution. In this method, the ill-posed inverse problem is replaced with a family of similar well-posed problems through the introduction of a regularization operator and a regularization parameter [18]. If some special method like L-curve is used to determine regularization parameter, the prior noise level is not required [2,3]. For a linear inverse problem, the uncertainty at some probability levels can also be obtained by the regularization method. Researchers have developed several regularization methods [19,20], which differ in their formulation of the regularization operator and selection of the regularization parameter. Among those, Tikhonov regularization is a widely applied technique for regularizing discrete ill-posed problems [21]. With Tikhonov regularization, the discrete form of the ill-posed equation is replaced with a well-posed minimization problem by adding a regularization term. Neupauer et al. applied Tikhonov regularization to recover the history of water contaminant [18]. Loris et al. applied nonlinear regularization techniques for 3D seismic tomography [22]. They reported that nonlinear L_1 method was much more efficient than classical L_2 minimization. Fan et al. presented a simplified Tikhonov regularization method for identifying the heat source [23]. In their regularization solution, the Hölder type stability estimate between the regularization solution and the exact solution was obtained. Kathirgamanath analyzed the feasibility of Tikhonov regularization for parameter estimation of atmospheric pollution source and found that the source parameters can be estimated easily by the solution of linear inverse problem with the knowledge of leakage rate [2]. However, the structure of his process for estimating source strength and location simultaneously was complex and negatively affected the computation efficiency. In this paper, an improved calculation method coupling Tikhonov regularization with particle swarm optimization (PSO) algorithm was presented to estimate the source parameters of hazardous gas emission in atmosphere.

2. Theory of Tikhonov regularization method

2.1. Basic theory of Tikhonov regularization

With the common least squares method to solve a problem of $\min\|\mathbf{G}m - \mathbf{d}\|_2$, a quadratic inequality constraint should be given because the noises do exist in the data,

$$\min\|\mathbf{G}m - \mathbf{d}\|_2 \le \delta \tag{1}$$

where $\mathbf{G}$ is the transfer matrix of linear problem $\mathbf{Gm} = \mathbf{d}$; $\mathbf{m}$ is the parameter matrix; $\mathbf{d}$ is measurement data; δ is related with data noises from measurements and model. In many common least squares methods, the value of δ is selected based on knowledge or a good guess of the noise level. However, with the Tikhonov's regularization, the problem of finding a solution is transformed into the following minimization problem [2,3]:

$$\min \boldsymbol{\phi}(\boldsymbol{m}) = \|\mathbf{G}_{M\times N}\boldsymbol{m}_{N\times 1} - \mathbf{d}_{M\times 1}\|_2^2 + \lambda^2\|\mathbf{L}_{M_L\times N}\boldsymbol{m}_{N\times 1}\|_2^2 \tag{2}$$

where M is the length of $\mathbf{d}$, and N is the number of estimation parameter; λ is the regularization parameter; $\mathbf{L}$ is an operator matrix and $\|\cdot\|$ denotes the Euclidian norm. Generally, the rank of $\mathbf{L}$ is M_L and it satisfies$M \ge N \ge M_L$. The first term on the right-hand side of Eq. (2) represents the square norm of the difference between the measured and the model-predicted system state. The second term represents the square norm of a specific property of the model which depends on the operator matrix, $\mathbf{L}$, where parameter λ determines how well the solution fits the data. The parameter λ has to be adjusted to make the solution fit the data in some optimal way. The error in the Tikhonov regularization solution depends on both the noise level and on the regularization parameter λ. A good regularization parameter should yield a fair balance between the data error and the regularization error in the regularized solution. The selection of the optimal regularization parameter is based on minimizing the total error. Generalized Cross Validation (GCV) [24] L-curve [25] and Quasi-optimality criterion [26] are two most popular methods, which do not require any information about the noise level.