Atmospheric dispersion prediction and source estimation of hazardous gas using artificial neural network, particle swarm optimization and expectation maximization

Sihang Qiu[1,2], Bin Chen[1]*, Rongxiao Wang[1], Zhengqiu Zhu[1], Yuan Wang[3], Xiaogang Qiu[1]

[1] *College of System Engineering, National University of Defense Technology, 410073 Changsha, China*

[2] *Faculty of Electrical Engineering, Mathematics and Computer Science, Delft University of Technology, 2628 XE Delft, the Netherlands*

[3] *College of Territorial Resources and Tourism, Anhui Normal University, 241003 Wuhu, China*

** Corresponding Author. Email address: nudtcb9372@gmail.com*

Highlights

- A dispersion prediction method based on artificial neural network is proposed.
- The method uses particle swarm optimization and expectation maximization to estimate the dispersion source.
- The method has high accuracy in dispersion prediction and source estimation.
- The method is verified by a field study.

Abstract

Hazardous gas leak accident has posed a potential threat to human beings. Predicting atmospheric dispersion and estimating its source become increasingly important in emergency management. Current dispersion prediction and source estimation models cannot satisfy the requirement of emergency management because they are not equipped with high efficiency and accuracy at the same time. In this paper, we develop a fast and accurate dispersion prediction and source estimation method based on artificial neural network (ANN), particle swarm optimization (PSO) and expectation maximization (EM). The novel method uses a large amount of pre-determined scenarios to train the ANN for dispersion prediction, so that the ANN can predict concentration distribution accurately and efficiently. PSO and EM are applied for estimating the source parameters, which can effectively accelerate the process of convergence. The method is verified by the Indianapolis field study with a SF_6 release source. The results demonstrate the effectiveness of the method.

Keywords: atmospheric dispersion; source estimation; neural network; particle swarm optimization (PSO); expectation maximization (EM).

1 Introduction

Hazardous gas leakage accident has brought huge damage to the society. For example, Bhopal accident caused thousands of deaths due to the methyl isocyanate gas leak accident (Varma and Guest, 1993). Consequently, it is of paramount importance to monitor industrial emission and use the monitoring data to estimate the release rate and location of emission source. To estimate the emission source, an atmospheric dispersion simulation (ADS) model and a parameter estimation algorithm with high accuracy and efficiency are necessary. The ADS model is used for predicting the concentration distribution, and the parameter estimation algorithm is used for finding the optimal source parameters to make ADS model output as close as possible to the actual measurement.

Many ADS modeling methods have been developed by researchers. Gaussian model is a typical and fast tool for atmospheric dispersion prediction, whose expression is quite simple. Usually, the Gaussian dispersion model is suitable for emergency management due to its high efficiency. However, its mechanism is too simple to give the accurate prediction, whose limitations are: it only supports low wind speed; it only supports straight-line trajectories; it assumes steady-state atmosphere; it has no memory of previous emissions. The Lagrangian model is very common in meteorological modeling tools based on random walk theory (Draxler and Rolph, 2012; Stein et al., 2015; Wilson and Sawford, 1996). It can simulate the atmospheric dispersion process in relatively complex meteorological conditions and global scale. This model is more suitable in large-scale scenarios, but the investigation area of hazardous gas leakage accident generally cannot reach that scale. Integrated model combines different dispersion model together, which is popular in commercial software for risk analysis such as PHAST (Connan et al., 2013; Hanna et al., 2008). However, the integrated models also need few minutes to calculate and the result is not always accurate. In complex environments, CFD model is currently the optimal option to obtain accurate prediction results (Hanna et al., 2009; Mazzoldi et al., 2008; Pontiggia et al., 2009). However, the CFD model needs long computation time, usually measured in hours or even days, which restricts the application of CFD in emergency management. Furthermore, a common problem of these methods is that some input parameters are quite difficult to measure and quantify. Therefore, researchers proposed the methods that can use pre-determined scenarios to train ANN for decision and bypass some troubling parameters (Krasnopolsky and Schiller, 2003; So et al., 2010). A previous study also used the integration of machine learning algorithms and traditional ADS models to predict the contaminant dispersion(Ma and Zhang, 2016). The high accuracy of these studies represents that the ANN could be a useful tool for pollution forecasting and risk analysis.

In terms of source parameters estimation, parameters could be determined by estimating their posterior distribution or finding the maximum likelihood estimate. Thus, most source estimation methods are based on Bayesian inference or optimization algorithms (Hutchinson et al., 2017). Markov Chain Monte Carlo (MCMC) algorithm is usually used for posterior distribution estimation in source estimation problem (Borysiewicz et al., 2012; Keats et al., 2007; Tierney, 1994; Yee, 2007). Some filtering methods also apply the Bayesian theory to update the source parameters (Huber, 2014; Wawrzynczak et al., 2014; Zhang and Wang, 2013). Optimization algorithms are widely implemented to find the solution of minimum cost or maximum likelihood, whose theoretical basis is maximum likelihood estimation (MLE) principle (Qiu et al., 2016; Sharan et al., 2009). Intelligent optimization methods are usually used, such as particle swarm optimization (PSO) (Eberhart and Kennedy, 1995; Qiu et al., 2016), simulated annealing (Thomson et al., 2007) and genetic algorithm (Allen et al., 2007). In dispersion source estimation problem, the release rate and location of source should be estimated. When the source location is known, these methods could be quite effective because we only have to estimate one parameter (release rate) (Chai et al., 2015; Eslinger et al., 2014; Katata et al., 2015). However, if the source location is unknown, the problem becomes more complicated because the algorithm may be difficult to converge. Even if the algorithm can converge successfully, estimating all these parameters together is a quite time-consuming task due to the huge search space. Therefore, expectation maximization (EM) algorithm is introduced to address this problem (Do and Batzoglou, 2008). In the E-step, the expected value of source location is estimated using ANN and PSO, while in the M-step, the estimated release rate is updated on the basis of MLE.

In this paper, the proposed method is able to estimate the emission source using ANN-based dispersion prediction and PSO-EM-based parameter estimation. To verify the proposed method, SF_6 dispersion data from Indianapolis field study is applied to validate whether the method is feasible in practice.

2 Methods

2.1 Workflow

In order to predict the concentration distribution and estimate the dispersion source, the workflow of the proposed method includes several steps:

A. Obtaining a large number of release scenarios covering nearly all possibilities from gas trace experiment. If it is difficult to control the variables of field experiment, release scenarios can also be obtained from simulation experiment.

B. Extracting input and target dataset from release scenarios. To predict the concentration of the interest point, the input data should contain the information including source term, meteorological parameters and the location of interest point. The target data should be able to present the value or level of gas concentration of the interest point.

C. Training and testing of the ANN. The input and target dataset extracted from release scenarios in step B is used for ANN training and testing to construct an ANN-based ADS model.

D. Configuration of the source estimation parameters. Both temporal and spatial investigation regions are defined in this step. Furthermore, initial parameters of the source estimation algorithm should be determined before inverse calculation.

E. Estimating the source of atmospheric dispersion using PSO or the combination of PSO and EM.

2.2 Structure of ANN

Generally, complicated ADS model such as CFD needs quite long time to compute the concentration distribution, while simple model can hardly give the accurate results. To address this problem, ANN is used to predict the concentration of the interest point with high efficiency and accuracy (Ma and Zhang, 2016).

Table 1 Common parameters for atmospheric dispersion model.

Parameters	Symbol	Unit
Downwind distance	D_x	m
Crosswind distance	D_y	m
Height of source	H	m
Height of interest point	z	m
Release rate	q	g s^{-1}
Atmospheric stability class	STA	/
Wind direction	d	deg
Wind speed	v	m s^{-1}
Mixing height	z_m	m
Cloud height	z_c	m
Cloud cover	p_c	%
Temperature	T	K

To satisfy the emergency requirements, the input data of the ANN should be easily to obtain. A rough idea is using all the measured parameters shown in Table 1 as the input of the ANN. However, it is quite difficult to train the ANN if we directly put these parameters into input layer because features of the atmospheric dispersion should be extracted before training. Generally, the concentration of hazardous gas follows Gaussian distribution on crosswind direction. Moreover, the concentration of a specific point is approximately proportional to the release rate and inversely proportional to the wind speed. Due to these features, as shown in Fig. 1, we use release rate q, reciprocal of the wind speed $1/v$, and two Gaussian parameters (G_y and G_z) on y- and z-axes as ANN input. The expressions of G_y and G_z are shown in Eq. (1) according to the experience of Gaussian dispersion model.

$$\begin{cases} G_y = \exp\left(-\dfrac{D_y^2}{2\sigma_y^2}\right), \\ G_z = \exp\left[-\dfrac{(z+H)^2}{2\sigma_z^2}\right] + \exp\left[-\dfrac{(z-H)^2}{2\sigma_z^2}\right] \end{cases} \tag{1}$$

where D_y and z represents the crosswind distance and the height of the interest point respectively. H is the height of the emission point. σ_y and σ_z, which represent the deviation of the Gaussian distribution, are the Gaussian dispersion coefficients affected by downwind distance D_x and atmospheric stability. Gaussian parameters, wind parameters and source term parameters are inputs of traditional Gaussian dispersion model. They are very common and easy-to-measure parameters (also simple to calculate in simulation software). Moreover, Gaussian dispersion model has already been extensively used in source estimation methods. Thus, by using these parameters as the input of ANN, we can directly substitute ANN-based atmospheric dispersion model for Gaussian model in source estimation, without changing inputs.

The number of neurons in the hidden layer could be determined by evaluating some important criteria (e.g. coefficient of determination). The output layer has only one neuron, meaning the concentration of the interest point. The algorithm and detailed process of ANN training is not in our research scope, so the ANN will be directly trained by MATLAB neural network toolbox in this paper (MATLAB, 2010).

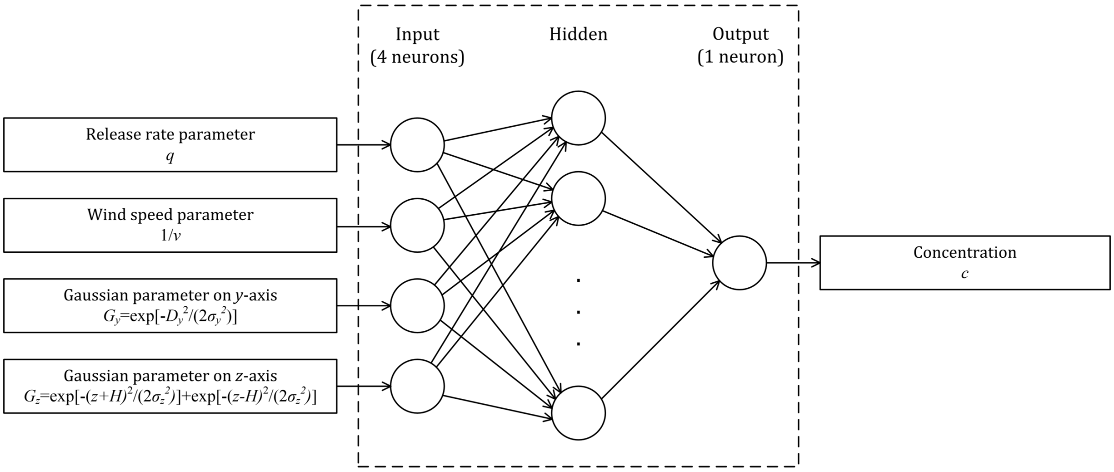

Fig. 1 Structure of the fitting ANN.

2.3 Quantifying release rate by PSO

The hazardous gas leak accidents can be classified into two categories. The category 1 is the accident that the source location is already known, while the category 2 is the accident that source location is unknown. For the category 1, we can just use PSO algorithm to quantify the release rate, which is explained in this section. As for category 2, the method used for estimating source will be introduced in section 2.4.

PSO algorithm uses specific rules to drive particles to quantify the emission source (i.e. find the optimal release rate). Because the theory and deduction of PSO are beyond the scope of this paper, we directly introduce the detailed steps to find the optimal release rate. First, generate N particles with random release rate $q_i^{(0)}$ in the appropriate range, where $i \in 1,2,\ldots,N$. Then, set the best known release rate of each particle q_p^i, whose value equals to its initial release rate $q_i^{(0)}$. After that, initialize a random velocity of each particle, and keep particles updating according to Eq. (2) until the algorithm converges.

$$\begin{cases} v_i^{(t+1)} = w \cdot v_i^{(t)} + c_1 r_1 (q_i^p - q_i^{(t)}) + c_2 r_2 (q_g - q_i^{(t)}) \\ q_i^{(t+1)} = q_i^{(t)} + v_i^{(t)} \end{cases} . \tag{2}$$

where v_i^t represents the velocity of particle i at step t. $q_i^{(t)}$ means the release rate of particle i at step t. r_1 and r_2 are random number follows $U(0,1)$. w, c_1, and c_2 are PSO parameters that can be adjusted to improve the performance of PSO algorithm. In this paper, c_1 and c_2 equal to 2, and w equals to $2/t$.

At each step, the best known release rate of each particle q_i^p will be updated if $p(q_i^{(t+1)}) > p(q_i^p)$, where $p(q)$ is likelihood function (as shown in Eq. (3)).

$$p(q) \propto \exp\left\{-\frac{1}{2\sigma_e^2}\left\|f(q)-D\right\|^2\right\} \quad (3)$$

where q is release rate; D is concentration measurements; $f(q)$ represents the output of ADS model with input q; σ_e is measurement error deviation. Because σ_e never changes when the algorithm is running, we only have to compare the cost function $J(q)=\left\|f(q)-D\right\|^2$.

Furthermore, the best known release rate of all particles q_g will be updated if $p(q_i^p) > p(q_g)$ at each step. When the algorithm meets the convergence condition and the iteration terminates, q_g becomes the optimal solution of PSO, which is also the rough expected release rate θ_q of the emission source based on MLE principle.

2.4 Estimating source by EM

It is also possible that people do not know the location of the emission source. To estimate the location (x, y), the release rate q should be estimated first. However, in order to estimate the release rate q, the location (x, y) should be determined before. If estimate all parameters together, the algorithm will become difficult to converge. Consequently, as shown in Fig. 2, EM algorithm is introduced to address this conflict.

First, the initial value of release rate should be estimated, denoted by $\theta_q^{(0)}$. This value can be determined according to prior information or the experience of expert. Then, the algorithm comes to the E-step. In this step, the source location should be updated if the release rate is assumed to be $\theta_q^{(i)}$. In this paper, we use the combination of ANN and PSO to find the optimal solution as the estimation of expectation. As shown in Eq. (4), the likelihood function is quite similar to Eq. (3), where the variable to be optimized is the source location now.

$$p(x,y) \propto \exp\left\{-\frac{1}{2\sigma_e^2}\left\|f(x,y)-D\right\|^2\right\} \quad (4)$$

After source location being estimated, the algorithm comes to the M-step. The target of this step is to find the release rate with maximum likelihood. In this step, we can use the method introduced in section 2.3 to maximize the likelihood for estimating the optimal release rate $\theta_q^{(i+1)}$. The estimated release rate $\theta_q^{(i+1)}$ is used as expected release rate in next iteration until the algorithm converges.

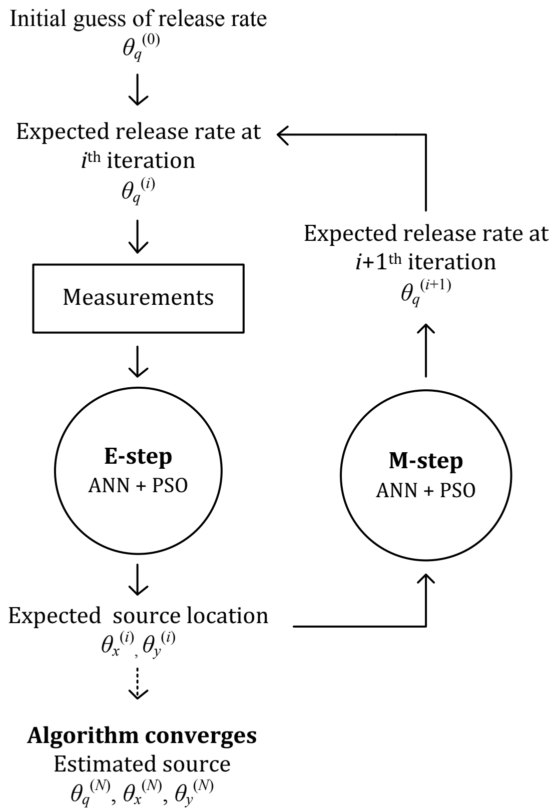

Fig. 2 Mechanism of EM algorithm for source estimation

3 Application: Indianapolis field study

The main target of the Indianapolis field study is to simply test whether the proposed method is feasible in real situation. The Indianapolis experiment was implemented during 16 September to 12 October in 1985 (Hanna et al., 2001). Researchers used sulfur hexafluoride (SF_6) to trace the dispersion plume emitted from an 83.8m height stack. The WGS84 coordinate of the emission source is (39.8N latitude, 86.2E longitude), and its Cartesian coordinate is set as $(0,0)$. During 16 September to 12 October, monitoring stations has sampled totally 170 hours. Meteorological data were sampled from a 94 m height monitoring tower in a bank and three other 10 m height monitoring towers at urban, suburban, and rural respectively. About 160 ground-level concentration monitoring stations were established at the distance ranging from 0.25 to 6.0 km to the emission source.

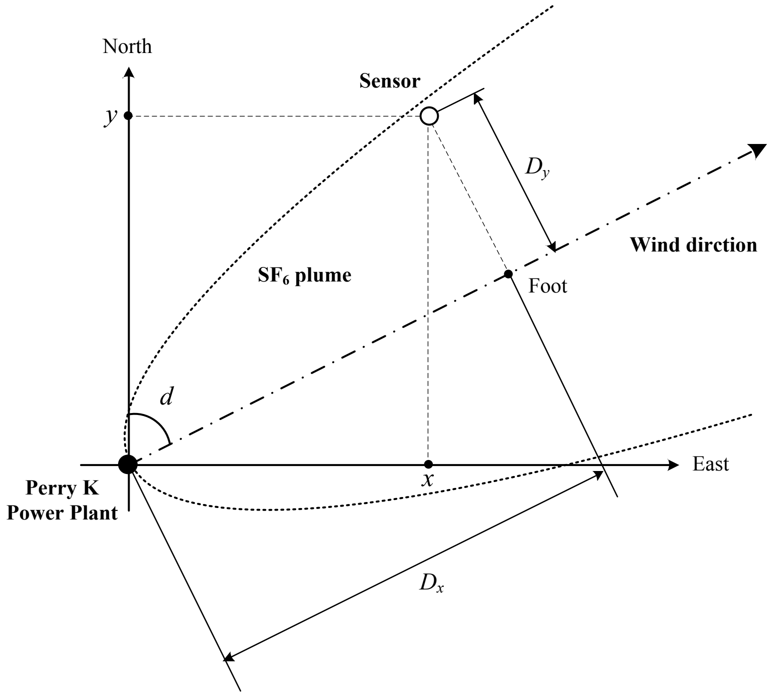

Fig. 3 The scenario of Indianapolis field study

Based on the range and size of the Indianapolis field data, the configuration of ANN and PSO can be consequently determined. In terms of the input of the ANN, the release rate parameter q and wind speed parameter $1/v$ can be directly calculated using Indianapolis field data. Turn to the expressions of Gaussian parameters G_y and G_z, it can be found that the values of D_x, D_y, σ_y and σ_z are not in the measured data. Therefore, the downwind distance D_x and crosswind distance D_y should be first calculated using wind direction d and Cartesian coordinates (x, y) of the sensor according to Fig. 3. After D_x and D_y being obtained, Gaussian dispersion coefficient σ_y and σ_z can also be calculated according to Vogt's scheme (Vogt, 1977). Afterwards, we use field data of 16 September for testing (1152 samples). Remaining data from 17 September to 12 October is used for training and validation (70% and 30% respectively, 25396 samples in total). The training algorithm of the ANN is Levenberg-Marquardt, whose maximum number of epochs is 1000 (if early stopping is not triggered). If validation accuracy shows no improvement more than 6 epochs, the early stopping will be triggered. Training process is conducted via MATLAB neural network toolbox. The unit of release rate is kg s^{-1} and the PSO algorithm in EM has 100 particles with initial random position satisfies that $(x_i^{(0)}, y_i^{(0)}) \in \{(x, y) \mid -6 < x < 6, -6 < y < 6\}$ (unit: km).

The number of neurons in the hidden layer can be adjusted by users. For Indianapolis experiment, by plotting the R^2 coefficient as a function of number of neurons in the hidden layer, we can find that R^2 increases at first and then basically follows downwards trend when the number of neurons in the hidden layer increases. We finally find that the ANN can obtain the highest R^2 when the hidden layer of the ANN has 18 neurons, as can be seen in Fig. 4.

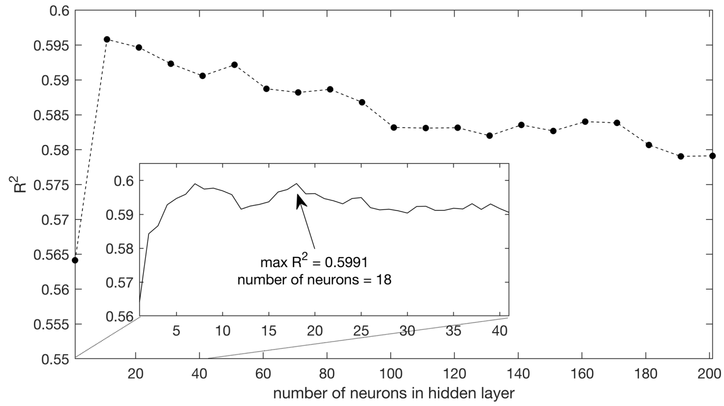

Fig. 4 The plot of R2 as a function of the number of neurons in hidden layer

Fig. 5 shows the prediction result of 16 September, 1985. Because the observed/predicted concentrations of lots of sensors are zero (sensors not in downwind direction), these unimportant samples could make performance artificially high. To evaluate the prediction result in a fair and reasonable way, these “zero” samples are removed before performance analysis. Fig. 5 (a) demonstrates the comparison between observed measurements and ANN prediction result. Obviously, the predicted concentrations are basically distributed around the perfect fitting line y=x. Except for R^2 (as can be seen in Fig. 4), the factor of two (FAC2), fractional bias (FB) and the normalized mean square error (NMSE) can also be used to evaluate the performance of atmospheric dispersion prediction (Lauret et al., 2016). The FAC2 of the prediction result is 0.582, proving that the prediction method has acceptable performance according criteria of a “good” model (FAC2 > 0.5) (Chang et al., 2004). The FAC2 over and under prediction lines (y=2x and y=x/2 respectively) are also shown in the figure. Furthermore, the FB of the result is -0.0292 and the NMSE is 0.6861, which are quite close to zero. Fig. 5 (b) shows the concentration distribution calculated by the ANN. The concentration distribution heat map can reflect the shape of the hazardous gas plume, which illustrates that the over-fitting problem does not happen on this ANN. Therefore, the trained ANN can be effectively used in further source estimation.

In terms of calculation duration estimation, when the number of neurons in the hidden layer equals to 18 (the optimal number according to R^2 plot), the program spends 197.729 seconds for training Indianapolis data (25396 samples) for 50 times (macOS High Sierra version 10.13.2, 3.1 GHz Intel Core i5, 8 GB 2133 MHz LPDDR3), which makes average training duration approximately equal to 3.955 seconds. When applying trained ANN to calculate concentration of all sensors over September 16th, 1985, the ANN spends 3.045 seconds for running 50 times. Therefore, the average calculation duration in this case equals to 0.061 seconds. Further, it is also quite important to estimate the concentration distribution in a specific area. When estimating the concentration distribution in a rectangular/square area (with 100×100 grids), the average calculation duration of 50-times running is 0.097 (4.828/50) seconds.

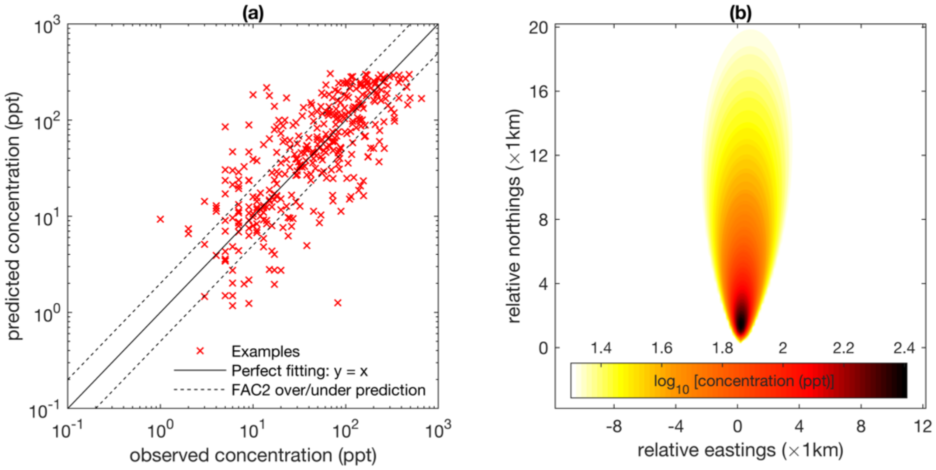

Fig. 5 The result of SF_6 dispersion prediction based on ANN. (a) Comparison of ANN output and measurements. (b) Concentration distribution generated by ANN.

If the source location is known, using 10 particles can make PSO converges very soon. To present the PSO process more clearly, in Fig. 6, only 3 particles are used to slow down the PSO convergence speed. Fig. 6 shows 20 iterations of PSO algorithm. The optimal release rate is finally stable at q_g = 5.118×10^{-3} kg/s. Compared to real release rate q_r = 4.940×10^{-3} kg/s, the relative error is only 3.61%. Therefore, the proposed source estimation method has high accuracy if the source location is known.

If the source location is an unknown parameter, the integration of ANN, PSO and EM is used to locate and quantify the emission source. The EM algorithm converges very soon within five steps. In the end, the estimated release rate is q_g = 5.507×10^{-3} kg/s (relative error is 9.99%), and the location error of the source is 2.116×10^{-3} km (only accounts for 1.76% of the investigate area length 12 km), which means the proposed method is also acceptable in practice if the source location is unknown.

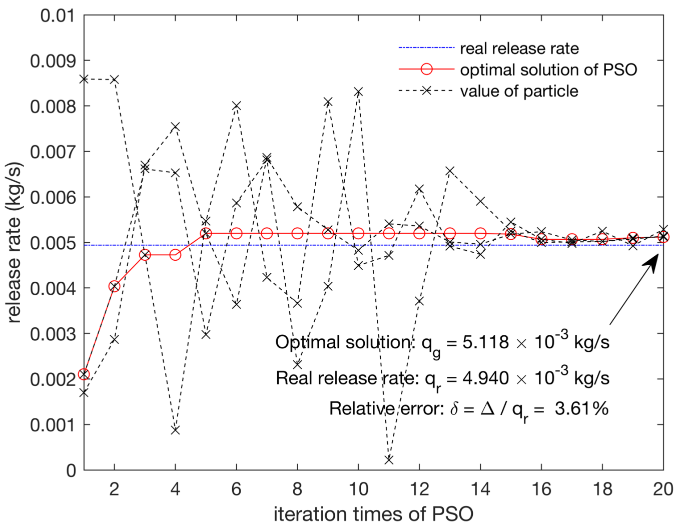

Fig. 6 Process of PSO algorithm when finding optimal release rate.

4 Conclusions

This paper proposed a novel method for quantifying and locating the emission source using ANN, PSO and EM. The Indianapolis field study is implemented to prove that this method is feasible in practice. The results of the field study show that the proposed method is able to estimate the emission source with acceptable accuracy and efficiency.

Hazardous gas leak accident needs quick response and high accuracy. The ANN-based prediction method is equipped with these two features. In terms of EM algorithm, the advantages of the proposed method are: (1) using ANN to predict gas dispersion accurately; and (2) applying EM to address the problem of source estimation efficiently.

Atmospheric dispersion prediction and source estimation based on ANN, PSO and EM could be used in emergency management by two ways in the future: (1) Field experiments could be conducted in chemical industry parks or nuclear power plants to sample enough data for ANN training. (2) If it is difficult (or even impossible) to collect sufficient data or parameters from field study, atmospheric dispersion simulation and risk analysis software could be used to generate "pseudo" scenarios and corresponding data for ANN training. Once the accident happens in these places (chemical industry parks or nuclear power plants), the integration of pre-trained ANN and source estimation methods can be applied to analyze the accident.

However, the method proposed in this paper also has some problems. The current method uses the average wind direction and wind speed as input, which requires that the meteorological condition should be relatively stable. Furthermore, the ANN prediction result beyond the training range is also not accurate enough. Future work will involve the complex release scenario containing terrain, plants and facilities. Current problems will also be addressed in the future.

Acknowledgements

This study is supported by National Key Research & Development (R&D) Plan under Grant No. 2017YFC0803300, the National Natural Science Foundation of China (Grant Nos. 71673292, 61503402 & 61673388), Guangdong Key Laboratory for Big Data Analysis and Simulation of Public Opinion, and Young Elite Science Sponsorship Program by China Association for Science and Technology (No. YESS20150082).

References

Allen, C.T., Young, G.S., Haupt, S.E., 2007. Improving pollutant source characterization by better estimating wind direction with a genetic algorithm. Atmospheric Environment 41, 2283-2289.

Borysiewicz, M., Wawrzynczak, A., Kopka, P., 2012. Bayesian-Based Methods for the Estimation of the Unknown Model's Parameters in the Case of the Localization of the Atmospheric Contamination Source. Foundations of Computing and Decision Sciences 37, 253.

Chai, T., Draxler, R., Stein, A., 2015. Source term estimation using air concentration measurements and a Lagrangian dispersion model – Experiments with pseudo and real cesium-137 observations from the Fukushima nuclear accident. Atmospheric Environment 106, 241-251.

Chang, J.C., Hanna, S.R., 2004. Air quality model performance evaluation. Meteorology and Atmospheric Physics 87, 167-196.

Connan, O., Smith, K., Organo, C., Solier, L., Maro, D., Hébert, D., 2013. Comparison of RIMPUFF, HYSPLIT, ADMS atmospheric dispersion model outputs, using emergency response procedures, with 85Kr measurements made in the vicinity of nuclear reprocessing plant. Journal of Environmental Radioactivity 124, 266-277.

Do, C.B., Batzoglou, S., 2008. What is the expectation maximization algorithm? Nat Biotech 26, 897-899.

Draxler, R.R., Rolph, G.D., 2012. Evaluation of the Transfer Coefficient Matrix (TCM) approach to model the atmospheric radionuclide air concentrations from Fukushima. Journal of Geophysical Research: Atmospheres 117, n/a-n/a.

Eberhart, R., Kennedy, J., 1995. A new optimizer using particle swarm theory, Micro Machine and Human Science, 1995. MHS '95., Proceedings of the Sixth International Symposium on, pp. 39-43.

Eslinger, P.W., Biegalski, S.R., Bowyer, T.W., Cooper, M.W., Haas, D.A., Hayes, J.C., Hoffman, I., Korpach, E., Yi, J., Miley, H.S., Rishel, J.P., Ungar, K., White, B., Woods, V.T., 2014. Source term estimation of radioxenon released from the Fukushima Dai-ichi nuclear reactors using measured air concentrations and atmospheric transport modeling. Journal of Environmental Radioactivity 127, 127-132.

Hanna, S., Dharmavaram, S., Zhang, J., Sykes, I., Witlox, H., Khajehnajafi, S., Koslan, K., 2008. Comparison of Six Widely-Used Dense Gas Dispersion Models for Three Actual Railcar Accidents, in: Borrego, C., Miranda, A.I. (Eds.), Air Pollution Modeling and Its Application XIX. Springer Netherlands, Dordrecht, pp. 443-451.

Hanna, S.R., Egan, B.A., Purdum, J., Wagler, J., 2001. Evaluation of the ADMS, AERMOD, and ISC3 dispersion models with the OPTEX, Duke Forest, Kincaid, Indianapolis and Lovett field datasets. International Journal of Environment and Pollution 16, 301-314.

Hanna, S.R., Hansen, O.R., Ichard, M., Strimaitis, D., 2009. CFD model simulation of dispersion from chlorine railcar releases in industrial and urban areas. Atmospheric Environment 43, 262-270.

Huber, M.F., 2014. On-line Dispersion Source Estimation using Adaptive Gaussian Mixture Filter. IFAC 2014.

Hutchinson, M., Oh, H., Chen, W.-H., 2017. A review of source term estimation methods for atmospheric dispersion events using static or mobile sensors. Information Fusion 36, 130-148.

Katata, G., Chino, M., Kobayashi, T., Terada, H., Ota, M., Nagai, H., Kajino, M., Draxler, R., Hort, M.C., Malo, A., Torii, T., Sanada, Y., 2015. Detailed source term estimation of the atmospheric release for the Fukushima Daiichi Nuclear Power Station accident by coupling simulations of an atmospheric dispersion model with an improved deposition scheme and oceanic dispersion model. Atmos. Chem. Phys. 15, 1029-1070.

Keats, A., Yee, E., Lien, F.-S., 2007. Bayesian inference for source determination with applications to a complex urban environment. Atmospheric Environment 41, 465-479.

Krasnopolsky, V.M., Schiller, H., 2003. Some neural network applications in environmental sciences. Part I: forward and inverse problems in geophysical remote measurements. Neural Networks 16, 321-334.

Lauret, P., Heymes, F., Aprin, L., Johannet, A., 2016. Atmospheric dispersion modeling using Artificial Neural Network based cellular automata. Environmental Modelling & Software 85, 56-69.

Ma, D., Zhang, Z., 2016. Contaminant dispersion prediction and source estimation with integrated Gaussian-machine learning network model for point source emission in atmosphere. Journal of Hazardous Materials 311, 237-245.

MATLAB, 2010. Version 7.11.0. The MathWorks Inc., Natick, Massachusetts.

Mazzoldi, A., Hill, T., Colls, J.J., 2008. CFD and Gaussian atmospheric dispersion models: A comparison for leak from carbon dioxide transportation and storage facilities. Atmospheric Environment 42, 8046-8054.

Pontiggia, M., Derudi, M., Busini, V., Rota, R., 2009. Hazardous gas dispersion: A CFD model accounting for atmospheric stability classes. Journal of Hazardous Materials 171, 739-747.

Qiu, S., Chen, B., Zhu, Z., Wang, Y., Qiu, X., 2016. Source term estimation using air concentration measurements during nuclear accident. Journal of Radioanalytical and Nuclear Chemistry, 1-14.

Sharan, M., Issartel, J.-P., Singh, S.K., Kumar, P., 2009. An inversion technique for the retrieval of single-point emissions from atmospheric concentration measurements. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Science 465, 2069.

So, W., Koo, J., Shin, D., Yoon, E.S., 2010. The Estimation of Hazardous Gas Release Rate Using Optical Sensor and Neural Network. Computer Aided Chemical Engineering Volume 28, 199-204.

Stein, A.F., Draxler, R.R., Rolph, G.D., Stunder, B.J.B., Cohen, M.D., 2015. NOAA's HYSPLIT atmospheric transport and dispersion modeling system. Bull. Amer. Meteor. Soc. 96, 2059-2077.

Thomson, L.C., Hirst, B., Gibson, G., Gillespie, S., Jonathan, P., Skeldon, K.D., Padgett, M.J., 2007. An improved algorithm for locating a gas source using inverse methods. Atmospheric Environment 41, 1128-1134.

Tierney, L., 1994. Markov Chains for Exploring Posterior Distributions. 1701-1728.

Varma, D.R., Guest, I., 1993. The Bhopal accident and methyl isocyanate toxicity. Journal of Toxicology and Environmental Health 40, 513-529.

Vogt, K.J., 1977. Empirical investigations of the diffusion of waste air plumes in the atmosphere. Nucl. Technol.; (United States) 34:1.

Wawrzynczak, A., Kopka, P., Borysiewicz, M., 2014. Sequential Monte Carlo in Bayesian Assessment of Contaminant Source Localization Based on the Sensors Concentration Measurements, in: Wyrzykowski, R., Dongarra, J., Karczewski, K., Waśniewski, J. (Eds.), Parallel Processing and Applied

Mathematics: 10th International Conference, PPAM 2013. Springer, Berlin, Heidelberg, pp. 407-417.

Wilson, J.D., Sawford, B.L., 1996. Review of Lagrangian stochastic models for trajectories in the turbulent atmosphere. Boundary-Layer Meteorology 78, 191-210.

Yee, E., 2007. Bayesian probabilistic approach for inverse source determination from limited and noisy chemical or biological sensor concentration measurements, Chemical and Biological Sensing VIII. Edited by Fountain, Augustus W., III. Proceedings of the SPIE, pp. 65540W-65540W-65512.

Zhang, Y., Wang, L., 2013. Particle Filtering Method for Source Localization in Wireless Sensor Network. Advanced Technology in Teaching: Selected papers from the 2012 International Conference on Teaching and Computational Science (ICTCS 2012), 517-523.