MSC 00A72 DOI: 10.14529/mmp230306

PARAMETERS IDENTIFICATION ALGORITHM FOR THE SUSUPLUME AIR POLLUTION PROPAGATION MODEL

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The article presents the method of identifying the parameters of a dynamic dispersion calculation model SUSUPLUME. It is supposed that the model parameters contain not only the characteristics of the atmosphere and the pollutant, but also information about the influence of other particular conditions such as terrain, building, background, etc. The model parameters are configured based on instrumental measurements of concentrations of pollutants in the atmospheric air in the surface layer (2 meters above ground level). Three identification strategies are considered: identification of parameters by all measurements, identification of parameters by measurements of a given source and identification of parameters using another approved model. A method for weighing these strategies is proposed in the issue. The article also provides objective functions for optimization criteria, an acceptable set of parameters, an algorithm for solving an optimization problem, a decision tree of a feasible set and a global optimization algorithm.

Keywords: SUSUPLUME model; global optimization; ecology; propagation of pollutants in the atmosphere.

Introduction

The economic activity of industrial enterprises is associated with the probability of damaging the environment. Currently, most of them do not have operational analysis systems to control environmental risks.

The authors have created a software system "Ecomonitor" for industrial enterprises, which allows you to visualize the current pollution propagation, predict the environmental risks and identify the sources that have the greatest influence on control points in a given area. This system is based on the developed mathematical model SUSUPLUME [1]. The model is created for practical use, which takes into account the limited computing resources of enterprises. The model also provides online monitoring of the spread of pollutants in the atmosphere in real time.

Mathematical models for calculating the spread of emissions in the atmosphere are divided into Gaussian, Lagrangian and Eulerian models [2–4]. The developed mathematical model SUSUPLUME is a trajectory Gaussian model. There is a large number of trajectory models around the world, the most known of which are CALPUFF [5,6], RAPTAD [7,8], HYSPLIT [9], RIMPUFF [10] and FLEXPART [11]. The question of setting up mathematical models is considered rather complicated in the practical part and the methodology of determining the model parameters depends on their accuracy and the scope of their use.

The most common approach to find model parameters is to determine physical quantities based on instrumental measurements. For example, meteorological parameters and the dimensions of the calculated grid can be involved. Another method of finding parameters is to find the coefficients characterizing the operation of emission sources.

In this article, the authors describe the implementation of the algorithm of determining the parameters of the SUSUPLUME model based on measurements of concentrations of pollutants at control points in the atmospheric surface layer. It is supposed that the model parameters contain not only the characteristics of the atmosphere and the pollutant, but also information about the influence of other particular conditions.

1. A Pollution Propagation Model from Point Sources

The SUSUPLUME model [1] is presented briefly in this section. Let the concentration of pollutants at point (x, y, z) at time t be written as $C(x, y, z, t) = k \sum_{i=1}^{N} C_i(x, y, z, t)$, where C_i is the concentration created by the i-th source, N is the total number of point sources, k is the coefficient of the model, which describes the conditions of pollutants accumulation. The concentration of pollution generated by the i-th source can be described by the relation

$$C_i(x, y, z, t) = \int\limits_{t-\frac{2D}{u_{min}}}^{t} \frac{m_{g,i}(t_0) e^{-\left(\frac{(x_i(t_0,t)-x)^2}{2\sigma_x^2(\hat{x})} + \frac{(y_i(t_0,t)-y)^2}{2\sigma_y^2(\hat{x})}\right)}}{(2\pi)^{3/2}\sigma_x(\hat{x})\sigma_y(\hat{x})\sigma_z(\hat{x})} \left[\begin{array}{c} e^{-\frac{(z_i(t_0,t)-z)^2}{2\sigma_z^2(\hat{x})}} + \\ +e^{-\frac{(-z_i(t_0,t)-z)^2}{2\sigma_z^2(\hat{x})}} \end{array} \right] dt_0,$$

where D is the diameter of the concentration calculation area, u_{min} is the minimum wind speed, $m_{g,i}(t_0)$ is the pollutants intensity created by the i-th source at time t_0, $\sigma_x, \sigma_y, \sigma_z$ are functions which describes the diffusion rate of pollutants depending on time. These functions can be calculated as

$$\sigma_x = \sigma_y = \frac{\hat{x}}{\sqrt{sA + sB\hat{x}}},\ \sigma_z = \frac{\hat{x}}{\sqrt{sC + sD\hat{x}}},\ \hat{x} = \int\limits_{t_0}^{t} \sqrt{u(s)^2 + v(s)^2}\, ds,$$

where (u, v) is the vector of wind direction depending on time.

The movement of center of mass of the single emission in the horizontal plane is described by the relations

$$x_i(t_0, t) = x_i + \int\limits_{t_0}^{t} u(t)\, dt,\ \ y_i(t_0, t) = y_i + \int\limits_{t_0}^{t} v(t)\, dt,$$

where (x_i, y_i) are the coordinates of the i-th source. The height of the single emission can be written as

$$z_i(t_0, t) = \max\left[h_i - \frac{c}{\gamma(a+\gamma)} + \left(w_i + \frac{b}{a} + \frac{c}{(a+\gamma)}\right)\left(\frac{e^{a(t-t_0)}-1}{a}\right) + \frac{ce^{-\gamma(t-t_0)}}{\gamma(a+\gamma)} - \frac{b(t-t_0)}{a}, 0\right],$$

$$a = -\mu, b = \left(\frac{M_a}{M_g} - 1\right) g, c = \frac{M_a(T_i - T_a) g}{M_g T_a},$$

where h_i is the height of the i-th source, w_i is the initial vertical speed of single emission from the mouth of the i-th source, m_g is the mass of single emission, m_a is the mass of displaced air, μ is the viscosity coefficient, which describes the dependence of the medium resistance to the movement of the single emission, T_a is the air temperature, T_g is the temperature of the single emission, M_a is the molar mass of the air, M_g is the molar mass of the single emission.

2. Problem of the SUSUPLUME Model Parameter Identification

There are many models of pollution propagation in the atmosphere. Most models are calibrated on a large amount of raw data. To improve the accuracy of the models, researchers introduce additional factors into consideration in order to take into account the relief, building and other characteristics. Such models work well, but at some points they will give an essential error, since the calibration of the model is carried out for the entire set of data.

Three strategies can be used to calibrate the SUSUPLUME model. The first strategy is standard calibration for the entire set of data. This implies the presence of a large number of real measurements at various locations and conditions for measuring concentrations. The second strategy involves calibrating the model based on data from only one location and involves a large number of real measurements for one specific point/area. The third strategy involves calibrating the SUSUPLUME model based on the results of another model simulation.

Using a combination of these strategies allows you to determine a set of parameters for the SUSUPLUME model, which will either be as accurate as possible at some point/area, or simulate all available measurements (requirements of normative models).

Simultaneous consideration of all three strategies leads us to the problem of multi-criteria optimization, for this reason we will use the following weighted criterion to determine the appropriate strategy

$$F(x) = w_1 f_1(x) + w_2 f_2(x) + w_3 f_3(x),$$

where $w_1,\ w_2,\ w_3 \in [0;1]$ are the weights of strategies and $f_1(x),\ f_2(x),\ f_3(x) : \mathbb{R}^n \to \mathbb{R}$ are the objective functions for each strategy.

3. Objective Functions for Optimization Criteria

Let (x_j, y_j, z_j) be the point coordinates, where the measurements were made, t_j is the time of the j-th measurement, x is the model parameter vector. Let $c^{meas}(x_j, y_j, z_j, t_j)$ be the measurements of pollutants and $c^{mod}(x, x_j, y_j, z_j, t_j)$ be the model calculations. Suppose we have M measurements. Measuring concentrations devices of pollutants have a number of features:

1. The measurement error is about 20–25%.

2. Each pollutant has its own approved threshold limit value (TLV). Concentration values of less than 1% TLV, as a rule, go beyond the measuring range of devices.

3. The measuring range of the device gains concentration values within the same order, but it can vary significantly more.

To solve the calibration problem, it is proposed to use several criteria that may be relevant in various situations.

1. Using the standard deviation criterion which can be written as

$$f(x) = \frac{1}{M} \sum_{j=1}^{M} \left(c_j^{\text{mod}} - c_j^{\text{meas}}\right)^2. \tag{1}$$

This criterion may be relevant if all measurements are in the measuring range of the device or they are received from another model.

2. Using the average absolute deviation criterion which can be calculated as

$$f(x) = \frac{1}{M} \sum_{j=1}^{M} \left|c_j^{\text{mod}} - c_j^{\text{meas}}\right|. \tag{2}$$

This criterion improves the previous one and can be used for the same conditions if there are significant pollutants.

3. Using the average relative deviation criterion which can be described by the relation

$$f(x) = \frac{1}{M} \sum_{j=1}^{M} \frac{\left|c_j^{\text{mod}} - c_j^{\text{meas}}\right|}{c_j^{\text{meas}}}. \tag{3}$$

This criterion can be applied only when all measurements are within the measuring range of the device.

4. As for the SUSUPLUME model, the objective function of the standard deviation can be improved by finding the coefficient k analytically. Let us describe the objective function with the coefficient

$$f(x) = \frac{1}{M} \sum_{j=1}^{M} \left(k \sum_{i=1}^{N} C_i(x_j, y_j, z_j, t_j) - c_j^{\text{meas}}\right)^2. \tag{4}$$

Note that the function depends quadratically on k. This function reaches its minimum when

$$k = \frac{\sum_{j=1}^{M} c_j^{\text{meas}} \sum_{i=1}^{N} C_i(x_j, y_j, z_j, t_j)}{\sum_{j=1}^{M} \left(\sum_{i=1}^{N} C_i(x_j, y_j, z_j, t_j)\right)^2}.$$

Then the objective function (4) can be calculated as

$$f(x) = \frac{1}{M} \sum_{j=1}^{M} \left(\frac{\sum_{j=1}^{M} c_j^{\text{meas}} \sum_{i=1}^{N} C_i(x_j, y_j, z_j, t_j)}{\sum_{j=1}^{M} \left(\sum_{i=1}^{N} C_i(x_j, y_j, z_j, t_j)\right)^2} \sum_{i=1}^{N} C_i(x_j, y_j, z_j, t_j) - c_j^{\text{meas}}\right)^2. \tag{5}$$

5. Using the quadratic residual. Let us describe the sets of measures: $A = \{j | c_j^{meas} \leq a_j\}$, where a_j is the lower measure limit of the device for the j-th measurement, $B = \{j | c_j^{meas} \leq b_j\}$, where b_j is the lower measure limit of the device for the j-th measurement, $C = \{j | a_j < c_j^{meas} < b_j\}$ which is a set of measures in range of device limits. While using the third strategy, a_j can be set as 0.01TLV and b_j can be infinite. Then the objective function can be written as

$$f(x) = \frac{1}{M} \left(\sum_{j \in A} \left(\left(a_j - c_j^{\text{mod}}\right)_+\right)^2 + \sum_{j \in C} \left(c_j^{\text{mod}} - c_j^{\text{meas}}\right)^2 + \sum_{j \in B} \left(\left(c_j^{\text{mod}} - b_j\right)_+\right)^2\right), \tag{6}$$

where $(x)_+ = \max(x; 0)$.

6. Using the average absolute residual. The function can be described as

$$f(x) = \frac{1}{M}\left(\sum_{j\in A}\left(a_j - c_j^{\text{mod}}\right)_+ + \sum_{j\in C}\left|c_j^{\text{mod}} - c_j^{\text{meas}}\right| + \sum_{j\in B}\left(c_j^{\text{mod}} - b_j\right)_+\right). \quad (7)$$

7. Using the average absolute residual. This can be estimated as

$$f(x) = \frac{1}{M}\left(\sum_{j\in A}\frac{\left(a_j - c_j^{\text{mod}}\right)_+}{a_j} + \sum_{j\in C}\frac{\left|c_j^{\text{mod}} - c_j^{\text{meas}}\right|}{c_j^{\text{meas}}} + \sum_{j\in B}\frac{\left(c_j^{\text{mod}} - b_j\right)_+}{b_j}\right). \quad (8)$$

The quality of the model is commonly evaluated by criterion (8), however, the use of this criterion for optimization algorithms is rather complicated. Initially, the function is non-smooth in the parameter space. There are also sums in the objective function that can be equal to zero.

Based on these considerations, the search for a solution is done in three stages: fitting parameters using a differentiable function (5), solving the problem using function (6) and solving the problem using function (8).

4. The Set of Admissible Parameters

It is assumed that the following identification parameters will be used for the SUSUPLUME model: molar mass of the gas-air mixture $M_g \in [3; 150]$ and the parameters of a single emission dynamics $\mu, \gamma \in \left[10^{-5}; 10\right]$, $sA, sC \in \left[10^{-6}; 10\right]$, $sB, sD \in \left[10^{-8}; 10^{-3}\right]$, $k \in [10^{-5}; 10^5]$. Some values have a linear scope, and some values are logarithmic. Therefore, variables with a logarithmic scope are optimized linearly, which is achieved by using the appropriate functional transformation.

The found optimal parameters may have no physical meaning and only describe the dynamics of the emission. If, after solving the problem, the parameters were on the border of the acceptable domain, then this domain should be expanded taking into account the physical meaning.

5. Solving the Optimization Problem Algorithm

Since the problem of selecting the parameters of the SUSUPLUME model is multidimensional and multi-extreme, it requires the use of multi-extreme optimization algorithms. It takes low time to count the objective function, as the calculation can be effectively parallelized. A parallel multistart algorithm in a hyperparallelepiped will be used to solve this problem.

The multistart algorithm is applied as a global optimization algorithm and the BOBYQA algorithm is used as a local optimization algorithm [12]. For guaranteed convergence of the global optimization algorithm, it is required to guarantee that the set of starting points for the BOBYQA algorithm is everywhere dense in X. A decision tree of feasible set will be used to apply the convergence.

6. A Dicision Tree of Admissible Set

Let us describe a decision tree of admissible set of parameters and the basic operations with this tree.

A decision tree of admissible set is a binary tree which consists of vertices that represent a hyperparallelepiped in a d-dimensional space. The vertex of the tree represents the entire admissible set X. The descendants of a vertex always represent two hyperparallelepipeds of dimension h mod d+1 (h is the level of the vertex in the tree (counting from the root)) which are obtained by splitting the hyperparallelepiped in half. The entire admissible set is always represented by the union of all the leaf nodes.

The operation of saving a point (a point where the calculations are done) consists of finding a leaf in the current tree in which the calculated point lies and saving it in this leaf. Such a leaf always exists and is the only one. The execution time of this operation is $O(\log(S))$, where S is the total number of leaves in the tree.

The operation of selecting the next point is more complicated. A hyperparallepiped with the largest diagonal is found. If this hyperparallepiped does not contain saved points, then the center of this hyperparallepiped is returned as an answer.

If the hyperparallepiped contains saved points, then it is divided into two descendants according to the rules described above and all the points saved in it come down into its descendants. The selection of the leaf with the maximum diagonal is repeated again. The search time of the leaf with the maximum diagonal is $O(\log(S))$.

7. Global Optimization Algorithm

The parallel multistart algorithm consists of the following steps:

Step 0. Set the number of parallel calculations. Let this number be P.

Step 1. Select P starting points for the BOBYQA algorithm from the decision tree of an admissible set.

Step 2. Run the BOBYQA algorithm for each selected point.

Step 3. Save all the points at which the BOBYQA algorithm calculated the value of the objective function in the decision tree of an admissible set.

Step 4. If the calculation time has exceeded the limit for calculation, then stop the algorithm.

The proposed algorithm makes it possible to construct an everywhere dense sequence of initial points. This is achieved because the sizes of hyperparallelepipeds decrease uniformly and an empty hyperparallelepiped with the maximum diagonal is always selected.

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Received May 11, 2023

УДК 004.942 **DOI: 10.14529/mmp230306**

АЛГОРИТМ ИДЕНТИФИКАЦИИ ПАРАМЕТРОВ МОДЕЛИ РАСПРОСТРАНЕНИЯ ЗАГРЯЗНЕНИЯ В АТМОСФЕРНОМ ВОЗДУХЕ SUSUPLUME

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В статье представлен метод идентификации параметров динамической модели расчета рассеиваний SUSUPLUME. Предполагается, что параметры модели содержат не

только характеристики атмосферы и загрязняющих веществ, но и информацию о влиянии других условий, таких как тип местности, застройка, фон и т.д. Настройка параметров модели осуществляется на основе инструментальных замеров концентраций загрязняющих веществ в атмосферном воздухе в приземном слое (2 метра над уровнем земли). Рассматриваются три стратегии идентификации: идентификация параметров по всем измерениям, идентификация параметров по измерениям заданного источника и идентификация параметров на основе другой утвержденной модели. В третьей стратегии предлагается идентифицировать параметры модели так, чтобы модель была максимально похожа на утвержденную модель. Также предложен метод взвешивания этих стратегий. В статье также представлены целевые функции для критериев оптимизации, множество допустимых наборов параметров, алгоритм решения оптимизационной задачи, дерево решений для допустимого множества и алгоритм глобальной оптимизации.

Ключевые слова: модель SUSUPLUME; глобальная оптимизация; экология; распространение загрязняющих веществ в атмосферном воздухе.

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Поступила в редакцию 11 мая 2023 г.