Identification of the pollution source in steel plant

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1 Introduction

This problem is posed by Mr. J. Nakagawa from Kimitsu Works of Nippon Steel. Kimitsu Works is among the biggest steel mills in the world with several big blast furnaces and other steelmaking equipments which is located near the sea. There are three high chimneys in the mill which produce plume pollution and there are a big coal yard and many dusty roofs which produce dust pollution when the sea wind brings the dust up. Unfortunately, the downtown is just located at the downwind direction about 4 km away (see Figure 1). To reduce the pollution to the downtown, the administrator of Kimitsu works wants to identify the main sources of the pollution then to adopt some methods such as fixing new dust filter on the top of the chimneys or spraying water to the locations where main dust pollution are produced. Some monitoring instruments which are placed somewhere not far from the pollution sources in the downwind direction is used to measure the concentrate of the plume and dust. During three very busy days, we set up some mathematical models for this problem, obtained some initial results and made clear what future work should be done.

In this report we will summarize the discussion and work of the study group during three days by introducing the problem and some assumptions, modeling of the direct and inverse problem, and discussing the initial results and the future work.

2 Assumptions and simplifications

We make some assumptions and simplifications as follows:

1. pollutant of plume and dust consist of very small particles;
2. There is only one high chimney in the mill which can be simplified to a point source, and the location of the coal yard and the dusty roofs (called secondary pollution source) is known and the height of secondary pollution source is relatively small and can be supposed on the ground;
3. We only investigate the steady situation, i.e. the wind direction and the wind speed do not change and the concentration of pollutant is time-independent;
4. For convenience, we suppose that the secondary pollution source are some point sources distributed into a known area (see Figure 2).

By taking a coordinate system with the bottom center of the chimney as the origin, the wind direction as the x axis and the up direction as z axis, we introduce following notations:

$c(x, y, z)$–pollutant concentration at position (x, y, z);

u–the wind speed;

k_x, k_y, k_z–diffusivity in x, y, z directions;

h–the height of the chimney;

Q–the quantity of pollutant goes out of the chimney during a unit time;

$q_j (j = 1, \cdots, N)$–the discrete flux of the secondary pollution sources.

3 Model of the direct problem

When pollutant consists of very small particles, the concentration c of pollutant is governed by the following convection-diffusion equation

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} + w\frac{\partial c}{\partial z} = \frac{\partial}{\partial x}(k_x\frac{\partial c}{\partial x}) + \frac{\partial}{\partial y}(k_y\frac{\partial c}{\partial y}) + \frac{\partial}{\partial z}(k_z\frac{\partial c}{\partial z}). \tag{3.1}$$

By assumption 2, we have $\frac{\partial c}{\partial t} = 0$. If we neglect the gravity and turbulence, the third and fourth terms of above equation vanish and by noticing that along x direction, the effect of convection is much bigger than that of diffusion and the term $\frac{\partial}{\partial x}(k_x\frac{\partial c}{\partial x})$ can be neglected and the governing equation becomes

$$u\frac{\partial c}{\partial x} = \frac{\partial}{\partial y}(k_y\frac{\partial c}{\partial y}) + \frac{\partial}{\partial z}(k_z\frac{\partial c}{\partial z}). \tag{3.2}$$

Let the contribution of the chimney with unit discharging of pollutant to the pollutant concentration c be c_0. Then c_0 is the solution of boundary value problem for heat equation

$$\begin{cases} u\frac{\partial c_0}{\partial x} = \frac{\partial}{\partial y}(k_y\frac{\partial c_0}{\partial y}) + \frac{\partial}{\partial z}(k_z\frac{\partial c_0}{\partial z}), x > 0, \\ c_0|_{x=0} = \frac{1}{u}\delta(y)\delta(z-h), \\ \frac{\partial}{\partial z}c_0|_{z=0} = 0, \\ \frac{\partial}{\partial z}c_0|_{z\to+\infty} = 0. \end{cases} \tag{3.3}$$

Let c_j be the contribution of the i-th secondary pollution point source with unit flux to the pollutant concentration, as $x > x_j, c_j$ satisfies

$$\begin{cases} u\frac{\partial c_j}{\partial x} = \frac{\partial}{\partial y}(k_y\frac{\partial c_j}{\partial y}) + \frac{\partial}{\partial z}(k_z\frac{\partial c_j}{\partial z}), x > 0, \\ c_j|_{x=0} = 0, \\ -k_z\frac{\partial}{\partial z}c_j|_{z=0} = \delta(x-x_j)\delta(y-y_j), \\ \frac{\partial}{\partial z}c_j|_{z\to+\infty} = 0. \end{cases} \tag{3.4}$$

Nevertheless,$c_j = 0$ as $x \leq x_j$. After solving (3.3) and (3.4), by superposition we obtain the concentration of pollutant at (x, y, z) located in downwind area of the pollution source as

$$c(x,y,z) = Qc_0(x,y,z) + \sum_{j=1}^{N} q_j c_j(x,y,z). \tag{3.5}$$

4 Solution of the direct problem

Suppose that k_x, k_y, k_z are constants. By use of Laplace transform (see[1]), or Fourier transform after even extension the unknown about $x-y$ plane([2],[3]), we obtain the explicit solution of (3.3)

$$c_0(x,y,z) = \frac{1}{4\pi x\sqrt{k_y k_z}}(\exp(-\frac{(z-h)^2 u}{4k_z x}) + \exp(-\frac{(z+h)^2 u}{4k_z x}))\exp(\frac{y^2 u}{4k_y x}), \tag{4.1}$$

and the explicit solution of (4)

$$c_j(x,y,z) = \frac{1}{2\pi(x-x_j)\sqrt{k_y k_z}} exp(-(\frac{z^2}{4k_z} + \frac{(y-y_j)^2 u}{4k_y})\frac{u}{x-x_j})(x > x_j). \tag{4.2}$$

The solution (4.1) is something similar to the Gaussian point source plume model in the literatures of environment science[4],[5]. Therefore, the explicit expression for pollutant concentration in the downwind domain is

$$\begin{aligned} c(x,y,z) = {} & \frac{Q}{4\pi x\sqrt{k_y k_z}}(\exp(-\frac{(z-h)^2 u}{4k_z x}) + \exp(-\frac{(z+h)^2 u}{4k_z y}))\exp(\frac{y^2 u}{4k_y x}) \\ & + \sum_{j=1}^{N} \frac{q_j}{2\pi(x-x_j)\sqrt{k_y k_z}} \exp(-(\frac{z^2}{4k_z} + \frac{(y-y_j)^2 u}{4k_y})\frac{u}{x-x_j})(x > x_j). \end{aligned} \tag{4.3}$$

5 Inverse problem and solution

Our main purpose is to identify the intensity of the pollution sources, namely to determine $Q, q_j(j = 1, \cdots, N)$ by the measurement of pollutant concentration somewhere in downwind area. Suppose that we measure the pollutant concentration at points $(X_i, Y_i, 0), i = 1, \cdots, M$ with $X_i > \max\{0, x_1, \cdots, x_N\}$ and $M \geq N$ and the measuring concentration data is $\bar{c}_i, (i = 1, \cdots, M)$. If there is no measuring error for $\{\bar{c}_i\}$, following equality should hold

$$c(X_i, Y_i, 0) = \bar{c}_i, (i = 1, \cdots, M)$$

that is

$$Qc_0(X_i, Y_i, 0) + \sum_{j=1}^{N} q_j c_j(X_i, Y_i, 0) = \bar{c}_i, (i = 1, \cdots, M). \tag{5.1}$$

This is a linear equation system of M equations for $N+1$ unknowns $(Q, q_1, \cdots, q_N)$.

By denoting

$$S = \begin{bmatrix} c_0(X_1, Y_1, 0) & c_1(X_1, Y_1, 0) & \cdots & c_N(X_1, Y_1, 0) \\ c_0(X_2, Y_2, 0) & c_1(X_2, Y_2, 0) & \cdots & c_N(X_2, Y_2, 0) \\ \cdots & \cdots & \cdots & \cdots \\ c_0(X_M, Y_M, 0) & c_1(X_M, Y_M, 0) & \cdots & c_N(X_M, Y_M, 0) \end{bmatrix}, \tag{5.2}$$

$$P = (Q, q_1, \cdots, q_N)^T, \tag{5.3}$$

and

$$B = (\overline{c}_1, \cdots, \overline{c}_M)^T, \tag{5.4}$$

equation (5.1) can be written as

$$SP = B. \tag{5.5}$$

By least square technique (5.5) is transform to solve

$$\min_P \{P^T(S^TS)P - 2P^T(S^TB)\}, \tag{5.6}$$

or to solve linear equation system

$$(S^TS)P = S^TB. \tag{5.7}$$

Nevertheless this problem is seriously unstable. It can be seen from that the condition number of matrix S is very poor. As we use measurement data without error obtained from formula (5.1) using given $(Q, q_1, \cdots, q_N)$, the inversion gives reasonable result. However, if we put some small white noise to the measurement the result of inversion drops far away from the exact (given) value of $(Q, q_1, \cdots, q_N)$.

To overcome this difficulty, we have to use the regularization technique, that is to modify problem (5.6) into

$$\min_P \{P^T(S^TS)P - 2P^T(S^TB) + \alpha R(P)\}, \tag{5.8}$$

where $\alpha R(P)$ is called regularization term and α is called regularization parameter. During the three days we tried some choices of regularization term such as the discrete H^1 and H^2 norm for $(q_1, \cdots, q_N)$, but they did not work well.

6 Model improvement and future work

In the discussion, we proposed to improve the partial differential equation model in several ways: Considering the settling speed, the PDE can be modified into

$$u\frac{\partial c}{\partial x} + w\frac{\partial c}{\partial z} = \frac{\partial}{\partial y}(k_y\frac{\partial c}{\partial y}) + \frac{\partial}{\partial z}(k_z\frac{\partial c}{\partial z}).$$

Suppose that the wind speed varys with height, the PDE is modified into

$$(u_0 + zu_1)\frac{\partial c}{\partial x} = \frac{\partial}{\partial y}(k_y\frac{\partial c}{\partial y}) + \frac{\partial}{\partial z}(k_z\frac{\partial c}{\partial z}).$$

If we consider the effect of turbulence the PDE should be revised into

$$u\frac{\partial c}{\partial x} = \frac{\partial}{\partial y}(k_y\frac{\partial c}{\partial y}) + \frac{\partial}{\partial z}(k_z(z)\frac{\partial c}{\partial z}).$$

We can combine the effect of the pollutant dispersion in the air and diffusion on the ground. In this case, we have two problems(in two dimensional situation) as follows

$$\begin{cases} (u_0 + zu_1)\frac{\partial c}{\partial x} = \frac{\partial}{\partial z}(k_z\frac{\partial c}{\partial z}), x > 0, \\ c|_{x=0} = \delta(z - h), \\ q = -k_z\frac{\partial}{\partial z}c|_{z=0} = -h(x, u_0, u_1)(c - c_g), \end{cases},$$

$$\begin{cases} u_0 \frac{\partial c_g}{\partial x} = \frac{\partial}{\partial z}(k_g \frac{\partial c_g}{\partial x}), x > 0, \\ c_g|_{x=0} = 0. \end{cases}$$

If $k_g \ll 1$, by combing above two problems, we finally have

$$\begin{cases} u_0 \frac{\partial c}{\partial x} = \frac{\partial}{\partial z}(k_z \frac{\partial c}{\partial z}), x > 0, \\ c|_{x=0} = \delta(z-h), \\ q = -k_z \frac{\partial}{\partial z} c|_{z=0} = -h(c - 1 + \int_0^\infty c dz), \end{cases}.$$

After study group we have to try to find suitable regularization term and regularization parameter to made the inversion stable.

Since the measuring instrument is heavy and expensive, It is difficult for us to acquire big measurement data. For a few fixed instruments, it is necessary to consider time-varying situation. In this case we should use the time-varying convection-diffusion equation. Maybe some traveling wave solution of form

$$\overline{c}(t, x, y, z) = c(x - vt, y, z)$$

can be useful.

References

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[2] Ockendon, J. et al. Applied Partial Differential Equations (2nd Edition), Oxford University Press, Oxford, 2003.

[3] Tan, Y. et al., Lecture note on mathematical models in economy, finance and management, High Education Press, Beijing, 2006.

[4] Gaussian plumes from point source, www.course.washington.edu /cewa567/plumes.PDF

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Figure 1

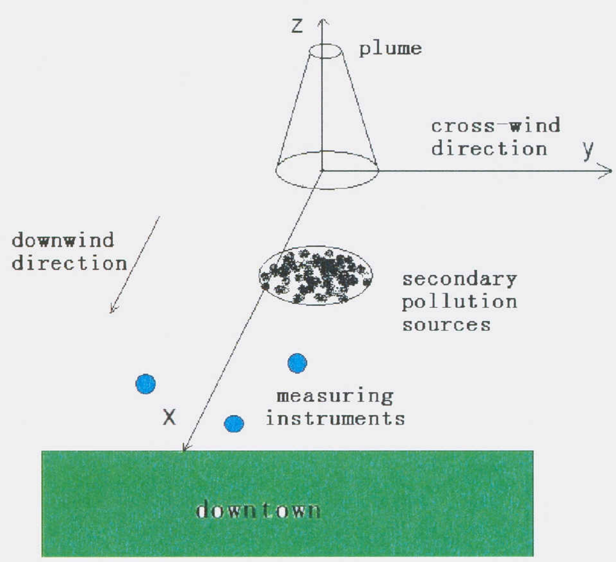

Figure 2