Mausam, (1987), 38, 2, 177-182

551.510.42 : 517.949

Optimal emission control of a transient air pollution source by the method of finite difference

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(*Received 8 January 1986*)

सार -- बुटकोविस्की (1969) का अनुसरण करते हुए वायुप्रदूषण की वर्गी कृत ईष्टतम नियन्त्रण समस्या को, हल करने का प्रयास किया गया है। यह कार्य अवकलन अंतर समीकरणों के समूह से स्थानिक अवकलनों के परिमित अंतर निरूपण पर आधारित स्थानीकृत मोटे अनुमानों का प्रयोग करके किया गया है । इस शोधपत्र में, क्षैतिज समांग सघन वितरण पर विचार किया गया है। जब भूसतह स्रोत को ऐसे समय से संबंधित करके नियंत्रण के रूप में माना जाता है कि यह प्रणाली निम्नतम संभव समय में, प्रारम्भिक अवस्था से एक बांछित अवस्था में पहुंच जाएगी ।

ABSTRACT. Following Butkovskiy (1969) an approach is made in solving distributed optimal control problem of air pollution by the use of lumped approximation based on finite difference representations of the spatial derivatives, yielding a set of differential difference equations. In this paper the diffusion of a horizontally homogeneous concentration distribution is considered, when the ground level source is taken as a control with respect to time such that the system will reach a desired state from an initial state in a lowest possible time.

1. Introduction

Increasing industrilization and urbanization rises the question of whether a further increase is tolerable from an environmental protection point of view. In most cases, new air pollution sources are built without sufficient knowledge of possible changes in the air pollution load of a given region. Only mathematical models and controls for air pollution transport and diffusion together with a deep knowledge of meteorological processes involved are able to solve a wide variety of problems of this kind (Omatu and Seinfeld 1982).

The problem of determining the optimal distribution of source of air pollution has received some prior attention (Seinfeld 1972, Seinfeld and Chen 1973, Seinfeld and Kyan 1982). From the practical point of view, it is useful to consider a possible distribution of emission sources which would be desirable from an air pollution standpoint. Thus, one of the central issues of air pollution turns out to be the distribution of new proposed emission sources which will maximise air quality subject to zoning restrictions.

Inversion occurs when temperature increases with height. This occurs frequently during the night or early morning hours. In addition, inversions occur more frequently during the fall of the year. Inversions are likened to putting a lid on a particular locale so that no pollution escapes by vertical diffusion (Howard 1974).

Low wind speeds less than 7 mph usually accompany inversions, so there is very little horizontal dispersion of pollution (Howard 1974). Inversion temperatures are usually limited to the first 500 metres and this, therefore, is the maximum inversion height (Howard 1974). Inversion heights are usually much lower than maximum mixing depth heights. Thus, it is more likely to presume that in certain meteorological conditions when the inversions occur low wind speed less than 7 mph, the horizontal diffusion may be neglected and vertical diffusion remains approximately constant. However, these realistic assumptions will, in turn, give some approximate solutions which can be set for obtaining solutions of optimal control problems from the engineering point of view.

Here, we consider the diffusion of a horizontally homogeneous concentration distribution, when the ground level source is taken as control with respect to time such that the system will reach a desired state from an initial state in the lowest possible time. Regland (1973) has considered atmospheric dispersion of air pollution emitted from an area source using an implicit finite difference scheme.

Here, an approach is made by looking at the problem as an distributed optimal control problem of air pollution using the well known lumped parameter approximation which in turn, is based on finite difference representations of spatial derivatives yielding a set of differential equations. We simply replace the partial derivative with respect to one independent variable by a finite difference approximation, reducing the system to a set of differential difference equations and consequently, the optimal control problem of distributed parameter system to lumped parameter system. This method of approximation is of great practical relevance since one can then use electrical and mechanical analog computers (Butkovskiy 1969).

2. Basic equations

The dispersion of passive contaminants in a turbulant medium is usually described by the diffusion equation, which reads (Pasquill 1974) :

$$\frac{\partial \chi}{\partial t} + u \frac{\partial \chi}{\partial x} + v \frac{\partial \chi}{\partial y} = k_x \frac{\partial^2 \chi}{\partial x^2} + k_y \frac{\partial^2 \chi}{\partial y^2} + \frac{\partial}{\partial z}\left(k_z \frac{\partial \chi}{\partial z}\right) \qquad (1)$$

where t is time, x, y and z the space coordinates, χ concentration of passive contaminant and u and v the velocity components of the horizontal mean wind. The vertical mean wind is taken as zero. k_x, k_y and k_z are turbulent diffusion coefficients.

We consider the diffusion of a horizontally homogeneous concentration distribution. Horizontal homogeneity is usually assumed for meteorological variables, so that wind speed and k-coefficient are functions of z only. In such case the diffusion Eqn. (1) reduces to an one dimensional form (Neiustadt 1980, Pasquill 1974)

$$\frac{\partial \chi}{\partial t} = \frac{\partial}{\partial z}\left[k_z(z) \frac{\partial \chi}{\partial z}\right] \qquad (2)$$

For simple case, let us take k is a constant (Kairulalam and Seinfeld 1980). Then Eqn. (2) gives,

$$\frac{\partial \chi}{\partial t} = k \frac{\partial^2 \chi}{\partial z^2} \qquad (3)$$

The initial and boundary conditions can be taken as (Omatu and Seinfeld 1982),

$$\chi(z, 0) = \chi_0(z) \quad ; \qquad (4)$$

$$-k \frac{\partial \chi}{\partial z} = u(t) - v\chi \quad \text{on } z = 0 \qquad (5a)$$

$$\frac{\partial \chi}{\partial z} = 0 \quad \text{on} \quad z = h \qquad (5b)$$

where $u(t)$ is the ground level emission source rate, v is the deposition velocity and h denotes the upper vertical boundary of the pollutant-containing region, for example, the base of the inversion layer (stable layer). The second boundary condition indicates that the flux of material through the upper boundary is equal to zero. For short time period of 24 hours, taking the meteorological conditions do not change rapidly as granted, one may assume this deposition velocity *as constant*. Here $v\chi(0, t)$ acts as a sink in the system.

3. Formation of the optimal control problem

To facilitate the analysis, we need to have a situation in which, at least a semblance of steady character, if not fully is ensured, this is, on the other hand, warranted by a physical set up in the inversion layer so as to bring about uniform and steady nature of the concentration of pollutants. This is corroborated by the findings and observations of (Kairul Alam and Seinfeld 1981 (Fig. 2).

Thus, one may formulate the optimal control given as follows — to obtain an optimal control $u(t)$, (rate of emission source), $0 \leqslant t \leqslant T$ satisfying the additional condition $0 \leqslant u(t) \leqslant A_2$, so that the controlled system described by Eqns. (3)-(5) will pass from the initial state described by the function $\chi_0(z)$ to the required desired state $\chi^*(z)$ (say) in the minimum possible time T. Thus,

$$\chi(z, T) = \chi^*(z) \qquad (5c)$$

4. Solution of the problem

Here we reduce the system with distributed parameters to system of lumped parameters with the aid of finite difference method as given by (Butkovskiy 1969).

Let us divide the segment $(0, h)$ on the z-axis into n equal intervals by the points $z_0 = 0$, $z_1 = S$, $z_2 = 2S, \ldots\ldots, z_n = h$ where $S = h/n$. Let us assume that the concentration of the pollutant in the middle point of each interval is determined by the quantity $\bar{\chi}_i$, $(i = 1, \ldots\ldots\ldots, n)$. In addition, the concentration of each surface from which contamination proceeds is equal to $\bar{\chi}_0$ at $z = 0$ and the concentration of the other surface is equal χ_{n+1} at $z = h$.

Then replacing in Eqn. (5a) the value of the partial derivative with respect to z of the function $\chi(x, t)$ at $z = 0$ by the first difference, we get, (Butkovskiy 1969)

$$-k \frac{\bar{\chi}_1 - \bar{\chi}_0}{S/2} = u(t) - v\bar{\chi}_0 \qquad (6)$$

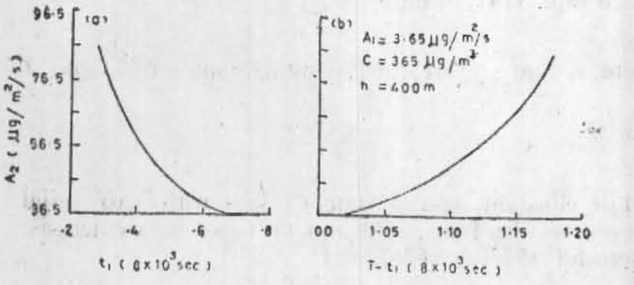
Similarly replacing in Eqn. (1) the second partial derivative with respect to z of the function $\chi(z, t)$ by the second difference we obtain the differential—difference equations, given by Butkovskiy (1969),

$$\frac{d}{dt}\bar{\chi}_1 = \frac{k}{S}\left(\frac{\bar{\chi}_2 - \bar{\chi}_1}{S} - \frac{\bar{\chi}_1 - \bar{\chi}_0}{S/2}\right) \qquad (7)$$

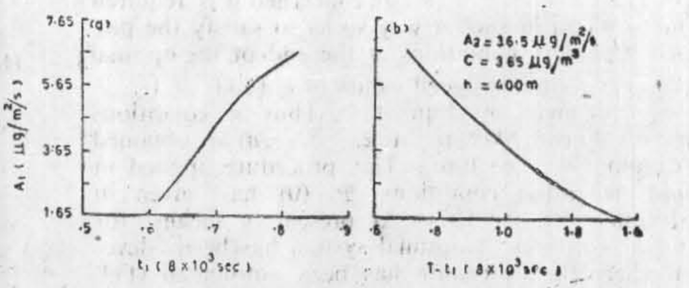
$$i.e., \frac{d}{dt}\bar{\chi}_1 = \frac{k}{S^2}\left(2\bar{\chi}_0 - 3\bar{\chi}_1 + \bar{\chi}_2\right) \qquad (7a)$$

$$\frac{d}{dt}\bar{\chi}_i = \frac{k}{S}\left(\frac{\bar{\chi}_{i+1} - \bar{\chi}_i}{S} - \frac{\bar{\chi}_i - \bar{\chi}_{i-1}}{S}\right) \qquad (8)$$

$$\frac{d}{dt}\bar{\chi}_n = \frac{k}{S}\left[\frac{\bar{\chi}_{n+1} - \bar{\chi}_n}{S/2} - \frac{\bar{\chi}_n - \bar{\chi}_{n-1}}{S}\right] \qquad (9)$$



Figs. 1 (a & b)



Figs. 2 (a & b)

Finally, replacing in Eqn. (5) the value of the partial derivative with respect to z of the function $\overline{X}(x, t)$ at $z = h$ by the corresponding first difference, we obtain (Butkovskiy 1969)

$$\frac{\overline{X}_{n+1} - \overline{X}_n}{S/2} = 0 \tag{10}$$

Considering the equality (10), the Eqns. (6) - (9) can be written as (Butkovskiy 1969) :

$$\overline{X}_0 = \frac{\beta}{2 + v\beta} u + \frac{2\overline{X}_1}{2 + v\beta} \tag{11}$$

$$\frac{d}{d\tau} = 2\overline{X}_0 - 3\overline{X}_1 + \overline{X}_2 \tag{11a}$$

$$\frac{d}{d\tau} \overline{X}_1 = \frac{2\beta}{2 + v\beta} u - \frac{2 + 3v\beta}{2 + v\beta} \overline{X}_1 + \overline{X}_2 \tag{12}$$

$$\frac{d}{d\tau} \overline{X}_i = \overline{X}_{i+1} - 2\overline{X}_i + \overline{X}_{i-1} ; \quad [(i = 2, 3, \ldots\ldots, (n-1)] \tag{13}$$

$$\frac{d}{d\tau} \overline{X}_n = \overline{X}_{n-1} - \overline{X}_n \tag{14}$$

$$\text{where, } \frac{kt}{S^2} = \tau, \ \beta = \frac{S}{k} \tag{15}$$

One can write the initial condition (4) of the systems (12)-(14) in the form (Butkovskiy 1969) :

$$\overline{X}_0(0) = X_0(0)$$

$$\text{and} \quad \overline{X}_i(0) = X_0\left(\frac{2i-1}{2} S\right) ; (i=1, 2, .., n) \tag{16}$$

Thus, one has to find the control $u(t)$ in $0 \leqslant t \leqslant T$ such that the systems (12)-(14) will move from the initial state to the desired state, given by [*see* Eqn. 5 (c)]

$$\overline{X}_0(T) = X_0^*(0),$$

$$\overline{X}_i(T) = X^*\left(\frac{2i-1}{2} S\right), (i = 1, 2, \ldots, n) \tag{17}$$

Now the problem described by Eqns. (12)-(17) can be solved with the aid of the maximum principle (Pontryagin *et al.* 1962). The Hamiltonian H thus stands,

$$H = -\Psi_0 + \Psi_1 \left[\frac{2\beta}{2 + v\beta} u - \frac{2 + 3v\beta}{2 + v\beta} \overline{X}_1 + \overline{X}_2 \right] + \sum_{i=2}^{n-1} \Psi_i (\overline{X}_{i+1} - 2\overline{X}_i + \overline{X}_{i-1}) + \Psi_n(\overline{X}_{n-1} - \overline{X}_n) \tag{18}$$

where the auxilliary functions $\Psi_1, \Psi_2, \ldots, \Psi_n$ can be written as (Pontryagin *et al.* 1962),

$$\frac{d}{d\tau} \Psi_0 = 0$$

$$\frac{d}{d\tau} \Psi_i = -\frac{\partial H}{\partial \overline{X}_i} ; \ (i = 1, 2, \ldots, n) \tag{19}$$

The maximum principle then yield (Pontryagin *et al.* 1962)

$$u(t) = \text{Sign } \Psi_1(t) \tag{20}$$

i.e., $u(t) = A_2$ for $\Psi_1(t) > 0$ and $= 0$ for $\Psi_1(t) < 0$. Let us consider the matrix of the homogeneous system described by Eqns. (12)-(14), given by (Pontryagin *et al.* 1962).

$$\begin{bmatrix} -\frac{2 + 3v\beta}{2 + v\beta} & 1 & 0 \ldots\ldots.0 & 0 \\ 1 & -2 & 1 \ldots\ldots.0 & 0 \\ \ldots & \ldots & \ldots\ldots & \ldots \\ 0 & 0 & 0 \ldots \ -2 & 1 \\ 0 & 0 & 0 \ \ldots\ldots 1 & -1 \end{bmatrix} \tag{21}$$

This is a symmetric matrix, so that its eigen values are real. It can be shown that they are negative. Therefore, by a Theorem [No. 10, of Pontryagin *et al.* 1962, p. 120)], the optimal control $u(t)$ takes on only the extremum values and does not have more than $(n-1)$ switching (*i.e.*, not more than n intervals on which it is a constant).

For solving the two systems of Eqns. (7)-(9) and (19)—fundamental and adjoint — it is necessary to know all the $2n$ initial conditions. The first n values are given by Eqn. (16).But as far as the n initial conditions of Ψ_i ($i=1, 2, \ldots\ldots\ldots\ldots, n$) are concerned it is required to choose them in such a way so as to satisfy the prescribed boundary conditions at the end of the optimal trajectory, *i.e.*, the assigned values of $\overline{X}_i(T)$ ($i = 1, \ldots\ldots\ldots\ldots, n$) given by Eqn. (17). Thus n conditions for the n unknown $\Psi_i(0)$ ($i=1, 2, \ldots\ldots, n$) are obtained (Fel'draum 1965, p. 106). The procedure applied in finding the initial conditions Ψ_i (0) has given in (Fel'draum 1965, p. 107). At present, a means for automatic synthesis of optimal system has been developed where the procedure has been automated (Fel'draum 1956). For systems with linear objects there are methods permitting the values Ψ_i (0) to be found with the aid of iteration (Byzova *et al.* 1983).

However, the greater number of intervals n in to which the segment (0, h) is divided, the more accurately the transient is approximated.

5. Particular case

To facilitate the analysis, we need to have a situation, in which, at least a semblance of steady character, if not fully, is ensured; this is, on the other hand, warranted by a physical set up in the inversion layer so as to bring about uniform and steady nature of the concentration of the pollutants. This corroborated by the findings and observation of Kairul Alam and Seinfeld 1981 (Fig. 2). Thus one may take the desired state $\chi^*(z)$ as a constant C (say). The rate of deposition, given by $\nu X(0, t)$ depends on meteorological conditions as well as on the emission sources. For constant rate of emission (since the control, the rate of emission, is singular and thus assume only extremum values 0 and A_2) and considering no change of meteorological conditions in 24 hours, one may assume this rate of deposition as constant A_1 (say). Also one may likely take the primary concentration of SO_2 in the ambient air as given by EPA as the desired state of cocentration of the pollutant.

For simple case let us take $n=2$. Let the control $u(t)$ assume the value A_2 $[0 \leqslant u(t) \leqslant A_2]$ on the interval $0 \leqslant t \leqslant t_1$ and $u(t)=0$ on the interval $t_1 \leqslant t \leqslant T$, where t_1 is the switching time when $u(t)$ switches from A_2 to 0 and T is the total time of completion of the desired state of the system. Then Eqn. (6) stands,

$$\overline{X}_0 = \frac{\beta}{2}(A_2 - A_1) + \overline{X}_1, \quad 0 \leqslant t \leqslant t_1 \qquad (22a)$$

$$\text{and} \quad \overline{X}_0 = \frac{-\beta}{2} A_1 + \overline{X}_1, \quad t_1 \leqslant t \leqslant T \qquad (22b)$$

Substituting (22a) and (22b) in Eqn. (11a) we get,

$$\frac{d}{d\tau}\overline{X}_1 = \beta(A_2 - A_1) - \overline{X}_1 + \overline{X}_2, \quad 0 \leqslant \tau \leqslant \tau_1 \qquad (23)$$

$$\text{and} \quad \frac{d}{d\tau}\overline{X}_1 = -\beta A_1 - \overline{X}_1 + \overline{X}_2; \quad \tau_1 \leqslant \tau \leqslant \Gamma \qquad (24)$$

Then Eqn. (14) stands, $\frac{d}{d\tau}\overline{X}_2 = \overline{X}_1 - \overline{X}_2$;

Here τ_1 and Γ are corresponding values of t_1 and T for $\tau = \frac{kt}{S^2}$.

For constant desired state C (say) with zero initial conditions the Eqns. (16) and (17) can be written as, (Netushil 1973, p. 636).

$$\overline{X}_1(0) = \overline{X}_2(0) = 0, \quad 0 \leqslant \tau \leqslant \tau_1 \qquad (25)$$

$$\overline{X}_1'(\tau_1) = \overline{X}_2(\tau_1), \; \overline{X}_2'(\tau_1) = \overline{X}_2(\tau_1), \quad \tau_1 \leqslant \tau \leqslant \Gamma \qquad (26)$$

$$\text{and} \quad \overline{X}_1'(T) = \overline{X}_2'(T) = C \qquad (27)$$

where, $\overline{X}_1'$ and $\overline{X}_2'$ designate the function $\overline{X}_1$ and $\overline{X}_2$ in the interval $\tau_1 \leqslant \tau \leqslant \Gamma$.

Then the Eqns. (23) and (24) under conditions (25) and (26) yield the solution, given by, (Netushil 1973, p. 636).

$$\overline{X}_1' = \tfrac{1}{2}\left[\beta(A_2\tau_1 - A_1\tau) - \frac{\beta A_1}{2} + \frac{\beta A_2}{2} e^{2(\tau_1 - \tau)} - \frac{\beta(A_2 - A_1)}{2} e^{-2\tau}\right];$$

$$\overline{X}_2' = \tfrac{1}{2}\left[\beta(A_2\tau_1 - A_1\tau) + \frac{\beta A_1}{2} - \frac{\beta A_2}{2} e^{2(\tau_1 - \tau)} + \frac{\beta(A_2 - A_1)}{2} e^{-2\tau}\right] \qquad (28)$$

Thus the condition (27) after manipulation give,

$$\Gamma = \tfrac{1}{2} \ln\left[\frac{A_2}{A_1}\left(e^{2\tau_1} - 1\right) + 1\right] \qquad (29)$$

$$\text{and} \quad \Gamma = \frac{A_2}{A_1}\tau_1 - \frac{2C}{\beta A_1}, \quad \text{where } \beta = S/k$$

Considering Eqn. (29), the plots can be constructed in a plane with coordinates τ_1 and Γ; their interaction defines the desired values of τ_1 and Γ (Netushil 1973).

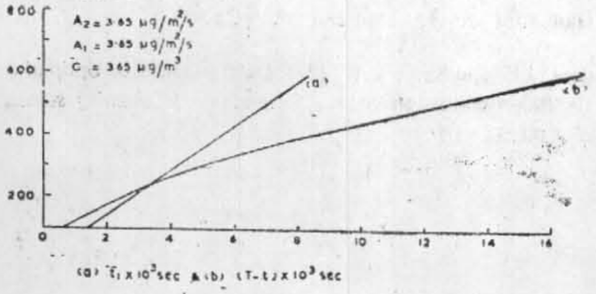
6. Numerical calculations

The parameters values used in numerical calculations are as follows (Kairul Alam and Seinfeld 1981) :

C (ambient aid quality of SO_2) $= 365 \mu g/m^3$ in 24 hours (National primary ambient air quality standard)

$k = 5\ m^2\ sec^{-1}$

$\nu = .1\ m\ sec^{-1}$



Figs. 3 (a & b)

A_2, A_1 = rate of emission source and deposition respectively.

With the help of Eqn. (29), we have obtained the values of t_1 and T for different values A_2, A_1 and h (height of inversion) in Figs. 1, 2 and 3 respectively.

7. Discussion

Here t_1 is the time during which both emission source and deposition (sink) are active and while $(T-t_1)$ is the time during which the emission source is the inactive, thereby allowing the deposition to be operative. The concentration of SO_2 in the ambient air is found to be greater than that of desired concentration (maximum tolerable concentration of SO_2 in air; National ambient air quality standard of SO_2) during the interval $(t_1, T-t_1)$. Thus this period $(t_1, T-t_1)$ may be taken as a potential hazard to human health. So once the total time of completion T is crossed, the concentration of SO_2 in the ambient air is found to be tolerable to human health and thus the period after the total time T may be termed as a safety time. It is noted that both t_1 and T depend on the the rate of emission, deposition and inversion height. However, some additional remarks can be made from the given figures. $(0, t_1)$ represents precisely the period of length t_1 during which both emission and deposition are active. From Figs. 1(a) and 1(b), we see that t_1 decreases and $(T-t_1)$ (during which only deposition takes place) increases with the increase of rate of emission source, while the increase of the rate of deposition increases the time t_1 and decreases the time $(T-t_1)$ (Fig. 2). The time t_1 and $(T-t_1)$ both increase with the increase of inversion height but $(T-t_1)$ increases from rapidly than that of t_1 in case of Fig. 3.

8. Conclusion

The estimation of species concentration distributions necessitates traverses over the region at different altitudes. There has been much recent interest in the air from measurement of pollutant concentrations at different altitude in which an aircraft with a downward looking instrument, such as, for example, the JPL Laser absorption spectrometer, is flown at different altitudes (Omatu and Seinfeld 1982). Thus the optimal control problem considered here can also be applied for estimation of optimal time of emission source and total time of completion to reach different specified (desired) concentrations at different altitude (Howard 1974).

Acknowledgement

The authors are grateful to U.G.C./D.S.A. for granting financial assistance and thank to Prof. J.H. Seinfeld, California Institute of Technology, for giving helpful suggestions.

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