On the Estimation of Contamination Sources from Downstream Concentration Measurements

A. Alekseev[1] J. M. Escobar[2] R. Montenegro[2] G. Montero[2]

Resumen

The estimation of contamination source parameters from concentration measurements at certain lines is considered in a variational statement. The corresponding optimality condition and the adjoint problem are formulated. Both direct and adjoint problems are calculated by a finite difference method. The optimization problem is solved in the iterative way. The non-uniqueness of the problem is considered and managed with using the additional information for sources. The numerical tests demonstrate the feasibility for the single source coordinates estimation.

Introduction

The estimation of contamination (air pollution) sources $Q_C(X,Y)$ from concentration measurements [4] is of obvious interest. Actually, there is a wide-ranging set of publications on Inverse Problems in general (see e.g. [6], [7]). Specifically in [5], an interesting study of the inverse source problems is developed.

First we present the state equation which defines our problem where the contamination sources are to be found, as well as propose the fitness function to be optimized. This function is constructed from the experimental measurements at certain lines inside the domain. Next, we establish the necessary adjoint problem to pose completely the problem. Finally we describe the numerical method for solving such problem and solve a numerical test, which led us to some preliminary conclusions.

State equation and fitness function

Herein, we consider using the measurements at certain lines in flow field or at boundaries. The problem is studied for the steady two-dimensional stream of viscous gas. The convection is assumed to be predominant along the direction (X) (see e.g. [10]). The contamination sources are supposed not to affect the flow parameters. So, the flow data $U(X,Y)$, $V(X,Y)$, $T(X,Y)$ may be obtained from external solvers. Herein, the flow data are calculated using the two-dimensional parabolized Navier-Stokes equations [1].

$$\frac{\partial U}{\partial X} + \frac{\partial V}{\partial Y} = 0 \tag{1}$$

$$U\frac{\partial U}{\partial X}+V\frac{\partial U}{\partial Y}+\frac{1}{\rho}\frac{\partial P}{\partial X}=\frac{\mu}{\rho}\frac{\partial^2 U}{\partial Y^2} \qquad (2)$$

$$U\frac{\partial V}{\partial X}+V\frac{\partial V}{\partial Y}+\frac{1}{\rho}\frac{\partial P}{\partial Y}=\frac{\mu}{\rho}\left(\frac{\partial^2 V}{\partial Y^2}\right) \qquad (3)$$

$$U\frac{\partial T}{\partial X}+V\frac{\partial T}{\partial Y}=\frac{1}{\rho C_p}\left(\dot{\lambda}\frac{\partial^2 T}{\partial Y^2}\right) \qquad (4)$$

Equations (1-4) provide the coefficients $U(X,Y)$, $V(X,Y)$ for solving contamination transfer equation

$$U\frac{\partial C}{\partial X}+V\frac{\partial C}{\partial Y}+Q_c(X,Y)=D\frac{\partial^2 C}{\partial Y^2} \qquad (5)$$

$$Q_C(X,Y)\geq 0;\quad (X,Y)\in\Omega=(0<X<1;0<Y<1);$$

The flow field scheme is presented in Figure 1. The entrance boundary (A, $(X=0)$) conditions $T(0,Y)=T_\infty(Y)$; $\rho(0,Y)=\rho_\infty(Y))$; $U(0,Y)=U_\infty(Y)$; $V(0,Y)=V_\infty(Y)$; $C(0,Y)=C_\infty(Y)$; the outflow conditions $\partial f/\partial y=0$ are used at B, D boundaries ($Y=0$, $Y=1$).

The contamination sources $Q_C(X,Y)$ will be determined from measurements $C^{exp}(X_m,Y_m)$ at a line (curve) within the flow field, such that the residual given by the fitness function (6) is minimized,

$$\varepsilon(Q_C(X,Y)=\int\int_Y\left(C^{exp}(X_m,Y_m)-C(X,Y)\right)^2\delta(X-X_m)\delta(Y-Y_m)dXdY \qquad (6)$$

Adjoint problem

The Lagrangian (7) is used for the adjoint problem statement

$$\varepsilon_0(Q_C(X,Y))=\varepsilon(Q_C(X,Y))+$$

$$+\iint_{X,Y}\left(U\frac{\partial C}{\partial X}+V\frac{\partial C}{\partial Y}+Q_C(X,Y)-D\frac{\partial^2 C}{\partial Y^2}\right)\Psi_C(X,Y)dXdY; \qquad (7)$$

Let the function $\Psi_C(X,Y)$ comply with Eq. (8) and boundary conditions (9):

$$\frac{\partial(U\Psi_C)}{\partial X}+\frac{\partial(V\Psi_C)}{\partial Y}+D\frac{\partial^2\Psi_C}{\partial Y^2}+$$

$$+2\left(C^{exp}(X,Y)-C(X,Y)\right)\delta(X-X_m)\delta(Y-Y_m)=0 \qquad (8)$$

$$\Psi_C\Big|^{X=0}=0;\ \Psi_C\Big|^{X=1}=0;\ \Psi_C\Big|^{Y=0}=0;\ \Psi_C\Big|^{Y=1}=0; \tag{9}$$

If Eqs. (8-9) hold, the residual variation equals:

$$\Delta\varepsilon(Q_C(X,Y))=\int\limits_{X,Y}\Delta Q_C(X,Y)\Psi_C(X,Y)dXdY; \tag{10}$$

while all other first order terms are equal zero. The Eq. (11) presents the residual gradient when the sources are distributed overall flow field.

$$grad(\varepsilon)=\Psi_C\,(X,Y) \tag{11}$$

Different iterative solvers may use the residual gradient [9]. Herein, the steepest descent was used:

$$Q_{ij}^{n+1}=Q_{ij}^{n}-\beta^{b}grad(\varepsilon^{n})_{ij};\ (i=1...Nx,j=1...Ny) \tag{12}$$

The present problem is obviously non-unique. The measurements at certain section may be engendered by the different sources (Figure 1).

Nevertheless, the additional information regarding sources may cure the problem. From heuristic viewpoint, some statements may be resolved. If the concentration field is engendered by single point source, the problem seems to be unique. More weak condition may demand the minimum number of point sources or their area. The adding of penalty terms proportional to source area seems the perspective for regularization [3]:

$$\varepsilon(Q_C(X,Y))=\int\int\limits_{Y}\left(C^{\exp}(X_m,Y_m)-C(X_m,Y_m)\right)^2\delta(X-X_m)\delta(Y-Y_m)dXdY+\int\limits_{X,Y}R(Q_C)dXdY$$

The less general approach may be used if the sources are described by some small set of parameters (location, amplitude etc.) $Q_C(X,Y)=F(A,X_0,Y_0,X,Y)$.

Numerical Experiments

Numerical tests demonstrated non-uniqueness in windward direction when all the field of sources was determined. Using of adjoint statement (with sources over total field) produces a single ravine with a slope to the outlet boundary. No success was obtained in problem solving with different $R(Q_C)$ penalizing the total area of sources. Nevertheless, for the single point source the problem is correct (although ill-conditioned). Fig. 2 presents the discrepancy contour lines for a single point source, which demonstrate the single minimum located in deep ravine. If the source is known to be single, the certain parameterization may be used with the corresponding gradients. Herein, the following expression for the source was used (X_0, Y_0 are the control parameters)

$$Q_C(X,Y)=A\exp\left(-\left(\frac{X-X_0}{D_X}\right)^2-\left(\frac{Y-Y_0}{D_Y}\right)^2\right)$$

$$\frac{\partial Q_C}{\partial X_0} = Q_C(X,Y)\left(-2\left(\frac{X-X_0}{D_X^{\,2}}\right)\right)$$

In finite differences the corresponding component of the gradient is of the form:

$\frac{\partial \varepsilon}{\partial X_0} = \Psi_{C_{ij}} \frac{\partial Q_C(X_i Y_j)}{\partial X_0}$; where the summation over i and j is performed.

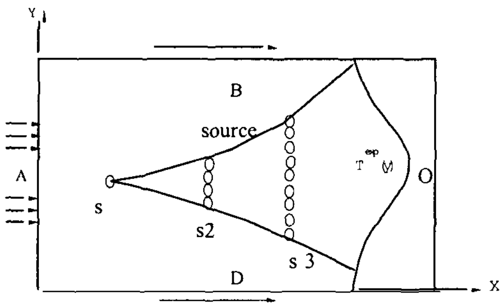

Figure 1. The scheme of flow region. A-inflow boundary. O- outflow boundary

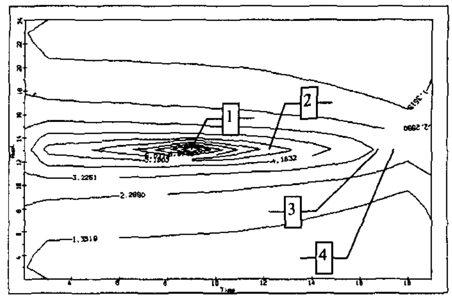

Figure 2. The discrepancy contour lines and solutions for the single point source

The numerical tests demonstrated successful estimation of the source location for exact data (with computer accuracy) and the data with simulated error. Fig. 2 presents results of numerical tests: 1 - exact position of source, 2- solution with data of computer accuracy, 3,4-solutions for error of standard deviation 0.01 and 0.05 correspondingly. The structure of sources in cross flow direction may be estimated with much greater success: two ravines are engendered by these data which corresponds to two separate sources.

Conclusions

The estimation of contamination sources from downstream measurements is a non-unique problem. The assimilation of additional information may cure this problem. If we know the number of sources (and this number is relatively small) we may search coordinates of point sources. For single source the problem has a unique solution. For a small number of sources the crosswind sources structure may be estimated. The utilization of adjoint approach provides quick and precise calculation of gradients for different forms of sources.

Evidently this technique becomes harder to be applied when we are solving nonlinear inverse problems. More research must be carried out in this direction where some initial results have been obtained by combining these type of iterative methods with Genetics Algorithms [8].

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1. RSC Energia, Korolev, Russia.

2. Department of Mathematics. University of Las Palmas de Gran Canaria. Edificio de Informática y Matemáticas, Campus Universitario de Tafira, 35017 - Las Palmas de Gran Canaria, Spain.