BALANCED AND ABSOLUTELY STABLE IMPLICIT SCHEMES FOR THE MAIN AND ADJOINT POLLUTANT TRANSPORT EQUATIONS IN LIMITED AREA

Yuri N. SKIBA*

Institute of Computational Mathematics, Russian Academy of Sciences, Moscow

(Recibido marzo 1993, aceptado agosto 1993)

Keywords: transport of pollutions, numerical solution, implicit scheme, splitting method, factorization method

ABSTRACT

Compatible, implicit, balanced and absolutely stable difference schemes of the second order aproximation in space and time are suggested for solving the main and adjoint pollutant transport equations in a limited area when there is a pollutant flux through the open lateral and top boundaries.

The differential operators of both the main and adjoint problems are positive definite, positive semidefinite or skew symmetric depending on the boundary conditions and the model parameters. The split 1-dim operators as well as the unsplit and split finite-difference operators have same properties. It enables us to apply the splitting-up method for constructing affordable implicit numerical schemes for the main and adjoint 3-dim problems.

RESUMEN

Se sugieren esquemas en diferencias finitas para resolver las ecuaciones de contaminación, principal y adjunta, en un área limitada en el caso de la existencia de un flujo contaminado a través de las fronteras lateral y superior abiertas. Estos esquemas son compatibles, implícitos, balanceados, absolutamente estables y de segundo orden de aproximación en espacio y tiempo.

Los operadores diferenciales de ambos problemas, el principal y el adjunto, son positivo definido, positivo semidefinido y asimétrico, dependiendo de las condiciones de frontera y de los parámetros del modelo. Los operadores separados, diferenciales y en diferencias finitas, son de 1-dimensión con las mismas propiedades del operador original. Esto permite aplicar el método de separación para construir esquemas numéricos implícitos para problemas de 3-dimensiones, el principal y el adjunto, que son económicos.

INTRODUCTION

Assuming that the wind, or current, velocities are known as a result of the solution of the corresponding dynamic model (Sawai 1978, Marchuk *et al.* 1979, Beniston 1987, Jauregui 1988, Buendia *et al.* 1992) the pollutant transport equation can be applied in a limited area to many interesting and important problems:

1) optimal allocation of new industrial plants in a given region with the aim to minimize the pollution concentration in certain ecologically significant zones (Marchuk 1986);

2) optimization of emissions from operating industrial plants (Marchuk 1982a, Penenko and Raputa 1983);

3) determination (on a basis of the air quality monitoring data) of the current level of pollutions coming from the industrial plants with the aim to identify the plant violating permissible sanitary norms (Penenko and Raputa 1982);

4) evaluation of the role of the emissions coming from the vehicle traffic including in the model

*Present address: Laboratorio de Teoría del Clima, Centro de Ciencias de la Atmósfera, UNAM, Ciudad Universitaria, Col. Coyoacán 04510 D.F., México

the linear pollution sources located along the main roadways (Heigorn *et al.* 1991, Sliggers 1992);

5) estimation of the oil pollution in various ecologically significant oceanic (sea) zones in case of the tanker wreck (Skiba 1993);

6) evaluation of the sea water desalination in ecologically significant zones when the fresh water is coming from a river estuary.

The above-listed problems can be studied by using the main and adjoint pollutant transport equations. The aim of this work is to formulate well posed main and adjoint pollutant transport problems in a limited area and construct balanced difference schemes. Moreover, the schemes for main and adjoint problems must be compatible, i.e. the finite-difference operators of these schemes must satisfy the Lagrange identity.

As it was pointed out by Forester (1977), Rood (1987), Dymnikov and Aloyan (1990), Allen *et al.* (1991), Smolarkiewicz (1991), Williamson (1992) and others, the most desirable transport scheme should be stable, balanced, transportive, monotonic, computationally affordable and of high order approximation. In addition, in case of limited area models when there is a pollutant flux through the boundaries, correct choice of the boundary conditions is also very important to obtain well posed problem in both the mathematical and physical sense. Indeed, typically all the absolutely stable schemes are implicit. In a multi-dimensional case, solving the implicit scheme is very costly. Geometric splitting of the original multidimensional problem into a few one-dimensional problems, greatly simplifies the numerical algorithm. However, application of the splitting-up method can be justified only when all the split operators are nonnegative. This property crucially depends on the choice of the boundary conditions. Thus construction of such operators for limited area models with the open boundaries is not trivial. In this work Marchuk's idea (Marchuk 1986) was applied not only to the lateral but also to the open top boundary. It allows to avoid putting the artificial condition w = 0 at the top of the domain where w is the vertical velocity component.

The schemes suggested are compatible, balanced, implicit, absolutely stable to initial perturbations and of second order approximation in time and space. The splitting-up method (Yanenko 1971, Marchuk 1982b) is used to obtain a solution of the original complex three-dimensional problem by solving a set of the simple one-dimensional split problems. The original and split operators of the main and adjoint pollutant transport equations are positive semidefinite both in the differential and difference form. Note that the same schemes can be applied to the thermodynamic models of the atmosphere and/or ocean in limited area (Adem 1991, Marchuk and Skiba 1992, Robertson 1992).

THE POLLUTANT TRANSPORT PROBLEM

Let us consider a 3-dimensional 'cylindric' domain $\mathbf{D}$ with the boundary $\Omega = \mathbf{S} \cup \mathbf{S}_0 \cup \mathbf{S}_H$ being the union of the cylinder lateral surface $\mathbf{S}$, the base $\mathbf{S}_0$ at z=0, and top cover $\mathbf{S}_H$ at z=H (Fig. 1).

The transport diffusion equation

$$\frac{\partial \phi}{\partial t} + \mathbf{U}\cdot\nabla\phi + \sigma\phi = \frac{\partial}{\partial z}\upsilon\frac{\partial \phi}{\partial z} + \nabla\cdot\mu\nabla\phi + \sum_{i=1}^{N} Q_i(t)\,\delta(\mathbf{r}-\mathbf{r}_i) \quad (1)$$

for the pollutant $\phi(r, t)$ in the domain $\mathbf{D}$ and time interval (0,T) is the common basis for most air quality models. Here $\mathbf{r}=(x, y, z)$; υ and μ are the diffusion coefficients; ∇ is the 2-dimensional gradient in (x, y) –direction; σ characterizes decreasing of $\phi(\mathbf{r}, t)$ because of different chemical processes; $Q_i(t)$ is the emission power of the *i*th pollution source located in the point $\mathbf{r}_i$ (i=1,...,N); $\delta(\mathbf{r})$ is the Dirac mass at the point $\mathbf{r}$; and $\mathbf{U}(\mathbf{r}, t) = \{u, v, w\}$ is the wind (or current) velocity vector satisfying the continuity equation

$$\operatorname{div}\mathbf{U} \equiv \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \quad (2)$$

where div (·) is the 3-dimensional divergence operator. Let $\mathbf{U_n}$ be the projection of the wind velocity component on the outward normal $\mathbf{n}$ to the

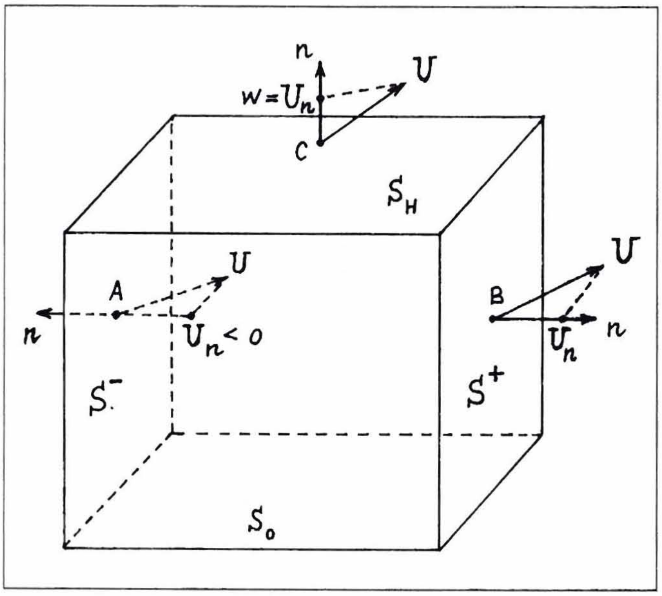

Fig. 1. The limited domain **D**. The boundary points A, B and C belong to the surfaces S^-, S^+ and S_H^+ respectively; U_n is the normal component of the velocity vector **U** to the boundary surface.

boundary Ω, besides, $\mathbf{U_n}= 0$ (or w=0) on $\mathbf{S_o}$. Then, given the horizontal components u(**r**, t) and v(**r**, t) of the velocity **U** in **D**, its vertical component w is determined as

$$w(x, y, z,t) = -\int_o^z \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)dz \qquad (3)$$

Hence, typically, w(x y, H) $\neq$ 0 on the top surface S_H, and there is a pollution flux from the inside of **D** through S_H. Thus our boundary condition on $\mathbf{S_H}$ are different from the Marchuk (1986) condition w(x y, H) = 0 which can be satisfied only in a special case.

Let us divide the lateral boundary **S** into two parts: the part $\mathbf{S^+}$ where $\mathbf{U_n} \geq 0$ and the pollutants are blown out by the wind from the inside of the domain **D**, and the part $\mathbf{S^-}$ where $\mathbf{U_n} \leq 0$ and the wind (or the current) is directed from the outside to the inside of **D** (see Fig. 1). Similarly, let $\mathbf{S_H^+}$ and $\mathbf{S_H^-}$ denote the parts of $\mathbf{S_H}$ where $\mathbf{U_n} \equiv w \geq 0$ and $\mathbf{U_n} \equiv w \leq 0$ respectively (Fig. 1). Since the boundary **S** consists only of parts of the surfaces x = Const or y = Const, the normal component $\mathbf{U_n}$ always coincides on **S** with either ±u or ±v where u and v are the components of the velocity vector **U**.

As the initial and boundary conditions for Eq. (1) in the time interval (0, T) and domain **D** we take

$$\phi(\mathbf{r}, 0) = \Phi^o(\mathbf{r}) \qquad (4)$$

$$\mu \frac{\partial \phi}{\partial \mathbf{n}} - \mathbf{U_n}\phi = 0 \text{ on } \mathbf{S^-} \qquad (5)$$

$$\mu \frac{\partial \phi}{\partial \mathbf{n}} = 0 \text{ on } \mathbf{S^+} \qquad (6)$$

$$\upsilon \frac{\partial \phi}{\partial z} = \alpha\phi \text{ on } \mathbf{S_o} \qquad (7)$$

$$\upsilon \frac{\partial \phi}{\partial z} - \mathbf{U_n}\phi = 0 \text{ on } \mathbf{S_H^-} \qquad (8)$$

$$\upsilon \frac{\partial \phi}{\partial z} = 0 \text{ on } \mathbf{S_H^+} \qquad (9)$$

where $\alpha \geq 0$ is a known function defining the interaction of the pollutant with the underlyng surface (for example, the pollutant settlement velocity). Note that the ground level emission sources from vehicle traffic can be included in the model through replacing (7) by

$$\upsilon \frac{\partial \phi}{\partial z} = \alpha\phi - \sum_{i=1}^{M} R_i(t)\, \delta(x - x_i)\, \delta(y - y_i) \text{ on } \mathbf{S_o} \qquad (7')$$

where (x_i, y_i) are the grid points belonging to the main roads.

The boundary conditions (5) and (8) mean that there is no pollutant flux from the outside of the domain **D** on the part $\mathbf{S^-} \cup \mathbf{S_H^-}$ of the boundary Ω, whereas the conditions (6) and (9) suppose that the turbulent flux of pollutants on the part $\mathbf{S}^+ \cup \mathbf{S}_H^+$ of Ω is negligible as compared to the advective pollutant flux by the wind $\mathbf{U}$ from the inside to the outside of the domain $\mathbf{D}$.

INTEGRAL PROPERTIES OF THE TRANSPORT PROBLEM SOLUTIONS

Let

$$\| \phi \| = \Big(\int_{\mathbf{D}} | \phi (\mathbf{r}) |^2 \, d\mathbf{r}\Big)^{1/2} \tag{10}$$

be the norm of the function $\phi(\mathbf{r})$ and let $\mathbf{H}$ be a Hilbert space of all such functions whose norm (10) is finite. We define the scalar product

$$(\phi, g) = \int_{\mathbf{D}} \phi(\mathbf{r})\, g(\mathbf{r})\, d\mathbf{r} \tag{11}$$

for any functions $\phi(\mathbf{r})$ and $g(\mathbf{r})$ from $\mathbf{H}$. The differential operator of Eq. (1) which can be written as

$$A\phi = \mathrm{div}(\mathbf{U}\phi) + \sigma\phi - \frac{\partial}{\partial z}\, \upsilon \frac{\partial \phi}{\partial z} - \nabla\cdot\mu\nabla\phi \tag{12}$$

due to (2) is defined for all sufficiently smooth functions $\phi(\mathbf{r})$ of $\mathbf{H}$ satisfying the conditions (5)–(9). We now show that

$$(A\phi, \phi) \geq 0 \tag{13}$$

for all such functions Φ, i.e., A is positive semidefinite: $A \geq 0$. Indeed, integrating by parts and using the Green formula and (5)–(9) lead to

$$(A\phi,\phi) \equiv \int_{\mathbf{D}} \phi\, A\phi\, d\mathbf{r} = \int_{\mathbf{D}} [\sigma\phi^2 + \upsilon \Big(\frac{\partial\phi}{\partial z}\Big)^2 + \mu\, | \nabla\phi |^2]\, d\mathbf{r}$$

$$+ \int_{\mathbf{S}_O} \alpha\, \phi^2 d\Omega + \frac{1}{2}\Big\{ \int_{\mathbf{S}^+ \cup\, \mathbf{S}_H^+} \mathbf{U_n}\phi^2\, d\Omega - \int_{\mathbf{S}^- \cup\, \mathbf{S}_H^-} \mathbf{U_n}\phi^2\, d\Omega\Big\} \geq 0 \tag{14}$$

where $d\Omega$ is the infinitesimal element of the corresponding part of the boundary surface Ω. Note that the last integral in (14) is non-negative since $\mathbf{U_n} \leq 0$ on the surface $\mathbf{S}^- \cup \mathbf{S}_H^-$. Moreover, A is positive definite ($A > 0$) if at least one of the next three conditions is satisfied: $\alpha \not\equiv 0$, $\sigma \not\equiv 0$ or $\mathbf{U_n} \not\equiv 0$. Beside, in the nondissipative case ($\mu \equiv \upsilon \equiv \sigma \equiv 0$) when, in addition, $\mathbf{U_n} \equiv 0$ on $\mathbf{S} \cup \mathbf{S}_H$ and $\alpha \equiv 0$, the operator A is skew symmetric:

$$(A\phi, \phi) \equiv 0 \tag{15}$$

Integrating (1) over $\mathbf{D}$ leads to the balance equation

$$\frac{\partial}{\partial t}\int_{\mathbf{D}} \phi\, d\mathbf{r} = \sum_{i=1}^{N} Q_i(t) - \int_{\mathbf{D}} \sigma\phi\, d\mathbf{r} - \int_{\mathbf{S}_O} \alpha\phi\, d\Omega - \int_{\mathbf{S}^+ \cup\, \mathbf{S}_H^+} \mathbf{U_n}\phi\, d\Omega \tag{16}$$

By Eq. (16), rise in the pollution concentration level within the domain $\mathbf{D}$ takes place because of the presence of the sources Q_i. At the same time, this level is decreased because of different chemical processes in $\mathbf{D}$, interaction of the pollutants with the underlying surface $\mathbf{S}_O$, and the pollutant flux from the inside of $\mathbf{D}$ through the boundary surface $\mathbf{S}^+ \cup \mathbf{S}_H^+$.

Let us consider the scalar product (11) of Eq. (1) written as

$$\frac{\partial\phi}{\partial t} + A\phi = \sum_{i=1}^{N} Q_i(t)\, \delta(\mathbf{r} - \mathbf{r}_i) \tag{17}$$

with the solution ϕ. Then taking into account (13), we obtain

$$\frac{1}{2}\frac{\partial}{\partial t} \|\phi(\mathbf{r}, t)\|^2 \leq \sum_{i=1}^{N} Q_i(t)\, \phi(\mathbf{r}_i, t) \qquad (18)$$

Thus the norm $\|\phi(\mathbf{r}, t)\|$ of the solution will not grow with time if all the sources $Q_i(t)$ are zero $(i=1,\ldots,N)$, and hence, the problem (1), (2), (4)–(9) is well posed in Hadamard's sense, i.e., the solution $\phi(\mathbf{r}, t)$ is stable to initial perturbations. Note that $\|\phi(\mathbf{r}, t)\|$ will be conserved if the operator A is skew symmetric and will tend to zero if A is strictly positive. In particular, when $\sigma \equiv 0$, $\alpha \equiv 0$, and $U_n \equiv 0$ on Ω, the operator A is positive semi-definite, and $\Phi(\mathbf{r}, t)$ tends to the constant $(\text{mes } \mathbf{D})^{-1/2} \int_{\mathbf{D}} \Phi^\circ(\mathbf{r})\, d\mathbf{r}$ where mes **D** is the volume of **D**, and $\Phi^\circ(\mathbf{r})$ is given by (4).

THE ADJOINT TRANSPORT PROBLEM

Using the Lagrange identity

$$(A\phi, g) = (\phi, A^*g) \qquad (19)$$

let us introduce the adjoint operator

$$A^*g = -\operatorname{div}(\mathbf{U}g) + \sigma g - \frac{\partial}{\partial z} \upsilon \frac{\partial g}{\partial z} - \nabla\cdot\mu\nabla g \qquad (20)$$

defined for all sufficiently smooth functions $g(\mathbf{r})$ of **H** satisfying the conditions

$$\mu \frac{\partial g}{\partial \mathbf{n}} = 0 \text{ on } \mathbf{S}^- \qquad (21)$$

$$\mu \frac{\partial g}{\partial \mathbf{n}} + \mathbf{U_n} g = 0 \text{ on } \mathbf{S}^+ \qquad (22)$$

$$\upsilon \frac{\partial g}{\partial z} = \alpha g \text{ on } \mathbf{S}_o \qquad (23)$$

$$\upsilon \frac{\partial g}{\partial z} = 0 \text{ on } \mathbf{S}_H^- \qquad (24)$$

$$\upsilon \frac{\partial g}{\partial z} + \mathbf{U_n} g = 0 \text{ on } \mathbf{S}_H^+ \qquad (25)$$

As the adjoint problem in the domain **D** and in the time interval (0, T) we consider the equation

$$-\frac{\partial g}{\partial t} - \operatorname{div}(\mathbf{U}g) + \sigma g = \frac{\partial}{\partial z} \upsilon \frac{\partial g}{\partial z} + \nabla\cdot\mu\nabla g + P(\mathbf{r}, t) \qquad (26)$$

with the forcing $P(\mathbf{r}, t)$, the initial condition

$$g(\mathbf{r}, T) = 0 \qquad (27)$$

and the boundary conditions (21)–(25).

Similar to (14), it can be shown that the adjoint operator (20) is also positive semidefinite:

$$(g, A^*g) \geq 0 \qquad (28)$$

If $P(\mathbf{r}, t) \equiv 0$, and the equation (26) is solved from t=T to t=0, then the adjoint solution norm $\|g(\mathbf{r}, t)\|$ goes down in the same way as the solution of the main equation (1). Besides, if $A^* > 0$ and $T \to \infty$ then

$$\lim_{t \to o} \| g(\mathbf{r}, t) \| = 0 \qquad (29)$$

Thus the adjoint problem (21)–(27) is well posed in the Hadamard sense only if it is solved in the opposite time direction. That is why the initial condition (27) is put at t=T.

Integrating (26) over **D** leads to the adjoint balance equation

$$-\frac{\partial}{\partial t}\int_{\mathbf{D}} g\,d\mathbf{r} = \int_{\mathbf{D}} \{P(\mathbf{r}, t) - \sigma g\}\,d\mathbf{r} - \int_{\mathbf{S}_o} \alpha g\,d\Omega + \int_{\mathbf{S}^- \cup \mathbf{S}_H^-} \mathbf{U}_n g\,d\Omega \quad (30)$$

Note that $\mathbf{U}_n \leq 0$ in the last integral of (30).

Let $P(\mathbf{r}, t) \equiv 0$ and $Q_i(t) \equiv 0$ for all $i=1,...,N$. Then the substitution $t'=T-t$ shows that Eq. (26) differs from Eq. (1) only by the sign of the velocity **U**. Hence, the part $\mathbf{S}^+$ of the boundary **S** in the main problem (1)–(9) serves as $\mathbf{S}^-$ in the adjoint problem and vice versa. That is why the conditions (5) and (6) are transformed to (21) and (22). These comments refer equally to the conditions (8), (9) and (24), (25). It also explains the difference between the last terms of the balance equations (16) and (30).

PRINCIPAL RELATION BETWEEN SOLUTIONS OF THE MAIN AND ADJOINT TRANSPORT PROBLEMS

Let us multiply Eq. (1) and Eq. (26) by g and ϕ respectively, integrate them over the domain **D** and time interval (0,T), and subtract the results one from another. Then taking into account the Green formula and the conditions (4)–(9), (21)–(25) and (27) give the identity

$$J_P(\phi) = \sum_{i=1}^{N} \int_o^T g(\mathbf{r}_i, t)\, Q_i(t)\, dt + \int_{\mathbf{D}} g(\mathbf{r}, 0)\, \Phi^\circ(\mathbf{r})\, d\mathbf{r} \quad (31)$$

where

$$J_P(\phi) = \int_o^T \int_{\mathbf{D}} P(\mathbf{r}, t)\, \phi(\mathbf{r}, t)\, d\mathbf{r}dt \quad (32)$$

The formulas (31) and (32) are dual and relate the basic and adjoint solutions. They allow to determine the pollution concentration level $J_P(\phi)$ in the domain **D** in two different ways. Unlike the formula (32) that uses the solution $\phi(\mathbf{r}, t)$ of the main pollution transport problem (1)–(9), the formula (31) uses the solution $g(\mathbf{r}, t)$ of the adjoint problem (21)–(27). It is the main formula for estimating the average pollution concentration within the interval (0, T) in some ecologically important zones located in the domain **D** (Penenko and Raputa 1982, Marchuk 1986, Skiba 1993).

The right-hand side of (31) explicitly demonstrates the role of the input data $Q_i(t)$ and $\Phi^\circ(\mathbf{r})$ in forming $J_P(\phi)$. Therefore this formula is especially efficient when many experiments should be carried out to estimate the sensitivity (or variability) of the functional $J_P(\phi)$ to various values $Q_i(t)$ and $\Phi^\circ(\mathbf{r})$. Indeed, in the case, for using (32) one need to solve Eq. (1) repetitively for each particular pair of the functions $Q_i(t)$ and $\Phi^\circ(\mathbf{r})$. Hence, it is more economical to solve Eq. (26) only once, and then use (31).

We now consider one example. Let $\mathbf{D}_e = \omega \times [o, z_o]$ be an ecologically important zone in **D** where $\omega \subset \mathbf{S}_o$ and $o < z_o < H$, and our aim is to estimate the average level of the pollution concentration in the zone $\mathbf{D}_e$ within the time subinterval $[T-\tau, T]$:

$$J_b(\phi) \equiv \int_{T-\tau}^{T} dt \int_o^{z_o} \int_{\omega} b\,\phi\, d\mathbf{r} \quad (33)$$

where $b(\mathbf{r}, t)$ is a positive weight function normalized by

$$\int_{T-\tau}^{T} dt \int_o^{z_o} \int_{\omega} b(\mathbf{r}, t)\, d\mathbf{r} = 1 \quad (34)$$

We choose the adjoint forcing $P(\mathbf{r}, t)$ as

$$P(\mathbf{r}, t) = \begin{cases} b(\mathbf{r}, t) \text{ if } \mathbf{r} \in \mathbf{D}_e \text{ and } t \in [T-\tau, T] \\ 0, \text{ otherwise} \end{cases} \quad (35)$$

Then the right-hand side of the formula (31) with the adjoint solution $g(\mathbf{r}, t)$ calculated for the forcing (35), gives us the estimate of $J_b(\phi)$. Note that if $A^*>0$ and the time interval $[0, T-\tau]$ is sufficiently large then, due to (29), the formula (31) can be simplified by ignoring the role of the initial value $\Phi^\circ(\mathbf{r})$:

$$J_b(\phi) \cong \sum_{i=1}^{N} \int_{o}^{T} g(\mathbf{r}_i, t)\, Q_i(t)\, dt \tag{36}$$

It is important to emphasize that finite difference approximations of the main and adjoint operators also must be compatible in the sense of validity of the Lagrange identity (see the formula (55) below). Only then the analogy of the formulas (31) and (32) can be obtained for main and adjoint finite-difference problems.

NUMERICAL SCHEME FOR THE MAIN POLLUTANT TRANSPORT EQUATION

Using (2) the equation (1) can be written as

$$\frac{\partial \phi}{\partial t} + (A_1 + A_2 + A_3)\phi = F \tag{37}$$

where

$$F(\mathbf{r}, t) \equiv \sum_{i=1}^{N} Q_i(t)\, \delta(\mathbf{r}-\mathbf{r}_i) \tag{38}$$

and the operator (12) is represented as a sum of three operators

$$A_1\phi = \frac{1}{2}\frac{\partial}{\partial x}(u\phi) + \frac{1}{2} u \frac{\partial \phi}{\partial x} - \frac{\partial}{\partial x}\left(\mu \frac{\partial \phi}{\partial x}\right) \tag{39}$$

$$A_2\phi = \frac{1}{2}\frac{\partial}{\partial y}(v\phi) + \frac{1}{2} v \frac{\partial \phi}{\partial y} - \frac{\partial}{\partial y}\left(\mu \frac{\partial \phi}{\partial y}\right) \tag{40}$$

$$A_3\phi = \frac{1}{2}\frac{\partial}{\partial z}(w\phi) + \frac{1}{2} w \frac{\partial \phi}{\partial z} - \frac{\partial}{\partial z}\left(\upsilon \frac{\partial \phi}{\partial z}\right) + \sigma\phi \tag{41}$$

It is shown in Appendix A that

$$A_m \geq 0\,,\ (m = 1, 2, 3) \tag{42}$$

if the boundary conditions (5)–(9) are taken into account (see Appendix A). Then the splitting method (Birkhoff and Varga 1959, Douglas and Rachford 1956, Yanenko 1971, Marchuk 1982b) can be applied for solving (39) within each small time interval (t_1, t_2): the equations

$$\frac{\partial}{\partial t}\phi_i + A_i\phi_i = F_i$$

$(i=1, 2, 3)$ are successively solved in (t_1, t_2) with $F_1=0$, $F_2=0$ and $F_3=F$, and the initial conditions $\phi_1(t_1) = \phi(t_1)$ and $\phi_i(t_1) = \phi_{i-1}(t_2)$ for $i=2, 3$. Then, eventually, $\phi(t_2) \cong \phi_3(t_2)$.

Note that the operator A also can be split by separating the advective and turbulent physical processes (Marchuk 1986, Salerno *et al.* 1992).

The net functions $\Phi_{ijk} \equiv \phi(x_i,y_j,z_k)$, $u_{ijk} \equiv u(x_{i-1/2},y_j,z_k)$, $v_{ijk} \equiv v(x_i,y_{j-1/2},z_k)$, $w_{ijk} \equiv w(x_i,y_j,z_{k-1/2})$, $\mu_k \equiv \mu(z_k)$ and $\upsilon_{ijk} \equiv \upsilon(x_i,y_j,z_{k-1/2})$ are defined on different grids (Fig. 2). For the sake of simplicity it is supposed in this section that the horizontal turbulent coefficient $\mu(z)$ is independent of x and y. The boundary nodes of the grid domain coincide with the boundary nodes of u_{ijk}, v_{ijk} or w_{ijk} (Fig. 3). We take

$$\{u_{i+1,jk} - u_{ijk}\}/\Delta x + \{v_{i,j+1,k} - v_{ijk}\}/\Delta y + \{w_{ij,k+1} - w_{ijk}\}/\Delta z = 0 \tag{43}$$

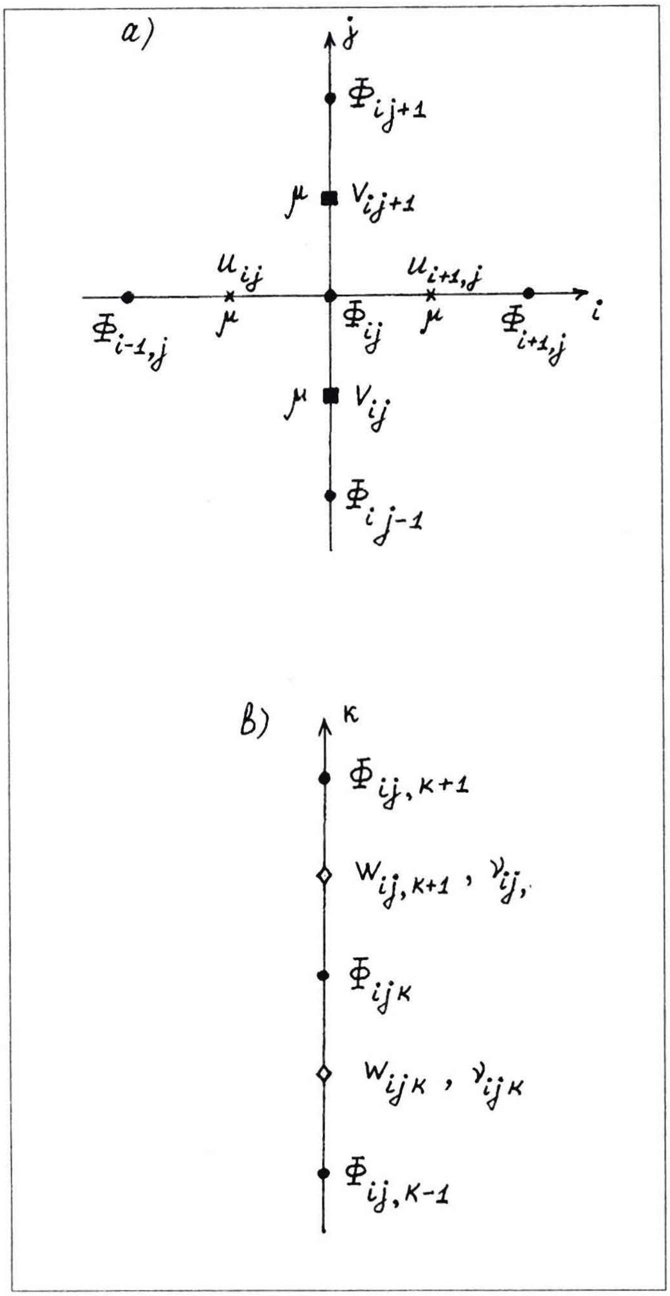

Fig. 2. Location of the grid functions in the case $\mu=\mu(z)$ at each horizontal level k=Const (a), and along each vertical line i=Const, j=Const (b).

as the difference form of the continuity equation (2). Further, let us rewrite (39)–(41) as

$$A_1\phi = \frac{1}{2}\phi\frac{\partial u}{\partial x} + u\frac{\partial \phi}{\partial x} - \frac{\partial}{\partial x}\left(\mu\frac{\partial \phi}{\partial x}\right)$$

$$A_2\phi = \frac{1}{2}\phi\frac{\partial v}{\partial y} + v\frac{\partial \phi}{\partial y} - \frac{\partial}{\partial y}\left(\mu\frac{\partial \phi}{\partial y}\right)$$

$$A_3\phi = \frac{1}{2}\phi\frac{\partial w}{\partial z} + w\frac{\partial \phi}{\partial z} - \frac{\partial}{\partial z}\left(\upsilon\frac{\partial \phi}{\partial z}\right) + \sigma\phi$$

It is known that the form $\frac{1}{2}\phi\frac{\partial u}{\partial x} + u\frac{\partial \phi}{\partial x}$ is approximated in the point(x_i, y_j, z_k) with the second order by

$$\{u_{i+1,jk}\Phi_{i+1,jk} - u_{ijk}\Phi_{i-1,jk}\}/2\Delta x$$

Therefore, the operators A_m are approximated by the matrices A_m^h defined as (Skiba 1978)

$$(A_1^h\Phi)_{ijk} = \{u_{i+1,jk}\Phi_{i+1,jk} - u_{ijk}\Phi_{i-1,jk}\}/2\Delta x$$
$$-\mu_k\{\Phi_{i+1,jk} - 2\,\Phi_{ijk} + \Phi_{i-1,jk}\}/\Delta x^2 \qquad (44)$$

$$(A_2^h\Phi)_{ijk} = \{v_{i,j+1,k}\Phi_{i,j+1,k} - v_{ijk}\Phi_{i,j-1,k}\}/2\Delta y$$
$$-\mu_k\{\Phi_{i,j+1,k} - 2\,\Phi_{ijk} + \Phi_{i,j-1,k}\}/\Delta y^2 \qquad (45)$$

$$(A_3^h\,\Phi)_{ijk} = \{w_{ij,k+1}\Phi_{ij,k+1} - w_{ijk}\Phi_{ij,k-1}\}/2\Delta z$$
$$+\,\sigma\,\Phi_{ijk}$$
$$-\,\{\upsilon_{ij,\,k+1}(\Phi_{ij,k+1} - \Phi_{ijk}) - \upsilon_{ijk}(\Phi_{ijk} - \Phi_{ij,k-1})\}/\Delta z^2$$
$$(46)$$

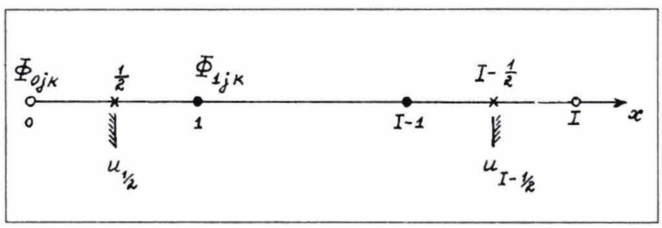

Fig. 3. Location of the grid nodes immediately adjacent to the boundary points $x_{1/2}$ and $x_{I-1/2}$ on the line j=Const, k=Const.

We now show how to approximate the boundary conditions. Consider, for example, a line along the axis x defined by y_j = Const, z_k = Const, and let $(x_{1/2}, y_j, z_k)$ and $(x_{I-1/2}, y_j, z_k)$ be the left and the right boundary points on this line respectively. Then (x_i, y_j, z_k) where i=1,...,I-1, are internal points of the grid domain. Due to (5), (6), two types of the boundary conditions are possible. If $u_{1jk} \equiv u(x_{1/2}, y_j, z_k) \geq 0$ then $\mathbf{U}_n = -u_{1jk} \leq 0$ and the boundary point $(x_{1/2}, y_j, z_k)$ belongs to the boundary $\mathbf{S}^-$. Besides, since $\frac{\partial\phi}{\partial\mathbf{n}}(x_{1/2}, y_j, z_k) \cong (\Phi_{ojk} - \Phi_{1jk})/\Delta x$, the boundary condition (5) is approximated as

$$\mu_k\,(\Phi_{ojk} - \Phi_{1jk})/\Delta x + u_{1jk}(\Phi_{ojk} + \Phi_{1jk})/2 = 0 \tag{47}$$

And if $u_{ijk} \equiv u(x_{1/2}, y_j, z_k) \leq 0$ then $\mathbf{U}_n = -u_{1jk} \geq 0$ and the point $(x_{1/2}, y_j, z_k)$ belongs to $\mathbf{S}^+$. Therefore the boundary condition (6) is approximated as

$$\mu_k\,(\Phi_{ojk} - \Phi_{1jk})/\Delta x = 0 \tag{48}$$

and hence, $\Phi_{1jk} = \Phi_{ojk}$. Thus the term $-u_{1jk}\Phi_{ojk}$ in the operator (44) for i=1 should be written as $-u_{1jk}\Phi_{1jk}$ to exclude the external point (x_o, y_j, z_k) from the consideration.

Further, if $u_{Ijk} \equiv u(x_{I-1/2}, y_j, z_k) \leq 0$, then $\mathbf{U}_n = u_{Ijk} \leq 0$ and the boundary point $(x_{I-1/2}, y_j, z_k)$ belongs to $\mathbf{S}^-$. Besides,

$$\frac{\partial\phi}{\partial\mathbf{n}}(x_{I-1/2}, y_j, z_k) \cong (\Phi_{Ijk} - \Phi_{I-1,jk})/\Delta x$$

and hence, the boundary condition (5) is approximated as

$$\mu_k\,(\Phi_{Ijk} - \Phi_{I\text{-}1,jk})/\Delta x - u_{I,jk}(\Phi_{I-1,jk} + \Phi_{Ijk})/2 = 0 \tag{49}$$

Finally, if $u_{Ijk} \equiv u(x_{I-1/2}, y_j, z_k) \geq 0$ then the boundary point $(x_{I-1/2}, y_j, z_k)$ belongs to $\mathbf{S}^+$, and (6) is reduced to

$$\Phi_{Ijk} = \Phi_{I-1,jk} \tag{50}$$

The boundary conditions for other lines along the axes x, y or z are approximated in the same way. Of course, number of inner grid points can vary for different lines. Thus, not only the differential equation (1), but also the boundary conditions (5)–(9) are approximated with the second order in the geometric variables. Taking into account (47) –(50) leads to

$$\Phi^T A^h_m \Phi \geq 0, \ (m=1, 2, 3) \tag{51}$$

where Φ^T is the transpose of the vector Φ with the components $\{\Phi_{ijk}\}$. Thus each matrix A^h_m is positive semidefinite and the finite-difference approximations conserve the important properties (42) of the differential operators A_m. Therefore numerical algorithm can be constructed on the basis of the splitting method (Birkhoff and Varga 1959, Douglas and Rachford 1956, Yanenko 1971, Marchuk 1982b).

Since the matrices A^h_m are noncommutative: $A^h_m\, A^h_l \neq A^h_l\, A^h_m$, the symmetrized variant of the splitting method suggested by Marchuk (1982b) is here applied to obtain the numerical scheme of the second order approximation in time. At each fractional time step, the Crank-Nicolson scheme is used to approximate the 1-dimensional split problems in time. Within each double time step interval $I_n \equiv (t_{n-1}, t_{n+1})$ the resulting numerical scheme has the form

$$\Phi\,[n-\tfrac{2}{3}] - \Phi\,[n-1] = -\frac{\tau}{2}\,A_1^h\,\{\Phi\,[n-\tfrac{2}{3}] + \Phi\,[n-1]\}$$

$$\Phi[n-\tfrac{1}{3}] - \Phi[n-\tfrac{2}{3}] = -\frac{\tau}{2}\,A_2^h\{\Phi\,[n-\tfrac{1}{3}] + \Phi\,[n-\tfrac{2}{3}]\}$$

$$\Phi[n+\tfrac{1}{3}] - \Phi[n-\tfrac{1}{3}] = -\tau\,A_3^h\,\{\Phi[n+\tfrac{1}{3}] + \Phi[n-\tfrac{1}{3}]\} + 2\tau\,F[n]$$

$$\Phi[n+\tfrac{2}{3}] - \Phi[n+\tfrac{1}{3}] = -\frac{\tau}{2}\,A_2^h\,\{\Phi[n+\tfrac{2}{3}] + \Phi[n+\tfrac{1}{3}]\}$$

$$\Phi[n+1] - \Phi[n+\tfrac{2}{3}] = -\frac{\tau}{2}\,A_1^h\,\{\Phi[n+1] + \Phi[n+\tfrac{2}{3}]\} \quad (52)$$

where $\Phi[n]$ is the column vector with the components $\Phi_{ijk}\,(t_n)$; $\tau = t_n - t_{n-1}$ is the scheme time step;

$$F[n] = 0{,}5\,\{F_{ijk}\,(t_{n+1}) + F_{ijk}\,(t_{n-1})\}, \quad (53)$$

is the forcing approximation, and $\Phi[n+p/3]$ with the fractional indices $p/3$ are the auxiliary functions ($n=1, 3, 5,\ldots$; $p=\pm1, \pm2$). Within I_n the scheme (52) is solved under the initial condition $\Phi[n-1] = \Phi(t_{n-1})$. Then the final solution $\Phi[n+1]$ in I_n is taken as the initial condition for the next interval I_{n+1} and so on. The initial vector $\Phi[0]$ has the components $\Phi^\circ\,(x_i, y_j, z_k)$ (see (4)).

Multiplying the first equation (52) from the left by the vector $\{\Phi[n-\tfrac{2}{3}] + \Phi[n-1]\}^T$ and taking into account (51) lead to

$$\Phi^T\,[n-\tfrac{2}{3}]\;\Phi\,[n-\tfrac{2}{3}] \le \Phi^T[n-1]\,\Phi[n-1] \quad (54)$$

Since $\Phi^T\Phi = \|\Phi\|^2$ ($\|\Phi\|$ is the Euclidean norm) and the inequalities like (54) are valid for all the equations (52) with $F[n] = 0$, the numerical scheme (52) is stable to initial perturbations for any time step τ.

Let us multiply each equation (52) from the left by the row vector $\mathbf{V}^T$ which has the same dimension as Φ, and equal components $\Delta x \Delta y \Delta z$. Summing all the results obtained gives a finite- difference version of the balance equation (16). It shows that the difference scheme (52) is balanced.

NUMERICAL SCHEME FOR THE ADJOINT POLLUTANT TRANSPORT EQUATION

Application of the Lagrange identity

$$G^T A \Phi = (A^T G)^T\,\Phi \quad (55)$$

(for real vectors and matrices) to A_m^h results in

$$\{(A_1^h)^T G\}_{ijk} = -\{u_{i+1,jk}\,G_{i+1,jk} - u_{ijk}\,G_{i-1,jk}\}/2\Delta x - \mu_k\{G_{i+1,jk} - 2\,G_{ijk} + G_{i-1,jk}\}/\Delta x^2 \quad (56)$$

$$\{(A_2^h)^T G\}_{ijk} = -\{v_{i,j+1,k}G_{i,j+1,k} - v_{ijk}G_{i,j-1,k}\}/2\Delta y - \mu_k\{G_{i,j+1,k} - 2G_{ijk} + G_{i,j-1,k}\}/\Delta y^2 \quad (57)$$

$$\{(A_3^h)^T G\}_{ijk} = -\{w_{ij,k+1}G_{ij,k+1} - w_{ijk}G_{ij,k-1}\}/2\Delta z + \sigma G_{ijk} - \{\upsilon_{ij,k+1}(G_{ij,k+1} - G_{ijk}) - \upsilon_{ijk}(G_{ijk} - G_{ij,k-1})\}/\Delta z^2 \quad (58)$$

for any inner grid point (x_i, y_j, z_k). Here $G_{ijk} = g(x_i,y_j,z_k)$. Thus the formulas (44)–(46) and (56)–(58) for the main and adjoint matrices differ only by the opposite signs of the velocity components u, v and w. The adjoint problem boundary conditions corresponding to (47)–(50) are

$$G_{ojk} = G_{1jk} \tag{59}$$

$$\mu_k(G_{ojk}-G_{1jk})/\Delta x-u_{1jk}(G_{ojk}+G_{1jk})/2 = 0 \tag{60}$$

$$G_{Ijk} = G_{I-1,jk} \tag{61}$$

and

$$\mu_k(G_{Ijk}-G_{I-1,jk})/\Delta x+u_{I,jk}(G_{I-1,jk}+G_{Ijk})/2 = 0 \tag{62}$$

respectively. It is easily checked that $(A^h_m)^T$ and (59)–(62) approximate the differential operators A^T_m and the corresponding boundary conditions with the second order in the spatial variables. As a result, we have

$$G^T(A^h_m)^T G \geq 0, \ (m=1, 2, 3) \tag{63}$$

The adjoint difference scheme has the form

$$G[n+\tfrac{2}{3}] - G[n+1] = -\frac{\tau}{2}(A^h_1)^T\{G[n+1] + G[n+\tfrac{2}{3}]\}$$

$$G[n+\tfrac{1}{3}] - G[n+\tfrac{2}{3}] = -\frac{\tau}{2}(A^h_2)^T\{G[n+\tfrac{2}{3}] + G[n+\tfrac{1}{3}]\}$$

$$G[n-\tfrac{1}{3}]-G[n+\tfrac{1}{3}] = -\tau\,(A^h_3)^T\{G[n+\tfrac{1}{3}] + G[n-\tfrac{1}{3}]\} + 2\tau P[n]$$

$$G[n-\tfrac{2}{3}] - G[n-\tfrac{1}{3}] = -\frac{\tau}{2}(A^h_2)^T\{G[n-\tfrac{1}{3}] + G[n-\tfrac{2}{3}]\}$$

$$G[n-1] - G[n-\tfrac{2}{3}] = -\frac{\tau}{2}(A^h_1)^T\{G[n-\tfrac{2}{3}] + G[n-1]\} \tag{64}$$

where $G[n]$ is the vector with the components $g(x_i, y_j, z_k, t_n)$, and $P[n]$ approximates the adjoint equation forcing. Since

$$G[n-1]G^T[n-1] \leq G[n+1]G^T[n+1] \tag{65}$$

for all n and $P[n] = 0$, the scheme (64) as well as the scheme (52) is stable to initial perturbations for any step τ. It is easy to show that (64) is the balanced scheme approximating Eq.(30).

Let us multiply from the left the equations (52) by the vectors $\{G[n-\tfrac{2}{3}] + G[n-1]\}^T$, $\{G[n-\tfrac{1}{3}] + G[n-\tfrac{2}{3}]\}^T$, $\{G[n+\tfrac{1}{3}] + G[n-\tfrac{1}{3}]\}^T$, $\{G[n+\tfrac{2}{3}] + G[n+\tfrac{1}{3}]\}^T$ and $\{G[n+1] + G[n+\tfrac{2}{3}]\}^T$ respectively. Further, multiply from the right the transposed equations (64) by the vectors $\{\Phi[n+1] + \Phi[n+\tfrac{2}{3}]\}$, $\{\Phi[n+\tfrac{2}{3}] + \Phi[n+\tfrac{1}{3}]\}$, $\{\Phi[n+\tfrac{1}{3}] + \Phi[n-\tfrac{1}{3}]\}$, $\{\Phi[n-\tfrac{1}{3}] + \Phi[n-\tfrac{2}{3}]\}$ and $\{\Phi[n-\tfrac{2}{3}] + \Phi[n-1]\}$ respectively. Combining the results obtained and using the Lagrange identity (55) lead to the difference version of the balance equation (31) for each time interval I_n:

$$G^T[n+1]\,\Phi[n+1] + \tau P^T[n]\,\{\Phi[n+\tfrac{1}{3}] + \Phi[n-\tfrac{1}{3}]\}$$
$$= \tau\,\{G[n+\tfrac{1}{3}] + G[n-\tfrac{1}{3}]\}^T F[n] + G^T[n-1]\,\Phi[n-1] \tag{66}$$

Emphasize that (66) can be obtained only if the scheme (64) is compatible with the s scheme (52).

FACTORIZATION METHOD

Each split one-dimensional equation of the schemes (52) and (64) represents a system of the three-point difference equations of the form

$$a_i W_{i-1} - b_i W_i + c_i W_{i+1} = f_i \tag{67}$$

with the corresponding two-point boundary conditions of the type of (47)-(50) or (59)-(62):

$$eW_o + rW_1 = 0 \tag{68}$$

$$hW_I + dW_{I-1} = 0 \tag{69}$$

The system (67)-(69) can easily be solved by the well known factorization method (see, for example, Marchuk 1982b) when the solution is sought in the form

$$W_i = \alpha_{i+1} W_{i+1} + \beta_{i+1} , \ (i=1,\dots,I-1) \tag{70}$$

Substituting (70) in (67) we obtain

$$\alpha_{i+1} = c_i (b_i - a_i \alpha_i) \tag{71}$$

$$\beta_{i+1} = (f_i + a_i \beta_i) / (b_i - a_i \alpha_i) \tag{72}$$

Due to the conditions (68) and (69) we have

$$\alpha_1 = - r/e, \ \beta_1 = 0 \tag{73}$$

$$W_I = \beta_I / (h/d - \alpha_I) \tag{74}$$

Thus the formulas (70)-(74) solve the problem (67)-(69).

ACKNOWLEDGMENTS

This work was supported by CONACYT (Mexico) through the visiting scientist fond. I am very grateful to my teacher Academician, Prof. G.I. Marchuk for many useful discussions on the problems considered in this work. I would also like to thank unknown reviewers for their criticism that resulted in improving the paper. Mrs. María Ester Grijalva was very kind to translate the abstract in Spanish.

APPENDIX A
POSITIVE SEMIDEFINITENESS OF THE OPERATORS A_i

We now show that the operators (39)-(41) are non-negative:

$$A_i \geq 0, \text{ or } (A_i\phi, \phi) \geq 0 \tag{A.1}$$

for each i=1, 2, 3. Obviously, it is sufficient to prove this assertion only for the operator

$$A_3\phi = \frac{1}{2}\frac{\partial}{\partial z}(w\phi) + \frac{1}{2} w\frac{\partial \phi}{\partial z} - \frac{\partial}{\partial z}(\upsilon \frac{\partial \phi}{\partial z}) + \sigma\phi \tag{A.2}$$

since the proof is the same for A_1 and A_2. To this end, let us calculate the scalar product (A.1). Integrating by parts and using the Green formula and the boundary conditions (7)–(9) lead to

$$(A_3\phi, \phi) \equiv \int_{\mathbf{D}} \phi\, A_3\phi\, \mathbf{dr} = \int_{\mathbf{D}} [\sigma\phi^2 + \upsilon\, (\frac{\partial\phi}{\partial z})^2]\, \mathbf{dr}$$

$$+ \int_{\mathbf{D}} \frac{\partial}{\partial z}\, [(\frac{1}{2} w\phi - \upsilon \frac{\partial\phi}{\partial z})\, \phi]\, \mathbf{dr} = \int_{\mathbf{D}} [\sigma\phi^2 + \upsilon\, (\frac{\partial\phi}{\partial z})^2]\, \mathbf{dr}$$

$$+ \int_{\mathbf{S_O}} \alpha\phi^2 d\Omega + \frac{1}{2}\{ \int_{\mathbf{S}_H^+} w\phi^2 d\Omega - \int_{\mathbf{S}_H^-} w\phi^2 d\Omega\} \geq 0 \quad (A.3)$$

because $w \leq 0$ on $\mathbf{S}_H^-$ (see the section 'Pollutant transport problem'). The assertion is proved.

REFERENCES

Adem J. (1991). Review of the development and applications of the Adem thermodynamic model. Climate Dynamics *5,* 145-160.

Allen D.J., Douglas A.R., Road R.B. and Guthrie P.D. (1991). Application of a monotonic upstream-biased transport scheme to three-dimensional constituent transport calculations. Mon. Wea. Rev. *119,* 2456-2464.

Beniston M. (1987). A numerical study of atmospheric pollution over complex terrain in Switzerland. Bounday-Layer Meteorology *41,* 75-96.

Birkhoff G. and Varga R.S. (1959). Implicit alternating direction methods. Trans. Amer. Math. Soc. *92,* 13-24.

Buendia E.C., Villicaña F.C., Delgado O.D. and Del Valle E.S. (1992). On the trajectory of cyclones likely to affect the Mexican republic. Atmósfera *5,* 21-30.

Douglas J. Jr. and Rachford H.H. Jr. (1956). On the numerical solution of heat conduction problems in two and three space variables. Trans. Amer. Math. Soc. *82,* 421-439.

Dymnikov V.P. and Aloyan A.E. (1990). Monotonic schemes for the solution of transport equations in problems of weather forecast, ecology and climate theory. Izvestiya, Atmos. Ocean. Physics *26,* 1237-1247.

Forester C.K. (1977). High order monotonic convective difference schemes. J. Comput. Phys. *23,* 1-22.

Heidorn K.C., Davies A.E. and Murphy M.C. (1991). Wind tunnel modeling of roadways: comparison with mathematical models. J. Air Waste Manage. Asses. *41,* 1469-1475.

Jauregui E. (1988). Local wind and air pollution interaction in the Mexico basin. Atmósfera *1,* 133-140.

Marchuk G.I. (1982a). Mathematical Issues of Industrial Effluent Optimization. J. Meteor. Soc. Japan *60,* 481-485.

Marchuk G.I. (1982b) *Methods of numerical mathematics.* Springer-Verlag, New York, 510 p.

Marchuk G.I. (1986) *Mathematical models in environmental problems.* Elsevier, New York, 217 p.

Marchuk G.I., Penenko V.V., Aloyan A.E. and Lazriev G.L. (1979). Numerical simulation of the urban microclimate. Sov. Meteorol. Hydrology No. 8, 1-10.

Marchuk G.I. and Skiba Y.N. (1992) Role of adjoint equations in estimating monthly mean air surface temperature anomalies. Atmósfera *5,* 119-134.

Penenko V.V. and Raputa V.F. (1982). Experiment planning in inverse problems of pollutant transport. Sov. Meteorol. Hydrology No. 8, 28-35.

Penenko, V.V. and Raputa, V.F. (1983). Some models for optimizing the operation of the atmospheric-pollution sources. Sov. Meteorol. Hydrology No. 2, 46-54.

Robertson A.W. (1992). Diagnosis of regional monthly anomalies using the adjoint method. Part I. Temperature. J. Atmos. Sci. *49,* 885-905.

Rood R.B. (1987). Numerical advection algorithms and their role in atmospheric transport and chemistry models. Rev. Geophys. *25,* 71-100.

Salerno R., Clerici G.C. and Sandroni S. (1992). Modelisation of pollutants dispersion in the Alpine region. In: *Air Pollution Modelling and Its Application IX.* (H. van Drop and G. Kallos, Eds.), Plenum Press, New York, vol. 17, pp. 187-194.

Sawai T. (1978). Formation of the urban air mass and the associated local circulation. J. Meteor., Soc. Japan. *56,* No. 3.

Skiba Y.N. (1978). Method of solving the atmosphere-ocean-soil heat interaction problem on a basis of the adjoint equations. Ph.D. Thesis, Computing Center, USSR Academy of Sciences, Novosibirsk, 124 p.

Skiba Y.N. (1993). On a method of estimating the pollution concentration. In: *Proccedings of International Symposium on Heat and Mass Transfer in Energy Systems and Environmental Effects.* Cancún, México, August 22-25, 167-172.

Sliggers J. (1992). The car model: calculation of air pollution from road traffic, a calculation method for the determination of air quality in city streets in the Netherlands. In *Air Pollution Modelling and Its Application IX.* (H. van Drop and G. Kallos, Eds.), Plenum Press, New York, vol. 17, pp. 39-48.

Smolarkiewicz P.K. (1991). On Forward-in-time differencing for fluid. Mon. Wea. Rev. *119,* 2505-2510.

Williamson D.L. (1992). Review of numerical approaches for modelling global transport. In: *Air Pollution Modelling and Its Application IX.* (H. van Drop and G. Kallos, Eds.), Plenum Press, New York, vol. 17, pp. 377-394.

Yanenko N.N. (1971). *Method of Fractional Steps.* Springer-Verlag, New York.