Jana Stará; Marta Tenčlová; Jiří Bubník; Svatopluk Fučík; Oldřich John

Gas exhalation and its calculations. I

Aplikace matematiky, Vol. 26 (1981), No. 1, 30–44

Persistent URL: http://dml.cz/dmlcz/103892

GAS EXHALATION AND ITS CALCULATIONS – Part I

JANA STARÁ, MARTA TENČLOVÁ, JIŘÍ BUBNÍK, SVATOPLUK FUČÍK, OLDŘICH JOHN

(Received January 11, 1979)

INTRODUCTION

The main goal of our paper is to suggest a (deterministic) mathematical method for effective calculation of the diffusion of gas exhalation (namely SO_2) in the boundary layer of atmosphere. This method (which we refer to as DM) is due to Sutton [9].

The equation for the concentration $\chi(t, x, y, z)$ is deduced from the continuity equation (the mass conservation law) in Section 2 under the assumptions which are collected and commented in Section 1. The description of the corresponding numerical method is given in Section 3. In Section 4 we describe the organization of calculation (wind velocity classes, stability classes and the definitions of the resulting quantities). We follow here the approach of Bubník [2] who introduced five classes of stability of the boundary layer of atmosphere. A concrete example is calculated in Section 5. There the results obtained by measurements, by the statistical method of Bubník [2] (which we refer to as SM*)) and by the method DM are compared.

After an attempt at discussing the results in Section 6 (the reader is asked to be very suspicious but at the same time not too intolerant when reading that part) we close the paper with an outline of possible generalizations of the DM model (Section 7).

In Part II of this article we will give the mathematical foundation of the boundary value mixed problem which appears as the mathematical description of the air-pollution problem considered in Section 2.

1. ASSUMPTIONS

We collect here the assumptions under which our model is deduced.

(I) Quasistationarity of the process ($\partial\chi/\partial t = 0$).

Since the mean values of the wind velocity are measured, this assumption seems

*) The SM method is the official method used for the forecast of the exhalation.

to be reasonable. In Section 4 we describe a practical way of calculating the real annual situation which takes account of the frequency of various values and directions of the wind velocity.

(II) The part of surface considered is flat and with no obstacles.

The coordinate system is chosen in such a way that the z-axis directs upwards perpendicularly to the surface which coincides with the (x, y)-plane. The origin is put at the foot of the source of exhalation. (Fig. 1).

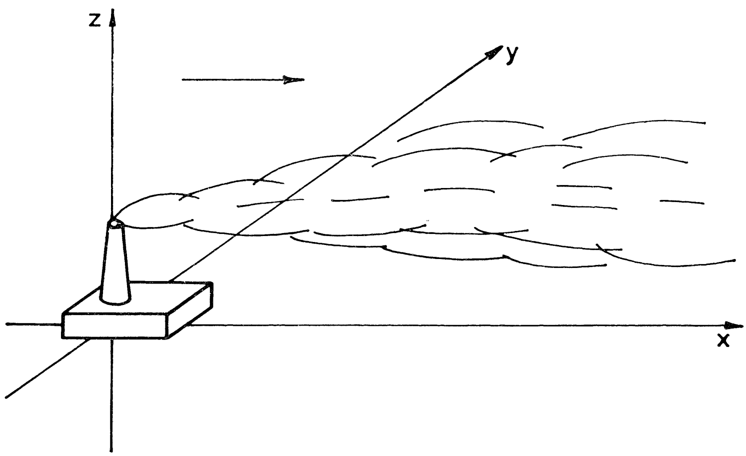

Fig. 1.

(III) The field of the wind velocity is given in the form $v_x = v_x(z)$, $v_y = v_z = 0$. The x-axis has the direction of the wind flow.

Assumption (II) is, clearly, very restrictive. As far as is known to the authors, isolated attempts have been made to deal with the situation of a hilly region but they have met with enormous difficulties concerning both the physical description and the numerical solvability of the problem. (See e.g. Hino [5], Jaňour [6].) In our calculations semiempiric corrections of the height are included as they were used in the SM method (Sec. 4).

Assumption (III) also idealizes the real situation because of the fact that the height of the source can reach the spiral layer where the velocity field "twists", i.e. changes its angle with the fixed x-axis along with the growing coordinate z. In Section 4 a semiempirical correction is described.

The transport of the gas exhalations is due to turbulent diffusion characterized by the so called eddy diffusivities K_x, K_y and K_z, as well as to the flow of the wind.

(IV) Transport in the direction of the x-axis is caused mainly by the flow of wind.

From the mathematical point of view it means that we can neglect the diffusive member $\partial/\partial x(K_x\, \partial\chi/\partial x)$ in comparison with the member $V_x(z)\, \partial\chi/\partial_x$.

(V) $$K_z = K_z(z)\,.$$

(VI) $$K_y = k_0\, v_x(z)\,, \quad k_0 \ldots \text{constant}\,.$$

While the assumption (V) is reasonable from the physical point of view (see Sutton [9]), the assumption (VI) enables us to reduce the dimension of the boundary value problem obtained (Sec. 2). Although this assumption has a purely mathematical character, many meteorologists use it without any embarassment. (See e.g. Berliand [1].)

(VII) No mass exchange between the earth surface and the atmophere takes place. Mathematically this means that $\partial\chi/\partial z = 0$ in the (x, y)-plane.

(VIII) The exhalated gas does not react chemically in the atmosphere.

Both these assumptions are unrealistic in case of high air moisture and big water areas in the region considered.

2. DEDUCTION OF A MATHEMATICAL MODEL

Our task is to describe the diffusion of the gas from a point source of an effective height H*). The source is characterized by its emission $\mathcal{M}$ for a time unit.

Taking account of (VIII) we have the general continuity equation for the density $\chi = \chi(t, x, y, z)$ in the form

$$\frac{\partial\chi}{\partial t} + v_x \frac{\partial\chi}{\partial x} + v_y \frac{\partial\chi}{\partial y} + v_z \frac{\partial\chi}{\partial z} = \frac{\partial}{\partial x}\left(K_x \frac{\partial\chi}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial\chi}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial\chi}{\partial_z}\right).$$

Using the assumptions (I), (III), (IV) and (V) we get the equation

(1) $$v_x(z)\frac{\partial\chi}{\partial x} = k_0\, v_x(z)\, \frac{\partial^2\chi}{\partial y^2} + \frac{\partial}{\partial z}\left(K_z(z)\, \frac{\partial\chi}{\partial z}\right)$$

for $\chi = \chi(x, y, z)$.

Let us formulate the boundary conditions for Equation (1) considered in the region

$$\Omega = \{(x, y, z)\,;\; x > 0,\; y \in \mathbb{R},\; z > 0\}\,.$$

The form of Ω follows from the assumptions (II), (III).

(2) $$\chi(0, y, z) = \frac{\mathcal{M}}{v_x(H)}\,.\,\delta(y)\,.\,\delta(z - H) \quad \text{for} \quad y \in \mathbb{R}\,, \quad z > 0$$

---

*) The effective height H does not coincide with the constructive height V. See Sec. 4.

(δ is the Dirac function);

$$\lim_{y \to +\infty} \chi(x, y, z) = \lim_{y \to -\infty} \chi(x, y, z) = 0 \quad \text{for} \quad x > 0, \quad z > 0\,; \tag{3}$$

$$\lim_{z \to +\infty} \chi(x, y, z) = 0 \quad \text{for} \quad x > 0, \ y \in \mathbb{R}\,; \tag{4}$$

$$\frac{\partial \chi}{\partial z}(x, y, 0) = 0 \quad \text{for} \quad x > 0, \quad y \in \mathbb{R}\,. \tag{5}$$

(Formula (5) is a mathematical formulation of the assumption (VII).)

In Part II of the present article it will be shown that under some conditions on the coefficients v_x and K_z the problem (1)–(5) is well posed. In concrete calculations all these conditions will be fulfilled.

The special form of Equation (1) enables us to look for the solution $\chi(x, y, z)$ of the problem (1)–(5) in the form

$$\chi(x, y, z) = \varrho(x, y)\, u(x, z)\,. \tag{6}$$

Substituting from (6) in (1)–(5) we split our problem (by means of a standard procedure) into two problems:

$$\frac{\partial \varrho}{\partial x} = k_0 \frac{\partial^2 \varrho}{\partial y^2} \quad \text{for} \quad x > 0, \quad y \in \mathbb{R}\,, \tag{7}$$

$$\lim_{y \to +\infty} \varrho(x, y) = \lim_{y \to -\infty} \varrho(x, y) = 0 \quad \text{for} \quad x > 0\,, \tag{8}$$

$$\varrho(0, y) = \delta(y) \quad \text{for} \quad y \in \mathbb{R}\,, \tag{9}$$

and

$$v_x(z) \frac{\partial u}{\partial x} = \frac{\partial}{\partial z}\left(K_z(z) \frac{\partial u}{\partial z}\right), \quad x > 0, \quad z > 0\,, \tag{10}$$

$$\lim_{z \to +\infty} u(x, z) = 0 \quad \text{for} \quad x > 0\,, \tag{11}$$

$$\frac{\partial u}{\partial z}(x, 0) = 0 \quad \text{for} \quad x > 0\,, \tag{12}$$

$$u(0, z) = \frac{\mathcal{M}}{v_x(H)} \,.\, \delta(z - H) \quad \text{for} \quad z > 0\,. \tag{13}$$

While the problem (7)–(9) is standard and has a unique solution

$$\varrho(x, y) = \tfrac{1}{2}(\pi k_0 x)^{-1/2} \exp\left(-y^2/4k_0 x\right), \tag{14}$$

the solution of the problem (10)–(13) cannot be expressed explicitly and we must use a numerical method to find it.

Up to now we have not made the character of the coefficients $v_x(z)$, $K_z(z)$ in Equation (10) (the wind velocity and the eddy diffusivity) clear. Meteorological considerations show that either

$$(15) \qquad v_x(z) = \begin{cases} \gamma \log \dfrac{z + \varepsilon}{\varepsilon} & \text{for} \quad 0 < z < h\,, \\ \gamma \log \dfrac{h + \varepsilon}{\varepsilon} & \text{for} \quad h \leqq z\,, \end{cases}$$

$$K_z(z) = \begin{cases} c.z & \text{for } 0 < z < h, \\ c.h & \text{for } h \leqq z. \end{cases}$$

whete γ, ε, h and c are positive constants, or

$$(16) \qquad v_x(z) = \begin{cases} \alpha z^{\omega} & \text{for} \quad 0 < z < h\,, \\ \alpha h^{\omega} & \text{for} \quad h \leqq z\,, \end{cases}$$

$$K_z(z) = \begin{cases} \beta z^{1-\omega} & \text{for} \quad 0 < z < h\,, \\ \beta h^{1-\omega} & \text{for} \quad h \leqq z\,, \end{cases}$$

where α, β, ω are positive constants.

More details will be given in Section 4. Here we remark only that the measurements of the wind velocity are carried out in a standard height of, say, ten meters, and the velocities in the other heights (the wind velocity profile) are calculated from the theoretically deduced formulas (15) and (16). The constants are determined by the velocity in the standard height, the quality (roughness) of surface and the thermodynamic state (stability class) of the atmosphere.

Both eligible forms of v_x and K_z are of the type

$$(17) \qquad v_x(z) > 0\,, \quad \lim_{z \to 0+} v_x(z) = 0\,,$$

$$K_z(z) > 0\,, \quad \lim_{z \to 0+} K_z(z) = 0\,,$$

so that (10) is the diffusion equation with variable continuous coefficients depending only on z, which vanish for $z \to 0+$.

3. NUMERICAL SOLUTION OF THE PROBLEM (10)–(13)

a) As we need to solve the problem in the domain $\Omega_1 = \{(x, z);\, x > 0,\, z > 0\}$, the finite difference methods seem to be the most suitable. For this purpose we replace the condition (11) by its approximation

$$(11') \qquad u(x, l) = 0 \quad \text{for} \quad x > 0\,,$$

where $l > H$. (Numerical experiments in practically calculated cases indicate that

$l = 3H$ is sufficient.) The initial condition (13) is replaced by

$$(13') \qquad u(0, z) = \frac{\mathcal{M}}{v_x(H)} \sqrt{\left(\frac{R}{\pi}\right)} \exp\{-R(z - H)^2\}$$

for $0 < z < l$. (The parameter R represents the "distension" of the δ-function.)

Consequently, instead of the problem (10)–(13) we are to solve the problem (10), (11'), (12) and (13').

b) Discretizing the domain Ω_1 in the form

$$\tilde{\Omega}_1 = \{(n \,.\, \Delta x, m \,.\, \Delta z); \quad n = 0, 1, \ldots, m = 0, 1, \ldots, Q\},$$

$$Q = \left[\frac{l}{\Delta z}\right] + 1,$$

we choose the implicit scheme of replacing (10), (11'), (12) and (13') by a system of algebraic equations. This choice is determined by the necessity of using a value Δx much bigger than Δz – it is a well known fact that the stability of the implicit scheme does not depend on the ratio $\Delta x/\Delta z$. (See e.g. Samarskij [8].)

c) Denote $u^n_m = u(n\,\Delta x, m\,\Delta z)$. According to the above considerations the numerical approximation of (10)–(13) has the following form:

$$(10'') \qquad v_x(m\,\Delta z)\,\frac{u^{n+1}_m - u^n_m}{\Delta x} =$$

$$= \frac{K_z((m + \frac{1}{2})\,\Delta z)\,(u^{n+1}_{m+1} - u^{n+1}_m) - K_z((m - \frac{1}{2})\,\Delta z)\,(u^{n+1}_m - u^{n+1}_{m-1})}{(\Delta z)^2},$$

$$(m = 1, \ldots, Q - 1;\ n = 0,1 \ldots),$$

$$(11'') \qquad u^n_Q = 0, \quad (n = 0, 1, \ldots),$$

$$(12'') \qquad u^n_1 = u^n_0, \quad (n = 0, 1, \ldots),$$

$$(13'') \qquad u^0_m = \frac{\mathcal{M}}{v_x(H)} \sqrt{\left(\frac{R}{\pi}\right)} \exp\{-R(m\,\Delta z - H)^2\}, \quad (m = 1, \ldots, Q - 1)$$

d) Remarks. The analysis of the scheme in case of degenerate coefficients (15) or (16) can be done similarly as in Samarskij [8]. Numerical experiments show that the scheme (11")–(13") is rather advantageous for our purpose.

From the algorithmical point of view, a system of linear algebraic equations with a tridiagonal matrix is solved for each n.

4. HOW THE CALCULATIONS ARE ORGANIZED

A) First we give a simplified description of calculations which are necessary to determine the concentration of exhalated gas in the region considered. For some omitted details see point C of this section.

Let I classes of wind velocities and M classes of thermodynamic situations of the boundary layer (the so called stability classes) be given. For each i, m ($i = 1, \ldots, I$; $m = 1, \ldots, M$) the coefficients v_x and K_z are determined.

The discrete function $\tau = \tau(m, i, s)$ ($m = 1, \ldots, M$; $i = 1, \ldots, I$; $s = 1, \ldots, S$) assigns to each index m, i, s the annual frequency (in per cent) of the state characterized by the m-th class of wind velocity in case that the angle contained between the direction of the wind and the half-line directed eastward (the positive x-axis of the fixed coordinate system) is $s \,.\, 360/S$ degrees.

(This description of the atmosphere is, of course, very rough one but, nevertheless, it is in good accordance with attainable exactness of meteorological measurements.)

Further, the sources X_j ($j = 1, \ldots, J$) and the check points Y_k ($k = 1, \ldots, K$) are given. Each source X_j is characterized by its effective height H_j, emission $\mathscr{M}_j$ and coordinates x_j, y_j, z_j in the fixed coordinate system described above. The points Y_k are characterized by their coordinates x_k., y_k, z_k.

For each source X_j, each velocity class and each class of stability the situation down the wind is calculated, i.e. the problem (10)–(13) is solved numerically according to Section 3 with the corresponding values of $\mathscr{M}_j$, H_j and the coefficients v_x, K_z. Thus we solve $M \times I \times J$ problems (10″)–(13″) to obtain all the information necessary for the solution of our main problem, which is to calculate the air pollution caused by the sources X_j ($j = 1, 2, \ldots, J$) at the check points Y_k ($k = 1, \ldots, K$). The number N_j of steps along the x-axis for each single problem (10″)–(13″) is determined by the maximal distance between X_j and Y_k ($k = 1, \ldots, K$).

Using the solutions of the problems (10″)–(13″) and the formulae (14) and (6) we calculate the quantities

$$(18) \qquad F(m, i, s, k, j) = \tfrac{1}{2}(\pi k_0 \bar{x}_s)^{-1/2} \,.\, \exp\left(-\bar{y}_s^2/4k_0\bar{x}_s\right) \,.\, u(\bar{x}, z_{k,j}),$$

where $(\bar{x}_s, \bar{y}_s)$ are the cartesian coordinates of the point Y_k with respect to the system whose origin is at the foot of X_j and the positive x_s-axis is directed so that the angle contained between itself and the half-line directed eastwards (the x-axis of the fixed coordinate system) is $s \,.\, 360/S$ degrees (Fig. 2). In (18) we put $z_{k,j} = 0$.

$F(m, i, s, k, j)$ is the contribution of the source X_j to the concentration at the check point Y_k for the m-th class of stability and for the wind blowing in the i-th class of velocity under the angle given by the index s. Instead of this field we store the values

$$F(m, i, s, k) = \sum_{j=1}^{J} F(m, i, s, k, j)$$

because we want to know the global situation at Y_k caused by the whole system $\{X_j; j = 1, \ldots, J\}$ of sources.

The field $\{F(m, i, s, k)\}$ is subjected to further transformations to obtain quantities we are interested in.

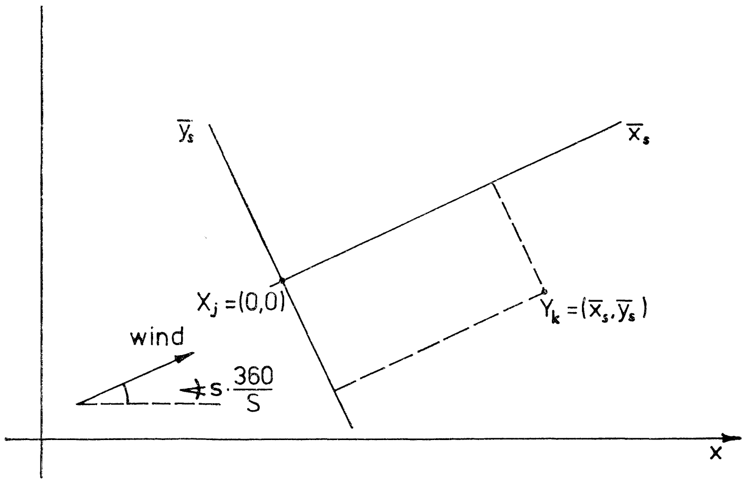

Fig. 2.

B) The following quantities are printed for the m-th class of stability:

(19) $$F(m, i, k) = \max\{F(m, i, s, k);\ s = 1, \dots, S\}, \quad (i = 1, \dots, I;\ k = 1, \dots, K).$$

(20) $$C(m, k) = \sum_{i=1}^{I} \sum_{s=1}^{S} F(m, i, s, k) \,.\, \tau(m, i, s), \quad (k = 1, \dots, K).$$

(21) $$F(m, k)\,\emptyset = C(m, k) \,.\, [\sum_{i=1}^{I} \sum_{s=1}^{S} \tau(m, i, s)]^{-1}, \quad (k = 1, \dots, K).$$

(22) $$F(m, i, k)\,\emptyset = \sum_{s=1}^{S} F(m, i, s, k) \,.\, [\sum_{s=1}^{S} \tau(m, i, s)]^{-1}, \quad (i = 1, \dots, I;\ k = 1, \dots, K).$$

(The meaning of $F(m, i, k)$ is clear; $C(m, k)$ is the so called total dose of concentration at Y_k corresponding to the m-th class and $F(m, k)\,\emptyset$, $F(m, i, k)\,\emptyset$ are the average quantities of concentrations at Y_k in the m-th class of stability.)

Further, the number $\nu(m, k, q)$ of hours a year during which the concentration at Y_k exceeds the given value β_q if the m-th class of stability takes place is printed for six prescribed values of β_q.

After that, the following quantities are printed which characterize the annual situation:

(23) $$F(i, k) = \max\{F(m, i, k);\ m = 1, \dots, M\}, \quad (i = 1, \dots, I;\ k = 1, \dots, K).$$

$$(24) \qquad C(k) = \sum_{m=1}^{M} C(m, k), \quad (k = 1, \ldots, K).$$

$$(25) \qquad F(k)\,\emptyset = C(k)/8760, \quad (k = 1, \ldots, K).$$

$$(26) \qquad F(i, k)\,\emptyset = \sum_{m=1}^{M} \sum_{s=1}^{S} F(m, i, s, k) \,.\, [\sum_{m=1}^{M} \sum_{s=1}^{S} \tau(m, i, s)]^{-1}, \quad (i = 1, \ldots, I;\ k = 1, \ldots, K).$$

Further, the number $\nu(k, q)$ of hours a year during which the concentration at Y_k exceeds the value β_q is printed for six prescribed values of β_q.

C) Here we present some details omitted in point A which, being unimportant for the algorithm itself, still may improve the quality of results.

a) As the frequencies $\tau(m, i, s)$ are given for fixed i, m usually for eight main directions N, NE etc., we interpolate this original function linearly to obtain a denser table of frequencies.

b) The effective height H_j of the source X_j depends on its constructive height V_j, the thermal substantiality Q_j and on the velocity of the wind at the constructive height V_j. In this way H_j depends also on the indices i, m. The empirical formulae are the following ones:

$$H_j = \begin{cases} V_j + \dfrac{1{\cdot}5V_j - 50}{v_x(V_j)}\, Q_j^{1/4} & \text{if} \quad V_j \geqq 100 \text{ meters}, \\ V_j + \dfrac{100}{v_x(V_j)}\, Q_j^{1/4} & \text{if} \quad V_j < 100 \text{ meters}. \end{cases}$$

c) Calculating the coordinates $(\bar{x}_s, \bar{y}_s)$ for formula (18) (see Fig. 2) we correct the angle $s \,.\, 360/S$ by taking account of the twisting of the wind with the increasing height. According to the convention that the wind twists linearly by four degrees between 0 and 1000 meters above sea-level we obtain the corrected angle φ as

$$\varphi = s \,.\, \frac{360}{S} + \frac{H_j - 10}{25}.$$

(This correction again approximates the real situation very roughly.)

d) The unrealistic assumption (II) from Section 1 was interpreted mathematically by inserting $z_{k,j} = 0$ in formula (18). The semiempirical correction consists in the use of $z_{k,j}$ in (18) given by the following formulae:

If $\qquad z_k \leqq z_j, \quad$ then $\quad z_{k,j} = 0$;

if $\qquad z_j < z_k \leqq z_j + 0{\cdot}8H_j, \quad$ then $\quad z_{k,j} = z_k - z_j$;

if $\qquad z_j + 0{\cdot}8H_j < z_k, \quad$ then $\quad z_{k,j} = 0{\cdot}8H_j$.

This correction has an obvious geometrical interpretation. It seems to be sufficiently reasobable except for the choice of the constant 0·8 which has no physical substantiation.

5. EXAMPLE

The real situation in an area characterized by 26 sources and 5 check points was calculated. The surface was not too hilly.

By the DM method the example was calculated by the computer EC 1040 in 143 minutes. The constants characterizing various classes of stability were calculated on the base of the theoretical background given by Sutton [9].

The quantities measured at the points $Y_1, \ldots, Y_5$ are, in fact, mean values of the day's measurements. So the only values which we can compare with these quantities are $F(k)\,\emptyset$, $k = 1, \ldots, 5$. (Tab. 1.) As for the maximal values $F(i, k)$, $i = 1, 2, 3$, $k = 1, \ldots, 5$, we can compare only the values calculated by DM and SM, having no technical possibility to measure the real maximal values at various Y_i. (Tab. 2.)

In Tab. 3 we bring the total doses of concentration $C(k)$ and, finally, in Tab. 4 we show the numbers $\nu(k, q)$ of hours a year during which at Y_k the given concentration β_q is exceeded. (For the sake of brevity we put $k = 1, 2$ only.)

Table 1

Calculated $F(k)\,\emptyset$ and measured quantities

Check point	Meas. value	DM	SM
Y_1	$4{\cdot}00 \times 10^{-2}$ mg/m^3	3·85	3·03
Y_2	3·50	3·32	5·08
Y_3	2·50	2·64	5·30
Y_4	3·50	4·74	4·59
Y_5	4·50	4·53	4·48

Table 2.

Maximal values $F(i, k)$ (in mg/m^3)

Check point	$i = 1$		$i = 2$		$i = 3$	
	DM	SM	DM	SM	DM	SM
Y_1	2·45	1·60	1·30	1·45	0·56	0·89
Y_2	3·34	2·00	1·14	1·16	0·68	0·92
Y_3	3·48	0·90	1·12	0·88	0·71	0·57
Y_4	2·94	1·47	1·33	1·38	0·72	0·88
Y_5	3·61	1·28	1·09	1·17	0·72	0·77

Table 3.

Total dose $C(k)$

Check point	DM	SM
Y_1	337·8	265·4
Y_2	291·4	444·9
Y_3	231·3	464·5
Y_4	415·5	402·1
Y_5	397·2	427·1

Table 4.

Numbers $\nu(k, q)$ of hours a year during which at Y_k the given concentration β_q is exceeded

Check point	Method	$\beta_1 = 0·01$	$\beta_2 = 0·05$	$\beta_3 = 0·15$	$\beta_4 = 0·30$	$\beta_5 = 0·50$	$\beta_6 = 1·00$
Y_1	DM	992·3	721·4	582·4	427·5	193·6	74·8
	SM	1026·5	787·4	609·8	341·0	181·7	40·1
Y_2	DM	1135·1	709·5	516·0	352·5	232·8	35·9
	SM	1808·7	1390·1	840·6	452·0	258·0	55·2

6. DISCUSSION

(i) Unless many real examples are calculated we must be very cautious in evaluating the DM method described in the previous text. Nevertheless, the comparison between the measured values and our results (Tab. 1) seems to be very encouraging.

(ii) In the example of Sec. 5 the check points and the sources practically have the same coordinates z. In an other example calculated the check points were considerably higher than the foots of the sources (the difference being approximately 500 meters). In that case the calculated values $F(k)\,\emptyset$ were almost 1·5-times bigger than the measured quantities. Even if this correspondence is not so bad, the fact indicates again that no semiempirical corrections can give us full satisfaction in the case of a hilly surface.

(iii) In the example described the values $F(k)\,\emptyset$ almost coincide with the values $F(m, k)\,\emptyset$ for $m = 4$. This index corresponds to the neutral stability class with a logarithmic field of velocities. If this were justified by more real examples, it would be possible to calculate the first approximation of the real situation much cheaper (by replacing $F(k)\,\emptyset$ by $F(4, k)\,\emptyset$ and saving in this way 4/5 of machine time).

(iv) We performed a number of numerical experiments which have confirmed the stability of the numerical process with respect to the choice of Δx, Δz and the parameter R representing the initial δ-function.

7. GENERALIZATIONS

By reducing some of the assumptions introduced in Section 1 it is possible to obtain more general approaches to the air-pollution problem. Without going into particulars we touch the mathematical aspects only. Figure 3 presents a scheme of the process of generalization. Concentrating our attention to the stationary models only we consider four models (i)–(iv) (circled in Fig. 3).

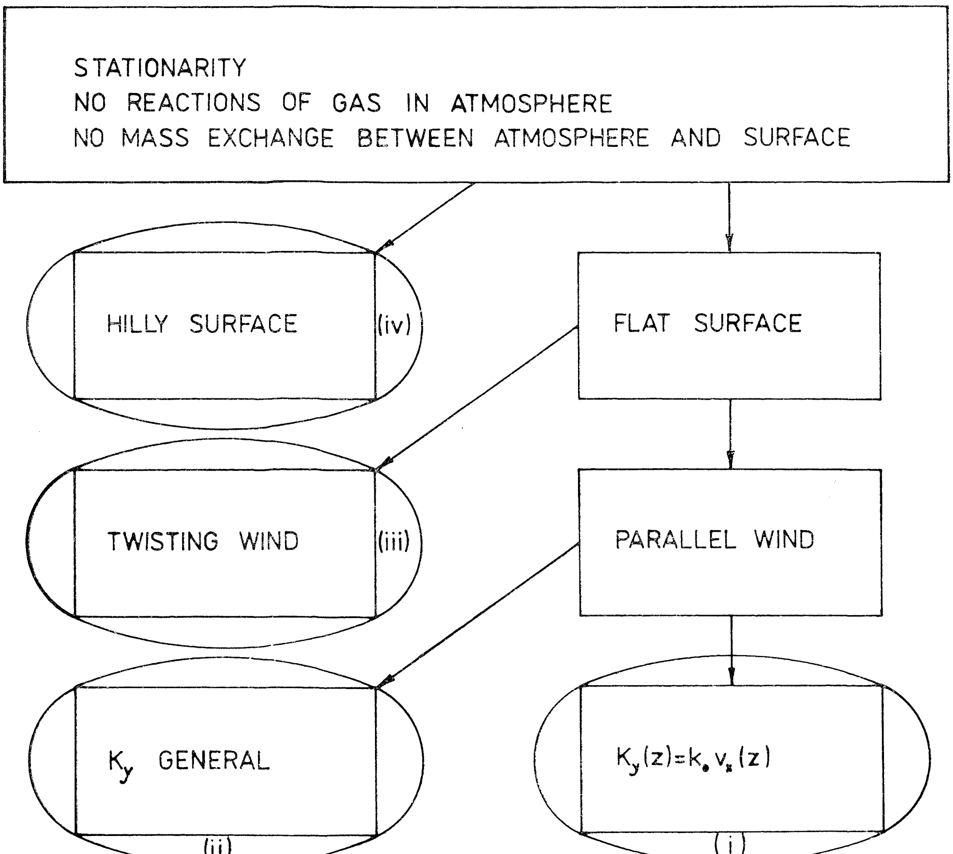

Fig. 3.

The question which remains open is whether the character of the meteorological measurements (their roughness and incompleteness) does not condemn the attempts at generalizations to the sphere of purely mathematical speculations. The importance of a reasonable answer to this question is emphasized by the presence of considerable difficulties connected with the numerical realization of the more general models.

Model (i) was treated in detail in the preceding sections. Recall that it led to a boundary value problem for the parabolic equation (1) with two spatial variables y and z. Thanks to the suspicious assumtion (VI) it splitted into two boundary value problems for parabolic equations with one spatial variable.

Considering model (ii) we obtain the equation

$$v_x(z)\frac{\partial\chi}{\partial x} = K_y(z)\frac{\partial^2\chi}{\partial y^2} + \frac{\partial}{\partial z}\left(K_z(z)\frac{\partial\chi}{\partial z}\right) \tag{27}$$

and the boundary conditions (2)–(5). From the numerical point of view this problem can be solved by means of some "economical" method for the parabolic boundary value problems. (See e.g. Samarskij [8], Richtmyer [7] etc.) Before applying this method we must transfer the zero condition from infinity to the lines $y = \pm L$, $z = Q$ with L and Q properly chosen positive numbers, and approximate the δ-function in the condition (2).

Model (iii) which takes account of the change of the direction of the wind velocity field with the increasing height could be much more suitable in the situation of sources higher than 60–100 meters, which is the approximate lower bound of the so called spiral layer of atmosphere. In this model, in general, there is no reason to neglect some of the diffusivity members. So we obtain the equation

$$v_x(z)\frac{\partial\chi}{\partial x} + v_y(z)\frac{\partial\chi}{\partial y} = K_x(z)\frac{\partial^2\chi}{\partial x^2} + K_y(z)\frac{\partial^2\chi}{\partial y^2} + \frac{\partial}{\partial z}\left(K_z(z)\frac{\partial\chi}{\partial z}\right), \tag{28}$$

which is of the elliptic type. The introduction of the source in the equation seems to be more convenable in this case than any attempt at formulating the influence of the source in the form of some artificially introduced boundary conditions. We obtain the equation

$$v_x(z)\frac{\partial\chi}{\partial x} + v_y(z)\frac{\partial\chi}{\partial y} = K_x(z)\frac{\partial^2\chi}{\partial x^2} + K_y(z)\frac{\partial^2\chi}{\partial y^2} + \frac{\partial}{\partial z}\left(K_z(z)\frac{\partial\chi}{\partial z}\right) + \tag{29}$$

$$+ M \,.\, \delta(x) \,.\, \delta(y) \,.\, \delta(z - H)$$

in the domain $\{(x, y, z);\, z > 0\}$ with the boundary conditions

$$\lim_{\substack{|x| + |y| + z \to +\infty \\ z > 0}} \chi(x, y, z) = 0\,, \tag{30}$$

$$\frac{\partial\chi}{\partial z}(x, y, 0) = 0\,. \tag{31}$$

The numerical solution can be carried out by some "economical" iterative method (see again Samarskij [8]). Before its application we must replace the δ-function $M \,.\, \delta(x) \,.\, \delta(y) \,.\, \delta(z - H)$ by its reasonable approximation while the unbounded domain $\{(x, y, z); z > 0\}$ is substituted by

$$\Omega = \{(x, y, z); x \in (-L_1, Q_1), \; y \in (-L_2, Q_2), \; z \in (0, Q_3)\}$$

with L_i, Q_i properly chosen positive numbers. The condition (30) is then transferred to the corresponding part of the boundary $\partial\Omega$ in the obvious manner.

The last generalization is the case (iv) of hilly surface. This problem was considered (under some simplifying assumptions) by Hino [5]. Physical analysis of some special cases was performed by Jaňour [6].

Under the assumption of a certain regularity and quasistationarity of the wind flow (which is realistic, perhaps, in the case of a very small curvature of the hills) we can write the equation

$$v_x(x, y, z) \frac{\partial \chi}{\partial x} + v_y(x, y, z) \frac{\partial \chi}{\partial y} + v_z(x, y, z) \frac{\partial \chi}{\partial z} =$$

$$(32) \qquad \frac{\partial}{\partial x} \left(K_x(x, y, z) \frac{\partial \chi}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y(x, y, z) \frac{\partial \chi}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_z(x, y, z) \frac{\partial \chi}{\partial z} \right) +$$

$$+ M \,.\, \delta(x) \,.\, \delta(y) \,.\, \delta(z - H) \,.$$

The domain in which we consider this equation is

$$\Omega = \{(x, y, z); \; (x, y) \in \mathbb{R}^2, \; z > \varphi(x, y)\} \,,$$

where the function φ describes the relief of the surface. The boundary conditions are then

$$(33) \qquad \lim_{\substack{|x| + |y| + z \to \infty \\ z > \varphi(x,y)}} \chi(x, y, z) = 0 \,,$$

$$(34) \qquad \frac{\partial \chi}{\partial n} (x, y, \varphi(x, y)) = 0 \,,$$

where n is the inner normal to the surface.

Notice that other generalizations are posible. For example, we can add the chemical reactions in the description of the process or calculate the velocity field as well as the concentrations using the complete system of equations describing the boundary layer.

References

[1] *M. E. Berliand:* Present problems of the atmospherical diffusion and the air pollution. Gidrometizdat, Leningrad 1975 (Russian).

[2] *J. Bubník:* A climatological model of calculation of the air pollution. Part 3. (Czech.) Research report.

[3] *J. Bubník, P. Doktor, S. Fučík, Z. Jaňour, O. John, J. Stará, M. Tenčlová:* Mathematical and numerical analysis of the problem of the gas exhalation diffusion in the lower layer of atmosphere (Czech). Research report.
[4] *J. Bubník, P. Doktor, S. Fučík, Z. Jaňour, O. John, J. Stará, M. Tenčlová:* Diffusion of gas exhalations in the lower layer of atmosphere (Czech). (A report for the year 1977.)
[5] *M. Hino:* Computer experiment on smoke diffusion over a complicated topography. J. Atm. Environm. 2, 541–558, 1968.
[6] *Z. Jaňour:* The resistance law for the atmospheric boundary layer over a Wavy surface. Boundary-Layer Met. 11. 1977.
[7] *D. R. Richtmyer, K. W. Morton:* Difference methods for initial-value problems. Second edition; Interscience Publishers, a division of John Wiley & Sons, 1967. (Russian translation, izd. MIR, Moskva 1972.)
[8] *A. A. Samarskij:* Introduction into the theory of difference systems. Izd. Nauka, Moskva 1971 (Russian).
[9] *O. G. Sutton:* Micrometeorology. McGraw-Hill Publishing Company, London 1953.

Souhrn

VYPOČET ŠÍŘENÍ PLYNNÝCH EXHALÁTŮ

JANA STARÁ, MARTA TENČLOVÁ, JIŘÍ BUBNÍK, SVATOPLUK FUČÍK, OLDŘICH JOHN

V článku je odvozen deterministický model šíření plynných exhalátů v přízemní vrstvě atmosféry. Při odvození se mimo jiné předpokládá, že: 1. Pole rychlostí je dáno, 2. proces šíření je kvazistacionární, 3. vítr se nestáčí s přibývající výškou nad povrchem, 4. povrch není kopcovitý. Matematickou formulací je pak okrajová úloha pro parabolickou rovnici s degenerovanými koeficienty. Je dána numerická metoda výpočtu této okrajové úlohy a popis programu kompletního výpočtu pro zadanou oblast. Dále je proveden výpočet konkrétního příkladu a výsledky jsou srovnány s měřeními. V závěru práce se diskutují možná zobecnění modelu s poukazem na potíže matematického i výpočetního charakteru, na něž se při těchto zobecněních naráží.

Author's addresses: RNDr. *Jana Stará*, CSc., doc. *Svatopluk Fučík*, CSc., RNDr. *Oldřich John*, CSc., MFF UK, Sokolovská 83, 180 600 Praha 8; *Marta Tenčlová*, MFF UK, Malostranské nám. 1, 11 800 Praha 1; RNDr. *Jiří Bubník*, CSc., Hydrometeorologický ústav, Na Šabatce 1, 140 00 Praha 4 - Komořany.