Journal of Engineering Physics and Thermophysics, Vol. 81, No. 5, 2008

HEAT AND MASS TRANSFER IN DISPERSE AND POROUS MEDIA

NUMERICAL MODEL OF THE SCATTERING OF A GASEOUS AND DISPERSED IMPURITY IN THE ATMOSPHERE

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UDC 551.511.61

A numerical model of the transfer of a gaseous and dispersed impurity in the atmosphere is described. The model is based on the semi-empirical stationary equation of turbulent diffusion in the boundary layer of the atmosphere with account for the gravitational deposition of particles. The altitude profiles of the coefficient of turbulent diffusion and of the wind velocity are approximated according to the Monin–Obukhov theory and the data obtained by Byzova with her coworkers. The atmosphere stratification is determined on the basis of standard meteorological data. The model is compared with experimental data and with well-known techniques used to calculate the propagation of impurity in the atmosphere.

Introduction. The transfer of an impurity in the atmosphere is a complex process that has not been adequately studied as yet. A fairly large number of methods have been developed to describe this process. Among them there are Gaussian simple models [1] that describe the propagation of an impurity from stationary and pulse sources in a local scale to distances of several tens of kilometers, when the direction and force of the wind can be considered constant. These models are also used to describe the transfer of an impurity in a regional scale involving a territory of size up to several thousands of kilometers. In this case the Gaussian distribution of impurity is formed around preliminarily calculated three-dimensional trajectories of the motion of air volumes in the variable field of the wind [2]. A more complex approach is that of Lagrange in which an impurity cloud is modeled by a large collection of particles moving in an averaged gas flow to which a random perturbation that models the effect of turbulence is added [3]. One of the most complete and laborious techniques is that based on mutual description of turbulent motion of atmospheric gases and scattering of impurity in them on the basis of the mass, momentum, and energy conservation laws [1]. In the present work we use the method that is being developed by Berlyand with his coworkers and which is based on the equation of turbulent diffusion [4]. To describe the altitude dependences of wind velocity and coefficient of turbulent diffusion that enter into this method, Byzova's experimental data were used [5, 6].

Mathematical Formulation of the Problem. We will assume that the concentration of a gaseous and disperse impurity $c(x, y, z)$ transferred by a turbulent wind stream can be presented in the form [4, 7]

$$c(x, y, z) = p(x, y)\, q(x, z) . \tag{1}$$

The quantity q, which is the integral of the concentration along the y axis, is determined from the equation

$$u(z) \frac{\partial q}{\partial x} - V_g \frac{\partial q}{\partial z} = \frac{\partial}{\partial z} k(z) \frac{\partial q}{\partial z} . \tag{2}$$

The initial condition for (2) with a source at the point $x = 0$, $z = h$ can be written in the form

$$u(h)\, q(0, z) = M\delta(z - h) . \tag{3}$$

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1062-0125/08/8105-0945

The boundary conditions are prescribed as follows: on the underlying surface

$$\left(k(z)\frac{\partial q}{\partial z}+V_g q\right)_{z=0}-V_d q(0)=0, \tag{4}$$

on the upper boundary $q(+\infty) = 0$.

An analysis of experimental data shows [4] that the distribution of concentration over the y axis is mainly determined by the fluctuations of wind direction. In this case the function of the transverse distribution of the concentration of the impurity p can be approximately presented in the form

$$p(x, y)=\frac{1}{\sqrt{2\pi}\,\Delta\varphi x}\exp\left(-\frac{y^2}{2\Delta\varphi^2 x^2}\right). \tag{5}$$

The angular dispersion of the wind direction fluctuations $\Delta\varphi$ depends on the atmosphere stratification, average wind velocity, and the time of observation t. Its coupling with the time of observation can be approximated by the relation $\Delta\varphi(t) \sim t^{1/4}$ [4].

To calculate the wind velocity profiles and the coefficient of turbulent diffusion in the ground boundary layer (GBL) of the atmosphere, the Monin–Obukhov theory was used [1, 8]:

$$\frac{\partial u}{\partial z}=\frac{u^*}{\chi z}\psi(\xi), \quad k(z)=\frac{\chi u^* z}{\psi(\xi)}; \tag{6}$$

$$\psi=\begin{cases}1+\beta\xi, & \xi\ge 0,\\ (1-\gamma\xi)^{-1/4}, & \xi\le 0,\end{cases} \qquad \xi=\frac{z}{L}, \quad L=-\frac{Tc_p\rho(u^*)^3}{\chi g H}. \tag{7}$$

To determine the wind velocity and the diffusion coefficient at the altitudes exceeding the GBL (~10–50 m), the following equations were used [9]:

$$u=u^*\bar{u}(\bar{z})/\chi, \quad k(z)=\chi u^*\lambda\bar{k}(\bar{z}); \tag{8}$$

$$\bar{z}=z/\lambda, \quad \lambda=\chi u^*/l, \tag{9}$$

where $\beta = 6$ and $\gamma = 16$. The universal profiles of the wind velocity $\bar{u}(\bar{z})$ and of the diffusion coefficient $\bar{k}(\bar{z})$ were suggested by N. L. Byzova and her coworkers [5, 6, 9] on the basis of the data obtained in observations of many years of the meteorological parameters on a 300-meters mast and numerical simulation of the structure of the atmospheric boundary layer. These universal profiles depend on the class of stability (stratification) of the atmosphere that was determined by the Terner — IEM technique [10].

Comparison of the Numerical Model with the Data of Full-scale Experiments and Other Models of Impurity Transfer. The input parameters of the numerical model are the meteorological data and characteristics of the source of ejections. For its testing the data of full-scale measurements give in [11–14] were used as well as the well-known computational techniques of determining the concentration of impurities [1, 15].

Table 1 contains the values of experimentally measured and numerically calculated normalized integral concentrations of impurity $qu(h)h/M$. These values were determined for different distances x from the source in the direction of wind, source height, wind velocities, and classes of stability. Moreover, the table also contains the values of integral concentrations calculated by the IAEA technique [15] and the Gaussian model [1].

Figure 1 presents a comparison of the predicted and experimental data. The graph a presents tabulated data in the form of the dependence of the ratio of calculated integral concentration of an impurity to the measured values on the distance to the source. The dashed lines show the region within which the difference between the prediction and experiment does not exceed two times. It is seen from the graph a that for all three techniques the indicated ratios are located symmetrically relative to unity and in the main lie inside the region bounded by the dashed lines. The excep-

TABLE 1. Comparison of Integral Concentrations of Impurity Calculated by the Numerical Model of the Present Work, the IAEA Technique, and the Gaussian Model with the Results of Measurements

No. of experiments	x, m	h, m	u, m/sec	Stability class	$(qu(h)h/M)_{pr}$	$(qu(h)h/M)_{IAEA}$	$(qu(h)h/M)_{G}$	$(qu(h)h/M)_{exp}$
1	3150	200	4	C	0.326	0.472	0.484	0.78
2	3160	200	4	C	0.327	0.473	0.484	0.34
3	3400	200	10	D	0.317	0.045	0.103	0.39
4	3310	200	10	D	0.307	0.041	0.095	0.39
5	3160	200	4	C	0.327	0.473	0.484	0.63
6	3160	200	4	C	0.327	0.473	0.484	0.48
7	3200	200	10	D	0.294	0.035	0.086	0.02
8	3230	200	10	D	0.298	0.035	0.089	0.04
9	3880	80	10	D	0.413	0.483	0.479	0.52
10	3880	80	10	D	0.413	0.483	0.479	0.45
11	3280	80	10	D	0.434	0.475	0.484	0.35
12	3250	80	10	D	0.435	0.474	0.484	0.34
13	3160	200	4	C	0.327	0.473	0.484	0.34
14	4100	200	10	D	0.382	0.088	0.163	0.34
15	4300	200	10	D	0.397	0.105	0.180	0.21
16	4250	200	4	C	0.442	0.481	0.464	0.37
17	4300	200	4	C	0.446	0.480	0.462	0.3
18	3250	200	4	C	0.339	0.481	0.484	0.23
19	3480	200	10	D	0.326	0.051	0.110	0.49
20	3850	200	10	D	0.361	0.071	0.142	0.27
21	4310	80	4	C	0.401	0.272	0.240	0.48
22	4250	80	10	D	0.399	0.484	0.473	0.68
23	4200	80	4	C	0.405	0.261	0.245	0.48
24	3950	80	4	C	0.415	0.289	0.255	0.52
25	3110	80	4	C	0.449	0.333	0.300	0.23
26	3200	80	4	C	0.446	0.329	0.295	0.12

tion is the ratio of calculations and results of measurements numbered 7 and 8 that go beyond the scale of the figure. These data were obtained for the source located at an altitude of 200 m at a wind velocity of 10 m/sec. The estimates show that measurements were made in those situations where the plume hardly reached the underlying surface. In that region the concentration is low and increases rapidly as the plume recedes. The accuracy of measurement of the integral concentration of impurity in the indicated region is low. This is also supported by a comparison of the results of measurements in the experiments numbered 4 and 8 in Table 1. At two close distances the measured concentrations differ by an order of magnitude, while calculations give values that differ little for these experiments. The results of the numerical method presented here are somewhat closer to experimental results than in other methods.

The graphs b–d compare axial concentrations calculated by different techniques and measured in three different experiments [12–14]. The experiments were carried out near the Dickerson and Morgantown thermal power stations, Maryland, USA and a nickel smelting plant in Sudbury, Ontario province, Canada. It is seen from the graphs that for axial concentrations the agreement between the calculation and experiment is much worse than for the values of concentrations that were integrated across the jet and which are presented in the graph a. On the average, the calculation differs from experiment roughly three times, which can be considered acceptable for such kind of objects [1].

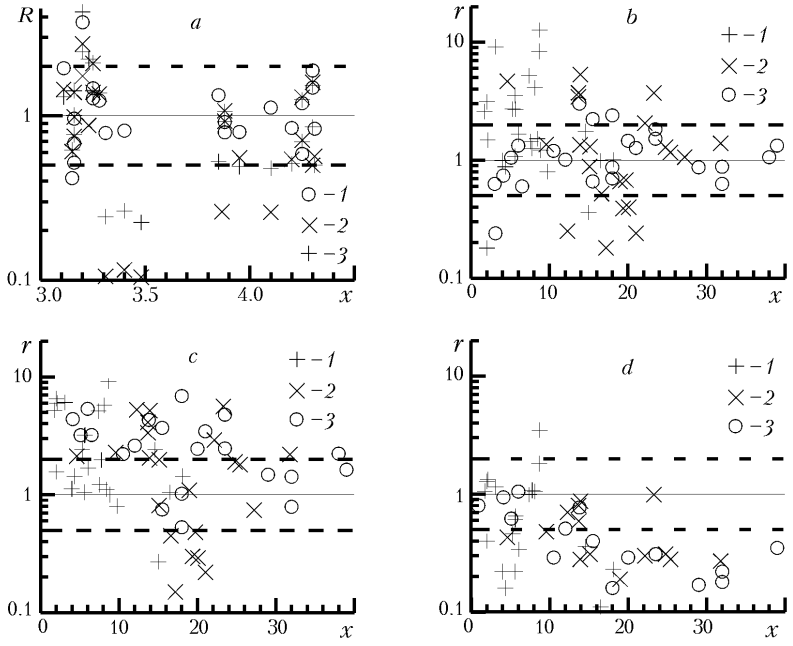

Fig. 1. Comparison between the predicted and measured concentrations: a) ratio of integral concentrations R calculated by different techniques (1) of the present work, 2) IAEA, 3) Gaussian) and measured in an experiment [9]; b, c, d) ratio of axial values of concentrations r calculated by the technique of the present work, Gaussian one, and the IAEA technique and measured in experiments, respectively [11, 12] (1, 2) near the Dickerson and Morgantoun thermal power stations; 3) in the region of the nickel smelting plant in Sudbury). x, km.

Conclusions. A numerical technique of calculation of the propagation of an impurity in the atmosphere has been developed. It allows one to uniquely describe the transfer of both a gaseous and dispersed impurity. A comparison of the calculations made by this technique with the data of four experiments gave a satisfactory agreement for the impurity concentrations integral across the jet and axial concentrations.

NOTATION

$c(x, y, z)$, impurity concentration at the point (x, y, z) of the Cartesian coordinate system, kg/m^3; c_p, heat capacity of air at a constant pressure, J/(kg·K); g, free fall acceleration, m/sec^2; h, height of the source, m; H, turbulent vertical heat flux, J/(m^2·sec); $k(z)$, coefficient of turbulent diffusion, m^2/sec; $\bar{k}$, dimensionless coefficient of turbulent diffusion; l, Coriolis parameter, sec^{-1}; L, Monin–Obukhov scale, m; M, source power, kg/sec; p, function of transverse distribution of impurity concentration; q, impurity concentration integral across the jet, kg/m^2; t, time, sec; T, air temperature, K; $u(z)$, wind velocity at an altitude z, m/sec; u^*, friction velocity, m/sec; $\bar{u}$, dimensionless velocity; V_d, velocity of dry precipitation, m/sec; V_g, velocity of gravitational precipitation of aerosol particles, m/sec; x, coordinate of the observation point relative to the horizontal axis directed along wind propagation, m; y, coordinate of the observation point relative to the horizontal axis directed perpendicular to wind propagation, m; z, coordinate of the observation point relative to the vertical axis, m; $\bar{z}$, dimensionless coordinate z; β, constant; γ, constant; δ, Dirac delta-function, m^{-1}; λ, scale of boundary-layer thickness, m; ξ, dimensionless variable; ρ, air density, kg/m^3; $\Delta\varphi$, angular dispersion of wind direction fluctuations; χ, von Karman constant; ψ, universal function the approximation of which is given by Eq. (7). Subscripts: d, dry precipitation; exp, experiment; G, Gaussian model; IAEA, International Atomic Energy Agency model; g, gravitational precipitation; p, pressure; pr, prediction by the numerical technique of the present work.

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