Verification of the Lagrangian stochastic model of smoke plume spread in the turbulent atmosphere

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A numerical method is proposed for solution of the problem on smoke plume spread in the turbulent atmosphere based on Lagrangian model. The algorithm proposed is adapted for use on a network of computers operated in parallel and implemented within the framework of the MPI system. The efficiency of the model and of the numerical method proposed is verified as applied to the problem of turbulent dissipation of perturbations from a linear heat source.

Introduction

As known turbulent fluxes often occur in nature and in the atmosphere in particular. It is also well-known that all models developed for describing of such fluxes are much more complicated than similar models for laminar fluxes by both the level of assumptions admitted during their derivation and by the laboriousness of obtaining the solutions. The validity of these general notes can be clearly seen in the history of the problem on the smoke plume spread in the turbulent atmosphere. The main peculiarities of this practically important problem are chemical reactions proceeding in the plume and the temperature difference between the smoke plume and the atmosphere that gives rise to intense mixing. The Table borrowed from Ref. 1 (Ref. 1 also gives a sufficiently detailed literature overview) compares different approaches to solution of this problem, their advantages and disadvantages, as well as domains of applicability.

In the first turn, it is interesting to note that automodel solutions based on the simplified consideration of all factors in combination with the simplest geometric models of dispersal do form still the basis for engineering methods of calculating the concentrations of smoke plume components in the vicinity of sources.[2]

Investigations of plume spread with the use of Reynolds averaged Navier–Stokes equations (RANS) employ simplified representations for the terms of the equations describing chemical reactions of smoke plume components and their mixing in the atmosphere. Such an approach, as automodel solutions, yields only mean characteristics of the plume and often gives rise to additional parameters, which cannot be measured experimentally.

In contrast to these approaches, the Lagrangian statistical models, namely, Lagrangian dispersion model (LDM) and Lagrangian turbulence model (LTM), yield not only the mean, but also statistical characteristics of a plume. The Lagrangian dispersion models imitate processes in the plume, but imply that the field of the main flux is known, i.e., calculated by other methods or approximated. Using the Lagrangian turbulence models, the flux field can be calculated at different altitude dependences of the wind velocity and temperature, which, as known, determine conditions of the smoke plume spread. An important advantage of these models is the possibility of accounting for even nonlinear chemical reactions proceeding in the smoke plume. One of such models will be considered in detail in this paper.

At direct numerical simulation and large eddy simulation, the Navier–Stokes equations are solved directly (LES). In LES, however, additional assumptions are used concerning the behavior of small-scale turbulence. Both these approaches are computationally expensive and impose certain restrictions on the Reynolds, Schmidt, and Damkohler numbers, as well as on the shape and size of an object. Therefore, they are now used for solution of simple problems, which can be then used as test ones for verification of other models.

Different methods for solution of the problem on smoke plume spread

Degree of allowance for mixing and reactions				
	Exact representation	–	LTM (reactions)	DNS
	Simulation	–	LTM (mixing)	–
	Parameterization	Automodel solutions	RANS LDM	LES
		Parameterization	Modeling	Exact representation
	Degree of allowance for mixing and reactions of flow in the plume and atmosphere			

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1. Description of the model

The Lagrangian turbulence model proposed in Ref. 1 is based on linear stochastic differential equations for the coordinates $\mathbf{x} = (x_1, x_2, x_3)$, velocities $\mathbf{u} = (u_1, u_2, u_3)$, and the potential temperature, θ, of gas particles:

$$\frac{\mathrm{d}}{\mathrm{d}t} x_i(t) = u_i(t),$$

$$\frac{\mathrm{d}}{\mathrm{d}t} u_i(t) = a_i + G_{ij}(u_j - \langle u_j \rangle) + G_i(\theta - \langle\theta\rangle) + b_{ij}\frac{\mathrm{d}W_j}{\mathrm{d}t},$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \theta(t) = a_4 + G_{4j}(u_j - \langle u_j \rangle) + G_4(\theta - \langle\theta\rangle) + b_4\frac{\mathrm{d}W_4}{\mathrm{d}t}.$$

Deterministic changes in the velocity and potential temperature of a particle are described by the first three terms in the right-hand sides with the unknown coefficients a_i, G_{ij}, and G_i. The first term reflects the effect of gradients in the flux field, whereas the second and third terms describe the difference in the velocity and temperature between the gas and the flux at the considered point. The last terms describe the effect of "stochastic forces." The "white noise" $\mathrm{d}W_i/\mathrm{d}t$ is a Gaussian process with zero mean $\langle \mathrm{d}W_i/\mathrm{d}t\rangle = 0$ and uncorrelated values at different moments in time $\langle \mathrm{d}W_i/\mathrm{d}t(t_1)\ \ \mathrm{d}W_j/\mathrm{d}t(t_2)\rangle = \delta_{ij}\,\delta(t_1 - t_2)$. The latter condition written for $i = 4$ means that the stochastic terms in the equations for the velocity and temperature do not give rise to the systematic effect on particle motion, if time steps are larger than the characteristic time introduced by Kolmogorov.[3]

To derive equations for the coefficients a_i, G_{ij}, and G_i (Ref. 1), the following procedure is used. First, the transport Fokker–Planck equation is derived for the probability density $\Psi(\mathbf{x}, t; \mathbf{u}, \theta)$. Multiplying this equation by the corresponding combinations of $\mathbf{u}$ and θ and integrating the right-hand and left-hand sides, Heinz and Van Dop[1] obtain the system of equations for probability density moments, which are compared with RANS. If it is assumed in making such a comparison that (1) the Boussinesq approximation is valid, (2) RANS is closed with the help of theories from Refs. 3 and 4, and (3) the functional form of the coefficients b_{ij} corresponds to those from Ref. 5, then for the model coefficients we have the following equations:

$$(b^2)_{ij} = C_0\, q^2\delta_{ij}/(2\tau);\ b_4 = C_1\,\langle(\theta - \langle\theta\rangle)^2\rangle/(2\tau);$$

$$C_0 = (k_1 - 2)/3;\ C_1 = 2k_3 - 2k_4 - k_1;\ G_{ij} = -k_1\delta_{ij}/(4\tau);$$

$$G_i = \beta g\delta_{i3};\ G_{4i} = 0;\ G_4 = -(2k_3 - k_1)/(4\tau);$$

$$a_i = \nu\frac{\partial^2\langle u_i\rangle}{\partial x_k \partial x_k} - \frac{\partial p}{\rho\partial x_i} - g\delta_{i3}\ (i = 1, 2, 3);\ a_4 = \alpha\frac{\partial^2\langle\theta\rangle}{\partial x_k\partial x_k},$$

where ρ, p, ν, α, and g are the mean values of density and pressure, kinematic viscosity and thermal conductivity coefficients, and the free fall acceleration, respectively; $q^2 = \langle(u_i - \langle u_i\rangle)\,(u_i - \langle u_i\rangle)\rangle$ is the doubled kinetic energy of turbulent pulsations; $\tau = q^2/(2\varepsilon)$ is the dissipation time; ε is the rate of dissipation of this energy; β is the thermal expansion coefficient; k_i are the closure coefficients.

Such a definition of the coefficients leads to the situation that the stochastic differential equations of the model depend on the function τ, which describes the process of mixing of the smoke plume with the atmosphere. According to Ref. 6, this function can be described by the equation

$$\frac{\mathrm{d}\tau}{\mathrm{d}t} = (C_{\varepsilon 2} - 1) - (C_{\varepsilon 1} - 1)\times$$

$$\times\frac{2\tau}{q^2}\left[\begin{array}{l} -\langle(u_k - \langle u_k\rangle)\,(u_l - \langle u_l\rangle)\,\dfrac{\partial\langle u_l\rangle}{\partial x_k} + \\ +\beta g\,\langle(u_3 - \langle u_3\rangle)\,(\theta - \langle\theta\rangle)\end{array}\right].$$

Having introduced this equation, the system of equations for LTM becomes closed for the given initial and boundary conditions, because all the parameters determining variations of the characteristics of gas particles (mean velocity and temperature, their covariations, and pressure gradient) can be calculated as mean values (following Euler) of the corresponding parameters of gas particles.[7]

2. Numerical method

The Lagrangian models, by their idea, are oriented at applying statistical solution methods (Monte Carlo methods). At the initial moment, the coordinates and velocities of N particles are specified in the computational domain. At the following moments in time, these particles move according to the model equations and the preset boundary conditions. At large values of time t, we obtain solution of the stationary problem. Let us consider briefly the main peculiarities in the applied algorithm for the case of a rectangular computational domain.

1. The accuracy, with which the results are obtained by the Monte Carlo methods, is usually proportional to $N^{-1/2}$ (N is the number of particles). This implies high time expenses and heavy demands imposed on the computer memory. These demands become less strict, if the problem is solved using computers operated in parallel with shared memory. In this case, for the algorithm multisequencing, it is the easiest way to use division of the computational domain into several subdomains. The exchange between processors reduces to transport of particles leaving the corresponding subdomain from one processor to another for a time step.

2. The speed distribution of incoming particles should be preset at the left boundary of the computational domain. Since the exact form of this function is usually unknown in the considered gas-

dynamic problems, some functional class (for example, local Maxwell distribution) is used, and the parameters of this distribution are calculated based on additional experimental information (for example, velocity and temperature and their variances) along the boundary.

3. The conditions reflecting the character of interaction of gas particles with surfaces should be specified at the upper and lower boundaries of the computational domain. These surfaces may be the Earth's surface or the surface of an experimental setup or some line in a flux, which serves as a boundary, in a particular consideration. Unfortunately, these conditions are unknown as well. Most often the condition of specular reflection is accepted at these boundaries. According to this condition, a particle interacting with the surface keeps the tangential component of momentum unchanged and alternates the sign of the normal component.

4. The equation for time of dissipation of turbulent pulsations τ includes derivatives of the components of the mean velocity vector with respect to coordinates. Since the components of the velocity vector are calculated as means of the corresponding components of velocity of gas particles being in the considered cell of the computational grid at a given moment and, consequently, include a statistical error, special measures should be undertaken for correct calculation of the derivatives. First, to decrease the statistical error, the components of the velocity vector are calculated as means for some number (on the order of several tens) of time steps. Second, before calculating the derivatives, the problem of a cubic spline minimizing the value of the smoothing functional is solved.[8]

5. When solving stationary problems by the methods of statistical simulation based on a correct model, the problems of solution stability and specification of the initial approximation are usually absent.

6. The considered Lagrangian model contains numerical parameters. Although these parameters obey some restrictions originating from the mathematical form and physical peculiarities of the model, the problem of searching the optimal set of these parameters is one of the most laborious components of the process of model verification.

3. Description of the test problem and discussion

For verification of the model and the numerical method, we have chosen Ref. 9, which studied experimentally the spread of temperature perturbations in the turbulent boundary layer. In a wind tunnel at some distance $z = h = 60$ mm from a rough wall, a wire was installed and electric current was passed through it. In some cross sections along the flow, temperature and two velocity components were measured. The measurements showed that the pressure gradient in the whole flow field is zero, and the mean velocity is well described by the equation $u/u_* = 2.63 \ln(500z/h)$, where $u_* = 0.48$ m/s. This flux was calculated by the Monte Carlo method based on the considered Lagrangian model. The local Maxwell speed distribution function was specified for incoming particles at the left boundary of the computational domain. The mean velocity was accepted equal to the measured one, and the factors in the exponents were determined from the measured values of rms deviations of the velocity components from the mean value. The condition of specular reflection was set on the upper and lower boundaries, and the free condition was taken at the right-hand side boundary: all outgoing particles were excluded from the consideration. The calculations were conducted on the massive parallel computer of the Institute of Mathematical Simulation RAS.

The comparison of calculations with measurements in two cross sections $x/h = 2.5$ and 15 is depicted in Figs. 1 and 2 as dependences of u/u_* and θ/θ_* on z/h. It can be seen that calculations closely agree with the experimental data far from the upper and lower boundaries. As a consequence of ill-posed boundary conditions, a peculiar "boundary layer" is formed near the lower boundary, and the speed of the flux in this layer increases. The behavior of the dependence $\theta/\theta_*(z/h)$ (see Fig. 2) near the wall at $x/h = 15$ is different than the experimental one, and this can be explained by two factors. First, the effect of the computational "boundary layer" on the wall is already marked in this cross section. Second, the energy exchange at the wall under conditions of the experiment and our computations was different: the condition of specular reflection implies the absence of exchange, whereas the surface used in the experiments had finite thermal conductivity.

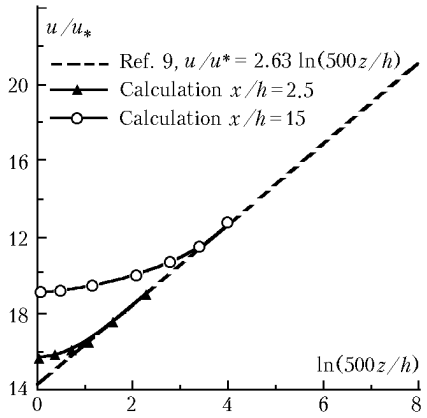

Fig. 1. Comparison of our calculations with the experimental data (speed of flux).

It should be noted that the computational "boundary layer" becomes more thin, if in place of the condition of specular reflection we use physically better

justified condition of reflection with the Maxwell speed distribution function having zero mean.

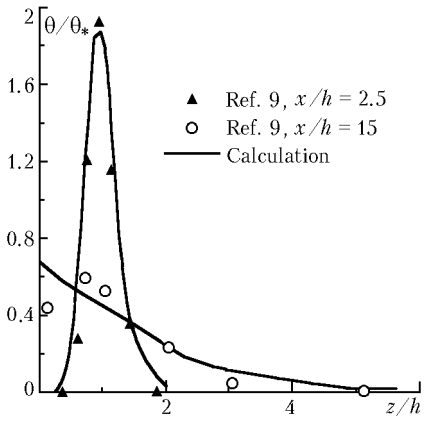

Fig. 2. Comparison of our calculations with experimental data (temperature within the flux).

Conclusions

Thus, our study has shown that

1. The considered Lagrangian stochastic model can be used to solve problems of plume spread from smoke stacks in the turbulent atmosphere.

2. The proposed algorithm of stochastic modeling has sufficient efficiency.

3. When solving practical problems, it should be taken into account that a computational "boundary layer" exists near the Earth's surface and the measures should be undertaken to decrease this layer.

Acknowledgments

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