A new model for boundary layer flows interacting with particulates in land surface on complex terrain

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(Manuscript received in final form January 29, 2007)

Abstract—This paper presents a model describing three-dimensional atmospheric flows with solid particles or aerosols. The model uses the Nigmatulin equations for two-phase atmosphere, which describes lifted atmosphere by ideal gas equations with variable equation of state. The Godunov numerical method based on solution of the one dimensional initial discontinuity decay problem on an interface of two cells of computational grid is applied in this work.

Key-words: boundary layer, Curant-Friedrichs-Levy condition, discontinuity decay problem, Godunov method, grid-scale function, Nigmatulin equations, scheme viscosity, single-velocity model, relaxation, two-phase atmosphere

1. Introduction

In the present work a new physical model of transport of atmospheric impurities (solid particles or heavy gases) by the wind in regions over non-homogeneous or variable in time surfaces is realized. This task is very important for solving the problems linked with preservation and optimal using of the nature. It is necessary to discuss fundamental difficulties, which prevent constructive solution of this problem. Essentially this task can be divided into two subtasks:

- Description of an atmospheric flow in planetary boundary layers under non-homogeneous and/or non-stationary conditions.
- Prediction of the space-time distribution of transported particulates concentration.

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Well-known traditional theories of boundary layers are applied to atmospheric flows along plane, homogeneous, and stationary surfaces. Along such ideal surfaces, atmospheric boundary layer is also horizontally homogeneous and it is in state of equilibrium. The problem of impurity transport reduces to solving the equation of passive scalar for turbulent flow in boundary layer in this simple situation. However, concentration of particulates or external factors can be beyond the limits of applicability of the passive scalar approximation (Barenblatt and Golitsin, 1974). In these cases the full system of thermo-hydrodynamic equations of boundary layer with parameterization of sub-grid scale turbulent flows in large eddy simulations method or in Reynolds averaged equations approach fails. Non-homogeneity of the Earth surface and its variations in time change the picture of the flow considerably. When flowing around various obstacles (mountains, buildings, and street canyons), the flow may change both dramatically and gradually. Usually, different space-time variations of planetary surface may appear simultaneously. In such situations it is impossible to create an adequate model of turbulent boundary layer.

The complicated topology of flows in such complex terrain may change the character of the impurity. In such a situation the initially passive impurity may be transformed into active one (affecting the hydrodynamic flow). A well-known example, which should be mentioned, is the origination of dust vortexes (devils) in domains with valleys. Moreover, an initially homogeneous cloud of particulates is transforming to complex non-homogeneous structure. Such structure includes regions with high concentration of impurities, which have its own dynamic behavior. As a result, besides the possibility of changing of impurity character, which was stated above, we face the necessity to analyze the interaction of such formations with the entire cloud of particles, and to predict duration of their life.

In the present work we develop the method describing the transport of particulates in atmospheric boundary layer over complex surface. This method is directed to overcome the difficulties of traditional methods, described above. Besides, it practically expands the opportunity of predictions of transportation of solid particles onto cases when it is impossible to use the approximation of passive scalar or in changes of impurity character in particular domains of cloud. Our model also permits to analyze phenomena, which are driven by complex topology of the flow above obstacles and can describe processes on interface between cloud of solid particles and pure atmosphere. In our model we use Nigmatulin equations (Nigmatulin, 1987) describing two-phase medium “gas-particles” by equations of ideal gas with variable equation of state. Effective equation of state for such medium depends upon characteristic size and concentration of spherical particles, and in the limit of absence of solid phase it is converted to usual equations of the ideal gas. Practically, the task to analyze the transport of particles in the atmosphere is reduced to solving equations of ideal gas with variable in space and time equations of state.
It provides the opportunity of describing the loaded and pure atmosphere by the same set of equations with different thermodynamic properties. In fact it means that this system of equations can be applied for modeling the boundary of clouds of solid particles and pure atmosphere. The use of the system of equations of ideal gas with a variable equation of state provides a direct dependence of hydrodynamic flow velocity upon the concentration of solid phase. Practically, it means that there is a possibility of overstepping the limits of applicability of passive impurity approximation.

The main idea of the suggested method is to use the non-viscous equations for modeling the transport of solid particles near a complex surface (Kulikovskii et al., 2001). For free atmospheric flows the Reynolds number, which characterizes the ratio of inertial force to viscosity force in hydrodynamic equations, is very large. That is why nonlinear inertial terms exceed significantly the molecular viscosity terms. The opposite situation appears for atmospheric flows near a surface, where viscosity mechanisms play the main role.

Flows in a viscous atmosphere with arbitrarily small viscosity coefficient have to satisfy non-slip conditions, which demand the full velocity of flow on solid surface to be zero. Undoubtedly, the hypothesis of Prandtl is satisfied (Schlichting, 1955). This means that the terms describing dissipation of energy in atmospheric flows are comparable with inertial force for a wide range of conditions in a layer boundering a solid surface. Thus, according to the Prandtl hypothesis, atmospheric flows, characterized by a high Reynolds number, formate a boundary layer. Within this layer a necessary transition from zero value of wind velocity to finite value on external side of a boundary layer is provided. In this case such values on external side of the boundary layer are very similar to the values that appear in an ideal atmospheric flow (Zilitinkevich, 1970). Within this layer, the high gradients of velocity field lead to the situation when viscosity effects are comparable to inertial force effects.

Thus, first we have to conciliate the concept of high gradients of wind in a boundary layer, and second, we have to ignore molecular viscosity in equations of the two-phase atmosphere. In this work we suggest to provide the high wind field gradients by means of the scheme viscosity of the numerical algorithm for modeling phenomena near a surface.

We use Godunov method (Godunov, 1976) for numerical solution of equations of the two-phase atmosphere. The main idea of Godunov method is to use the generalized solutions of initial discontinuity decay problem with discretization of impulse, mass, and energy conservation laws in each cell of the computational domain. These solutions include local tangential gaps, which do not appear on outer scales, and none the less provide dissipation of kinetic energy, as it is necessary for flows in a boundary layer. Thus, the structure of the used finite difference scheme provides diffusion of ranges with high entropy on all space coordinates and represents qualitatively effects of molecular viscosity. It should be mentioned that influence of the scheme
viscosity is shown more considerably in the situation when boundary layer is loaded with solid particles and in regions with considerable variations of surface relief. In such cases the influence of molecular viscosity also increases in reality. The value of molecular viscosity depends on gradients of sub-grid flows and has a finite limit as the grid of discretisation decreases. Thus, it can be regulated by a choice of the size of the grid. It is clear that for a turbulent flow, the scheme viscosity exceeds one for laminar flows, demonstrating a well-known relation between the turbulent and laminar viscosity.

2. Model of the effective ideal gas for atmosphere with solid particles

The effects of inhomogeneities seriously complicate the investigations of the processes in the atmospheric boundary layers. If we suppose that the size of particles is much smaller than the characteristic scale of those of atmospheric flows, we may describe macroscopic processes in such atmosphere with averaged parameters. We will use the same mass, impulse, and energy conservation equations for the atmosphere lifted by solid particles as for a single-phase medium. In this case it is necessary to take into account boundary conditions on the interface between the phases.

We suppose that volume concentration of solid phase is small enough. Let $\alpha_i (i = 1,2)$ be the part of particulates volume which is occupied by each phase: $\alpha_1 + \alpha_2 = 1$ ($\alpha_i \geq 0$). Hence, $\alpha_2 \leq 1$. The solid phase is represented by spherical particles of the radius $a$. In our model $\rho_1^0$ and $\rho_2^0$ are the density of the atmosphere and the solid particles, respectively, $n$ is the number of particles of dispersed phase in a unit volume of particulates. Thus, according to our assumption, we have $\alpha_2 = \frac{4}{3} \pi a^3 n$, $\alpha_1 = 1 - \alpha_2$. Weights of phases in a unit volume of the atmosphere are denoted as $\rho_i (i = 1,2)$, and $\rho = \rho_1^0 \alpha_1$, $\rho_2 = \rho_2^0 \alpha_2$, $\rho = \rho_1 + \rho_2$. We ignore the effects of inertia for moving solid particles, their interactions and collisions, and the process of subdivision and sticking of particles. Viscosity and heat-conduction of fluid and solid phase do not appear in the macroscopic transport of impulse and energy. The values of viscosity and heat-conduction are needed only to describe processes in inter-phases interaction. It allows using non-slip boundary conditions near the solid surface to find parameters of the fluid phase. The density of the atmosphere with solid particles is much less than the density of the substance of solid particles.

Under these conditions the atmosphere with solid particles allows hydrodynamic description. If velocities, $\mathbf{v}$, and temperatures of these phases are equal to each other, we can describe such impurity by equations of nonviscous and non-heat-conducting medium of ideal gas. For three-dimensional atmosphere, these equations can be written as:
\[ \frac{\partial \rho}{\partial t} + \frac{\partial (\rho v_x)}{\partial x} + \frac{\partial (\rho v_y)}{\partial y} + \frac{\partial (\rho v_z)}{\partial z} = 0, \]

\[ \frac{\partial (\rho v_x)}{\partial t} + \frac{\partial (p + \rho v_x^2)}{\partial x} + \frac{\partial (\rho v_x v_y)}{\partial y} + \frac{\partial (\rho v_x v_z)}{\partial z} = 0, \]

\[ \frac{\partial (\rho v_y)}{\partial t} + \frac{\partial (\rho v_y v_x)}{\partial x} + \frac{\partial (p + \rho v_y^2)}{\partial y} + \frac{\partial (\rho v_y v_z)}{\partial z} = 0, \]

\[ \frac{\partial (\rho v_z)}{\partial t} + \frac{\partial (\rho v_z v_x)}{\partial x} + \frac{\partial (\rho v_z v_y)}{\partial y} + \frac{\partial (p + \rho v_z^2)}{\partial z} = 0, \]

\[ \frac{\partial e}{\partial t} + \frac{\partial (e + p) v_x}{\partial x} + \frac{\partial (e + p) v_y}{\partial y} + \frac{\partial (e + p) v_z}{\partial z} = 0. \]  

Here \( e \) is the total energy per unit volume of mixture: \( e = \rho (e + \frac{v_x^2 + v_y^2 + v_z^2}{2}) \), \( \varepsilon(\rho, p) \) is the internal energy determined by the equation of state. In accordance with Nigmatulin's model (Nigmatulin, 1987), rheology of mixture can be described by the equation of state of ideal gas with the effective gas constant \( R \):

\[ \varepsilon = cT, \quad p = \rho RT, \quad \text{where } R = x_1 R_1, \quad c = x_1 c_1 + x_2 c_2, \quad x_i = \rho_i / \rho, \quad x_1 + x_2 = 1, \]

\( R \) and \( R_1 \) are the specific ratios of atmosphere gas mixture and solid particles, respectively, and \( c, c_1, c_2 \) are the heat capacities of the atmospheric gas mixture and solid phase under constant pressure accordingly. Thus, to close the system Eq. (1), we add a complimentary equation of change of mass of solid particles:

\[ \frac{\partial \rho_2}{\partial t} + \frac{\partial (\rho_2 v_x)}{\partial x} + \frac{\partial (\rho_2 v_y)}{\partial y} + \frac{\partial (\rho_2 v_z)}{\partial z} = 0. \]  

The described model of the atmosphere with solid particles is especially useful for modeling processes near a solid surface, because it formally coincides with classic hydrodynamic equations of ideal gas with the recalculated adiabatic index \( \gamma \) (Ovsyannikov, 1981): \( \gamma = (c + R) / c \leq \gamma_1 \), and with the recalculated velocity of sound wave: \( C_s = \sqrt{\frac{\gamma p}{\rho}} = C_{1s} \sqrt{\frac{\gamma x_1}{\gamma_1}} \leq C_{1s} \). The formal coincidence of the equations of clear and lifted atmosphere provides a possibility of modeling nonstationary processes of the particle transport in the atmosphere and motion of dust clouds. In particular, it allows to investigate stability and dynamics of the propagation of a dust cloud and its boundary.
The main limitation of the model is related to ignoring the two-speed effects due to relative motion of the solid phase. It is interesting that the decreasing of the size of solid particles and retaining the same parameters of the atmosphere naturally result in a decrease of relaxation time of velocity and temperature of each phase. If characteristic time scale of the investigated flow is much smaller than the velocity inter-phase relaxation time, we can use a one-speed scheme. According to Nigmatulin (1987), for small characteristic Reynolds numbers \( Re_1, 2 \leq 1 \), describing the atmospheric stream flow over the individual particle, the relaxation time is determined only by viscosity of flowing phase \( \mu_1 \), by the size and density of the particles substance \( \rho_2^0 \):

\[
t_1 = \frac{2a^2 \rho_2^0}{9\mu}.
\]

In the other limit case of high Reynolds numbers \( Re_1, 2 \geq 50 \), the relaxation time is determined by the density of the ambient atmosphere phase \( \rho_1^0 \), its flow velocities \( v_0 \), and the velocities of particles \( v_2 \):

\[
t_2 = \frac{16a}{3} \frac{\rho_2^0}{\rho_1^0} \frac{1}{|v_0 - v_2|} << t_1.
\]

### 3. Computational method

To build the finite difference scheme, we use a cubic orthogonal grid with constant step. Initially we have calculation domain size \( (X + 2) \times (Y + 2) \times (Z + 2) \) with given cell size \( L \). The internal part of the calculation region has the size \( XYZ \) and is filled with gas and solid particles with arbitrary initial conditions.

Internal part of the calculation region is surrounded by a layer of gas with arbitrary boundary conditions. We suppose that boundary cells are “infinite” – if any part of the ambient gas or gas with solid particles flow in or flow out from the cell, the thermodynamic parameters of the boundary conditions do not change. Inside of any internal cell, all thermodynamic parameters are isotropic through one time step.

Procedure of digitization of the computational domain consists of putting the space grid with constant step on this domain. In this case, for a cell, which contains elements of relief we set in the following criterion:

- If a volume filled with gas is less than one half of the total volume of the cell, we suppose that this cell completely consists of relief, otherwise we suppose that this cell is completely filled by gas or gas with admixture. In latter case, values of thermodynamic parameters for all cells are supposed to be equal to thermodynamic parameters in real range.

Calculation of all thermodynamic parameters in studied region is carried on the base of integral form of the equations, which in this case looks as follows:
\[
\begin{align*}
\rho_1 \frac{d}{dt} dydz + \rho_1 v_x dydz dt + \rho_1 v_y dydz dt + \rho_1 v_z dydz dt &= 0, \\
\rho_2 \frac{d}{dt} dydz + \rho_2 v_x dydz dt + \rho_2 v_y dydz dt + \rho_2 v_z dydz dt &= 0, \\
\rho_1 v_x dydz + (p + \rho_1 v_x^2) dydz dt + \rho_1 v_y v_x dydz dt + \rho_1 v_x v_z dydz dt &= 0, \\
\rho_1 v_y dydz + \rho_1 v_x v_y dydz dt + (p + \rho_1 v_y^2) dydz dt + \rho_1 v_y v_z dydz dt &= 0, \\
\rho_1 v_z dydz + \rho_1 v_x v_z dydz dt + \rho_1 v_y v_z dydz dt + (p + \rho_1 v_z^2) dydz dt &= 0, \\
ev dydz + (e + p)v_x dydz dt + (e + p)v_y dydz dt + (e + p)v_z dydz dt &= 0. 
\end{align*}
\]

Suppose that the integration can be implemented on any close surface in four-dimensional space \((x,y,z,t)\). We consider integrals in expressions of Eq. (3) as surface integrals of the second type, i.e., as integrals on oriented surface. Using the mean theorem we obtain the following equations:

\[
\begin{align*}
R_1^* &= R_1 + \frac{\tau}{S} (R_1^{(1)} v_x^{(1)} - R_1^{(3)} v_x^{(3)} + R_1^{(2)} v_y^{(2)} - R_1^{(4)} v_y^{(4)} + R_1^{(5)} v_z^{(5)} - R_1^{(6)} v_z^{(6)}), \\
R_2^* &= R_2 + \frac{\tau}{S} (R_2^{(1)} v_x^{(1)} - R_2^{(3)} v_x^{(3)} + R_2^{(2)} v_y^{(2)} - R_2^{(4)} v_y^{(4)} + R_2^{(5)} v_z^{(5)} - R_2^{(6)} v_z^{(6)}), \\
R_1 v_x^* &= R_1 v_x + \frac{\tau}{L} ((P^{(1)} + R_1^{(1)} v_x^{(1)}^2) - (P^{(3)} + R_1^{(3)} v_x^{(3)}^2)), \\
R_1 v_y^* &= R_1 v_y + \frac{\tau}{L} ((P^{(2)} + R_1^{(2)} v_y^{(2)}^2) - (P^{(4)} + R_1^{(4)} v_y^{(4)}^2)), \\
R_1 v_z^* &= R_1 v_z + \frac{\tau}{L} ((P^{(5)} + R_1^{(5)} v_z^{(5)}^2) - (P^{(6)} + R_1^{(6)} v_z^{(6)}^2)), \\
E^* &= E + \frac{\tau}{L} ((E^{(1)} + P^{(1)}) v_x^{(1)} - (E^{(3)} + P^{(3)}) v_x^{(3)} + (E^{(2)} + P^{(2)}) v_y^{(2)}), \\
&\quad - (E^{(4)} + P^{(4)}) v_y^{(4)} + (E^{(5)} - P^{(5)}) v_z^{(5)} - (E^{(6)} + P^{(6)}) v_z^{(6)}). 
\end{align*}
\]

The obtained formulas have simple physical meaning and they determine the stream of flowing phase and solid particles, impulse, and energy through a plane surface. In the set of equations of Eq. (4) symbols with superscripts are used to denote the values of thermodynamic parameters at corresponding sides of the cell. Symbols with asterisk denote the values of parameters inside the cells after time \(\tau\).

Starting from the initial conditions, our task consists of computing the value of all parameters inside the computational domain after a fixed time \(\tau\). Common computation scheme of the single time step, i.e., transition from the state of task on time moment \(t_0\) to the state on time moment \(t_0 + \tau\), in general consists of three parts:
• We have to compute the values of thermodynamic parameters on all sides of all cells in our computational domain, as a solution of the corresponding Riemann problem.

• It is necessary to find the maximum value of time step $\tau$, which satisfies the Courant-Friedrich-Levy condition of stability (Rogdestvenskiy and Yanenko, 1987).

• Finally, we have to compute the values of thermodynamic parameters inside all cells in our computational domain at the next time step, which guarantees the stability of computation.

To finish the description of this method, we describe an algorithm of computation of flux values. The value of hydrodynamic parameters in neighbor cells is assumed to be an initial condition for one-dimension Cauchy problem for two infinite domains of gas. The concentration of dispersion phase in each of the gases is constant during one step of time and accordingly, effective value of polytrophic constant also stays constant during a computation step of time. Thus, our task is to solve the initial discontinuity decay problem for two polytrophic gases with different polytrophic constants. This task is Cauchy problem with constant initial conditions or Riemann problem. The solution of this task is well-known (Landau and Lifshic, 1988; Kochin et al., 1963; Billett and Toro, 1997).

4. Modeling results

To illustrate the capabilities of the developed theory, we have carried out numerical computations. These model computations are directed to show main effects, described by the model. We have created a computer code, which computes the problem with any complex relief. It demonstrated strong influence of admixture on the character of flow and formation of the boundary layer due to scheme viscosity on non-homogeneous surface. The computations are carried out for two different types of obstacles and for conditions characteristic for earth winds: the wind velocity is 10 m/s, the pressure is 100 000 Pa, the density of medium and density of admixture are equal to 1.2 kg/m$^3$ and 0.01 kg/m$^3$, accordingly. In all cases, the size of the computational domain is chosen in such a way, that the number of cells within the relief or obstacles is about 10% of all cells in the computational domain. Boundary conditions are the following:

• Non-slip condition on solid surface,
• Constant values of stream on boundaries far from obstacle.
Nontrivial influence of particulates (which was taken to be SiO$_2$, i.e., sand in the experiments) has been obtained and graphically shown in the following figures of distribution of impurity and velocity field. As Figs. 1 and 2 show, in the region of particulates, there is a zone with increasing and decreasing, horizontal component of the velocity compared to the average value. This fact is explained by the influence of admixture, because admixture has an active influence on forming boundary layer. Figs. 1 and 2 show two-dimension visualization of moving steam of admixture over different kind of reliefs. Digits mean:

1. stream of particulates,
2. elements of relief,
3. wind direction,
4. domain of turbulence.

*Fig. 1.* Dynamics of the particulate cloud moving over a “crater”. Tcomp = 2, 30, 70, 150c.

*Fig. 3* shows the profiles of the $x$-component of the velocity at the different grids of computational domain near a surface. It clearly represents the gradients of wind velocity due to scheme viscosity.
Fig. 2. Dynamics of the particulate cloud moving over “mountains”. Tcomp = 1, 20, 40, 92c.

Fig. 3. Profile of the $x$-component of the velocity ($v_x$) in different layers.

5. Conclusions

At present work a three-dimension model of transport of solid particles and aerosols near a solid surface is proposed. This model is based on two main physical ideas:
• Description of two-phase atmospheric flows on the base of Nigmatulin equations (equations for perfect gases with renormalized equation of state),
• Use of the Godunov method, which has a scheme viscosity, for numerical solution of model equations.

The main advantage of our model the possibility of modeling of two-phase atmospheric flows in a range, where the vertical scale of inhomogeneousness is much higher than the horizontal scale. This is because of using initial fluid equations in integral form, and the idea of scheme viscosity provides good conditions for the stability of computations. As usual, in this case traditional modeling methods as LES and method based on Reynolds averaging face difficulties due to the modeling of turbulence in fractional grids, and these methods are still in the beginning of development. We will provide results of such computations with our method in subsequent papers. We showed, the that presence of two mechanisms of scheme viscosity in the created algorithm, namely, presence of homogeneities of surface and gradients of concentration of solid admixture, allows reproducing dynamic transport of admixture in boundary layer.

References