Numerical modelling of pollution dispersion in complex terrain

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Abstract

The aim of the presented work is to develop a mathematical model for prediction of flow and pollution dispersion in Atmospheric Boundary Layer (ABL). Three different mathematical models based on the system R²-NS equations and its simplifications are introduced and solved. Systems are completed by the transport equations for passive impurities and potential temperature. A simple turbulence closure is used. Resulting systems of governing equations are solved by explicit finite-volume or semi-implicit finite-difference schemes on structured boundary fitted mesh. Results of simple test computations are presented and discussed.

1 Introduction

The air pollution resulting from the rapid industrialization has became a serious public environmental problem. The accurate evaluation of environmental impact has received an increased attention during the past decades and is now one of the key points in further development of any industrial region. Thus it is a grave importance to have a method that is able to select an optimum site for an industrial complex to minimize the pollution impact on the neighboring areas.

There are two basic possible approaches to this problem.
The first one is the physical modelling that involves the use of geometrically scaled-down model in a wind-tunnel. However it is nearly impossible to satisfy all the similarity requirements in this case because of large scaling factors $(1/500-1/1000)$ and complexity of atmospheric conditions.

The second method is based on mathematical modelling. The classical pollution models deal with the Gaussian plume model. This methodology is simple and is widely used in the environmental engineering. However the Gaussian plume models applicability is restricted to the pollution dispersion over a flat terrain. In the case of flow over complex topography the predicted results could contain unacceptable errors. The dispersion characteristics of pollutants in complex geometries are sensitively influenced by the local flow field as well as by the thermal stability conditions. In this situation (where the analytical solution is not possible to obtain) the numerical methods of solution of models based on systems of partial differential equations seem to be a promising tool for understanding the local flow and dispersion characteristics.

There are some significant attributes of ABL modelling that urge us to develop special numerical methods for this case. We mention at this place just the most important properties:

- Anisotropic turbulence
- Large scale vorticity
- High Reynolds numbers flows
- Influence of Coriolis forces
- Thermal stratification
- Large computational domains
- High resolution requirements
- Large time-scales of changes

The most important characteristic of ABL is that the flow is turbulent. The equations that represent these turbulent characteristics are non-linear and so the mathematical difficulty in parametrizing the boundary layer lies in solving these non-linear partial differential equations.

The aim of this work is to establish a mathematical and numerical method for prediction of the atmospheric wind flow and the pollutant dispersion over complex terrain. The following steps are taken to achieve the objectives of the present investigation:

i) The proper choice of mathematical model is the key point for the further investigation. The system must be general enough to be able to fully resolve the complex terrain phenomenology but should be also relatively easy to solve.

ii) Development of numerical method and solver. In this step is necessary to chose numerical scheme that is accurate on one hand and simple, fast and easy to implement on the other hand.

iii) Validation of presented method on simple test cases where the solution can be compared with the measurements or with numerical results obtained using another method.
In the following text each of these parts will be discussed in the detail.

2 Mathematical model

2.1 Reynolds Averaged Navier-Stokes equations

2.1.1 System of governing equations

\[ \bar{R}W_t + F_x + G_y + H_z = [R_x + S_y + T_z] + \bar{f} \]  

(1)

Where \( W = (p, u, v, w)^T \), \( \bar{R} = \text{diag}(0, 1, 1, 1) \), \( \bar{f} = (0, \lambda v, -\lambda u, g)^T \)

\[ F = (u, u^2 + p, uv, uw)^T, \quad G = (v, uv, v^2 + p, vw)^T, \quad H = (w, uw, vw, w^2 + p)^T \]

\[ R = (0, Ku_x, Kv_x, Kw_x)^T, \quad S = (0, Ku_y, Kv_y, Kw_y)^T, \quad T = (0, Ku_z, Kv_z, Kw_z)^T \]

The \( \lambda \) denotes the Coriolis parameter and \( g \) is the magnitude of gravity acceleration.

2.1.2 Numerical solution

The artificial compressibility method can be used. In such a case the \( \bar{R}' = \text{diag}(\varepsilon, 1, 1, 1) \), \( \varepsilon > 0 \) stands instead of \( \bar{R} = \text{diag}(0, 1, 1, 1) \). This modified system may be solved using finite volume semidiscretisation and Runge-Kutta multistage scheme.

2.1.3 Model characterization

This is the classical concept used in many recent works. The advantage of this method is in its generality. There are no restrictions to the smoothness of the surface geometry. Just the turbulence model limitations must be respected. In the case of using the above proposed numerical method, some other problems will appear. Firstly, the explicit scheme has relatively strong time-step restrictions. From this and also from the fact that all the terms in the RA-NS equations are used (nothing is a priori neglected) follows the high consumption of computational time. The second problem follows from the artificial compressibility concept which makes this method almost unusable for unsteady flows.

2.2 Boussinesq approximation of RA-NS equations

2.2.1 System of governing equations

\[ \nabla (\rho_0 V) = 0 \]  

(2)

\[ V_t + (V \cdot \nabla)V = - \frac{\nabla p'}{\rho_0} + \frac{1}{\rho_0} \nabla[K \nabla V] + \bar{f} \]  

(3)

The vertical background pressure field gradient is given by the hydrostatic balance

\[ \frac{\partial \rho_0}{\partial z} = -\rho_0 g \]  

(4)
2.2.2 Numerical solution
There are two basic concepts of solution of the above systems:

i) Artificial compressibility method
Here the time-derivative of pressure perturbation \( p' \) is added into the continuity equation (2). The solution proceeds in two steps. Firstly the velocity components are computed from the momentum equations. Then in the second step the pressure is evaluated from the modified continuity equation. It is a time-marching method and can be used in steady cases.

ii) The method with Poisson equation for pressure
As above also in this case the first step of the numerical solution consists of evaluation of velocity field from momentum equations. The difference is in the second step where the Poisson equation for pressure is solved. This equation can be derived as a sum of corresponding partial derivatives of the momentum equations. This method is especially designed for unsteady flow solution.

2.2.3 Model characterization
The Boussinesq approximation is still very general model, which allows to do computations on many geometries without significant restrictions. The main advantage is in the proposed numerical solvers. The semi-implicit finite differencing used in both, time-marching and time-dependent method, has more favorable stability conditions. The time-step in both cases can be larger and the methods are more efficient.

2.3 Approximation of ABL equations

2.3.1 System of governing equations

\[

d_1 + v_2 + w_3 = 0 \tag{5}
\]

\[
u_1 + uu_1 + vv_1 + ww_1 = [Ku_1]_z + \lambda(v - v^g) + f_1^g \tag{6}
\]

\[
v_1 + uv_1 + vv_1 + vv_1 = [Kv_1]_z + \lambda(u - u^g) + f_2^g \tag{7}
\]

Here \( u^g, v^g \) is the velocity of geostrophic wind and \( f^g \) is a function depending on the velocity field on the upper boundary (respectively on its gradient).

2.3.2 Numerical solution
The same type of finite difference discretization and semi-implicit scheme as in the previous case can be used. The solution has also two steps. In the first step the horizontal velocity components are solved from the momentum equations and then the vertical component is determined by numerical integration of continuity equation.

2.3.3 Model characterization
The advantage of this model is in the reduction of number of equations and the amount of terms in them. Due to the absence of pressure gradient in the system, the simplified transport equations will adopt the same form as the momentum equations and can be thus solved simultaneously by the same numerical solver. Also the time step can be large enough due to the
semi-implicit discretization. The disadvantage of this model is in its restriction on smooth enough geometries. Some problems may be caused by the numerical integration, due to its inconsistency with the physical boundary conditions.

2.4 Transport equations

\[ \Theta_t + (V \cdot \nabla) \Theta = \frac{1}{\rho_0} \nabla \left[ \frac{K}{\sigma_\Theta} \nabla \Theta \right] \]  
\[ C_t^i + (V \cdot \nabla) C^i = \frac{1}{\rho_0} \nabla \left[ \frac{K}{\sigma_\Theta} \nabla C^i \right] \]

where the \( \sigma_{\Theta}, \sigma_C \) denote the turbulent prandtl's number for potential temperature and concentration.

2.5 Turbulence model

In our work we deal with the classical algebraic turbulence closure model based on the Boussinesq's hypothesis. Diffusion coefficient \( K \) is equal to sum of the molecular viscosity \( \nu \) and the turbulent viscosity \( \nu_T \).

\[ K = \nu + \nu_T \quad \text{where} \quad \nu_T = l^2 \left[ u_z^2 + v_z^2 \right]^{1/2} G \]

For the mixing length \( l \) we use the classical Blackadar's formula:

\[ l = \frac{\kappa(z + z_0)}{1 + \kappa \frac{(z + z_0)}{l_\infty}} \quad l_\infty = \frac{27 \| V_g \| 10^{-5}}{\lambda} \]

Here the parameter \( \kappa = 0.36 \div 0.41 \) is von Kármán's constant. The \( z_0 \) is roughness parameter which depends on the aerodynamic quality of the surface over which the wind flows.

The stability function \( G \) is given by:

\[ G = (1 + \beta Ri)^{-2} \quad \text{for} \quad Ri > 0 \]
\[ G = (1 - \beta Ri)^2 \quad \text{for} \quad Ri \leq 0 \]

where \( Ri \) is Richardson's number characterizing the thermal stratification of atmosphere \( \beta \) is a constant \((\approx 3)\).

3 Numerical solution of Boussinesq approximation

In order to resolve correctly the boundary layer in the near wall region it is necessary to refine the mesh in the surface-normal direction. This results into a very thin mesh cells and consequently into a very strong time-step restriction. The need to use very short time-step makes the classical explicit methods unefficient and at least difficult to use for ABL flows. One of the
possible ways how to improve the stability of numerical scheme is the use of implicit or semi-implicit discretization rather than the explicit one.

In the following text we present a simple semi-implicit finite-difference scheme for the Boussinesq approximation of RA-NS equations in the above presented form.

3.1 Numerical scheme

To simplify notation of discretized equations we introduce operators of differences. The symbol \( \delta_s \) denotes the central difference with respect to \( s \). Similarly \( \delta^+_s \) and \( \delta^-_s \) denote the forward and backward differences (See Fig.1).

\[
\delta^-_s = \frac{V_i - V_{i-1}}{\Delta s^-} \\
\delta^+_s = \frac{V_{i+1} - V_i}{\Delta s^+} \\
\delta_s = \frac{1}{2}(\delta^-_s + \delta^+_s)
\]

Figure 1: Local mesh scheme

The left-hand side of momentum equations is discretized by the following way:

\[
V_t \sim \frac{\delta^+_s V^n_{i,j,k}}{\delta t} \\
\ddot{u} V_{s_1} \sim \frac{1}{2} \left( \frac{\ddot{u}^n_{i+1/2} \delta^+_s V^n_{i,j,k} + \ddot{u}^n_{i-1/2} \delta^-_s V^n_{i,j,k} + 1}{\delta s_1} \right) \\
\ddot{u} V_{s_2} \sim \frac{1}{2} \frac{1}{2} \left( \frac{\ddot{u}^n_{j+1/2} \delta^+_s V^n_{i,j,k} + \ddot{u}^n_{j-1/2} \delta^-_s V^n_{i,j,k} + 1}{\delta s_2} \right) \\
\ddot{w} V_z \sim \frac{1}{2} \frac{1}{2} \left( \frac{\ddot{w}^n_{k+1/2} \delta^+_z V^n_{i,j,k} + \ddot{w}^n_{k-1/2} \delta^-_z V^n_{i,j,k} + 1}{\delta z_1} \right)
\]

The dissipative terms on right-hand side are approximated by a similar way. The pressure is updated from the modified continuity equation.

\[
p_t = -(u_x + v_y + w_z) \tag{13}
\]
In order to improve the convergency of this method for high Reynolds numbers we add the artificial viscosity terms $DV_{i,j,k}^n$.

3.2 Artificial viscosity terms

This additional terms are especially designed to suppress high frequency numerical oscillations in computational field. For both schemes the combination of artificial dissipation of second and fourth order is used.

$$DW_i^n = D^2W_{i}^n + D^4W_{i}^n$$

$$D^2W_i^n = \tilde{\varepsilon}_2 \Delta x^3 \frac{\partial}{\partial x} |W_x|W_x$$

$$= \tilde{\varepsilon}_2 \Delta x^2 (\varepsilon_{i+1/2} W_x - \varepsilon_{i-1/2} W_x)$$

$$\varepsilon_{i+1/2} = \begin{cases} |W_{i+1} - W_i| & \text{for } |W_{i+1} - W_i| < \frac{K}{10} \\ \frac{K}{10} & \text{for } |W_{i+1} - W_i| \geq \frac{K}{10} \end{cases}$$

$$D^4W_i^n = \tilde{\varepsilon}_4 \Delta x^4 W_{xxx}$$

$$= \tilde{\varepsilon}_4 (W_{i+2} - 4W_{i+1} + 6W_i - 4W_{i+1} + W_{i+2})$$

Symbol $W$ denotes here the vector of state variables including also the concentration and potential temperature. The $K = \nu + \nu_t$ is coefficient of turbulent diffusion. The coefficients $\tilde{\varepsilon}_2, \tilde{\varepsilon}_4 \in R$ are constants of order $\Delta x^2$ respectively $\Delta x^4$.

4 Numerical tests, results

4.1 Computational domain

Domain $\Omega \subset \mathbb{R}^3 : \Omega \equiv \Omega_b \setminus \Omega_g$ where $\Omega_b \equiv \{[0, a] \times [0, b] \times [0, c]\}$ $a, b, c \in \mathbb{R}^+$ and $\Omega_g$ is the space under the graph of function $g : ([0, a] \times [0, b]) \to \mathbb{R}$, which describes the surface of the earth.

For numerical tests we used domain with the "Single hill" ground profile. The hill has a sinusoidal shape. The dimensions of computational domain are $a = 4000 m$, $b = 2000 m$, $c = 1000 m$.

For this test case we used a structured body-fitted mesh $80 \times 40 \times 40$ points.

4.2 Boundary conditions

The following boundary conditions were used:

(a) $x = 0 \ldots u = "power law" \ a = 1/7", \ v = 0.0, \ w = 0.0, \ p' = 0.0$

(b) $z = g(x, y) \ldots u = 0.0, \ v = 0.0, \ w = 0.0, \ \frac{\partial p'}{\partial n} = 0$

(c) $x = a \ldots (u, v, w, p')_x = 0$.

(d) $z = c \ldots V = V^g, \ V^g = (1.0, 0.0, 0.0)^T$

(e) $y = 0, \ y = b \ldots \text{Periodic boundary conditions for } u, v, w, p'$
4.3 Numerical results

The flow structure in complex terrain may be very complicated. A massive flow separation appear behind the hills with high slopes. The three-dimensionality of flow over 3D-hill is shown at Fig.2. The streamlines are drown at the low level approx. $z=20\text{m}$.

![Figure 2: Streamlines at the near-ground level](image)

The influence of terrain profile on the flow and corresponding ground-level concentration distribution is demonstrated on Fig.3 and Fig.4.

![Figure 3: Ground-level concentration from point source on flat plate](image)

![Figure 4: Ground-level concentration from point source on 3D hill](image)
Also the vertical concentration profiles differ due to the topography as shown at Fig.5 and Fig.6.

![Figure 5: Concentration distribution in \( x - z \) section. Flow over flat plate.](image1)

![Figure 6: Concentration distribution in \( x - z \) section. Flow over 3D hill.](image2)

The importance of 3D modelling is demonstrated on the Fig.7 and 8. In 2D case the separation is much larger then in the 3D. In both cases the vortices behind the hill are well resolved. The basic characteristics of the separation region is the position of reattachment point. This position is measured from the top of the hill. In our 2D test case the reattachment point has position \( x_R = 5.3h \) where the \( h \) is the height of the hill. The experimental measurement data are available for this case. In [5] the measured position is given for this case \( x_R = 5.25 \pm 0.5h \). It means the agreement with experiment seems to be quite good.

![Figure 7: Streamlines behind 2D and 3D hill](image3)

![Figure 8: Velocity vectors behind 2D and 3D hill](image4)
5 Conclusions, remarks

The numerical experiments showed the efficiency and robustness of the presented solver. In the case for which the with experimental data are available an excellent agreement was achieved. Also in other test computations the results seems to be realistic.

In the framework of this project was developed full software package for solution of pollution dispersion in ABL. This numerical software includes mesh generation, discretization and solution of governing system and finally also includes the visualization layouts. The solver is simple, fast and robust enough for general use in environmental engineering.

To achieve more realistic results will be necessary to determine more precisely the boundary conditions. Also the turbulence modelling can be improved using the k-ε or LES techniques. Some complications will be also connected with the use of real hilly surface profiles, where the surface must be carefully approximated. This will be the subject of future development.

Acknowledgements

The financial support for the present project is partly provided by the Czech Grant Agency under the Grant No.101/98/K001, Grant No.205/01/1120, Grant No.201/99/0267 and by the COST Grant No. OC 715.70 and Research plan MSM 210 000 003. Joint work between universities of Prague and Toulon has been made possible by the PhD program "Mathematiques Numeriques et Environnement" of the French Ministry of Education.

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