High-resolution simulation of particle transport in the urban atmospheric boundary layer

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Abstract. This paper presents a model simulating the transport of particles of various sizes and masses in complex atmospheric boundary layer domains over urban areas by using a Lagrangian approach. The model takes input fields of air velocity and turbulence characteristics from various external RANS, LES, or DNS models (in this study, ENVI-met model is used), and includes a parameterization of subgrid stochastic velocity fluctuations. It allows us to estimate the movement of particles, their sedimentation, accumulation on the surface, and the variability of these processes depending on meteorological conditions. The results of test numerical experiments for aerosol transport over an idealized urban canopy are presented. The model has shown a good degree of qualitative conformity with the ENVI-met model.

1. Introduction

Air is a crucial resource of human life with a complex gas composition. It contains a multitude of different suspended particles, whose influence on people and nature is of great importance. In pristine nature, the phenomenon of particle transport rarely poses a serious danger to humans or ecosystems. In contrast, urban environment is a significant source of technogenic emissions, including various solid and liquid particles that are involved in the airflow and often have a stronger (compared to natural particles) negative impact on human, animal, and plant health.

Spatial heterogeneity of emission sources and complex geometry of the urban surface greatly complicate the process of particle transport. Thus, it can lead to overall high concentrations and the accumulation of particles in limited areas [1]. In the urban environment, both anthropogenic and natural aerosols are present and, therefore, the atmospheric transport becomes intricate for natural particles (plant pollen, snow, water drops, dust, and others) as well. Also, burning of various substances and the release of harmful combustion products into the atmosphere are typical for industrial areas and landfills. Under high wind speed conditions, the emission rate of heavy particles, such as sand, soil particles, and road dust, can significantly increase. The capabilities of modern measurement techniques to provide the spatiotemporal pattern of aerosols in an urban atmospheric boundary layer are limited because of high variability of particle concentrations on all scales. Therefore, the direct influence of the particle transfer in large cities on human health and the environment motivates the development of computational tools for modeling and, ultimately, forecasting the air quality determined by the aerosol content.
Due to the present-day fast increase of computer performance, the spatial and temporal resolution of hydrodynamic models of atmosphere steadily improves. However, the available microscale models of particle transport do not always allow one to adequately reproduce the transfer in the atmosphere of the entire diversity of particles characterized by different shapes, sizes, masses, and chemical compositions, since only a limited number of aerosol parameters are typically taken into account. It limits the possibilities of these models for studying the transport and deposition of particles. Also, computational modules implementing the transport of various pollutants which are integrated in complex microclimatic or meteorological models are linked to a specific software product and, hence, inherit possible limitations of the mathematical formulation and programming technologies chosen by the code developers. Most of such modules follow the Eulerian approach – disabling the possibility of tracking trajectories of individual particles, whereas the latter provides useful information in many studies. Taking into account the above, this work is aimed at developing a new Lagrangian model for the motion of particles in geophysical media, especially in the urban atmospheric boundary layer, with different options to parameterize turbulence, microscale physical and chemical processes. This paper presents first results of the model development.

2. Model description

2.1. Governing equations

In this model, the movement of particles and their interaction with the surrounding medium is described on the basis of known axioms and laws of physics using semi-empirical parameterizations.

The simplest concept to represent a particle suspended in the air is a material point. The mathematical formulation of how a material point or body moves in the three-dimensional space is the equation of motion, which describes the dependence of the spatial coordinates of a point on time:

$$\mathbf{r}(t) = x(t)\mathbf{e}_x + y(t)\mathbf{e}_y + z(t)\mathbf{e}_z,$$

where $\mathbf{r}$ is the material point position, $t$ is the time, $x$, $y$, $z$ are the Cartesian coordinates, and $\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$ are unit basis vectors.

The equation of motion for particles suspended in the air and affected by the buoyancy and air resistance forces is as follows:

$$\frac{d\mathbf{u}_p}{dt} = \mathbf{g}(\rho_p - \rho)/\rho_p + F_D(\mathbf{u} - \mathbf{u}_p),$$

where $\mathbf{u}_p = d\mathbf{r}/dt$ is the particle velocity, $\mathbf{g}$ is the gravitational acceleration, $\rho_p$ is the particle density, $\rho$ is the density of air (or other medium), $F_D$ is the drag coefficient, and $\mathbf{u}$ is the ambient flow velocity.

The drag coefficient $F_D$ is given by the following expression [2]:

$$F_D = \frac{3\mu C_D Re}{4\rho_p d_p^2},$$

where $\mu$ is the dynamic air viscosity, $C_D$ is the drag coefficient, $Re$ is the Reynolds number for a particle, and $d_p$ is the particle diameter.

Usually the Stokes law is used instead of this formula, but it does not take into account the flow turbulence. In the lower troposphere at the microscale level the influence of turbulence becomes very important. Hence, in equation (3) the Reynolds number accounts for the turbulence created by the particle motion relative to the ambient flow:

$$Re \equiv \frac{\rho d_p |\mathbf{u}_p - \mathbf{u}|}{\mu}.$$

To calculate the drag coefficient $C_D$, different methods are used depending on the shape of particles. In our model, particles are assumed to be spherical, and formulas from [3] are used:

$$C_D = a_1 + \frac{a_2}{Re} + \frac{a_3}{Re^2},$$

where $a_1$, $a_2$, $a_3$ are the empirical coefficients depending on the range of Reynolds numbers.

Various explicit and implicit finite-difference schemes are available for approximate solution of differential equations. In this model, to solve the equation of particle motion (2), an explicit 4-order Runge-Kutta method is used, which is chosen for high accuracy and ease of implementation.
2.2. Model structure and operation scheme

The model is implemented in a limited three-dimensional area with a given boundary geometry and continuous medium characteristics. The model computes the motion of an arbitrary number of particles, tracking the trajectory of each particle, diagnosing the particle concentrations and the surface deposition rate. The model code is implemented in C++.

The dynamic and thermodynamic properties of the air are assumed to be stationary and are read from the input file. The influence of the transported particles on the characteristics of the medium is taken negligibly small in comparison with the influence of external factors, the initial and boundary conditions.

The model algorithm is a sequence of iterations limited by a given modeling period. At each iteration, a cycle of logical blocks takes place, and each of them is responsible for a certain function. The first step in the algorithm chain is the reading of the input data and the initialization of the computational domain. Then the particle characteristics are calculated during the simulation period in a time-stepping cycle and, in the end, the results are written in files for subsequent analysis and visualization.

Input data (stationary air velocity field, turbulence properties) are assigned to the computational grid nodes. The last one is attached to the Cartesian coordinate system. Trilinear interpolation is used to calculate medium’s parameters at the current location of each particle.

The domain boundary conditions for the particles in the model are realized as follows. When there is no solid surface at the boundary, the periodic conditions or transparent boundary conditions are applied. The interactions of particles with solid surfaces are divided into two types: deposition and elastic rebound (the velocity component normal to the boundary reverses the sign after the interaction) – the type of interaction can be set for each solid surface.

2.3. Parameterization of turbulent velocity fluctuations

In turbulent flows of fluid or gas the velocity may be represented as the sum of the averaged and fluctuation components:

\[ \mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}' , \]

where \( \mathbf{u} \) is the flow velocity, \( \bar{\mathbf{u}} \) is the averaged flow velocity, and \( \mathbf{u}' \) is the fluctuation component of the flow velocity.

The averaged velocity in the model depends only on the spatial coordinates and is taken from the input data. The velocity fluctuation characterizes the effects of subgrid turbulent vortices and depends on both the coordinates and time. Since these vortices are not resolved explicitly, various parameterizations can be used to take into account their influence.

Two different parameterizations are realized in the model. In the first one (hereafter referred to as “simple parameterization”), the fluctuation component is a Gaussian random variable generated at each time step along a particle trajectory. Its mean value is zero, and the standard deviation is calculated as follows:

\[ \sigma = \sqrt{2k/\epsilon} , \]

where \( \sigma \) is the standard deviation, \( k \) is the turbulent kinetic energy, and \( \epsilon \) is the turbulent kinetic energy dissipation rate.

The second option to parameterize turbulence implemented in this work is a discrete random walk (DRW) model [4]. In this method, the fluctuation component is the Gaussian random variable, too; it has zero mean, and equation (7) is employed for the standard deviation, but the new value of this variable is not generated at each time step. The time of interaction of a particle with a turbulent eddy is introduced, during which the fluctuation component acting on the particle is considered constant. This time is calculated by the following equation:

\[ t_{\text{int}} = \min (t_e, t_R) , \]

where \( t_{\text{int}} \) is the time of interaction of a particle with an eddy, \( t_e \) is the eddy lifetime, and \( t_R \) is the time for the particle to cross the eddy (transit time scale).

The eddy lifetime \( t_e \) is estimated as follows:
where \( l_e \) is the characteristic size of a randomly sampled vortex, which is assumed as the dissipation length scale given in [4].

The transit time scale \( t_R \) is estimated by the following expression:

\[
t_R = -\tau \ln \left( 1 - \frac{l_e}{(\tau |u - u_p|)} \right),
\]

(10)

where \( \tau \) is the droplet “relaxation” time defined in [4].

The parameterizations described above require accurate turbulent flow characteristics. Recent studies show that sufficient accuracy of such data for the particle transport problem is provided only by large eddy simulation (LES) models and direct numerical simulation (DNS) [5]. Therefore, careful analysis of the results is required if using this model with the input data obtained from Reynolds-averaged Navier-Stokes (RANS) models.

3. Results

The model has been tested in a number of idealized experiments, including a circular flow with a known analytical solution for trajectories, with the presence and absence of turbulence. In what follows we present the results of a particle transport simulation in a two-dimensional urban canyon.

To provide the Lagrangian model with external data on wind velocity, turbulent kinetic energy and dissipation rate, ENVI-met, a holistic microclimate modelling system [6] was used. Inter alia, this system includes a block for particle concentration transport, which uses the Eulerian approach [7].

The developed Lagrangian model showed qualitative agreement with the ENVI_MET Eulerian model in terms of concentrations and sedimentation rates in experiments with a flat surface, a single point source of particles, and a steady unidirectional wind.

For 2D modeling of the particle transport in an urban canyon, the inflow wind speed was set in the ENVI-met by a logarithmic profile with 5 m/s at 10 m and directed perpendicular to a set of parallel canyons. The atmosphere stratification was set neutral. Six buildings 30 meters high and 18 meters wide were placed in the domain. All buildings were separated by intervals of 30 meters, which formed five consecutive identical city canyons with an aspect ratio of 1. A point source was placed inside the second downwind canyon to simulate the automobile emissions and study the quality of ventilation of the canyon with this aspect ratio and perpendicular flow velocity. All particles had a diameter of 2.5 \( \mu \)m and a density of 1000 kg/m\(^3\). The simulation period was set to 600 seconds.

The results of the simulations show (Figure 1.a and 1.b) that most of the particles emitted into the air remain in the source canyon, and maximum concentrations are observed there. The model also shows that a small part of the particles rises above the canyon and spreads further, flowing and settling in the downwind canyons. The ability of the particles to enter downwind canyons is also found when using more accurate large eddy simulation models [8]. The developed Lagrangian model with simple parameterization of turbulence demonstrates (Figure 1.a) the capture of particles by a large vortex inside the canyon and their uneven rise to the roof level. The more advanced DRW method shows (Figure 1.b) an uneven distribution of the concentrations within the canyon. In addition, the plume is wider when using this stochastic parameterization, because of longer influence of each generated speed fluctuation on the particle, which seems more realistic in specified conditions. However, the advanced method is more sensitive to input data on turbulence characteristics and, therefore, it may not be applicable in some cases due to the suppression of other effects by turbulence. This indicates the sensitivity of the model to the turbulence parameterization being used and the need to explore this aspect of Lagrangian modelling more.
Figure 1. Particle concentrations calculated by Lagrangian model using two turbulence (stochastic) parameterizations: a) simple parameterization; b) discrete random walk model.

4. Conclusions
This work presents first steps in the development of a Lagrangian model of particle advection in the urban atmospheric boundary layer with the possibility of receiving fields of hydrodynamic and thermodynamic variables from various possible sources (RANS, LES, DNS models) and simulating aerosols in a wide range of physical and chemical properties.

The model has been tested in a number of idealized flow cases with input data from the ENVI-met model. The results of modeling and comparison showed a high degree of conformity between the above-developed technology and the ENVI-met model. Two parameterizations of subgrid turbulent (stochastic) velocity fluctuations were introduced, and simulations of aerosol transport in a 2D domain over a sequence of parallel canyons demonstrated the sensitivity of model results to the choice of stochastic parameterization.

Further steps in the development of the Lagrangian model will be in coupling to a RANS urban boundary layer model parallelized for supercomputers in order to run simulations in larger domains and in wider ranges of boundary layer parameters and surface geometries. Another direction of the model improvement is more accurate accounting for the physical properties of specific classes of particles, both natural and anthropogenic, e.g. their shape and size distributions.

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