A three-dimensional numerical model of air pollutant dispersion

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Abstract

The authors propose a model of air pollutant dispersion over Lodz, the city located in Central Poland. In a 3D calculation domain, topographic features were differentiated using an available digital map. Having a topographic map, sub-areas of similar average building heights were selected which allowed the authors to refer to changes in the character of the buildings. Main traffic roads constituting ventilating ducts for the city were specified in the urbanised area. In the calculation process, Navier-Stokes equations and a continuity equation were integrated which enabled determination of an airflow velocity field. Next, the equation for pollutant transport was solved to obtain continuous concentration fields and their evolution in time. In the calculations the finite element method was applied. The model operation was presented using, as an example, the hypothetical point emissions of hazardous substances.

The evolution of air pollutant concentration fields can be observed for different meteorological conditions including the strength and direction of air mass flow over the tested area. Moreover, the tested pollutants can get into the environment in any point in the city either from point or surface sources. The proposed model can be used in the testing of the concentration fields of typical urban pollutants, provided the measuring data relevant to the position and intensity of emissions are available. The above method can also be applied in the case of accidental releases that can be a result of terrorist attacks, for example.

Keywords: air pollutant dispersion, urban air quality, finite element method.

1 Introduction

A feature of the climate in big cities is a poor state of the atmosphere which is a result of developed road transport, industrial activities and fulfilment of
inhabitants needs. Consequently, a big number of people are exposed to pollutants and their negative effects are accumulated (Mayer [1]). Above average concentrations may be hazardous for health, and sometimes even for life. Therefore, in the management of an urban environment quality, a significant role is played by the diagnostic and predictive models of aero-sanitary conditions. In order to describe the concentration field in urbanised areas it is necessary to have a big number of measuring points because of significant changes of concentrations in time and space on a relatively small area. However, in many regions the air quality monitoring network does not exist or is insufficient.

An alternative seems to be the assessment of concentrations made on the basis of numerical modelling. A mathematical description enables estimation of the existing state, and additionally allows us to predict effects of possible air pollutant concentration fields. It can also be used to predict hazards induced by serious accidental emissions. Numerical models are applicable in the case of big cities, however due to specificity of urbanised areas, it is a complicated task to construct them. The concentration field formation is determined by various factors, e.g. characteristic features of emission sources, elevation of emission points, topographic features, and finally the type and amount of emitted pollutants. Important is also the structure of residential housing and streets. Additionally, meteorological conditions and air circulation are also significant (Kaminski and Skrzypski [2]). Lower layers of the atmosphere are characterised by significant dynamics and nonlinearity of the processes that occur there.

In this study, a model of pollutant dispersion in the lower air layers over Lodz, a city in Central Poland, is presented.

2 Calculation domain of the model

Processes occurring in the atmosphere can be modelled using deterministic and empirical mathematical models. Solution of equations that describe processes occurring in the lower layer of atmosphere requires numerical methods. Due to the reference system in which the occurring phenomena are described, the models can be divided into Euler type models and Lagrange type models (Zanetti [3]).

A mathematical, deterministic model of pollutant dispersion in the air is discussed in the paper. This is an Euler type model which uses the finite element method (FEM). FEM is the method of computer-aided solution of differential equation systems that describe the law of mass, momentum and energy conservation. This is an universal technique which enables simulation of real systems with complex geometry (Zienkiewicz and Taylor [4]). It enables application of the three-dimensional network of the calculation domain, which takes into account the layout of the land resulting from topography and character of buildings over the tested area, and also specification of main arterial roads. The specified elements have a significant effect on the dispersion of air pollutants, and taking them into consideration makes the model closer to reality and allows to avoid simplifying assumptions.
2.1 Average height of buildings

Boundaries of the area considered in the model were imposed by the range of the available digital map that contained the coordinates of natural layout of the land in Lodz and its neighbourhood. On this area, basing on a topographic map, sub-regions of a similar character and building heights were marked. They are shown in Figure 1. This approach is simplified as compared to reality. It would be ideal to take particular buildings into account in the building structure on the basis of
the information taken for instance from aerial photographs. However, it is worth noting that the calculation domain would be then very complicated. A problem would be overlapping of boundary and initial conditions in the case of simulated situations. Additionally, enormous processor capacity would be necessary which would undermine universal character of the model and its applicability in practice. The proposed approach is a compromise and allows to take into account the features of building structure that are most important for the urbanised region.

The sub-regions were coupled to three levels of average building height as shown in Figure 2. This procedure enabled determination of faults resulting from changes in the building type, e.g. between modern housing estates (25 m) and compact residential housing in the form of apartment houses in the city centre (12 m). In the sub-regions with scattered housing, which were mainly green areas or arable lands, the height equal to 0 m was assumed. The faults were obstacles for the advection and they affected the wind field on the urban area.

2.2 Main arterial roads

Sub-regions with a uniform building character were identified taking into consideration most important traffic roads that constitute ventilation ducts for the city (Kaminski and Skrzypski [2]).

![Arterial roads](image)

Figure 3: Arterial roads (main ventilation ducts; streets that have lesser importance for city ventilation; ventilation ducts of a relatively lowest importance).

Roads situated in the built-up area were distinguished because only then they fulfilled ventilating functions. To better represent a complicated character of the arterial roads in an urbanised area, they were divided in view of their type (railroad, street) and width (e.g. one- or two-lane street). As a result, three types
of ducts were classified for airflow induced by natural winds, which are of different importance for Lodz ventilation. Figure 3 illustrates this system.

In the calculation domain, the arterial roads were taken as lines on the building surface, which is a simplification assumed in the model. Pollutant dispersion in real street canyons is modelled by smaller scale models. In the described case, an object of interest is the evolution of ambient pollutant concentration fields in the entire city. Introduction of canyons would not cause big changes in the shape of the simulated air pollutant concentration fields, but it would greatly increase calculation costs and make the calculation network geometry very complicated.

2.3 Natural layout of the surface

The space of calculation domain was filled with a net of hexagonal elements according to the FEM principles. The altitude 160 m from the ground surface, i.e. 135 m from the level of the tallest building, was considered. All nodes of the calculation network were given real altitudes above sea level on the basis of the digital map. Due to the fact that the digital map contained over 2 million points and the calculation network included almost 20 thousand nodes, this operation was made automatically. A program written specially for this purpose in Fortran was used. In this way the calculation domain geometry was proposed as shown in Fig. 4, which was a starting point in further operations. Owing to multiplication of the vertical dimension in Fig. 4, it was possible to follow topographic features of the tested area. It could be observed that the highest ground elevations are in northeast part of the city which results mainly from the natural configuration of the surface and to a lesser extent from building structure.

![Figure 4: Calculation domain mesh (vertical dimension extended for better visualisation).](image)

2.4 Mass balance

To solve equations of mass, energy and momentum conservation in three-dimensions, it is required to determine relevant boundary conditions that ensure
conservation of the mass of airflow within the calculation domain. To fulfil this condition, a procedure enforcing zero velocity components in the direction normal to the faults resulting from difference in the height of neighbouring buildings was placed in the solver code. Additionally, on surfaces delimiting the calculation domain from the bottom, typical Dirichlet boundary conditions, in the form of zero velocities for all three directions were defined. Lines corresponding to arterial roads, which were assumed to constitute ventilation ducts for the city, required a separate approach. On these lines a zero velocity component was forced in the vertical direction, assuming at the same time a free flow in horizontal directions. If a communication route is on the border of the change in the neighbouring buildings, then an additional fault is taken into account.

Due to the fact that in the model only the altitude of 160 m from the ground level was considered, on surfaces limiting the calculation domain from the top a condition of zero velocity in the vertical direction was imposed. It is also possible to use different boundary conditions, for example taken from mesoscale models. A solution may be offered by the use of a vertical wind component, taken from numerical mesoscale predictive models such as e.g. MM5.

2.5 The assumed correction factors

Geometry of the calculation domain contains simplifications concerning the construction described earlier. An immediate solution of mass transfer and balance equations would lead to erroneous results. In fact, there are no uniform faults in the character of a built-up area and arterial roads are the real ducts in its structure. Factors correcting velocities of airflow were introduced in the above fragments of the calculation network. They were estimated on the basis of multiple simulations and are universal for the model.

Additionally, by analogy to the flow of fluids in porous bodies, a resistance on the building-air interface was introduced. It was assumed to be proportional to the coefficients attributed to each category of the arterial roads. Coefficients for particular classes of the arterial roads depended on the duct width. Their values are described by 7:3:1 ratio. The highest value corresponding to the highest interfacial resistance refers to the arterial roads of the least importance for the ventilation of Lodz, which at the same time are the narrowest ones.

3 Mathematical basis of the model

In numerical calculations our own software written in Fortran was applied. Access to the software code allowed us to implement many elements which made the model closer to reality. The calculation process consisted of two main stages.

First, both Navier-Stokes equations, eqn (1), and continuity equation, eqn (2), were integrated under the assumption of liquid incompressibility. The equations of motion referred to three directions because a three-dimensional calculation domain was used.
\[
\rho \left( \frac{\partial u}{\partial t} + \nabla u \cdot u \right) = \rho g - \nabla p + \nabla \cdot \left[ \mu (\nabla u + (\nabla u)^T) \right].
\]

(1)

\[
\nabla \cdot u = 0.
\]

(2)

It is possible to calculate in the model a turbulent viscosity determined by the kinetic energy of fluctuation velocities according to Prandtl-Kolmogorov concept. Literature data show that the K-model is sufficient for geophysical applications requires low calculation cost, and quality of results is comparable to more complicated relations, e.g. k-ε Axell and Liungman [5]. However, the simulations revealed that the values of velocity vectors were overestimated using this model of turbulence. This follows probably from the algebraic form of the applied scale of turbulence proportional to the distance from building walls. Presumably, simplifications related to the sub-regions with similar building heights and streets in the model network are also significant. Therefore, turbulent viscosity was not taken into account in the calculations. Velocity fields obtained from the solution of eqn (1) and eqn (2) determine the process of pollutant transport due to advection and diffusion in lower layers of the atmosphere.

At the second calculation stage, using the previously determined velocity field, the equation of pollutant dispersion, eqn (3), was solved. To solve eqn (3), original Lagrange’s approach was used in transport analysis Petera et al. [6], according to which substance concentration in liquid element in motion is the function of time, eqn (4). As a result, continuous concentration fields and their evolution in time were obtained.

\[
\frac{Dc}{Dt} = \nabla \cdot \left[ (D + D') \nabla c \right] + \Delta.
\]

(3)

\[
c = c[x(t), y(t), z(t), t].
\]

(4)

where: \(D=\begin{bmatrix} D_x & 0 & 0 \\ 0 & D_y & 0 \\ 0 & 0 & D_z \end{bmatrix}\) – dispersion coefficients [m²/s], \(\Delta\) – pollutant release rate [kg/s].

4 Simulation of a hypothetical accidental release

The model operation was presented taking as an example a hypothetical random release of a hazardous substance. It was assumed in the scenario that emissions took place simultaneously in two points in the city of Lodz. They were localised at the ground level, at the crossing of main streets in the city of Lodz (Fig. 6, point 1) and in the industrial district (Fig. 6, point 2). The shape of released substance concentration field in the atmosphere was tested in four hours since the event. It was assumed that pollutants got to the environment at the constant rate of 0.2 kg/s during the first two hours of the period considered. In the simulation, southeast wind of velocity 4 m/s was assumed. Due to the lack of data concerning wind profile, this information was used as the boundary condition - advection.
4.1 Results and analysis

When analysing the results, a remarkable effect of anthropogenic obstacles on the released substance dispersion was observed. Changes in the type of buildings and arterial roads have also an important influence on the shape of simulated velocity fields of flowing air masses (Fig. 5).

![Figure 5: Wind field: a) view from top, b) field from the bottom of a calculation domain.](image)

Communication routes constitute ducts for airflow that improve ventilation of the city. On the other hand, they cause a more intensive penetration of pollutants into the regions of a relatively compact development. It was found that division of the main communication routes into categories had no effect on the shape of simulated fields of ambient air pollutant concentration, but it was important for the obtained wind fields. In reference Kaminski et al. [7], it was proved that the natural layout of the land differentiated directions of the obtained velocity vectors. Consequently, the substance is better dispersed in the lower layers of the atmosphere.

The model can also be applied in surface emission sources. In earlier investigations an attempt was made to predict daily average particulate matter concentration fields. As a surface source the area with old apartment houses equipped with coal-burning stoves contributing to high concentrations of this pollutant in winter was selected. Measurements of daily average particulate matter concentration from 23 stations operating in the past in the city and data available from Lodz meteorological station were used in the research. As an initial condition the ambient air pollutant concentration field over the city was used. It was obtained using an interpolation procedure that applied biharmonic spline curves (Sandwell [8]). However, results were not satisfying. A problem was an insufficient information on meteorological conditions changing over the day and lack of the record of low power-plant emission sources and vehicle exhaust emissions.
Figure 6: Evolution of released substance concentration fields in time. Emissions take place in points 1 and 2 marked by an asterisk, $[\mu g/m^3]$. 

5 Conclusions

This research justified the use of complicated three-dimensional calculation domain in the investigation of evolution of ambient air pollutant concentration fields over an urbanised area. The proposed model takes into account topography, three types of arterial roads classified according to their type and width and faults caused by changes in the type of housing. All these elements have influence on the shape of simulated wind fields and evolution of air pollutant concentration fields in time.

The proposed model enables prediction of the dispersion of air pollutants penetrating the environment in any place in Lodz, either from point or surface sources. The method can be useful in the case when places and size of emissions are known, e.g. during accidental release in the city. The results are helpful in indicating the regions that are especially exposed to the impacts and can be taken into account in planning rescue actions.

At the present stage it is possible to make simulations for different directions and velocities of air masses flowing over the tested area. Isothermal
conditions can be considered at any average ambient temperature and under the assumption that the tested substance is not a subject of chemical reactions. To make results of the simulations reliable, it is necessary to use the data on changes in the direction and velocity of flowing air masses in time and with altitude. Then, the presented mathematical model will become a universal tool for modelling pollutant concentration fields over Lodz. The method can be applied also in other cities, provided relevant information on topography and urban system of the area is available.

References