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Urban air pollution modeling: a critical review

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Industrial and transport emissions are the main sources of air pollution in large cities, causing significant risks to human health. Minimizing risks requires information on the distribution and physico-chemical characteristics of emissions. Spatial and temporal detailed data are required because the intensity and composition of emissions varies greatly with time of day and local variations in wind, traffic composition and flow. There are modern mathematical models that simulate the behavior of emissions from industrial plants and traffic flows with a high degree of resolution. The chemistry of the simulated emissions has also been largely resolved by taking into account photochemical reactions as well as dry and wet deposition processes. This review presents concepts of urban air pollution monitoring, and analyses and summarizes new insights of real-time air pollutants concentrations. This research is expected to open a door for creating smart cities and digital twins for effective management of environmental risks in an urbanized area. The reviewed studies were classified by various modeling approaches such as statistical and analytical models which give the best prediction results. We find that air pollution monitoring and assessment techniques for calculating air concentrations were successfully used to study temporal and spatial changes in pollutant concentrations. In the same time, it is impossible to create a universal analytical model for predicting the concentrations of pollutants anywhere and for any condition. The outcome of this study will help engineers and researchers develop air pollution forecasts concept.

Keywords: mathematical models, air pollution, types of pollutants, environmental monitoring methods, air quality.

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Моделирование загрязнения воздуха в городской среде: критический обзор

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Промышленность и автотранспорт являются основными источниками загрязнения воздуха в крупных городах, вызывая значительные риски для здоровья человека. Минимизация рисков требует информации о распределении и физико-химических характеристиках выбросов. Требуются подробные пространственные и временные данные, поскольку интенсивность и состав выбросов сильно варьируются в зависимости от времени суток и местных изменений состава движения и потока ветра. Существуют современные математические модели, моделирующие поведение выбросов промышленных предприятий и транспорта с высокой степенью разрешения. Химический состав смоделированных выбросов также в значительной степени решён за счёт учёта фотохимических реакций, а также процессов сухого и влажного осаждения. В обзоре представлены концепции мониторинга загрязнения воздуха в городах, а также проанализированы и обобщены новые данные о концентрациях загрязнителей воздуха, полученные в режиме реального времени. Ожидается, что это исследование откроет дверь для создания умных городов и цифровых двойников для эффективного управления экологическими рисками в урбанизированной зоне. Проанализированные научные работы были классифицированы на основании различных подходов к моделированию, таких как статистические и аналитические модели, дающие наилучшие результаты прогнозирования. Отмечено, что расчётные методы оценки и мониторинга концентрации загрязняющих веществ в атмосферном воздухе могут успешно использоваться для выявления пространственных и временных закономерностей динамики загрязнения городской атмосферы. В то же время невозможно создать универсальную аналитическую модель для прогнозирования концентраций загрязняющих веществ в любом месте и для любых условий. Результаты этого исследования помогут инженерам и исследователям разработать концепцию прогнозов загрязнения воздуха.

Ключевые слова: математические модели, загрязнение воздуха, типы загрязняющих веществ, методы экологического мониторинга, качество воздуха.

The state of the surface layer of atmospheric air is of great importance for the flora and fauna, as well as for human health [1]. The deteriorating air quality in large cities is of particular concern. Changes in the chemical and aerosol composition of urban air occur due to anthropogenic impact: emissions from industrial enterprises and exhaust gases from vehicles. Air quality monitoring in an urban environment can be estimated from air monitoring stations. However, these point measurements may be insufficient due to their low spatial representativeness. To monitor and predict the ecological state of the city atmosphere, along with instrumental studies, methods of mathematical modeling can be successfully applied.

This review was prompted by the need to better understand the main sources of air pollution in large cities, especially at the scale of individual streets. This is true for typical Russian large cities, which are characterized by the location of large industrial enterprises in close proximity to residential buildings, as well as increased traffic density, for which the existing highways were not designed. Though in many large cities there is a state air monitoring network, but it is not sufficiently well distributed. Another serious problem is the inability to determine the source of pollution leading to exceeding the maximum permissible concentration (MPC). For example, Chelyabinsk showed heavy air pollution, having about 30% of pollution days in the whole year when there are the excesses of the established MPCs of air pollutants [2]. The sources of pollution are not always clear, but it is very important to know them for making decisions to reduce the amount of days. One solution could be to expand the monitoring network by using low cost wireless sensors for real-time air quality monitoring system [3, 4]. But currently there are only very few pollutants that can be measured well without expensive equipment [5]. In most cases, complex and expensive physicochemical methods of analysis are required. Therefore, modern scientific modeling of emissions from industrial plants and vehicles makes it possible to assess air pollution in real time [5]. Air pollution models make it possible to predict the situation through the implementation of a scenario approach saving the considerable expense of monitoring equipment [6].

The aim of the present review was to focus on the state of the science of modelling air pollutant concentration from a large number of sources in the urban environments.

Statistical air pollution models

The mathematical models can be generally classified into statistical and analytical. Statistical models are a simplified mathematical representation of the process leading to the generation of the observed values of the variable of interest. A statistical model can be used for simulation that simulates the operation of a simulated process. This allows you to artificially generate new values of the studied variable, which have the properties of real data.

In the literature, among numerous statistical approaches, there are two that are most useful and often used to assess air pollution:

– simplified dispersion models, in which the dynamic transfer equations are reduced to a series of formulas;

– models based on GIS technologies.

Simplified dispersion models. Simplified dispersion models (SDMs) represent an attempt to reduce the complex dynamic equations inherent in a true variance model to a simpler and generally static form. Simplification is achieved mainly by ignoring local, time-varying processes that affect short-term concentrations of air pollutants (for example, associated with changes in meteorology), and instead models average long-term patterns.

Among numerous examples of statistical models, two are the most widely used in Europe: the Calculation of Air pollution from Road (CAR) traffic model [7] and the Design Manual for Roads and Bridges (DMRB) model. However, they are inevitably limited so that they are not designed to deal with non-transport emissions, and in terms of the number of sources and the ability to simulate long-range transport of pollutants.

GIS-based models. Geographic information systems (GIS) are important tools for air pollution modeling. They are characterized by the ability to extract and process spatial data required as input to air pollution models and then display the results of the models.

However, in recent years, GIS technology has also been used to independently develop air pollution models. One of such approaches is land use regression (LUR) [8]. It is based on empirically derived regression equations linking land cover to measured air pollutant concentrations at a number of monitoring sites.

Recently, an alternative to LUR modeling has been developed using focusing techniques in GIS [9].

In general, it should be noted that a dense air quality monitoring network is required to develop a statistical model. These models find the greatest application for the analysis of relatively long-term (e. g., seasonal, annual) concentrations of local pollutants. The main limitation is that the models do not directly represent the processes that determine air pollution.

Analytical models

Analytical models are functional relationships: systems of algebraic, differential, integro-differential equations, logical conditions. The construction of an analytical model for the dispersion of pollutants in the atmospheric air of cities is associated with certain difficulties. The main problems of modeling the state of atmospheric air are due to the complexity and interconnectedness of the processes of propagation, dispersion and chemical transformation of the components of impurities. The urban environment induces a complex flow field, which generates heterogeneity of pollutant concentration fields and very strong concentration gradients in certain streets or squares [10].

All scientific analytical models have limitations of applicability due to different conditions. The following types of analytical models can be distinguished below.

Computational Fluid Dynamics (CFD) models are able to explicitly resolve complex air currents and dispersions induced by urban obstacles. Computing domains range from a fraction to one or two square kilometers.

Analytical models provide better calculation results than statistical models. Let us consider each type of analytical models in more detail.

Mesoscale models. Mesoscale models are mainly used in forecasting weather and other climatic phenomena. The same can be used to model air quality in cities.

By integrating the numerical mesoscale modeling of the Weather Research and Forecasting (WRF) model and the parameterization of information on urban development, a large number of atmospheric air pollution models have been proposed, such as the WRF/ LSM/ Urban modeling system [11], NU–WRF model [12] and others. Also, the mesoscale approach included the formation of atmospheric aerosols and chemical transformations with their participation, which was implemented in the WRF/ Chem–NCSU [13, 14] and WRF/ Chem–ROMS [14] models. An example of the use of mesoscale modeling taking into account chemical transformations and aerosols is to simulate atmospheric air pollution in Sydney [15] within the framework of the Australian government-funded project The Clean Air and Urban Landscapes Hub.

Empirical models. Empirical models include the composition of regulated methods and regulations, such as standard models developed at the Main Geophysical Observatory by A.I. Voeikov. In Russia, to calculate the dispersion of pollutants , the OND-86 [16] method was used (until January 1, 2018), and the MMP–2017 [17] method is used at present. Empirical models can be successfully used to analyze quasi-stationary processes when the time of emissions of substances exceeds the time of movement of air masses in the analyzed area of space. These models make it possible to calculate the field of impurity concentrations for a given direction and wind speed and a combination of meteorological parameters that is most unfavorable for dispersion of impurities. But the models have low accuracy due to too “rigid” structure and a large number of accepted simplifications.

The numerous correction factors [18] do not lead to an increase in accuracy. In addition, the model is not applicable for forecasting in specific weather conditions.

Parameterized semi-empirical models. Micro-scale semi-empirical models, which are currently considered as the most accurate ones among those reflecting the situation of atmospheric air pollution in the urban environment, have been independently developed. Gaussian models assume a normal distribution of impurities along three axes. They have found great practical application for local problems. Gifford [19] proposed a scheme for determining the variances of the Gaussians Diffusion Model (GDM) in accordance with the Pasquill stability classes. The model based on this scheme is called the Pasquill–Gifford model. This model was recommended in 1986 as the basis for the creation of national local models in the IAEA member countries [20]. On its basis, the NPO Typhoon [21, 22] models have been developed for radionuclides in our country. The disadvantage of the GDM in comparison with the OND-86 is the lack of a rigorous algorithm for selecting meteorological conditions for normalizing one-time concentrations to the maximum ones. The advantage is the possibility of calculating under actual weather conditions and calculating long-term concentrations, including average annual [23]. Basic equation of GDM composed of two probability density functions of the normal distribution law:

$$q(x,y,z)=\frac{Qf_F f_W}{2\pi\sigma_y(x)\sigma_z(x)\underline{U}}\exp-\left[\frac{y^2}{2\sigma_z^2(x)}\right]\left\{\exp\left[-\frac{(z-h)^2}{2\sigma_z^2(x)}\right]+\exp\left[-\frac{(z+h)^2}{2\sigma_z^2(x)}\right]\right\} \quad (1).$$

In world practice, the Gaussian model AERMOD is widely used [25], it is recommended by the American Environmental Protection Agency (EPA). It is suitable for solving local problems at a distance of no more than 50 km from the source. The model is successfully used to simulate atmospheric air pollution [24, 25] and has not lost its relevance to this day. Currently, the model is being supplemented with new approaches. The hybrid model AERMOD LUR was also developed [26]. A meaningful solution was obtained for the emissions from the Pittsburgh steel mill. The railroad was considered as an additional source of pollution.

The EPA recommends the CALPUFF computational complex for modeling the distribution of impurities on a regional scale [27]. It is based on Lagrangian–Gaussian model (LGM):

$$C(x,y,z)=\frac{Q(x_i,y_i,z_i)}{2\pi\sigma_x\sigma_y u}\cdot\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right]$$

This model takes into account the height of the source (H) and the average wind speed (u) in the direction of the x axis, which leads to obtaining more reliable results in comparison with GDM. The main disadvantages of the LGM is the complexity of determining σ_x, σ_y, σ_z.

The model is widely used in Europe and Asia [28, 29].

The Air Pollution Model (TAPM) [30, 31] was proposed and developed in Australia. The mean wind is determined for horizontal components u and v (m s^{-1}) from the momentum equation and the terrain following vertical velocity σ (m s^{-1}) from the continuity equation.

The model is based on the solution of the Euler and Lagrange equations for different cases.

The Eulerian Grid Module (EGM) consists of nested grid-based solutions of the prognostic equation for concentration χ, and is similar to that for the potential virtual temperature and specific humidity variables, and includes advection, diffusion, and terms to represent pollutant emission S_χ and chemical reaction R_χ:

$$\frac{d\chi}{dt}=\frac{\delta}{\delta x}\left(K_\chi\frac{\delta\chi}{\delta x}\right)+\frac{\delta}{\delta y}\left(K_\chi\frac{\delta\chi}{\delta y}\right)-\left(\frac{\delta\sigma}{\delta z}\right)\cdot\frac{\delta}{\delta\sigma}\left(\omega'\chi'\right)+S_\chi+R_\chi$$

The Lagrangian Particle Module (LPM) can be used on the innermost nest for selected point sources to allow a more detailed account of near-source effects, including gradual plume rise and near-source dispersion.

In the vertical direction, particle position is updated using:

$$\frac{d\sigma_{particle}}{dt}=\sigma^{\bullet}+\sigma^{\bullet\prime}+\sigma^{\bullet\prime}_p$$

where $\sigma_{particle}$ is the particle position in terrain following coordinate $\sigma^{\bullet}$, is the mean ambient vertical velocity, $\sigma^{\bullet\prime}$ is perturbation of vertical velocity due to ambient turbulence, $\sigma^{\bullet\prime}_p$ is perturbation of vertical velocity due to plume rise effects.

In order to calculate total pollutant concentration for use in chemistry calculation and time-averaging, particles are converted to concentration at grid points of the EMG using the equation for concentration increment of a particle at a grid point:

$$\Delta\chi=\frac{\Delta m}{2\pi_c\sigma_y^2\Delta z}\exp\left(-\frac{r^2}{2\sigma_y^2}\right) \quad (2).$$

The model takes into account photochemical reactions, dry and wet deposition, urban development, terrain and can be adapted for real-time modeling.

In the technical description of the model [31], it is noted that the model consists of plugins, each of which is responsible for the influence of certain parameters. There is also a fairly detailed block diagram describing the connection sequence for each of the modules, as well as a list of numerical methods used to perform calculations on the model.

This approach to identify the source of pollution was used in Karabash, Chelyabinsk region, Russia [32].

Most of the TAPM publications were used for Southeast Asia and Australia regions [33–36]. The calculation accuracy has been improved using TAMP with the chemical transport model (CTM) [35].

The first serious attempts to account urban building were made in parametrized semi-empirical models developed since 2000, such as OSPM [37], SIRANE [38] or ADMS-URBAN

[39]. Street-scale systems were applied in Madrid [40].

Computational Fluid Dynamics models. Computational Fluid Dynamics (CFD) models are able to explicitly resolve complex air currents and dispersions induced by urban obstacles using this resolution over computational domains that range from a fraction to one or two square kilometers [41–44]. CFD–based models use high-resolution emission estimates from microscale emission models. However, for real applications (air quality assessment, network design, micro-level air pollution abatement strategies, etc.) they lack the computing power. It is impossible to use them to simulate long periods.

In a number of studies by Russian scholar [45], the Navier-Stokes equation was used for mathematical modeling of atmospheric aerodynamics and the propagation of pollutants over a complex underlying surface, the Poisson equation was used to take into account the pressure, and the pollutant was described by the diffusion equation, the source was taken to be linear (Karmadon Gorge).

Conclusion

Analysis of mathematical models of atmospheric dispersion showed that the most known modern models are designed to solve narrow problems. To improve the accuracy of calculations, models often include several submodels and form complex systems of software complexes. Many modern models contain elements of various previously studied models. They are hybrid varieties of existing ones. The complication of models by introducing a large number of variable factors and requires significant software resources and training of highly qualified specialists. Thus, new universal software complexes are greatly needed.

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