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Review and analysis of the modelling of the atmospheric air pollution for urban air basins

Abstract. The paper considers the main stages of modelling of urban air basins pollution. It determines the following main stages: calculation of background concentration; modelling of pollution in an "urban canyon"; calculation of point, linear, and areal pollution sources; and summation of concentration values.

As a method of calculating the conditional background concentration and also a method of forecasting the meteorological conditions changing, two different methods are considered: time series analysis and use of artificial neural networks.

Classification of existing models by using the solvable problems principle and mathematical basics is carried out. Two models are used as a mathematical basis: the Gaussian model of the pollutant plume dispersion and the Lagrange model of the layer. From the point of view of solvable problems and solution completeness, model screening, expanded models and dispersion models in conditions of urban canyons are emphasized.

Keywords: air pollution; urban pollution sources; The Gaussian dispersion model; Lagrangian model layer; urban canyons; modeling of air pollution; screening model; advanced models.

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Introduction

The most rational method of assessing and forecasting an urban atmospheric air pollution is the method of modelling. This method is notable for its significant complexity since the complex analysis requires solving some questions.

In the general case, for cities with a large population density and size, calculation of atmospheric air pollution requires solving 4 questions:

- Calculation of the background concentration;
- Calculation of dispersion of pollutants from other point, linear, and areal sources;
- Modelling of dispersion of pollutants from the road traffic in urban street canyons;
- Calculation of the total concentration level.

Solving this sort of questions requires taking into account the following: the most valuable models are the models that can be used for other territories, time intervals, etc. That is the models that can be adjusted, corrected, or the models that take these parameters into account by default. Constant correction of the model, carried out by the researcher manually, complicates the modelling process. However, now this problem can be solved by processing the data by means of neural networks.

Dispersion models differ in the approach to their mathematical construction and, therefore, in the set of the model parameters. The parameters most often include the following:

- Meteorological conditions: wind velocity and direction, atmospheric pressure, amount of precipitations, cloudiness, solar radiation, etc.
- Parameters of the emissions: source location (including height) and type, velocity and mass flow of pollutants.
- Landscape of the location of the pollution sources and the points of perception.
- Obstacles to spreading of the pollutants, tall buildings, surface roughness, etc. In the general case, for simplification of the assessments, only two values are taken: "city", "village".

In the general case, calculation of the pollutants concentration includes the following stages:

1. Preliminary processing of the meteorological and other data used in the models.
2. One of the concentration calculation algorithms is started, based on the data derived from the processing.
3. Output of the average pollutant concentration for the source of perception (calculation of the pollution in a concrete point, area, etc.).
4. Overlaying of the concentration values over the conditional background accepted for this area.

1. Mathematical basics of the dispersion process

Gaussian air pollutant dispersion equation

Scientific and technical literature that covers dispersion of pollutants in air is quite extensive. One of the first papers in this area is the paper by Bosanquet and Pearson [1]. The dispersion equation derived by the authors did not include Gauss distribution and the effect of reflection of the ground-level plume. In 1947, Graham Sutton assumed that there was the Gauss distribution for vertical and crosswind dispersion of the plume and also the ground-level plume reflection effect [2].

Clean Air Acts enacted in 1956 and 1968 in Great Britain [3, 4] served as a basis for formation of the air dispersion models. The basis for computer modelling of the dispersion processes was the complete equation for Gaussian dispersion modelling of continuous air pollution flows according to which the emission concentration C (g/m³) at any receptor located x meters downwind from the emission source point, y meters crosswind from the emission plume centerline, z meters above ground level is calculated by the following formula [5, 6]:

$$C = \frac{Q}{u} * \frac{f}{\sigma_y \sqrt{2\pi}} * \frac{g_1 + g_2 + g_3}{\sigma_z \sqrt{2\pi}} \quad (1)$$

where f – crosswind dispersion parameter $f = \exp\left[\frac{-y^2}{2\sigma_y^2}\right]$;

g_1 – vertical dispersion parameter with no reflections $g_1 = \exp\left[-\frac{(z-H_e)^2}{2\sigma_z^2}\right]$;

g_2 – vertical dispersion parameter taking into account the ground-level reflections;

$$g_2 = \exp\left[-\frac{z+H_e}{2\sigma_{z2}}\right];$$

g_3 – the vertical dispersion parameter taking into account the ground-level reflections from an inversion aloft;

$$g_3 = \sum_{m=1}^{\infty}\left\{\exp\left[-\frac{(z-H_e-2mL)^2}{2\sigma_z^2}\right] + \exp\left[-\frac{(z+H_e+2mL)^2}{2\sigma_z^2}\right] + \exp\left[-\frac{(z+H_e-2mL)^2}{2\sigma_z^2}\right] + \right.$$
$$\left. + \exp\left[-\frac{(z-H_e+2mL)^2}{2\sigma_z^2}\right]\right\};$$

Q - emission intensity (g/s);

u - horizontal wind velocity along the plume centerline (km/s);

H_e - emission plume height above the ground (m);

σ_z - standard vertical deflection of emissions (m);

σ_y - standard horizontal deflection of emissions (m);

L - height from the ground level to the bottom of inversion aloft (m).

This equation includes not only ascending reflection from the ground, but also descending reflection from the bottom of the inversion aloft.

The sum of the four summands in the exponential component g_3 converges to the final value quite quickly. In most cases, summation of the series of the three values of m from 1 to 3 gives an adequate solution of the equation.

The parameters of vertical *(σ_y)* and horizontal *(σ_z)* deflection of emissions are functions of the atmospheric stability class (for example, a measure of the turbulence). These values alongside with the source height are the main values in taking into account the dispersion.

The Briggs plume rise equation

The Gaussian equation presented above requires calculation of the parameter H_e. It is actually a sum of the emission source height H_s and the plume rise Δh due the plume's buoyancy and is described by the following equation:

$$H_e = H_s + \Delta h \tag{2}$$

Figure 1 demonstrates the graphic description of the equation (2).

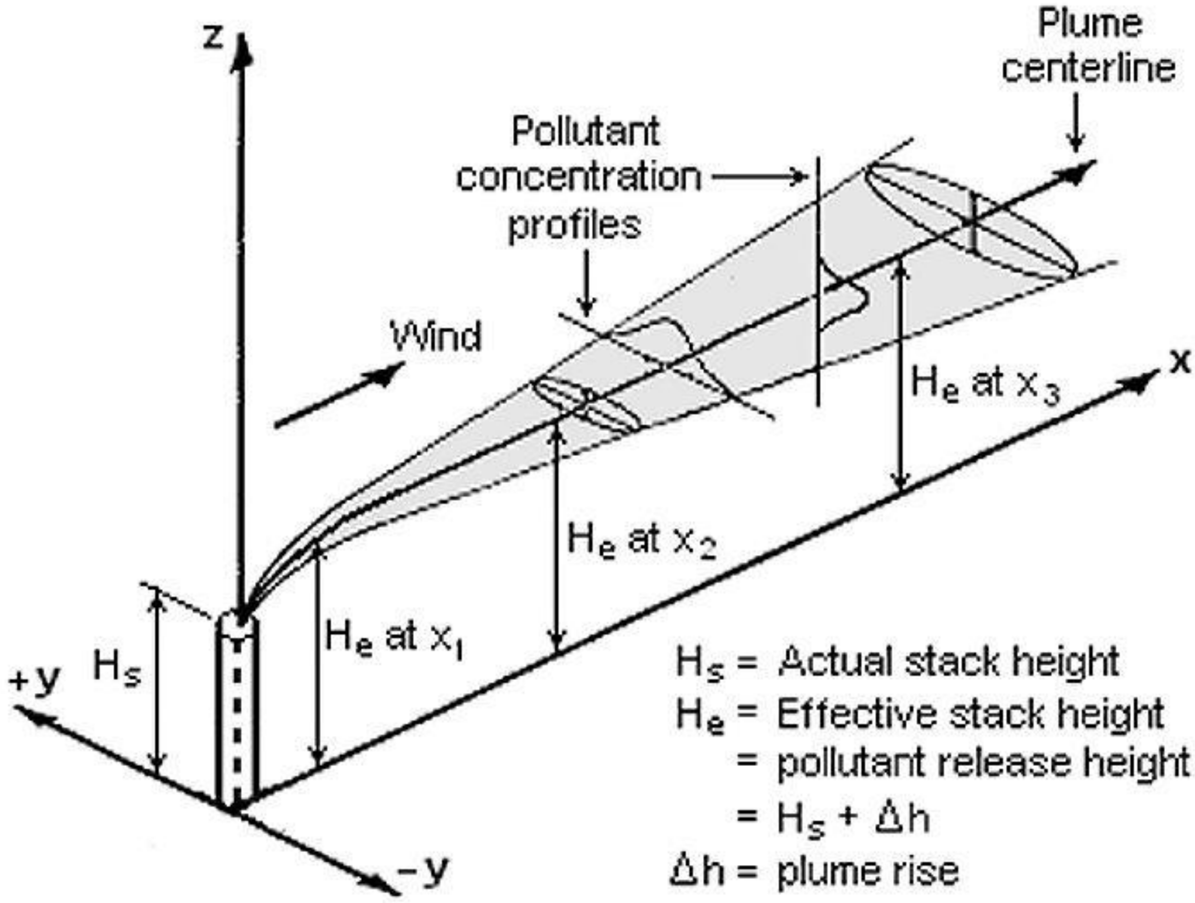

Figure 1. *Visualization of a buoyant Gaussian air pollutant dispersion plume [6]*

From the end of 1960s to the beginning of 2000s, the plume rise was determined by the Briggs equation (2).

Briggs for the first time published his plume rise observations in 1965 [7]. Then he compared many plume rise models available at the time in CONCAWE [8] and in the published work edited by Slade [9].

In 1969, Briggs proposed a set of plume rise equations that became widely known as "Briggs equations" [10]. Subsequently, he modified them in 1971 and 1972 [11, 12].

Briggs divided air pollution plumes into the following four general categories:

- Cold jet plumes in calm ambient air conditions;
- Cold jet plumes in windy ambient air conditions;
- Hot, bent-over buoyant plumes in calm ambient air conditions;
- Hot, bent-over buoyant plumes in windy ambient air conditions.

In spite of the fact that he proposed the plume rise equation for each of the plume categories stated above, it is important to note that the equation most frequently used in calculations is the equation for hot, bent-over buoyant plumes in windy ambient air conditions. These equations are based on observations and data regarding plumes from typical pollution sources such as smoke-stacks, large power plants burning fuels that frequently contribute to the pollution level above all other sources. Stack exit velocities in such conditions are usually range from 6 to 30 km/s and the exit temperatures range from 120 to 260°C.

A bent-over buoyant plume can be calculated according to the Briggs' formula on the basis of the Beychok's logic diagram presented in Figure 2.

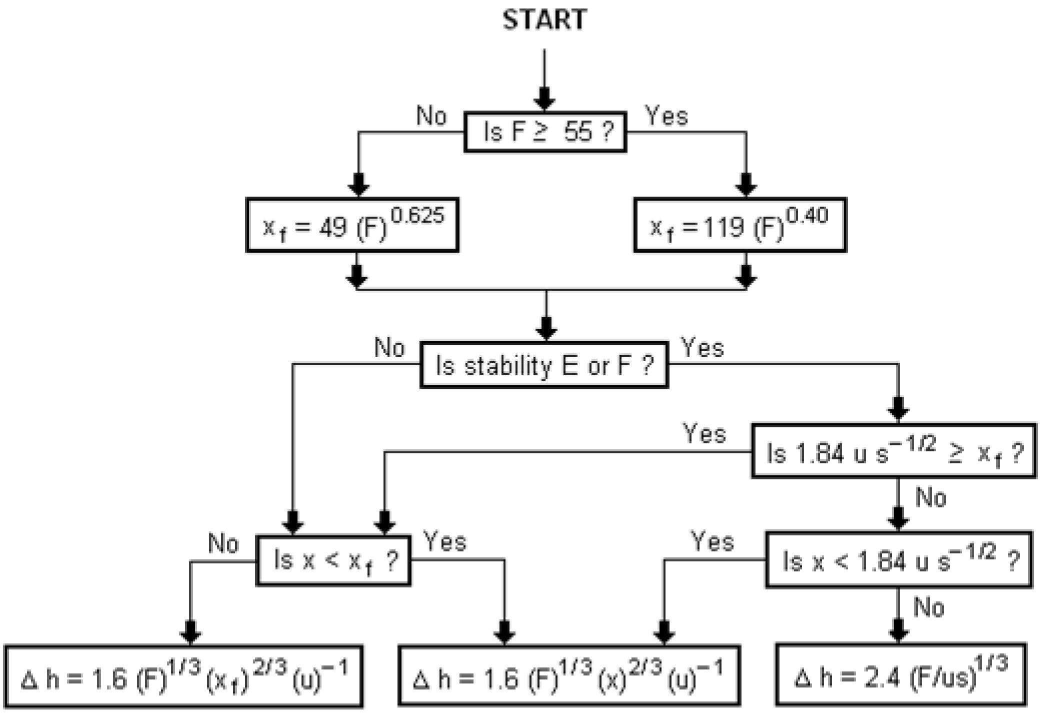

Figure 2. *Logic diagram for using the Brigg's equation [6]*

F - buoyancy factor (m^4s^{-3});

x - downwind distance from the plume to the measuring point (m);

x_f - downwind distance from plume source to point of maximum plume rise (m);

u - wind velocity at the actual exit height (m/s);

s - stability parameter (s^{-2}).

2. Calculation of the conditional concentration background

Background level of concentration is the concentration value observed in an area unaffected by human activity and which is a sum of a set of natural components.

When considering real conditions and contribution of the real pollutants, it is most appropriate to talk about the conditional background i.e. about pollutant concentration without taking into account contribution of the local components for their subsequent calculation, i.e. taking into account both natural and the anthropogenic factors acting during a significant amount of time [13].

Thus the conditional background concept includes also the set of unorganized sources that can influence local substance concentration. Besides, their description can be carried out by the stochastic methods.

In the first stage of modelling, it is important to decide on the necessary degree of the measurement accuracy. In the general case, the conditional background can influence considerably the total pollution level. The data on environmental conditions are quite difficult for simulating due to a great number of interacting factors and variables that are to be taken into account in calculations that, therefore, give a great number of value combinations.

To simplify the calculations, the two following methods are used most frequently: time-series analysis and artificial neural networks.

Time-series analysis

Time series is a set of data elements obtained by means of repeated measurements during a long period of time. Time-series data have a natural time order of distribution that, in its turn, introduces a number of special features for analysis. The main distinctive feature is the close interrelation of data connected with their natural closeness [14].

Artificial neural networks

Artificial neural networks (ANNs) are a mathematical presentation of biological neural networks i.e. some kind of emulation of a biological nervous system. ANNs have a high degree of adaptability to nonparametric data distributions and do not give preliminary hypotheses about interrelation between variables. ANNs also have a low sensitivity to mistakes and can solve such questions as noise reduction and exclusion of abnormal chaotic values. ANNs consist of the input layer, several neuron (mathematical objects whose behavior is regulated by a predetermined function) layers and the output layer. At first, each network is trained by means of an input and output data set to be able to take into account behavior of the parameters for subsequent forecasting [15].

The presented methods considered for analysis of the primary pollutant concentration data can be used for determination and forecasting of meteorological parameters, including for specifying of missing data.

3. Existing atmospheric dispersion models

The European Topic Centre on Air and Climate Change, which is a part of the European Environment Agency, maintains an online Model Documentation System that currently (August 2015) includes 142 dispersion models developed in Europe.

The most part of the models can be divided into two categories:

1. Gaussian plume models;
2. Lagrangian layer models.

In essence, the hypothesis about the Gaussian plume model assumes that the pollutant concentration in the plume is proportional to the emission intensity and inversely proportional to the wind velocity in the emission point. Thus at the wind velocity close to zero, the assumed concentration tend to infinity and the Gaussian plume presentation is invalid. One more problem arises from the "stationary assumption" according to which meteorological conditions between the emission source and the observer are constant for each modeled hour. This assumption can be invalid in two cases [16]:

Non-uniform meteorological conditions. If there are territories inside the modelling area that have considerable differences in the mode of use (for example, city and village inside one area of research), the assumption of the wind field uniformity for the entire modelling object is incorrect.

Dispersion at large distances. Gaussian models allow calculating pollutant concentration in the modelling area along the direct line between the source and the measurement point for each hour. However, they do not take into account the time necessary for the pollutant plume to move from the source to the measurement point. So, at sufficiently low wind velocities, the maximum distance for which the calculation can be carried out is no more than 10 km. For this reason, the Gaussian models confine themselves only to this distance when forecasting pollutant concentration.

The Lagrangian layer models describe mathematically the process of pollutants transmission through the movement of parcels (aggregate of pollutant particles). Parcel movement modelling corresponds to the random walk process. Then the Lagrangian model calculates the air pollution dispersion by calculating the continuous plume trajectory as series of discrete pollutant parcels. This model uses a moving reference system relative to its initial location. The total pollutant concentration in a point is calculated on the basis of contributions of all component plumes. A layer model can also include Gauss distributions for describing pollutant dispersion in each plume. This approach has a higher degree of accuracy in comparison with the Gaussian dispersion models, but requires more time for the model realization.

From the point of view of application, all models can be divided into three groups:

1. Screening models;
2. Expanded models;
3. Models of urban street canyons.

Screening models

The first group includes the models for assessment of maximum concentrations that are calculated with taking into account standard sets of meteorological conditions and simplified assumptions describing relative position of the pollution source and the analysis point. The primary task of the screening modelling is to eliminate the sources whose influence on the pollution process is insignificant and, therefore, which do not endanger the environment. Another task of the screening models is determination of the worst scenario, i.e. determination of the maximum level of concentration from the source or the group of sources, depending on the maximum possible emission and the meteorological conditions that are worst for dispersion. Of course, this set of circumstances is hardly probable, however exceeding of national or other air pollution standards is a reason for application of more exact modelling methods including expanded models.

AERSCREEN. It is the Gaussian plume distribution model using worst meteorological data for forecasting pollutant concentration from a single source with continuous pollutant emission, based on the AERMOD model.

The model forecasts the highest pollutant concentration for one source with an averaging period of 1 hour. Recalculation for other time intervals (3 hours, 8 hours, 24 hours, and average annual concentration) is carried out on the basis of the correction coefficients [17]. AERSCREEN is intended for assessment of concentrations that are equal or higher than the assessments performed by means of AERMOD with taking into account a full meteorological data set and the relief.

Requirements to the model, specified in its manual:

- Data on the source: emission intensity (g/s), emission source height (m), mouth diameter(m), gas exit velocity (m/s) or volume flow rate (m^3/s), temperature (K);
- Meteorological parameters: minimum and maximum ambient temperature (K), wind velocity (m/s), height at which velocity of air masses is measured, surface characteristics;
- Settlement type: urban settlement / rural settlement;
- Relief: digital terrain model (DTM), the file for starting AERMAP;

- Buildings' features: buildings' sizes and location of the emission source relative to the buildings;
- Output concentrations: 1 hour (conversion to other average values by using correction coefficients).

ADMS-Screen. By analogy with the previous model, this model calculates the Gaussian pollutant plume distribution by using worst meteorological data. Besides, the data used are not theoretical worst meteorological conditions, but the real worst ones [18].

The plume dispersion relative to the buildings is calculated by the algorithms built in the ADMS 3 model [19]. The model is intended for forecasting pollutant concentrations in the environment that are equal or higher than ones forecasted by the ADMS 3 model.

Requirements to the model, specified in its manual:

- Data on the source: emission intensity (g/s), emission source height (m), mouth diameter(m), gas exit velocity (m/s) or volume flow rate (m^3/s), temperature (°C);
- Meteorological parameters: no parameters for short-term forecasts, long-term forecasts require specifying of coordinates (calculation only for Great Britain);
- Settlement type: no choice;
- Relief: digital terrain model (DTM), the file for starting AERMAP;
- Buildings' features: buildings' sizes and location of the emission source relative to the buildings;
- Output concentrations: 1 hours, average daily value, average annual concentrations, and also percentiles.

As can be seen from the necessary data sets for two screening models presented above, each of the models assumes certain simplifications. Both of these models have also advanced versions.

Expanded models

Expanded dispersion air pollution models use more modern scientific theories and more sophisticated complex mathematical methods in comparison with screening models. Expanded models can consider pollution distribution from many sources and take into account many obstacles such as buildings.

Detailed meteorological and spatial data used in such models allow describing atmospheric processes of pollutants distribution more representatively. However, expanded models have a number of limitations that are not present in screening models since, depending on the prevalent source types, some of them are too complex in realization. Models taking into account industrial influence, such as AERMOD and ADMS 4, are of the greatest interest.

AERMOD. AERMOD is an air mass dispersion model based on planetary structure of the boundary turbulence layer. It also includes surface data processing and uses two initial data types for calculation:

AERMET, meteorological data for preprocessing, which include the data on air dispersions, based on the turbulence structure of the planetary boundary layer.

AERMAP, terrain data.

ADMS 4. ADMS 4 is an expanded pollutant dispersion model based on the Gauss distribution that can take into account several emission sources. By analogy with AERMOD, ADMS 4 also uses the meteorological conditions data and terrain data. Besides, the data source is the British Weather Bureau. The main AMDS 4's distinctive feature is the Lagrangian layer model algorithms.

Expanded models have one common feature: setting up of such models requires a large amount of meteorological and spatial characteristics of the researched object. Each of the models uses some knowledge base maintained by scientific or governmental organizations of the developer country.

Models of urban street canyons

A special urban pollution type is a pollution of central streets due to specificity of buildings arrangement. As a rule, center of the city is developed with high buildings whose heights are very disproportionate to the widths of the streets between them that prevents free movement of the wind. Thus buildings form a special sort of "urban canyons" (Figure 3).

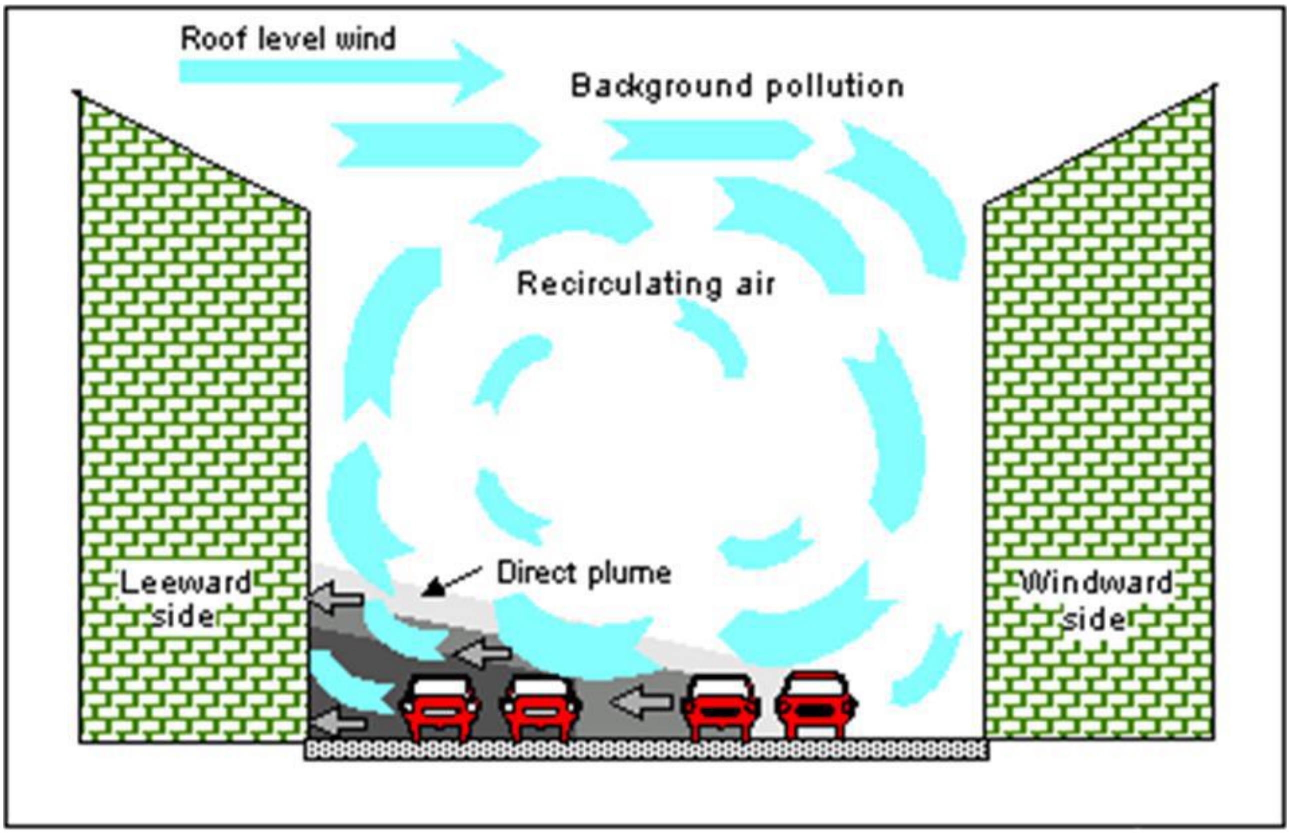

Figure 3. *Urban street canyon model [20]*

Pollutants concentration in such formations exceeds considerably the average concentration in the city that increases the risk of pedestrians' illness [21].

Now the following models for calculation of urban canyons are realized: STREET, CPBM, AEOLIUS, SLAQ, ADMS Urban, OSPM.

All the models presented are calculated on the basis of the motor transport quantity and specificity of the buildings geometry.

Conclusion

The stages and elements of the urban air pollution modelling considered above allow to make a conclusion about specificity of this pollution type and, therefore, specificity of solving modelling process problems. Many existing models solve certain problems and perform certain functions. Creation of a universal pollution calculation model for various cities is extremely difficult due to complexity of assessing a great number of factors.

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Обзор и анализ процесса моделирования загрязнения атмосферного воздуха воздушных бассейнов городских территорий

Аннотация. В статье рассматриваются основные этапы моделирования загрязнения воздушных бассейнов городских территорий. В качестве основных этапов выделены: расчет фоновой концентрации, моделирование загрязнения в «городском каньоне», расчет точечных, линейных, площадных источников загрязнения и суммация значений концентрации. В качестве метода расчета условного фона концентрации, а также метода прогнозирования изменения метеорологических условий рассматриваются два отличных друг от друга метода: анализ временных рядов и использование искусственных нейросетей. Проводится классификация существующих моделей по принципу решаемых задач и по математическим основам. В качестве математической основы выделяется две модели: Гауссова модель дисперсии шлейфа загрязнителя и Лангранжева модель слоя. С точки зрения решаемых задач и полноты решения выделяются скрининг модели, расширенные модели и модели рассеивания в условиях городских каньонов.

Ключевые слова: загрязнение воздуха; городские источники загрязнения; Гауссова модель дисперсии; Лагранжева модель слоя; городские каньоны; моделирования загрязнения воздуха; скрининг модели; расширенные модели.

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