Approach to modeling the spread of pollutants in air by the example of Volgograd

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Abstract. The article provides an overview of the systems for modeling the spread of pollutants, discusses their advantages and disadvantages. An approach to modeling the spread of pollutants in the atmospheric air of an urbanized area on the basis of the Calpuff software suite is proposed. The processes and sources of data on the terrain, meteorological parameters, etc., necessary for the generating concentration maps for Russian cities are described in detail. The approach consists of three main stages: modeling meteorological parameters, modeling pollution spread and visualization of the data obtained. An example of modeling of pollutants spread in the atmospheric air for Volgograd is given.

1. Introduction
For a sustainable integrated development of environmental monitoring of the Russian Federation it is necessary to use decision-support information systems, including mathematical models, databases, information analysis tools, graphical interfaces. It is necessary to leverage the opportunities of rapid development of information technologies using geographic information systems, data networks, the artificial intelligence theory and much more for the introduction of decision-support systems (DSS) in the field of environmental monitoring[1,2].

In order to solve the objectives, it is necessary to provide information on the concentrations of pollutants in the urban area. In the US, EU and China, information is obtained from stationary environmental monitoring stations. In Russia, the regions face with insufficient funding, therefore it is impossible to expand the network of monitoring stations.

Methods of artificial intelligence, data analysis, and knowledge engineering can be used to obtain the missing data and refine the modeling results.

2. Analysis of pollutant spread modeling systems
A review of modern pollutant spread modeling systems was carried out, this article presents a fragment of the review [3-11].

The MOVES model estimates emissions from road and off-road sources, covers a wide range of pollutants and enables multi-scale analysis. The approach, which uses several scales, is based on a common set of modal emission levels broken down by driving modes.

The American AERMOD model is a model of a Gaussian plume in a stable state. It is used to estimate the dispersion of inert pollutants from point, area, volume and open sources. If the roadway is
modeled from multiple area or volume sources, the coordinate set that determines the location of each source is the same. The AERMOD model is designed for a distance of no more than 50 km.

The CALPUFF model is a non-stationary Lagrangian model, which models the emissions as a series of continuous feeds of fuel through the supercharger and is most suitable for emissions in the range from 50 to 200 km [12].

It can model linear sources with constant emissions as well as point and volume sources.

After the analysis, preference was given to the Calpuff modeling system. The advantages of this system include the following:

- the terrain of a particular area is taken into account;
- meteorological parameters are taken into account: wind speed and direction at different heights; air temperature; atmospheric pressure; air humidity, etc.
- it is possible to work with different sources of pollution: stationary sources; linear sources; area sources; motor transport, etc.
- open-source software product;
- the project is being developed, updates and new versions are released.

The disadvantages of the Calpuff modeling system include the following:

- it is difficult to find the necessary source data [13];
- long calculation time.

It should be noted that the above disadvantages arise from the fact that the modeling takes into account many factors that increase the accuracy of the result.

When using the Calpuff software, the modeling is performed in two stages: at the first stage, a three-dimensional meteorological map is constructed, at the second stage, the dispersion of pollutants is simulated.

3. Approach to modeling the spread of pollutants

This article describes an approach to modeling air pollution for a particular urban area (the city of Volgograd), taking into account the terrain, land use and meteorological parameters.

The modeling process consists of three main stages:

- modeling of meteorological parameters;
- pollution modeling;
- visualization of the results (both historical and predictive).

At the first step, it is necessary to run the WRF modeling system. The process of using the system is shown in figure 1.

The Weather Research and Forecasting Model (WRF) is a mesoscale numerical weather prediction system used to model atmospheric processes at scales ranging from several tens of meters to hundreds of kilometres.

Components of WPS:

- geogrid.exe. The program extracts static data about the ground surface from the obtained archives, creates modeling areas (domains) and interpolates the data onto the modeling grid.
- ungrib.exe retrieves the required weather data from files in the GRIB format.
- metgrid.exe horizontally interpolates meteorological fields created by ungrib.exe onto the grid created by geogrid.exe.

To run the software, the user needs to prepare two data archives:

- archive of static data on the ground surface. The archive can be obtained for free at [14]. It is used by geogrid.exe.
- archive of meteorological data in the GRIB format. Access can be obtained for free at [15] after registration. It is used by ungrib.exe.

Components of WRF:

- real.exe initializes the system to work with real data.
- wrf.exe – numerical integration program.
The software modules of the WRF system for the prepared source data archives and configuration files are run using the scripts developed by the author and do not require any user actions.

At the second stage, the Calpuff modeling system is used. The process of working with the system is shown in figure 2.

Let's take a closer look at the process of launching the Calmet preprocessor.

Calmet is a preprocessor that simulates meteorological processes, including 3D wind and temperature maps, and calculates 2D maps of the micro-meteorological variables needed to simulate the dispersion of pollutants [16].

Modeling is carried out in two stages. At the first stage, winds are modeled depending on the terrain (various kinematic effects, wind flow slopes, blocking effect). At the second stage, the obtained result is superimposed with observational data.

The first step requires information about the terrain and land use. This information can be obtained at the EarthExplorer [17] web service (registration is required). To obtain the necessary data, you must specify the coordinates of the area, as well as the size of the plot of interest. Information about the terrain (the global digital terrain model with the grid spacing of thirty corner nodes - about 1 kilometer) is available in the section “Digital Elevation -> GTOPO30”. The information obtained is the input to the terrel.exe preprocessor.

In section “Land Cover -> GLCC” you can obtain information about land use. This information is required to launch the “ctgproc.exe” preprocessor.

For the second stage of the Calmet preprocessor, the following meteorological observations obtained at a frequency of one hour on the surface are required: wind speed, wind direction, temperature, atmospheric pressure, humidity, cloudiness and some others. Data from the upper atmosphere (wind speed and direction, pressure, temperature and altitude of observations) are also needed.
The above data can be obtained from the following resources (registration is not required, but you need to know the ID of the observation station):

- NOAA/ESRL Radiosonde Database [18] - data on the state of the upper atmosphere from radiosondes. Data are processed using the “read62.exe” preprocessor.
- ncdc.noaa [19] - data from ground weather stations, they are used by “smerge.exe”.

![Diagram of the process of using the Calpuff modeling system.](image)

**Figure 2.** The process of using the Calpuff modeling system.

It is also necessary to prepare the output data obtained in the WRF model using the “calwrf.exe” preprocessor.

The second stage of using the Calpuff modeling system is to run the preprocessor for modeling the dispersion of pollutants.

Calpuff [20] is a pollutant spread model that takes into account the impact of various meteorological effects happening at various points in time and space.

Data on pollution sources are recorded in the general input file ptemarb.dat. The system takes into account point, line, plane and volume sources for several types of pollutants.

The third stage is post-processing. Calpuff will generate many output files. To analyze the spread of pollutants, a .CON file is required. This file contains data on the concentration of pollutants within the time interval specified in the simulation.

To visualize the data using a 2D map, the “calpost.exe” postprocessor is necessary. However, visualization in this format is extremely inconclusive, since this display of the concentration matrix is not tied to the terrain map. Therefore, there is a need to visualize the results using a geographic information system.

The QGIS geographic information system was chosen to visualize the simulation results (figure 3).
For visualization of concentration maps in the QGis geographic information system, the data obtained from the Calpuff modeling system have to be pre-processed.

![Diagram of data processing](image)

**Figure 3.** Visualization of the results of modeling the spread of pollutants

The computational experiment was conducted for the cities of Volgograd and Volzhskiy. The terrain parameters were determined: date and time - June 01, 2016, 07:00 AM; atmospheric air temperature - +12.3 °C; atmospheric pressure - 748 mm Hg; air humidity - 77%; wind direction and speed - northeast, 8 m/s; precipitation - none; cloudiness - significant cloudiness (70%); latitude and longitude of origin - 48.414373, 44.317071; size of the modeling cell - 500 x 500 meters; size of the modeling matrix - 100 x 100 cells. Figure 4 shows a visualization of SO2 pollution.

![Visualization of SO2 pollution](image)

**Figure 4.** Results of a computational experiment for SO2.

4. Conclusion
The analysis of modern methods of modeling the spread of pollutants in the air, as well as software systems based on them, showed the expediency of using the Calpuff pollutant spread model to predict the quality of atmospheric air for a particular region. Calpuff provides the best results at the lowest computational cost.

The proposed approach to modeling the spread of air pollution for a particular urbanized area, adapted for Russian cities (by the example of Volgograd) on the basis of the Calpuff software package will provide more information necessary for making managerial decisions to ensure the quality of the atmospheric air in urban environment.

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