Surface ozone forecasting in a big city (by the example of Moscow)

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The variations of trace gas admixtures on the territory of a big city were analyzed based on the data on routine measurements at the "Mosecomonitoring" network, which allowed us to get new ideas about the inhomogeneity of the field of trace gas admixtures, including surface ozone. The regression models of the daily maximum surface ozone concentration are elaborated for the first time for four types of urban territories, which differ in the level of man-caused stress. Maximum ozone concentration in previous day (inertia) and meteorological pollution potential (MPP) turned out to be the most significant predictors. It is determined that the inertia contribution attains 80–90%, but the MPP index becomes more informative in the events of high ozone concentrations. The MPP index, included in calculation equations, showed its advantage over the use of individual meteorological parameters in statistic models. The calculation equations are obtained for the warm season. A comparison of the calculated maximum ozone concentrations with the inertia forecast showed a success of the methodical forecast.

Introduction

In the last decade, the increased attention is given to monitoring and forecasting of surface ozone. This attention is due to several objective causes.

First, ozone is a toxic air pollutant and in high concentrations it adversely affects the human health and vegetation.[14] It relates to the matter of the first class of hazard. Since the bad air quality is mostly connected with high ozone concentrations,[6,21] the World Health Organization includes ozone in the first five pollutants, concentrations of which are to be controlled when air quality monitoring.

Second, ozone is a key participant of chemical and photochemical reactions in the troposphere, conditioning its oxidation capacity.

Third, total increase of tropospheric and surface ozone is of common concern, as well as the increasing number of events of its enhanced levels observed in wide continental areas of the northern hemisphere. Events of ozone concentrations, exceeding its maximum permissible values (MPC), have become more frequent in Moscow region since the end of 90th of XX century as well.[5,13,20]

Sharp intensification of ozone investigations in the last 15 years is largely connected with appearance of comparatively cheap high-precision off-line operating instruments for ozone measurements.[5,8]

Ozone monitoring system in Western European countries operates under the aegis of the European Environment Agency (EEA). The majority of the stations are situated in contaminated areas. The events of photochemical ozone generation are frequently registered just in such conditions. In 2003, EEA presented data on ozone measurements from 1805 stations, 1624 of them are situated on the territory of the European Union: 497 in rural areas, 857 in urban ones, 139 in industrial regions.

A part of the stations monitors ozone within the EU background monitoring programs (EMEP project "The co-operative program for monitoring and evaluation of the long range transmission of air pollutants in Europe").[17,26] EMEP network was formed in 1979; its activity is aimed at the study of atmospheric composition variability and environmental situation over Europe. At present, the number of stations is over 200, about 100 of them have been operated during more than 10 years. The data quality is examined regularly and thoroughly. The percent of series filling is between 79 and 99%. A similar monitoring network operates also in the USA.

On the territory of Russia, the ozone monitoring is conducted only in a few points. Routine ozone measurements have been carried out by IAP RAS in the region of Kislovodsk (since 1989)[3] and in Moscow (since 2002).[4] IAO SB RAS conducts the measurements in Tomsk since 1991;[23] PGI KSC RAN in cooperation with IAP RAS measure ozone near Apatity town (Murmansk Region) since 1992. Routine measurements in the forest-park suburb of Moscow are conducted since 1991 at the Central Aerological Observatory (CAO) of RosHydroMet. In Moscow, the State Environmental Agency "Mosecomonitoring" monitors ozone since 2002, using the Automated Air Pollution Network (AAPN).

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At present, AAPN includes about 30 observation stations situated virtually in all districts of the city at territories with different technogenic stresses. AAPN monitors trace gas admixtures: carbon oxide, nitrogen oxide, nitrogen dioxide, etc.; 9 stations measure ozone.

In this work, regularities of time ozone variations in different districts of Moscow are analyzed, their correlation with meteorological parameters and AAPN-measured pollution levels is revealed.

The state of the art in the problem

The ozone forecast in countries of Western Europe and Northern America is carried out with the use of the empirical models, based on correlations between ozone levels and meteorological parameters,[25] as well as models of atmospheric ozone transport, including the blocks of photochemical transformations. Well-known foreign models sufficiently good forecast ozone concentrations in Western and Central Europe with an advance time of 1–3 days. Some models disseminate their forecasts to the European part of Russia as well, but according to the expert estimates, model calculations for Russia often have high errors, first of all, due to lack of data on emissions at the Russian territory.

In 1982, regression methods for forecast of surface ozone maxima were suggested in the USA.[15] The regression models are based on correlations between daily maximum ozone concentrations and meteorological parameters; totally, 40 predictors are used.

In Russia, the empirical model for forecasting daily maximum ozone concentrations has been elaborated for the first time at CAO.[10] It is based on linear regression relationships between deviations from ozone concentration "norms" and meteorological predictors. To calculate the "norms" (precisely, their assessments), two complete observation years are enough; it is important that ozone "norms" and all predictors were calculated in the same period. Maximum ozone concentration in previous day, maximum surface temperature, and minimum relative air humidity are the most significant predictors for Moscow. The model is effective if anthropogenic emissions of ozone precursors vary slightly from day to day and from year to year and their scattering is mainly caused by meteorological parameters.[10]

The coefficients of regression between ozone and predictors in the improved version of the model[8,11] depend on the season. To define the quantitative indices of the model, first of all, a good quality of ozone measurements is required, which is provided by modern optical gas analyzers.

Ozone forecasts accounting for only meteorological predictors are more effective for territories distant from considerable sources of pollutants (highways, industrial enterprises), where ozone levels are defined by comparatively well forecasted meteorological parameters, because the effect of pollutants is less.

The quality of the prognostic model was confirmed by its testing on data from the Moscow region and several German stations, participating in the EMEP Program.[6,9,11,22] The most significant predictors in the improved model are the forecasted maximum temperature of the surface air, deviation of ozone level from the "norm" in previous day, relative humidity, and wind speed.

The comparison of the model forecast with measurement data for the Moscow region for 2002 showed that the 24-hour forecast error exceeded 0.032 mg/m^3 (20% of single-time maximum permissible concentration) for the period of the highest seasonal ozone levels not more than in 7% of cases.

In scientific literature, devoted to comparison of ozone in rural and urban areas, the difficulties related to interpretation of measurement results at the territory of a big city are often emphasized.[16,18,19] In this work, the regression model is described, elaborated for Moscow at the RosHydroMet. To analyze spatial ozone variability at the territory of Russia, the data of routine measurements of trace gases were used for the first time; it was shown that the quality of the measurements in Moscow is sufficient for improving the model characteristics. The model was elaborated for the warm season. As distinct to models from Refs. 8 and 11, we approved predictors describing emissions of ozone precursors along with meteorological parameters as predictors. First results of the study are considered in this work.

The used data

The "Mosecomonitoring" AAPN data of routine trace gases measurements in Moscow are first used for elaboration of the urban ozone model.[24] Specifications of the network instruments are described in detail in Ref. 2. Data from AAPN stations with the longest observation series (Kutuzovskiy ave., Mar'inskiy park, Novokosino, and MSU) were used for the elaboration.

Meteorological predictors were calculated from the data of standard ground-based observations and aerological sounding; data of microwave measurements of temperature profiles with MTP-5 instruments were also used.[12]

Variations of trace gases in the city

At the initial stage of the model elaboration, the quality of AAPN data was checked and the uniformity of series was estimated. The division of the city territory into 4 types according to the level of technogenic stresses (adjacent to city transport mains, mixed, dwelling, and reference[1]) was taken into account when analyzing the spatial distribution of trace gases. The AAPN stations, chosen for the analysis, refer to different types: Kutuzovskiy ave. is the area adjacent to the city transport main, Mar'inskiy park is the territory exposed to transport and industrial pollution; Novokosino is the dwelling zone in the east of the city; and MSU is the reference area, i.e., non-affected directly by emissions.

To estimate the degree of inhomogeneity of the surface air pollution in Moscow, mean season concentrations of different pollutants have been calculated for these four territory types. Mean diurnal CO variations at different stations illustrate the inhomogeneity of pollution levels in Fig. 1.

As is seen, pollution levels differ slightly for the territories of different types at late night and day minima while the difference increases 2–2.5 times at the hours of morning and evening maxima.

Diurnal variability of CO concentration (one of the most important ozone precursor) is significant in the city (see Fig. 1) due to, first of all, remoteness of emission sources and microclimate peculiarities. Figure 1 illustrates territorial differences of both absolute values and trends of diurnal variations. Similar patterns are observed also for NO and NO_2 in all seasons. Note that initial concentrations of pollutants (CO, NO) in industrial areas can exceed several times the corresponding concentrations in areas, distant from the pollution sources.

In contrast to ozone precursors, maximum concentration of which is observed at the morning or evening hours, maximum ozone concentrations in the surface air are usually observed in the afternoon. The most interesting maximal contrasts of ozone concentrations in the city fall on the same time. Daily maximum ozone concentrations measured at the four stations in summer 2004 are shown in Fig. 2.

The data analysis has shown, that variations of ozone concentrations at the stations reflect the influence of atmospheric processes of different scales. Day-to-day fluctuations are mainly synchronized at the stations, but sometimes they can essentially differ in absolute value probably due to local emissions.

Selection of meaningful predictors

As it was noted in Refs. 10 and 11, the most meaningful predictor is the inertia factor, i.e., ozone concentration for the day before forecasting. High ozone inertia reflects the standard seasonal variability. According to our assessments, the forecast accuracy is 80–92%. Hence, the factor of inertia is the first in the list of significant predictors. In contrast to the known models, a set of significant parameters includes data on CO and NO concentrations for each station at 9 a.m. of a current day, mean concentrations for the period from 9 a.m. of the previous day to 9 a.m. of the current one, and concentration variations in 6–9 h for each of the three components. Being the ozone precursors, these trace gases determine the rate of ozone generation.

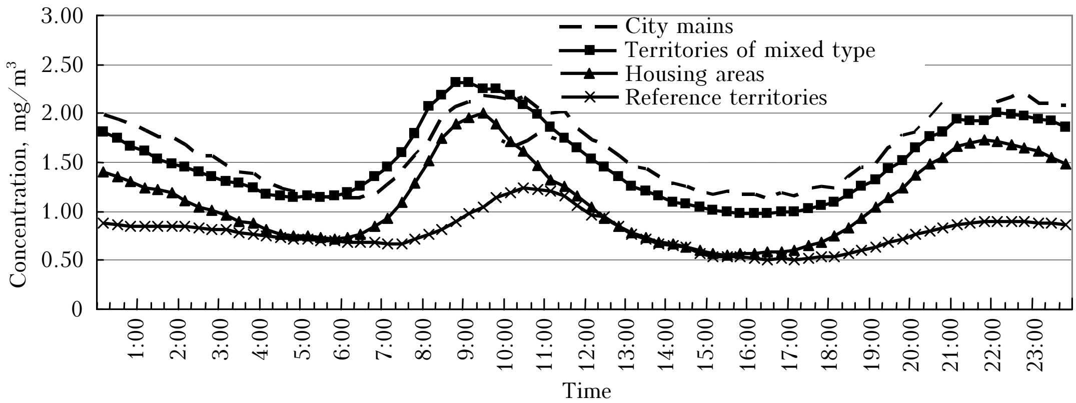

Fig. 1. Mean diurnal variations of CO concentrations. Moscow, September – October, 2005.

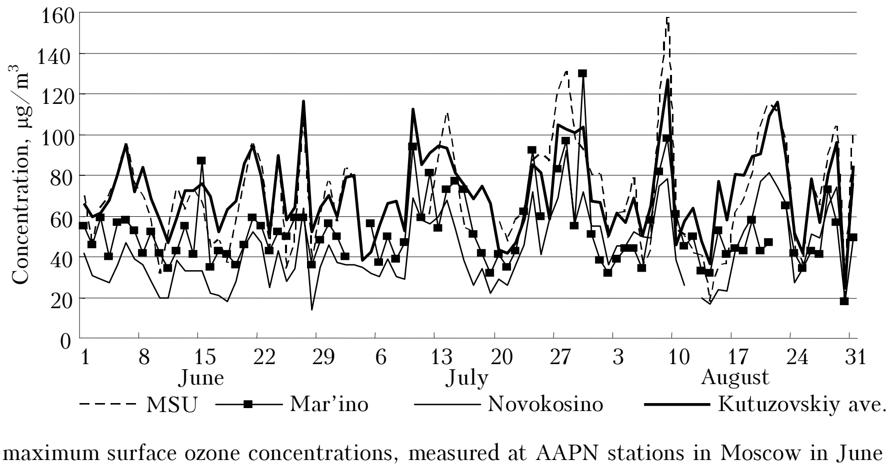

Fig. 2. Daily maximum surface ozone concentrations, measured at AAPN stations in Moscow in June – August, 2004.

Also the city average concentrations of CO, NO, and NO_2, calculated by AAPN stations data, were considered as possible predictors.

To select significant meteorological predictors eight parameters representing the state of the boundary atmospheric layer and large-scale circulation were considered: maximal and minimal surface air temperature, minimal relative air humidity, as well as temperature and wind speed on the 925-GPa constant-pressure surface (about 750 m) in two times: 0 and 12 hours (UT). The numerical value of meteorological pollution potential (MPP) was first use as a predictor; it is based on identification of the combination of weather conditions favorable for formation of abnormal ozone level in the air of Moscow.

It was ascertained, that ozone anomalies, i.e., concentrations exceeding seasonal variations, are connected with some definite type of weather conditions and are observed in the periods of anomalous weather as well. The frequency of ozone anomalies is not high and regular from year to year. Thus, no events of excess of $O_{3\max}$ seasonal levels were observed in June, 2002–2005, while increased ozone concentrations were recorded during six days in June, 2006 in the weather conditions, favorable for the abnormal ozone level.

Recently, the maximal number of abnormal ozone events was recorded in 2002 because of long-term drought and export of combustion products from forest fire cites. Note, that the events of abnormal ozone concentrations are preceded by the weather conditions unfavorable for air purification and are accompanied by the concentration increase of ozone precursors (CO, NO, and NO_2) at night and morning hours.

Taking into account high territorial inhomogeneity of ozone precursors, ozone models were elaborated separately for each station. The most informative predictors for all stations were determined by the step-wise method. The daily maximum ozone concentration is a predictand in the regression models. The most significant predictors entering into the calculation equations are:

1) maximum ozone concentration in the previous day, mg/m^3;

2) MPP index;

3) maximum temperature T, °C;

4) difference between minimum and maximum surface temperature T, °C;

5) minimum relative air humidity, %;

6) 925-GPa temperature at 12 p.m. and 12 a.m. T, °C;

7) 925-GPa wind speed at 12 p.m., m/s.

As was expected, the maximum ozone concentration in the previous day (inertia predictor) turned out to be the most significant predictor for all equations. This agrees with the most effective predictor in the ozone forecast models,[10,11] as well as maximum surface temperature $T_{\max}$ and minimum relative humidity H. Note, that the MPP index was the second by significance predictor. A set of meteorological predictor and predictors – ozone precursors in the obtained calculation equations was individual for each station, i.e., a unique calculation equation for the city was not obtained.

In general, sets of meteorological predictors at the stations are similar, but the contribution of each predictor can vary for different stations. Ozone precursor predictors are individual for each station.

Discussion of the results

The suggested synoptic statistical model is based on correlations between daily maximum ozone concentrations with meteorological parameters and anthropogenic emissions of ozone precursors.

The calculations were carried out for the warm season (from April to September), when diurnal ozone variability is the highest. In the cold season, daily maximum ozone concentrations vary insignificantly in Moscow, maximum values virtually never exceed 0.08 mg/m^3, which is half as low as $MPC_{o.-t}$ (0.16 mg/m^3).

Several models have been elaborated for each station using the method of multiple step-by-step linear regression. The most relevant models have been chosen from the analysis results and by model statistical factors. The general form of the equations is the following:

$$O_{\max} = a_1 O_{3\max}(d-1) + \\ + a_2 \mathrm{MPP} + a_3 T_{\max} + a_4 H + \ldots + a_5 P + a_0,$$

where $O_{3\max}$ is the calculated daily maximum ozone concentration; $O_{3\max}$ $(d-1)$ is the daily maximum ozone concentration in the day before the forecast; MPP is the MPP index; H is the minimum relative air humidity; P is the CO, NO, and NO_2 concentration/variation in the period 6–9 h; a_0, a_1, ... are the regression coefficients.

Prognostic equations with local and city-average levels of CO, NO, and NO_2 have been obtained for each station for the warm season as a whole and for spring and summer separately.

The most effective calculation equations have been obtained for the MSU station distant from direct pollutant sources; they describe from 72 to 80% of $O_{3\max}$ dispersion. Less than 50% of the variability falls on the inertia. Ozone precursors describe up to 6% of the variability. The comparison of measured and model $O_{3\max}$ concentrations for the MSU station in June–August, 2002 are given in Fig. 3.

As is evident, the model, accounting for the local level of $O_{3\max}$ precursors (RM_{loc}), reflects $O_{3\max}$ variability better than the model with city-average levels of precursors ($RM_{c.-av}$). The latter noticeably overestimates $O_{3\max}$ values except for several days in July, 2002 (8, 13, and 29–31) when extremely high surface ozone concentrations were recorded due to advection of precursors and photochemical ozone generation.[7]

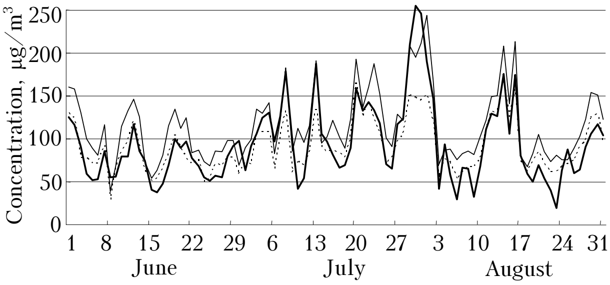

Fig. 3. Measured and model ozone concentrations at the MSU station (thick line corresponds to the measured O_{3max} concentrations, thin line – to the values calculated by the RM_{loc} model, and the dashed one – to the values calculated by the $MP_{c.-av}$ model).

The comparison of calculated and measured ozone concentrations has shown that the calculation errors exceeding 0.032 mg/m^3 (20% of the single-time $MPC_{o.-t}$) for the RM_{loc} model cover 3–6% of cases; the calculation errors for the $RM_{c.-av}$ model sharply change from year to year: they make up less that 1% in 2005 and 33% in 2002.

Inertia at the Mar'inskiy park station (mixed type of the territory) has been the most significant comparative to all other stations, it describes up to 60% of O_{3max} variations. The introduction of predictors (ozone precursors) allows the prognostic properties of the equations to be enhanced by 4–6%; in this case, the use of precursors of both local and city-average levels gives similar results showing that the station is close to "city average" ones by the air pollution. In contrast to reference territories, seasonal models (individually for spring and summer) have shown that the contribution of the inertia factor during spring is higher (63–70%) than in summer months, when it decreases to 47–54%. High inertia contribution in spring period reflects the principal mechanism of ozone export from the upper troposphere into the surface layer through vertical exchange. The decrease of the inertia contribution in summer along with the increase of significance of meteorological predictors and ozone precursors (from 6 to 17%) confirms the essential influence of ozone photochemical generation in summer, when the weather conditions, favorable for the surface air pollution increase, become more frequent.

The estimates of calculation errors show that forecast errors, exceeding 20% of $MPC_{o.-t}$, made up 2% with accounting for both local and city-average predictors in 2005, when the weather conditions, favorable for abnormally high ozone concentration, were not observed. In other years, the errors with the above allowance vary between 5 and 8.5%.

The Novokosino station (dwelling area in the east of the city) is the only station, where the accounting for ozone precursors of the city-average level gave better results in comparison with the local one. This indicates that ozone formation in this area is often influenced by the city pollution plume. This model describes up to 71% of ozone variations, where 56% falls on the factor of inertia, 2–3% determine the pollution parameters. In average, forecast errors exceeding 20% of the single-time MPC, are about 6% for the model using the precursors of the moderate city level and 7.5% for the model using the local-level ones.

According to model estimations, meteorological predictors describe up to 22% of maximum ozone concentration variations at the station situated near the city mains (Kutuzovskiy ave.) while the factor of inertia – up to 34–50%, i.e., less than at the other stations. Such a low inertia share reflects the fact that fluctuations of both primary and secondary pollutants near city mains depend on the traffic intensity, while significant variations are influenced mainly by large-scale atmospheric processes. In average, the model errors, exceeding 20% of the single-time MPC, make 2–7% for this station. There were not revealed essential differences in the accuracy between the models accounting for ozone precursors of city-average and local levels.

Finally note that calculation equations, obtained for all stations, have advantages over the inertia forecast. The accuracy of methodical and inertia forecasts for 3 years are presented in the Table below.

Table. Accuracy of the inertia (column 1) O_{3max} forecast and values calculated with the local-level precursors (2), %

Year	MSU		Mar'inskiy park		Novokosino		Kutuzovskiy ave.	
	1	2	1	2	1	2	1	2
2003	82	94	91	92	91	92	–	–
2004	89	95	88	92	88	92	86	98
2005	84	97	97	98	97	98	83	93

The table data show that the calculation methods mostly surpass the inertial forecast at the reference station (MSU) and the most "polluted" one (Kutuzovskiy ave.) – up to 10–13%. At a general high accuracy of the inertia forecasts, they differ by 3–9% from year to year while this difference is 1–6% for the methodical ones. Such essential variability of the inertial forecast is due to, first of all, a variety of weather conditions in different years. Thus, in 2005, when the weather conditions, favorable for abnormal ozone, were not observed, the inertia was 97% at two of the four stations, while in anomalous 2002, the accuracy of the inertial forecast was not more than 74% at the MSU station.

It is stated, that the accuracy of the inertia forecast decreases just in the period of high ozone concentrations. Figure 4 shows the measured O_{3max} concentrations and the deviations of the calculated values from those, measured in July–August, 2004 at four city stations.

O_{3max} concentrations, measured at the stations, are evidently well agree, reflecting general regularities of O_{3max} variations under the influence of significantly varying weather conditions. The highest concentrations were measured at the reference station while the lowest ozone content in the afternoon was recorded at the Novokosino station, which can be connected with the location of this station in the "climatic" pollution plume of the city.

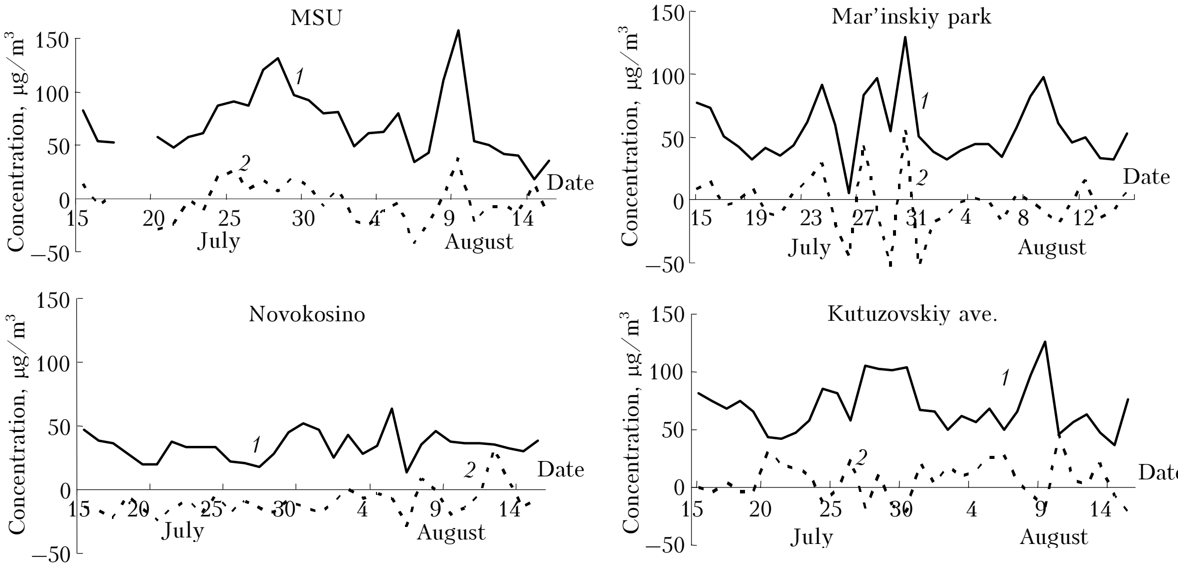

Fig. 4. Measured maximum O_3 concentrations (curves *1*) and model calculation deviations in the period from July 15 to August 15, 2004 (curves *2*).

The calculation errors for the Novokosino station never exceeded 20% of the single-tine MPC (32 mg/m^3); at the MSU station, it exceeded this threshold only on August 9. Note that simultaneous increase of ozone content in the surface air was recorded this day at all stations under anomalous weather conditions (see Fig. 4). A maximum calculation error took place at the station, where the highest O_{3max} level (close to $MPC_{o.-t}$) was recorded; maximal values at other stations were forecasted by the calculation equations with a high accuracy.

Next day, August 10, the weather conditions sharply changed. The deviations of calculated values from the real ones significantly increased due to the contribution of the inertia predictor; the calculation error at the Kutuzovskiy ave. station exceeded 20% of the single-time MPC; the smallest error was at the MSU station where the inertia contribution to the calculation equation was the smallest.

This episode shows that the variability of ozone content on the city territory is insignificant under typical-for-season weather conditions and is well identified by the inertia forecast. The range of city ozone concentrations extends on the city territory in the weather conditions favorable for seasonal anomalies; in this case, the accuracy of inertia forecast sharply decreases.

Conclusions

Data of routine monitoring of trace gases in Moscow allows us to obtain some new ideas about inhomogeneity of the field of surface air pollution in a big city. It has been shown, that ozone concentrations at the city territory can significantly differ from the mean values; under the weather conditions, favorable for abnormal ozone level formation, differences in surface ozone concentrations between districts can attain 0.07 mg/m^3 and even more.

Calculation equations have been obtained for the warm season for four types of territory differing in the level of technogenic stress. We failed to obtain a universal equation for all territory types. This indirectly points out to the fact that ozone variability in a big city depends not only on large-scale processes and local weather conditions, but on the intensity of technogenic stresses in the area, where the station is situated. The obtained calculation equations represent the characteristic variability of maximum ozone concentrations at the city territory subject to, first of all, the factor of inertia and ozone precursors.

It has been shown that the contribution of the inertia factor to the ozone variability is 45–60%; the contribution of inertia decreases from reference territories to the most polluted ones. The complex identification of meteorological conditions of pollution, used as a pollution predictor for the first time, has shown its advantage over the use of individual meteorological parameters. The MPP index describes from 5 to 20% of ozone variability. The most significant predictors in the calculation equations serve the inertia factor and MPP. Predictors, describing ozone precursors, increase the calculation accuracy of maximum ozone concentration in the city from 2 to 6%; their role becomes more important in conditions favorable for formation of abnormal ozone levels.

The obtained equations are supposed to be used for calculating maximum ozone concentrations in the warm season in Moscow in periods of anomalous weather conditions. It is important that all predictors from the calculation equations can be obtained from on-line data.

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