Evaluation of Background Concentrations of Tropospheric Ozone Using Dynamic Phase Portrait Methodology

Aleksandr Khaustov and Margarita Redina

Abstract

The study aims to estimate the applicability and precision of a methodology for identifying the background concentration of ozone. These values are necessary to estimate a maximum permissible emission value, understand the population's health risk level, and evaluate the activity of ozone sources (first of all man-made). Currently applied state-approved methods have some limitations; thus, applying a new methodology based on the time variations of impurity concentration is of research and practical interest. Research objects are concentrations of tropospheric ozone in Moscow (anthropogenic polluted atmospheric air, mostly because of the transport activity) and in the settlement with relatively low pollution levels. Initial data are the results of the continuous records of concentrations of ozone, its precursors, and meteorological parameters from the ozone monitoring network. The methodology tested in this study to identify a background ozone concentration is the dynamic phase portrait method, considering variations of changes in concentration during the time. The value obtained presents the concentration of tropospheric ozone most characteristic of the studied location. The background concentration value obtained using the tested methodology is more consistent with the values calculated using the state-approved methodology the longer the observation period is. Furthermore, the values identified make it possible to consider the peculiarities of the distribution of pollutants and the complex meteorological factors in a particular territory and to abandon the standard values assigned.

A. Khaustov (✉) · M. Redina
Peoples' Friendship University of Russia (RUDN University), Moscow 117198, Russia
e-mail: khaustov-ap@rudn.com

Keywords

Ozone · Background concentration · Tropospheric · Monitoring · Phase portrait

1 Introduction

Tropospheric ozone is one of the strongest toxicants, causing significant negative effects on human health and ecosystems. Its sources in the troposphere are natural and anthropogenic; a complex set of factors causes the concentrations.

The purpose of the study was to determine background concentrations of tropospheric ozone. This is a basis for assessing the well-being of territories and establishing norms for acceptable emissions of pollutants that are precursors of ozone or potential sources of dangerous pollutants during oxidation processes with the participation of ozone. A currently applied state-approved method has a set of limitations (size of a data set, averaging algorithm). For the locations where the monitoring system is not developed enough, some prescribed values are to be applied for the environmental regulation. Thus, a new approach will be suggested and tested for this particular task.

2 Objects of the Study

The objects of the study are the characteristics of atmospheric air of urban areas in the European part of Russiawith different levels and sources of pollution—concentrations of tropospheric ozone. Two locations are considered: Moscow (mainly emissions of precursor substances by transport) and the district center Krasnye Polyany (emissions of precursors by industrial and municipal facilities). The data were obtained from the continuous measurements by the ozone monitoring network stations (every 20 min, records of concentrations of ozone, nitrogen oxide, PM_1, PM_4, PM_{10}, hydrocarbons total, methane, and meteorological

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parameters, as presented in the study (Andreev et al., 2020)) for November 1–30, 2021. Thus, the total data sets counted 2160 measurements for each parameter for each location. Such a data set size allows us to obtain reliable statistical estimations.

3 Methods of the Study

The background ozone concentration in our study is determined using the method of dynamic phase portraits (Trofimchuk, 2018): the trajectory of changes in the O_3 concentration C and the speed of this process dC/dt is analyzed. This allows us to identify stable and unstable states of the system (the distribution of O_3 in the troposphere), time characteristics, critical points (indicators of the system's transition from one stable state to another), and attractors on the O_3 changes trajectory. The method of phase portraits is common in the study of natural systems. The essence of this method is to estimate the dynamics of the analyzed value over time: a spline function is constructed that reflects the ratio of the concentration increment per unit of time (Y-axis) and the actual concentration (X-axis). In addition, the attractor points to which the O_3 concentration tends are identified; the intersection point of the approximation line for the constructed phase portrait with the abscissa axis corresponds (in our case) to the desired value of the background concentration.

To build the dynamic phase portrait, the initial data sets were processed, and the median values of the ozone concentration were calculated:

- the daily to identify the monthly background concentration, and
- the hour medians—to identify the daily background concentration.

The daily background concentrations for both the studied locations were calculated for the typical date. A cluster analysis (single linkage method, Euclidean distances) was applied to determine such a date. These are representative days, during which variations in meteorological parameters and measured concentrations of substances reflect the changes in these values for each of the 30 days (November 1–30, 2020) considered. For Moscow and Krasnye Polyany, a typical day was selected for November 30. On the cluster dendrograms, this day is in the center of the group of considered dates.

The obtained value presents a *local background*: this is the most typical value of the O_3 concentration for the vicinity of the control point (and not the value formed on the “background, that is, clean territory”).

4 Results

As a result of the data processing, patterns of daily and monthly dynamics of ozone concentrations for both cities were identified. The reasons for their differences from the dynamics of other regions were evaluated. A slight dependence of the concentration variations on the solar radiation intake in both cities was revealed.

The values of the average monthly (median) background O_3 concentrations were obtained. They were relatively close (about 0.015 mg/m^3 in Moscow and Krasnye Polyany), despite the differences in the volume of anthropogenic loads in both urban areas (Fig. 1a, b). The data processing operations can probably explain such a matching: in this case, we analyze the daily median concentrations.

Similar estimations were obtained for “typical days” (Fig. 1c, d), November 30.

As can be seen from the graphs, the values of the background ozone concentration for the technogenically loaded territory (Moscow; Fig. 1c) was 0.029 mg/m^3, and for the “background” one, 0.024 mg/m^3 (Krasnye Polyany; Fig. 1d).

5 Discussion

In all the considered cases, the values of background concentrations in both settlements do not exceed the national values of the maximum permissible concentration for residential areas (0.030 mg/m^3).

Estimations of the correlation of O_3 concentrations with meteorological parameters and concentrations of other controlled substances showed significant and strong relationships: negative—with NO, CO, dust particles, and air humidity (probably, O_3 is consumed for the oxidation of gaseous, dissolved, and sorbed on the PM impurities); positive—with wind speed (probably due to the intensification of gas exchange and the influx of new precursor substances).

At the same time, the dependence of the ozone concentration on the magnitude of the arrival of solar radiation was not revealed. One of the possible reasons is the generally low solar activity during the study period for both points. Also, the analysis of the daily dynamics showed clear peaks of concentrations in the morning for both monitoring points. On the other hand, some studies show morning lows, especially in Asian regions (Arshinov et al., 2015; Héroux et al., 2013; Zhamsueva et al., 2013). Therefore, a possible explanation is the differences in the receipt of solar radiation in the European and Asian territories.

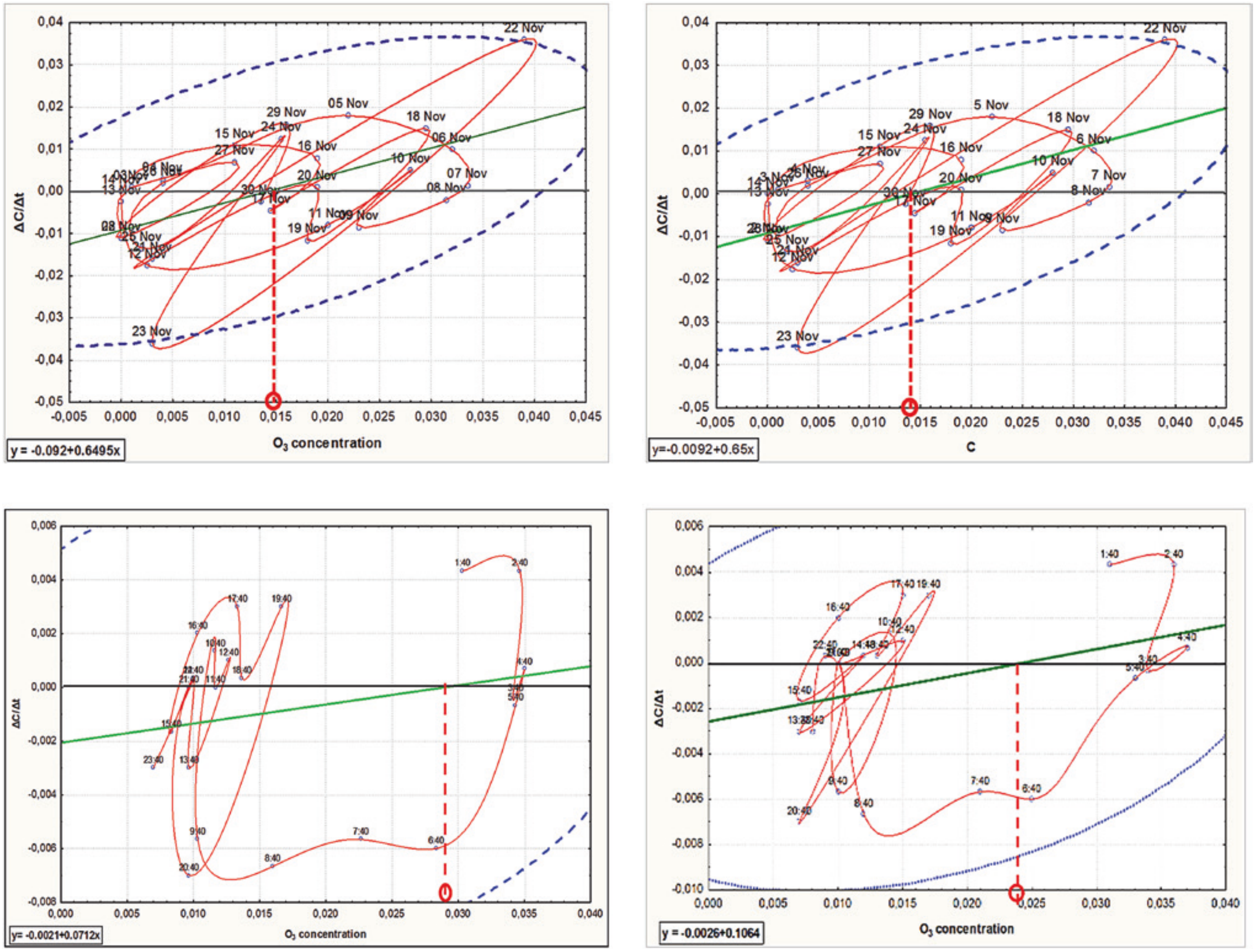

Fig. 1 Phase portrait of ozone concentrations by median values: for November 1–30, 2020, for a technogenically loaded (**a**) and relatively safe (**b**) territory and for a typical day (November 30, 2020) for a technogenically loaded (**c**) and relatively safe (**d**) territory

6 Conclusions

No excess of background values over the MPC was established for both considered locations. However, in the conditions of a large city, the concentrations are higher due to the presence of precursor substances (mainly nitrogen oxides and hydrocarbons) coming from anthropogenic sources (transport), which is proved by the complexity of the phase portraits.

This leads to the need for more detailed studies and monitoring of tropospheric ozone to understand the chemical processes of atmospheric transformation, especially under anthropogenic influences on air quality.

The results obtained in this study present a state of atmospheric pollution for only one month and for one typical day as "test periods". Nevertheless, the study shows this method's applicability for identifying the most typical atmospheric situations—forming local background concentrations of substances.

The phase portrait method demonstrates its effectiveness for these purposes based on continuous observations. Furthermore, it can be used in practice to regulate local anthropogenic loads. This allows us to consider the peculiarities of the distribution of pollutants and the complex meteorological factors in a particular territory and to refuse the assigned regulatory values. This can be a new flexible air quality regulation approach depending on local conditions.

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