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A model for calculation of the air quality index for ozone

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Abstract
In the present paper, the influence of the atmospheric photochemical process and the products formed on pollutants concentrations were studied and analyzed. Models were developed for calculation of the air quality index (AQI) for ozone using the data on the total solar radiation at three monitoring sites in the municipality of Burgas: Automatic measuring station (AMS) Meden Rudnik, AMS Dolno Ezerove and OPSIS DOAS. The comparatively high levels of ozone concentration are an important problem for the while district which requires new quantitative methods to be develop for studying and control of the AQI with respect to this quite important pollutant or our city. The tests and measurements performed showed that the model developed provides suitable way for quantitative estimation of the relationship between the total solar radiation and the ground level concentrations of ozone in the atmospheric air.
Keywords: *Atmospheric chemistry, Air pollution, Ozone, Air quality index (AQI), Total solar radiation, Coefficient of determination, F - statistics.*

1. Introduction

Air pollutants can have serious consequences for human health and environment deterioration. The overall state of the atmospheric air is determined using the properties defined in article 4 of the Clean air act [1]. The AQI for the municipality of Burgas [2] is calculated on the basis of 6 of the controlled air pollutants: nitrogen dioxide, sulfur dioxide, particulate matter, hydrogen sulfide and styrene.
Preservation of atmospheric air purity is one of the main tasks and major concern of the whole society [3,4]. As far as air is one of the main components of the environment, monitoring and control of its quality is of crucial importance. In this respect, the main goals are preservation of air quality in “clean” areas and taking measures to improve its quality in areas where the standard requirements are not met [5].
The preservation of air quality is based on the principles of sustainable growth and Bulgaria, as member state of the European Union, has synchronized its national regulation acts in the field of AQI preservation with the European directives [6]. However, the influence of the atmospheric photochemical processes and the products formed on the concentrations of the pollutants was not studied and analyzed.
The studies on the effects of the total solar radiation on some atmospheric air pollutants and the photochemical processes taking place are important for the preservation of both human health and the environment.
In the present paper, an analysis of the interrelation between the ozone concentration In the atmosphere and the total solar radiation is made. Models were developed for calculation of the air quality index (AQI) for ozone using the values of the total solar radiation measured at three monitoring sites in the municipality of Burgas: AMS Meden Rudnik, AMS Dolno Ezerovo and OPSIS DOAS. An important problem for the region is the high level of ozone which requires the development of new quantitative methods to study this air pollutant.

2. Materials and Methods

The air quality index (AQI) is focused on the possible concequances fo the human health which can appear within couple of hours or days after breathing the polluted air. For the municipality of Burgas, the AQI index is calculated using six air pollutants monitored: nitrogen dioxide, sulfur dioxide, particulate matter, hydrogen sulfide, ozone and styrene. The methods of the US Environment protection agency were used [7,8]. The values of AQI, the corresponding requirements of the Standards for protection of human health and the colors used for visualization are according to the definitions of the US EPA. AQI values higher than 300 indicate for critical risks for human health and high possibility that all the population will be affected.
The AQI is determined by the formula [1]:

$$x = \frac{a}{M}, \qquad (1)$$

where: a – measured concentration, $\mu g/m^3$ or mg/m^3; M – Standard for protection of human health. AQI value for the six main air pollutants is shown at the web page of the municipality of Burgas [2] and it is refreshed every other hour.
The intensity of the solar radiation decreases by ca. 25–30% while passing through the earth atmosphere. The reasons for this are the dispersion and absorption by the atoms and ions of atmospheric gases (oxygen, hydrogen, nitrogen, ozone, carbon dioxide, etc.). The degree of decrease of the solar energy flow can be described by the law of Bouquer-Lambert [9], which can be written as follows:

$$\frac{G_i}{G_0} = c_i + f_i.e^{-\frac{P_i}{sinh}}, \; i = 1, 2, 3 \qquad (2)$$

where: G_i – the total solar radiation at monitoring site i, W/m^2; i = 1, 2, 3 (for AMS Dolno Ezerovo, AMS Meden Rudnik and DOAS OPSIS);

G_o – the total extraterrestrial solar radiation (Total global insolation), W/m^2;

$P_i = \frac{C_i}{180}$ – AQI for ozone at site i;

C_i – monthly average concentration of ozone for 2012 at site i, $\mu g/m^3$;

C_o = 180 $\mu g/m^3$, standard for protection of human health for measurement period of 1 h, Threshold for informing the population (TIP);

h – height of the Sun, *degree*;

c_i and f_i – coefficients.

The total global insolation G_o can be determined from the relationship of Klein [10,11]

$$G_0 = \frac{24}{\pi}.I_{sc}.\left(1 + 0.033.cos\left(\frac{360.d}{365}\right)\right).\left(cos\,\phi.cos\,\delta + \frac{\pi.\omega_s}{180}sin\,\phi.sin\,\delta\right)$$

(3)

where: ϕ – longitude, *degree*;

δ – declination, *degree*;

I_{sc} – solar constant, (I_{sc} = 1367.7 W/m^2);

ω_s – hour angle of the sunrise, *degree*;

d – day of the year. Usually, d is assumed to be the 15th day of the month and solar declination is calculated for that date.

After some mathematical transformations, formula (2) can be written as follows:

$$P_i = -sinh.ln\left(b_i + a_i\frac{G_i}{G_0}\right), \qquad (4)$$

where: $a_i = 1/f_i$ and $b_i = -c_i/f_i$.

The coefficients b_i and a_i taking part in eq.(4) are determined by regression analysis from experimental data [12,13,14].

For the calculation of the air quality index for ozone and the total solar radiation, regression models of power of 11 and 6, respectively, were developed:

$$G = a_1t + a_2t^2 + a_3t^3 + a_4t^4 + a_5t^5 + a_6t^6 + b, \qquad (5)$$

$$P = a_1t + a_2t^2 + a_3t^3 + a_4t^4 + a_5t^5 + a_6t^6 + a_7t^7 + a_8t^8 + a_9t^9 + a_{10}t^{10} + a_{11}t^{11} + b, \qquad (6)$$

where: G – total solar radiation per unit area per unit time, W/m^2;

b, a_1, a_2, ..., a_6 – regression coefficients;

t – time; P is the AQI for ozone, %.

For the estimation of the quality of the regression models, the coefficient of determination R^2 was used which shows the proportionality of the linear dependence between the regressors included in the model and the predicted value of the initial variable. The significance of R^2 is checked by the criterion of Fisher [15,16]

$$F = \frac{R^2}{(1-R^2)}.\frac{(N_1 - k)}{(k-1)}, \qquad (7)$$

where: k – number of the estimated parameters of the model;

N_1 – the size of the sample of experimental data.

The Fisher criterion has degrees of freedom $v_1 = k - 1$ and $v_2 = N_1 - k$.

At $F > F(\alpha, v_1, v_2) = F_{crit}$, the value of R^2 is considered to be significant and it can be used for estimation of model adequacy. The higher the calculated value of R^2 the more reliable is the regression model.

3. Results and discussion

In the present paper, models for calculating the air quality index (AQI) for ozone from the total solar radiation measured at three monitoring sites in the municipality of Burgas: AMS Meden Rudnik, (European code BG0063A), AMS Dolno Ezerovo (European code BG0044A) and OPSIS DOAS (European code BG0056A). The comparatively high ozone concentrations are an important problem of the region so new quantitative methods for studying and controlling the AQI for this important for the city pollutant must be developed.

For the calculation of the total solar radiation at the monitoring sites in the municipality of Burgas, data obtained from Solar Radiation Databases [17] were used. The measured values cover a period of 12 years and the interval from 4.87 to 19.87 *h* at steps of 0.25 *h*.

The regression model for the total solar radiation includes one factor – time, but with regressors up to power of 6. The regression coefficients were determined for the individual monitoring sites for each month of the year.

For the calculation of the AQI for ozone by regression equation (6), data on the hourly average values of ozone concentration at the three monitoring sites on monthly basis. The monthly average concentrations were calculated for the interval from 8 to 17 h which is the minimal monthly average of sunshine.

The coefficients of determination R^2 for the estimation of the quality of models (5) and (6) for the three monitoring sites in the municipality of Burgas studied (AMS Meden Rudnik, AMS Dolno Ezerovo and OPSIS DOAS) on monthly basis are presented in Table 1.

Table 1. Coefficients of determination for models (5) and (6) for AMS Meden Rudnik, AMS Dolno Ezerovo and OPSIS DOAS

Month	AMS Meden Rudnik		AMS Dolno Ezerovo		OPSIS DOAS	
	AQI for ozone	Solar radiation	AQI for ozone	Solar radiation	AQI for ozone	Solar radiation
January	0.9415	0.9976	0.9739	0.9988	0.9563	0.9977
February	0.9801	0.9951	0.9564	0.9951	0.9135	0.9958
March	0.9590	0.9967	0.9503	0.9963	0.9164	0.9964
April	0.9602	0.9964	0.9841	0.9964	0.9182	0.9962
May	0.9273	0.9968	0.9540	0.9968	0.9475	0.9967
June	0.9533	0.9969	0.9960	0.9969	0.9839	0.9968
July	0.9663	0.9973	0.9887	0.9974	0.9782	0.9975
August	0.9791	0.9970	0.9937	0.9970	0.9801	0.9969
September	0.9707	0.9965	0.9773	0.9965	0.9677	0.9964
October	0.9887	0.9966	0.9530	0.9966	0.9448	0.9967
November	0.9603	0.9968	0.9933	0.9969	0.9424	0.9970
December	0.9723	0.9967	0.9680	0.9964	0.9118	0.9965

It can be seen from Table 1 that the values of the coefficients of determination are very close to unity (R^2 > 0.99) which was considered enough to conclude that the models are of good quality and reliability. The values of the F-criterion obtained were higher than the critical value. At AMS Dolno Ezerovo, for instance, the total solar radiation for January was 5802.31 and the AQI for ozone – 407.19. The critical value is from 2.27 to 2.42. The orders for the other months and the other sites are similar.

The statistical estimation performed means that the regression equations (5) and (6) derived are suitable for use to predict the AQI for ozone and the total solar radiation.

To calculate the AQI for ozone as a function of the degree of dissipation of the energy flow (expressed by the ratio total solar radiation / total global insolation), formula (4) was adapted individually to the data obtained from the three monitoring sites in the municipality of Burgas.

The values of the regression coefficients calculated for eq.(4) for AMS Dolno Ezerovo, AMS Meden Rudnik and OPSIS DOAS are given in Table 2.

Table 2. Regression coefficients in eq.(4) for the monitoring sites

Monitoring site	Model 4

AMS Dolno Ezerovo	$P_1 = -sinh.ln\left(-0.6269807848\dfrac{G_1}{G_o} + 0.9710363805\right)$
AMS Meden Rudnik	$P_2 = -sinh.ln\left(-1.1907960702\dfrac{G_2}{G_o} + 1.3380350164\right)$
OPSIS DOAS	$P_3 = -sinh.ln\left(-0.4910842098\dfrac{G_3}{G_o} + 0.8420852738\right)$

Table 3. Coefficients and quality parameters of model (4) for the individual monitoring sites in the municipality of Burgas.

Monitoring site	Coefficients	Standard error	Fisher coefficient F	Coefficient of determination R^2
AMS Dolno Ezerovo	b = 0.117301 a = -0.690685	0.0106 0.0232	887.04	0.9042
AMS Meden Rudnik	b = 0.072172 a = -0.75386	0.0119 0.0246	936.19	0.9096
OPSIS DOAS	b = 0.066555 a = 0.747874	0.0123 0.0236	998.33	0.9148

In Table 2, P_1, P_2, P_3 – AQI foe ozone for the corresponding sites, %; G_1, G_2, G_3 – the total solar radiation for the sites, W/m^2; G_0 – total global insolation calculated by formula (3), W/m^2.

Table 3 shows the values of the coefficient together with the quality parmeters of the models derived for the sites, calculated by the Fisher criterion (7).

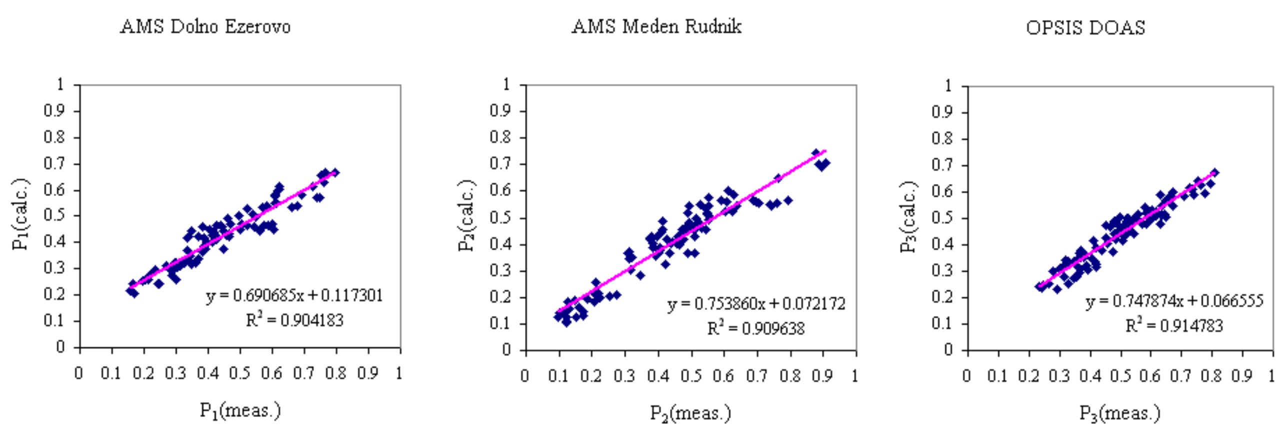

Fig.1. Values of AQI for ozone measured and predicted by model (4) for the three monitoring sites in the municipality of Burgas (AMS Dolno Ezerovo, AMS Meden Rudnik and OPSIS DOAS)

For all the monitoring sites, the coefficient of determination R^2 was significant and its value is higher than 0.9 which indicates that the method can be used for analysis and prediction.
Fig.1 illustrates the comparison between the values of AQI for ozone measured and predicted by model (4) for the three monitoring sites in the municipality of Burgas (AMS Dolno Ezerovo, AMS Meden Rudnik and OPSIS DOAS).
The models developed clearly shows the tendencies and the relationship between the ozone concentration (AQI for ozone) in the atmosphere and the total solar radiation and can successfully be used for quantitative estimation and prediction.
Ozone is a major air pollutant and, furthermore, as far as practically all of it is product of atmospheric processes, its concentration (AQI for ozone) indicates for the degree of air pollution in a region.

4. Conclusions

Based on the results obtained and the discussion above, the following conclusions can be made:
The paper presents models derived for calculation of the air quality index (AQI) for ozone using data on the total solar radiation at three monitoring sites (AMS Dolno Ezerovo, AMS Meden Rudnik and OPSIS DOAS) in the municipality of Burgas. Values of AQI for ozone measured and predicted by model (4).
A statistical estimation of regression models for the total solar radiation (5) and AQI for ozone (6) was made. The values of the coefficients of determination were close to unity ($R^2 > 0.99$) which was enough to conclude that the models are of good quality and reliability. The valus obtained for the F-criterion were higher than the critical value. For AMS Dolno Ezerovo, for instance, the total solar radiation for January was 5802.31 and the AQI for ozone – 407.19. The critical value is from 2.27 to 2.42. The orders for the other months and the other sites are similar.
The statistical estimation obtained means that the equation derived (5) and (6) can be used to predict the values of the AQI for ozone and the total solar radiation.
To calculate the AQI for ozone as a function of the degree of dissipation of the energy flow (expressed by the ratio total solar radiation / total global insolation), formula (4) was adapted individually to the data obtained from the three monitoring sites in the municipality of Burgas.
For all the monitoring sites, the coefficient of determination R^2 was significant and its value is higher than 0.9 which indicates that the method can be used for analysis and prediction.

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