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Development of a short–term ozone prediction tool in Tirana area based on meteorological variables

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ABSTRACT

The short–term prediction of near surface ozone levels is very important due to the negative impacts of ozone on human health, climate and vegetation. The objective of this paper is to develop and test an analytical model that could be applied to predict next day's maximum ozone concentration for the first time in Tirana, Albania, where ozone's monitoring has been recently started. The relationship of the daily maximum hourly ozone values with meteorological variables, including near surface air temperature and relative humidity and with air pollution variables like the persistency of ozone levels and its seasonal variation is examined. The data analysis reveals that the pollution persistency and the near surface air temperature are the factors that mainly affect the peak ozone levels. Multiple linear regression analysis has been performed to establish the relationship between the above mentioned parameters and peak ozone concentration. The agreement between observed and predicted daily maximum hourly ozone values is very good, with a correlation coefficient (R) of 0.87. The model slightly under–predicts the ozone concentration while no significant mispredictions are observed. Additionally, the model's ability to predict the exceedances of a specific ozone limit value is examined. The model successfully predicts the exceedances of 105 μg m^{-3}, a value that corresponds to the 75th percentile, in the 86% of the cases applied.

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1. Introduction

Ozone is a highly reactive chemical oxidant that induces various adverse health effects, generating also significant economic consequences. It can affect the respiratory system of humans and animals and can cause lung inflammation (Cole, 1996; Heinsohn and Kabel, 1999). It also impacts on agricultural yields, as even low ozone concentrations are associated to foliar injury and crop loss (Krupa et al., 1998). Moreover, ozone can accelerate materials' decay and discoloration (Heinsohn and Kabel, 1999). Additionally, ozone is a greenhouse gas and can lead to global warming by trapping infrared radiation emitted by the earth surface (National Research Council, 1991).

European Union (EU) has established air quality standards regarding the ambient ozone concentration. Directive 2008/50 defines information and alert thresholds that refer to hourly values and equal to 180 and 240 μg m^{-3}. The same Directive also defines a guideline for the protection of human health. According to the Directive, the daily maximum 8–hour mean value should not exceed the target value of 120 μg m^{-3} on more than 25 days per calendar year in a three–year period.

Several studies have been conducted aiming to develop tools capable to achieve short–term forecast of ozone levels. Some of them are cited in Table 2, later in this paper. The analysis often focuses on investigating whether or not a threshold is exceeded. Such information could be exploited by environmental and medical authorities to announce public health warnings. A common method widely used when developing prediction models is to correlate meteorological and pollution data with the concentrations of a certain pollutant. The parameters used in analytical modeling are chosen so as to represent the meteorological conditions that don't favor the dispersion of pollutants and to a certain degree, the short–term variations in emissions.

The objective of this study is to develop an analytical model in order to produce the forecast of the next day's daily maximum hourly value (DMHV) of ozone concentration in Tirana. The model relates the forecasted DMHV of ozone concentration in Tirana with various meteorological and pollution variables. Moreover, this study provides statistical information about the ozone levels in the suburbs of the capital city of Albania. This is the first paper in the international literature that deals with the ozone levels and their prediction in Tirana, where ozone monitoring has just recently been started. Additionally, it is the first study that examines the relation between ozone levels and meteorology in the area. The study of this relationship in Tirana is interesting as the greater area is characterized by complex topography that influences air flows and consequently pollution levels.

2. Study Area and Observational Data Used

2.1. Study area description

Tirana is located at the central part of Albania. Approximately 800 000 inhabitants live in the greater urban area (Nurja, 2010), which occupies ~31 km^2 and extends approximately 25 km far away from the Adriatic Sea. At a distance of ~7 km to the east of the city, there are the foothills of Dajti Mountain, (1 612 m maximum height). The western part of the city is surrounded by small hills with mean height of ~400 m. Therefore, air from the sea could reach the urban area, when the wind in Adriatic Sea blows from westerly directions. The main pollution problems in Tirana city are attributed to vehicular traffic, to the increasing rate of construction activity, to waste dumps and to the use of small generators due to the lack of electricity.

2.2. Observational dataset

Air quality and meteorological variables are monitored by an automatic station operated by the Institute of Energy, Water and Environment (ex–Hydrometeorological Institute), the only one in Tirana area during the study period. The station is situated at a suburb, at a distance of 3 km to the west of the city center (latitude: 41˚20′, longitude: 19˚48′, height: 97 m a.s.l.). The main source of pollution in this area is the construction activity; therefore no significant sources of ozone's precursors are identified in the area. Ozone levels in Tirana area are monitored on a regular basis since 2006. Air quality data are collected by a Rhode & Schwarz ML8810 analyzer that applies the UV photometry method, while meteorological data are collected by a Vaisala stationary meteorological station situated at 7 m a.g.l. The analysis is carried out by exploiting the data that are collected during a two–year period (April 2006 – April 2008). The missing data are found to be ~10% and they are attributed to electricity break-downs.

2.3. Ozone levels

Ozone concentrations in the greater Tirana area remain at relatively low levels (Banja, 2008). The maximum hourly value and the maximum 8–hour mean value observed at the monitoring site during the study period equal to 157 and 130 μg m^{-3} respectively, while the daily maximum 8–hour mean value exceeds the target value of 120 μg m^{-3} in 9 days. Since the station is located at the city suburbs, it is expected to detect ozone concentrations that are higher compared to the respective in the city centre. It is well known that ozone levels are higher in the suburbs than in the city centers. Ozone is a secondary pollutant. Ozone precursors are usually released in the city center and are usually transported by the wind to the suburbs where ozone is produced. Additionally, the absence of significant local sources of nitrogen monoxide in the suburbs results to the weakening of ozone destruction processes.

The frequency distribution of the DMHVs of ozone concentration is presented in Figure 1. The highest frequency of occurrence is observed around the 75th percentile value that equals to 105 μg m^{-3}. The skewness and kurtosis of the distribution are both –0.3. Since they are not zero, the normal distribution does not fit well the distribution of ozone concentrations. This conclusion is in accordance with other studies that have concluded that the most popular distribution used for fitting air pollutant concentration including ozone is the log–normal distribution (Ott, 1990; Nali et al., 2001; Lu, 2003). Additionally, the value of the 25th percentile is quite high (66 μg m^{-3}) and exceeds the phytotoxicity limit of 64 μg m^{-3}, indicating that the background ozone levels can be relatively high.

Ozone levels at the suburbs of Tirana do not present a significant weekly variation (not shown here), a fact indicating that they are not strongly affected by the weekly variation of the city activities. Ozone levels appear to be higher during weekends, when the DMHVs of ozone concentration are on average 9.4% higher than the values recorded during week days (Banja et al., 2009). As road traffic is less intense during the weekends, the emissions of nitrogen oxides are reduced. Consequently, ozone destruction processes are weakened and ozone levels are elevated.

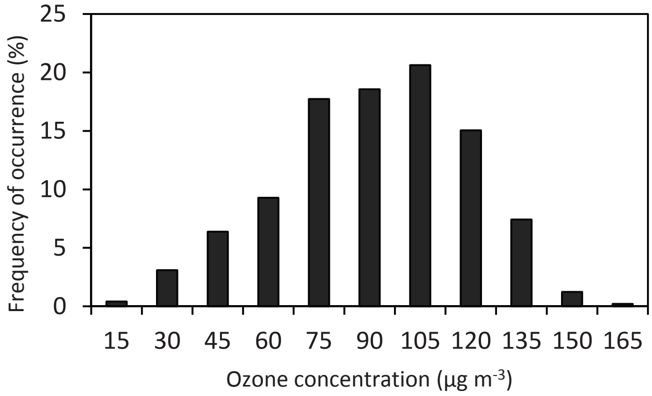

Figure 1. *Frequency distribution of DMHVs of ozone concentration.*

3. Predictors of Ozone Levels

In addition to emissions, the following atmospheric processes are influencing ozone concentrations: (1) the chemical reactions between the ozone precursor species (emitted from anthropogenic activities and natural processes) which occur under the effect of solar radiation, (2) the dry and wet deposition, (3) the advection by the horizontal wind, and (4) the vertical dilution within the boundary layer due to turbulence. It is thus important that the variables considered as predictors of maximum ozone levels can cover these atmospheric processes. Following is the description of the variables considered in the development of the maximum ozone levels forecasting tool. The variables were selected in order to represent most of the above atmospheric processes while taking into consideration at the same time the meteorological and air quality variables measured at the monitoring station located in the suburbs of Tirana.

3.1. Air temperature

Air temperature can be considered as a reasonable surrogate for the combined effects of wind speed, wind direction, inversion height and chemical reaction rate on ozone levels for two main reasons: (1) high air temperatures are an indication of environmental conditions conducive to ozone production and accumulation (i.e., anticyclonic conditions with associated clear skies and light winds) and (2) the rate constants of chemical reactions are highly temperature dependent (Robeson and Steyn, 1990).

Ozone levels are also strongly affected by the intensity of the incoming solar radiation in the troposphere being related with the complex photochemical cycles that produce ozone and with the growth of the atmospheric boundary layer (ABL) which in turn exerts a complex influence on pollutant levels in the lower troposphere. Figure 2 shows that the DMHVs of ozone concentrations are strongly related to the DMHVs of total solar radiation, with a correlation coefficient R being equal to 0.70. Figure 2 verifies that increased solar radiation flux is associated to higher ozone concentrations. Despite this fact the solar radiation is not selected as one of the variables included in the forecasting tool developed. Instead, the near–surface air temperature is selected as a surrogate of the solar radiation that reaches Earth's surface given also the more complete temperature dataset available compared to that of the solar radiation. The above suggest that air temperature may have the strongest correlation with ozone concentrations of all meteorological variables and can be considered as one of the most important variables for forecasting the ambient ozone levels. This assumption is verified by Figure 3, where the DMHVs of ozone are plotted in relation to the DMHVs of near surface air temperature. The correlation coefficient between the two parameters is equal to 0.72.

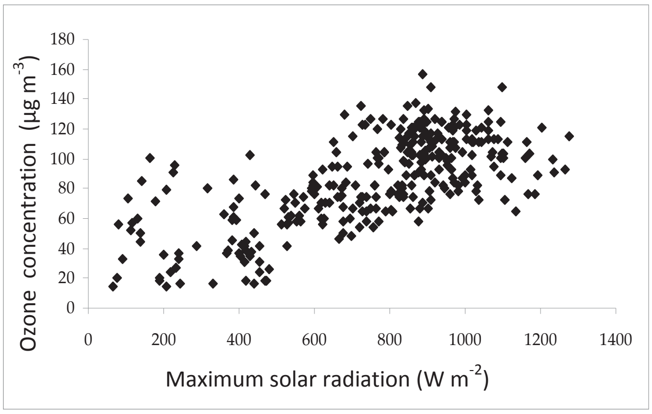

Figure 2. *Scatter plot of DMHVs of ozone concentration versus DMHVs of total solar radiation.*

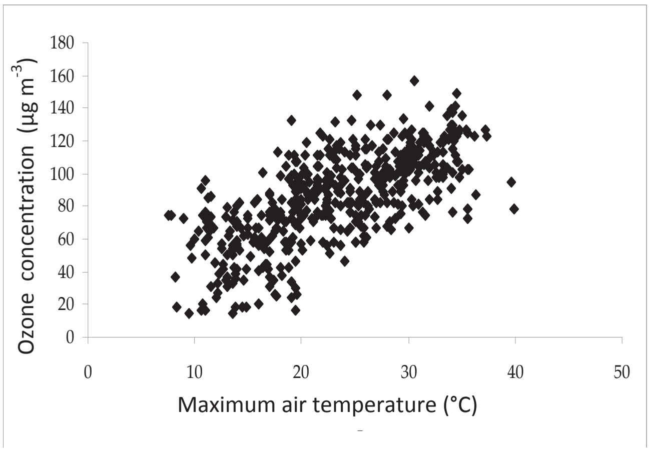

Figure 3. *Scatter plot of DMHVs of ozone concentration versus DMHVs of near surface air temperature.*

3.2. Relative humidity

High relative humidity and wet and rainy weather are usually associated with low ozone concentrations due to a reduction of photochemical efficiency and an increase of ozone deposition on water droplets (Lelieveld and Crutzen, 1990; Di Carlo et al., 2007). It is well known that relative humidity is negatively correlated with temperature, which can be considered as one of the primary ozone predictors. Ambient humidity affects the minimum temperature via two mechanisms (Hubbard and Cobourn, 1998). Firstly via the absorption of long–wave radiation emitted by the earth that would otherwise, under dry and cloudless conditions, be lost to space and secondly via the release of the latent heat of condensation as the sensible temperature falls to the dew point. Figure 4 shows that high values of ozone concentrations are associated with low relative humidity values (R = –0.40).

3.3. Seasonal variation of ozone concentration

Ozone concentration presents a clear seasonal cycle with its maximum values being observed during the warm period of the year. The average of the DMHVs of ozone concentration during winter, spring, summer and autumn equals to 67, 99, 108 and 64 μg m^{-3}, respectively. This seasonal variation is mainly attributed to the increase in the amount of solar radiation that reaches to the Earth during this period. The maximum values of total solar radiation that were observed in the summers of 2006 and 2007 were 1 277 and 1 186 W m^{-2}, respectively. In order to take into account the annual variation of ozone, an index Y is defined by the Equation (1), where M_i is a number ranging from 1 to 12 that refers to the month of the year.

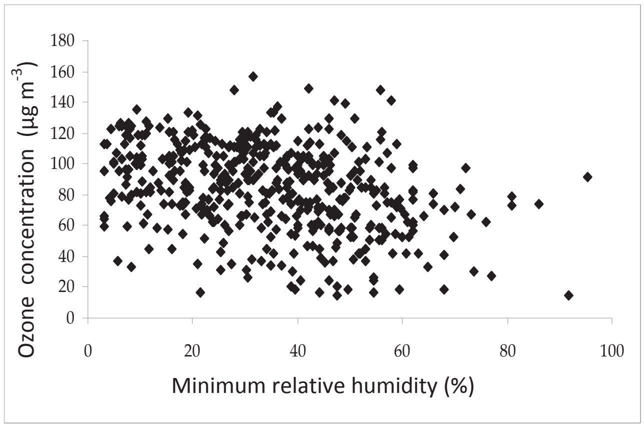

Figure 4. *Scatter plot of DMHVs of ozone concentration versus daily minimum hourly values of relative humidity.*

$$Y = \cos\left[\left(2\pi M_i\right)/12\right] \quad (1)$$

3.4. Ozone persistency

As it has already been mentioned above, meteorology plays an important role in determining pollution levels. However, except for the meteorological factors, there are some other variables that could also be considered as predictors of pollution levels. Earlier studies have shown that the possibility of occurrence of a pollution episode is increased when the previous day's pollution levels were higher than normal (Robeson and Steyn, 1990; Ziomas et al., 1995). This is attributed to the fact that pollution episodes are "built up" when meteorological conditions favoring high pollutant concentrations occur during successive days. The persistency of pollution levels could be also attributed to the daily cycle of the ABL.

Atmospheric pollutants are usually retained within the residual layer after the ABL's destruction at the end of the previous day. After sunrise, when the nocturnal boundary layer starts to be destructed and the ABL starts to develop, a mixing of the low atmospheric layers air with that of the upper layers occurs. Near surface air is less polluted than the air aloft as city activities have just started. Therefore, this vertical mixing can result in an increase in the near surface pollution levels. The more polluted the air that is trapped within the residual layer, the more significant the physical processes described above are. Additionally, the downward transport of ozone or ozone precursors from aloft could result in the production and increase of near surface ozone values.

Figure 5 reveals that the DMHVs of ozone concentration in Tirana are significantly correlated to the respective values of the previous day, as the correlation coefficient equals to 0.85. Therefore, the persistency of ozone levels is an important atmospheric process that has to be accounted for in the forecast of the peak ozone concentrations.

4. Development and validation of the forecasting tool

Data were split into two sets, the development and the evaluation set. The first one consists of the two thirds of the available data (i.e. 439 days) and it is used to develop the model, while the latter one consists of the rest one third (i.e. 220) of the available data and is used to evaluate the model. For three consecutive days, the first two were included in the development set and the third was included in the evaluation set.

4.1. Development of the model

The quantitative estimation of next day's maximum hourly values of ozone concentration is based on an analytical expression

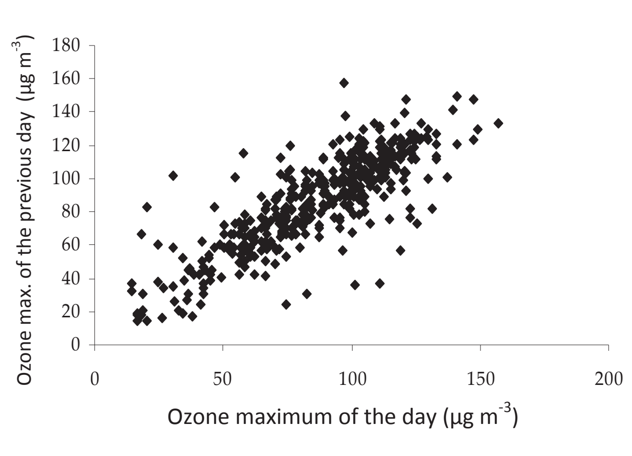

Figure 5. *Scatter plot of DMHVs of ozone concentration versus those of the previous day.*

[Equation (2)] derived by performing multiple linear regression analysis (MLRA):

$$y = m_1 x_1 + m_2 x_2 + m_3 x_3 + b \quad (2)$$

where y is the forecasted DMHV of ozone concentration (μg m^{-3}), x_1 is the previous day's maximum hourly value of ozone concentration (μg m^{-3}), x_2 is the DMHV of the near surface air temperature (°C), x_3 is the value of the index *Y,*and m_1, m_2, m_3, b are constants.

The independent variables that are included in the model are selected by applying the partial least squares (PLS) analysis, which is a method that has been widely applied in environmental studies (Massart et al., 1998; Wold et al., 2001). PLS regression is a recently developed technique that generalizes and combines features from principal component analysis and multiple regression analysis (Abdi, 2003). It is particularly useful when analyzing a large set of data with strongly correlated variables. This multivariate statistical technique transforms the original data set into a set of linear combinations of the original variables. The uncorrelated new variables, designated by principal components, account for the majority of the original variance. The modeling process is iterated n times, where n is the number of observations. In every iteration, one of the observations is left out and the model is updated using the rest n – 1 values.

As it emerges from PLS analysis (Figure 6), a simple model involving the previous day's maximum hourly value of ozone concentration, the DMHV of air temperature and the index *Y*, which accounts for the annual variation of ozone, is capable to provide a satisfactory prediction of the peak ozone levels. As it is shown in Figure 6, the introduction of other variables, such as the previous day's maximum hourly value of air temperature and the daily minimum hourly value of relative humidity does not improve the forecasting ability of the model. However, the inclusion of other independent variables in the model that are not taken into account in the present study due to data unavailability or sparseness, such as wind speed and direction, rain, etc, may improve the accuracy of the forecast.

The values of the four constants, m_1, m_2, m_3, b, which are included in the prediction tool, are equal to 0.652, 0.182, –8.578 and 25.164, respectively.

4.2. Validation of the model

The scatter plot of observed and predicted DMHV of ozone concentrations is presented in Figure 7. This Figure shows that the agreement between predicted and observed data is very good. The results of the developed model are evaluated against observational ozone data with the estimation of several statistical indexes that have been used in previous studies (Papanastasiou and Melas, 2008; Poupkou et al., 2009). These indexes are the mean bias error (MBE), the mean absolute error (MAE), the root mean square error (RMSE), the correlation coefficient (R) and the index of agreement (d). MBE defines whether the model over (positive value) or under (negative value) predicts the observations, MAE and RMSE illustrate the presence of significant mispredictions, R reflects the linear relationship between the observed and predicted values and d reflects the degree to which the model's predictions are error free. Their values also reveal that the agreement between the observed and the predicted DMHVs of ozone concentration is very good. This conclusion is supported by the high value of the correlation coefficient R, which equals to 0.87. This result indicates that the developed model is capable to explain the 76% of the variability of ozone's concentration. The above conclusion is also verified by the high value of the index of agreement that equals to 0.93, which is considered to be more unbiased, as it is based on squared differences between predicted and observed values. MBE takes a small negative value (–1.6 μg m^{-3}) since the mean of the observed and the predicted values are 87.8 and 86.2 μg m^{-3} respectively, revealing a minor under prediction of the obser-

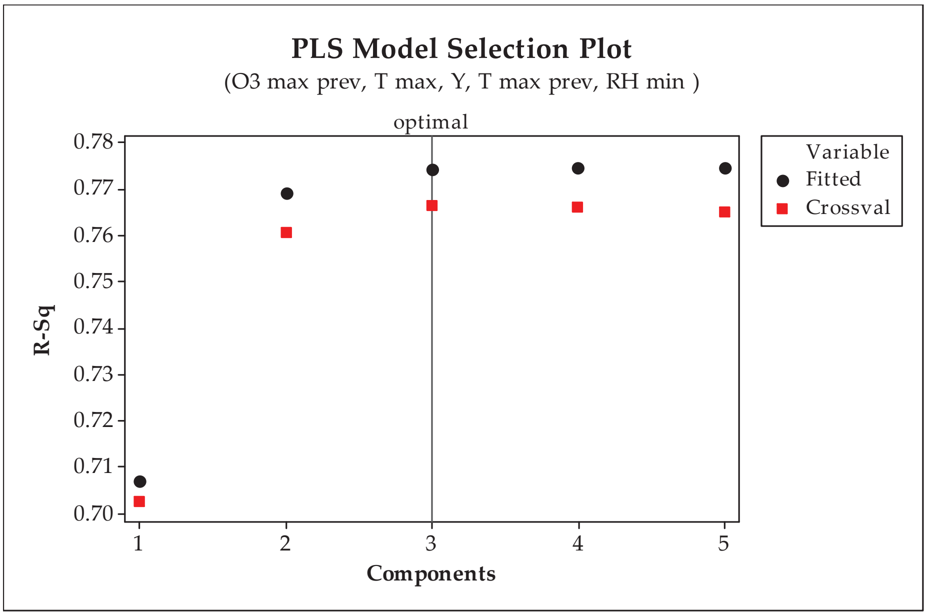

Figure 6. *Selection of independent variables by applying PLS analysis.*

vations by the model. The corresponding standard deviations are 27.1 and 23.4 µg m^{-3} respectively, showing that the model succeeds in reproducing the variability of the observed data. The values of MAE and RMSE are found equal to 11.8% and 15.0% of the observed mean ozone concentration respectively and they take values which are less than the standard deviation of the observations. As a result, they suggest a good performance of the forecasting model developed.

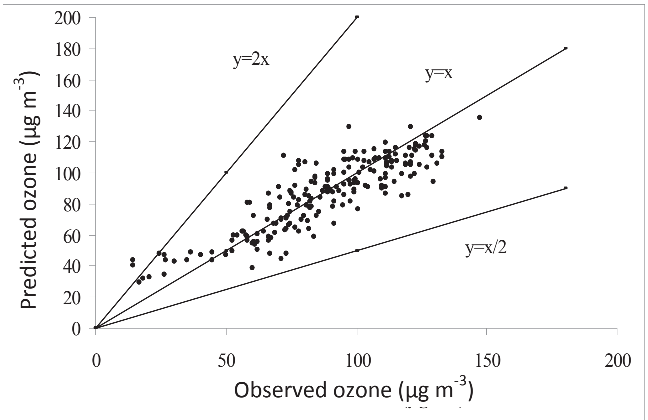

Figure 7. *Comparison between predicted and observed DMHV of ozone concentration.*

The ability of the developed model to predict the exceedances of a specific threshold is also examined. For this purpose, three statistical indexes are estimated, namely the probability of detection (POD), the false alarm rate (FAR) and the success index (SI), which have already been utilized in similar studies (Comrie, 1997; Chaloulakou et al., 2003; Papanastasiou and Melas, 2008). Their definitions are presented in Table 1, where A is the number of exceedances that are observed and predicted, B is the number of exceedances that are observed but not predicted, C is the number of exceedances that are predicted but not observed and D is the number of non–exceedances. The value of the threshold could be the limit value of 180 µg m^{-3} that is established by the relevant EU Directive. However, as is mentioned in Section 2.3, ozone concentrations in the suburban monitoring station of Tirana do not exceed this limit value, so another value has to be determined. It is decided to select the value of the 75th percentile, which equals to 105 µg m^{-3}.

Table 1. *Statistical indexes used to assess the ability of the model to predict the exceedances of a given threshold*

Index	Definition	
	Equation	**Meaning**
POD	A/(A +B)	Fraction of correct predictions over total observed exceedances
FAR	C/(C+A)	Fraction of false predictions over total predicted exceedances
SI	[A/(A+B)]+[D/(D+C)]-1	Relation between the correct predictions of the exceedances and non-exceedances

According to the definition of POD and FAR, their best values are 1 and 0 respectively. So, they should be reasonably high and low respectively, in order to support that a model can predict accurately the exceedances of the selected threshold value. The developed model fulfils this condition, as the POD and FAR indices are 0.86 and 0.11 respectively, taking values which are very close to their best values. Moreover, the value of SI is estimated equal to 0.75 (values range between –1 and 1, best value is 1), a fact that demonstrates that the predictions of the exceedances are well balanced with the predictions of non–exceedances.

The forecast capability of the present study developed tool is compared with similar studies for Southern Europe. The study areas as well as information on the forecasting capability of previous models that were developed by applying regression analysis are presented in Table 2. Table 2 confirms that the developed tool for Tirana is included among the most successful ones, as it explains 76% of ozone observed variability. Additionally, the present study is in line with that of Kovac–Andric et al. (2009) regarding the number of predictors used. Both studies suggest that the short term ozone levels can be sufficiently predicted even if a small number of independent variables are utilized. Kovac–Andric et al. (2009) using solar radiation time, temperature and wind speed in their model achieved to explain 77% of ozone variance during summer. Moreover, the present study is in line with those studies that report the correlation coefficients between ozone concentrations and independent variables. In all studies the ozone concentrations are better correlated to the previous day's concentrations rather than to temperature values.

Table 2. *Review of studies that aimed to predict short term ozone levels in South Europe*

Reference Paper	Site Information		Number of predictors used	Correlation of ozone with		Variance Explained (%)
	City	Country		Temperature	Previous day's ozone	
Kovac-Andric et al., 2009	Osijek	Croatia	3	Not reported	Not reported	77
Chaloulakou et al., 1999	Athens	Greece	7	Not reported	Not reported	43
Ziomas et al., 1995	Athens	Greece	6	Not reported	Not reported	59
Papanastasiou and Melas, 2008	Volos	Greece	7	0.75	0.90	86
Sousa et al., 2007	Oporto	Portugal	5	Not reported	Not reported	49
Barrero et al., 2006	Errenteria	Spain	6	0.38	0.70	60
Tecer et al., 2003	Istanbul	Turkey	8	0.48	0.48	71.5
Di Carlo et al., 2007.	L'Aquila	Italy	4	0.43	Not reported	62

5. Conclusions

This study provides information about ozone levels in the suburbs of Tirana during the period April 2006 – April 2008 and presents the development of a short–term forecasting tool that could be exploited to predict peak ozone levels in the area. It is worth mentioning, that to the knowledge of the authors, this is the first relevant study conducted for Albania. The main conclusions of this study are the following:

- Ozone levels in Tirana do not exceed the EU's air quality standards in force.
- The PLS analysis reveals that the most significant variables in predicting the DMHV of ozone concentration is the previous day's maximum hourly ozone value, followed by the near surface air temperature.
- The developed model is capable of explaining 76% of the variability in the observed ozone concentrations. Its reliability was evaluated against observational ozone data with the calculation of several statistical indexes (MBE, MAE, RMSE, R, d). All the statistical measures examined take very satisfactory values suggesting a good agreement between modeled and observed values. Both the levels and the variance in observed ozone values are well reproduced by the model.
- The estimation of additional indexes like POD, FAR and SI showed that the developed model is capable to predict adequately the exceedances of 105 $\mu g\ m^{-3}$, a threshold value which was selected since it represented the 75^{th} percentile of the available ozone concentrations dataset measured at the monitoring station. The POD, FAR and SI measures take values which are close to their best values. The fraction of correct predictions over total observed exceedances is high (POD equals to 0.86), the fraction of false predictions over total predicted exceedances is low (FAR equals to 0.11), while the relation between the correct predictions of the exceedances and non–exceedances is well balanced.

The use of simple meteorological variables, available from routine measurements, together with pollution measurements, may give rather good ozone level predictions in the study area. Since the model equation derived is simple, it can be used easily for operational forecasts. It should be noted though that the success of the predictions depends strongly on the accuracy of the temperature forecast. However, since forecasted meteorological data were not available, this factor of uncertainty was not possible to be further examined in our study.

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