FORECASTING DAILY MAXIMUM OZONE CONCENTRATIONS IN THE ATHENS BASIN

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Abstract. In the work ozone data from the Liossion monitoring station of the Athens/PERPA network are analysed. Data cover the months May to September for the period 1987–93. Four statistical models, three multiple regression and one ARIMA (0,1,2), for the prediction of the daily maximum 1-hour ozone concentrations are developed. All models together, with a persistence forecast, are evaluated and compared with the 1993's data, not used in the models development. Validation statistics were used to assess the relative accuracy of models. Analysis, concerning the models' ability to forecast real ozone episodes, was also carried out. Two of the three regression models provide the most accurate forecasts. The ARIMA model had the worst performance, even lower than the persistence one. The forecast skill of a bivariate wind speed and persistence based regression model for ozone episode days was found to be quite satisfactory, with a detection rate of 73% and 60% for O_3 >180 μg m^{-3} and O_3 >200 μg m^{-3}, respectively.

Keywords: air pollution in Athens, ozone concentration, prediction of episodes, statistical modelling

1. Introduction

The atmospheric pollution problem in the Athens Basin has become quite serious during recent years. This densely populated and industrialised area of Greece is a region of high susceptibility to photochemical smog (Gusten, *et al*., 1988; Abatzoglou *et al*., 1996). The Athens Basin lies on a northeastern axis, is surrounded at three sites by fairly high mountains and at its southern extremity is bounded by the Saronic gulf (Figure 1). Between these mountains there are narrow geographical openings. The formation of air-pollution episodes in the Athens Basin is due to the synoptic conditions and the general physiographic characteristics of the area (mountains, hills, valleys, land–sea distribution, orientation of the coastline, land use etc.).

During the warm season (1 May–30 September) high photochemical activity, combined with the prevailing adverse dispersion conditions in the Basin, leads to high ozone concentrations measured at some monitoring stations (Liossion, Geoponiki, Maroussi).

A number of previous works have used different statistical models to forecast ozone air-pollution concentration. Regression techniques for both model formula-

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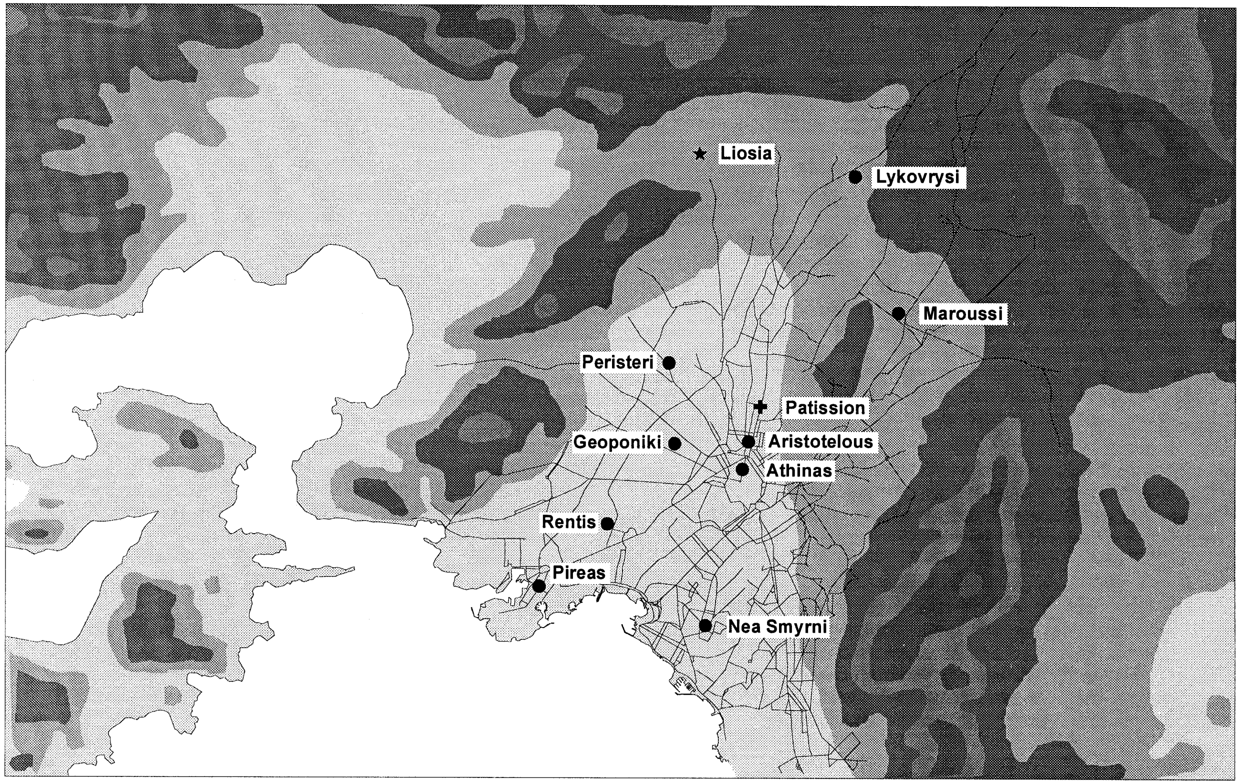

Figure 1. Map of the Athens Metropolitan area. Locations of the PERPA monitoring sites, main road system and mountains.

tion and estimation are commonly used (Revlett, 1978; Prior *et al*., 1981; Lalas *et al*., 1985; Robeson and Steyn, 1989; Lorenzini, *et al*., 1994). Another common approach among environmental scientists if the purely stochastic ARIMA technique of Box and Jenkins. Many investigators have used this time series technique for forecasting ozone concentrations (Mertz *et al*., McCollister and Wilson, 1975; Chock *et al*., 1975; Simpson and Layton, 1983; Robeson and Steyn, 1989).

The development and application of deterministic, as well as stochastic, statistical models to the *same data sets* is still quite infrequent in the literature. The development of different types of models in parallel gives an excellent opportunity to evaluate and compare their relative forecasting accuracy.

The work in this paper is concerned with the development and application of three multiple-linear regression models and one ARIMA model to seven years (1987–93) of ozone data from Liossion monitoring station in Athens. A broad array of statistics indicative of model forecast performance has been used, selected from previous works (Willmott *et al*., 1985; Rao and Visalli, 1981; Simpson and Layton, 1983; Wolf and Lioy, 1978; Robeson and Steyn, 1989). The analysis is focused on the ozone high season (1 May–30 September) and is concerned with the *daily maximum one hour ozone* concentration. All models are evaluated and compared as far as their forecasting ability is concerned graphically and statistically using 1993's data, not used in the model development. In addition, their ability to forecast real ozone episodes has been estimated.

2. Data Sets and Study Region

The data sets for the various chemical and meteorological parameters used in this study are drawn from the monitoring network operated by the Branch of the Ministry of Environment, City Planning and Public Works (PERPA) and from the National Observatory Meteorological Institute monitoring network.

The Liossion monitoring station is located in the northwest area of Athens Basin, well away from traffic and is not influenced by any specific pollutant source. Ozone concentrations in the Liossion station have been found to frequently exceed WHO air quality guidelines (200 μg m^{-3} hourly average) and national health protection thresholds (250 μg m^{-1} daily 1-hour maximum concentration, for the warning stage) during the high season (Gusten *et al*., 1988; Abatzoglou *et al*., 1996). Measurements from PERPA continuous monitoring system recorded as 1-hour average include concentration of ozone, CO, NO_x and SO_2. The ozone automatic analysers are operating on the UV absorption method. The sampling manifold used by all gaseous monitors has an intake at about 8 m from the ground. Figure 1 displays the locations of the PERPA monitoring sites on a land use map of the Athens Metropolitan area. The percentage of data capture is very good (>85%) and the length of continuous data records is seven years. Preference was given *to daily 1-hour maximum concentration*, as this is often used as an air-quality standard. A

TABLE I

List of selected explanatory variables by order of estimated correlation coefficient

$[O_3]24$	Previous day's maximum 1-hour ozone concentration, (μg m^{-3})
$[NO_2]$PAT	Average of the maximum concentration for the [6 p.m.–2 a.m.] interval of the previous day and the maximum concentration of the [6 a.m.–9 a.m.] interval of the same day in Patission station, (μg m^{-3})
[CO]PAT	Maximum concentration for the [6 a.m.–9 a.m.] interval of the same day in Patission station (mg m^{-3})
WS^{-1}	Inverse of daily average wind speed, same day, (s m^{-1})
WS	Daily average wind speed, same day, (m s^{-1})
WD	Predominant wind direction, same day (deg)
T_{max}	Daily maximum temperature, same day, (°C)

large number of available chemical and meteorological variables were tested for their ability to explain some of the ozone variability. The explanatory variables, expressed in a formula selected according to the estimated correlation coefficient with ozone values at the Liossion station, are presented in Table I. Unfortunately data on solar radiation and mixing-height were not available. However, T_{max} with SR are closely related and so the inclusion of both is not expected to substantially improve the overall correlation. A multi-linear regression analysis of the maximum O_3 hourly means, on the available chemical and meteorological variables, is performed. Only the significant linear regression coefficients are given in Table II (according to *f*-statistics). Data on relative humidity (RH), dew point temperature, and concentrations of NO_2 and CO at the same station were also tested and not found significant.

The previous day's one-hour maximum ozone concentration has the strongest correlation followed by NO_2 concentration at Patission station. The latter is a city core station, where the highest values of NO_2 and CO concentrations in Athens Basin are recorded. The 6–9 a.m. CO concentration at Patission station is an indicator of prevailing morning-dispersion conditions and, thus, of high or low morning ozone precursors concentrations. Patission station is located about 10 km far from the Liossion station (usually in the upwind direction during the episode days); the high NO_2 concentrations (recorded in the Patission station) are indicative of ozone formation later on the same day (Revlett, 1978). On the other hand, as Liossion monitoring station is located away from traffic and is not influenced from any specific emissions source, it records some of the lowest CO and NO_2 concentrations in the area.

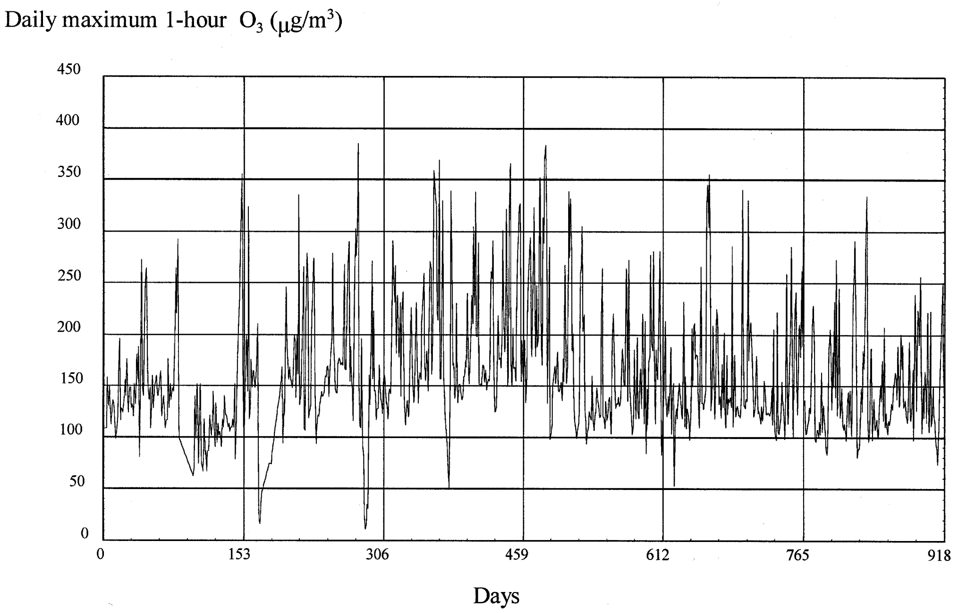

Figure 2. O_3 time series. Liossion station, 1987–92.

3. Statistical Forecast Models for O_3

A deterministic approach (multiple linear regression analysis, MLR) and a stochastic approach (ARIMA time series analysis) were used for forecasting daily-one-hour-maximum ozone concentrations at the Liossion station. The historical series cover the time period 1987–92 and it was used for developing the model. The data for the year 1993 were used for validation and evaluation purposes.

3.1. Regression Models

A large number of linear regression models was developed using various combinations of the independent variables shown on Table I. Three models were finally selected; a typical one with six explanatory variables and the best R-coefficient (REGLING) and two bivariate models, named TEMPER with variables T_{max} $[O_3]24$, and WISPER with variables WS, $[O_3]24$. The last two models give a lower explanation of variance but are attractive for their simplicity; the names used, TEMPER (according to (Robeson and Steyn, 1989)) and WISPER, indicate their bivariate (temperature or wind speed and persistence) structure.

The corresponding linear equations together with their coefficients are given in Table II. It appears that the inverse of daily average wind speed is one of the more important single factors and its contribution is much higher than others, a fact already observed elsewhere (Wolff and Lioy, 1978) and strongly supported by the prevailing conditions in the study area during episode days. The ability

TABLE II

Equations and coefficient estimates of forecasting models

REGLIN6	$[O_3]$ = a + b*$[O_3]$24 + c*T_{max} + d*WS^{-1} + e*WS^{-1} + f*$[NO_3]$PAT + g*[CO]PAT							
	a	b	c	d	e	f	g	
	–55.374	0.348	1.835	3.002	111.323	0.210	1.928	R = 0.66
St. error	21.719	0.030	0.369	2.883	23.590	0.048	0.462	R^2 = 0.43
WISPER	$[O_3]$ = a + b*$[O_3]$24 + c*WS^{-1}							
	a	b	c					
	35.697	0.478	123.719	R = 0.610				
St. error	6.011	0.028	11.148	R^2 = 0.37				
TEMPER	$[O_3]$ = a + b*$[O_3]$24 + c*T_{max}							
	a	6	c					
	43.079	0.507	1.255	R = 0.537				
St. error	11.557	0.030	0.388	R^2 = 0.289				
ARIMA (0,1,2)	$[O_3]$ = $[O_3]$24 + b(1)*z(t.l) + b(2)*z(t-2)							
	b(1)	b(2)						
	0.487	0.324						
St. error	0.031	0.035						

of regression models to forecast daily-ozone-maxima is discussed in a following paragraph.

3.2. ARIMA MODELS

Many investigators have used time series analysis methods (Box and Jenkins, 1976) to develop stochastic models for forecasting ozone concentrations (Mertz *et al*., 1972; McCollister and Wilson, 1975; Chock *et al*., 1975; Simpson and Layton, 1983; Robeson and Steyn, 1989). Plots of the *original* ozone concentration time-series (Figure 2) and of the corresponding auto-correlation function (ACF, Figure 3), indicate that the series is non-stationary and needs to be differenced. The plots of the *first differenced* time-series and of the corresponding ACF and partial auto-correlation function (PCF) are shown in Figures 4, 5, 6, respectively.

Inspection of these diagrams and taking into account the principle of parsimony suggests that a second order moving average model, ARIMA (0,1,2), is the most

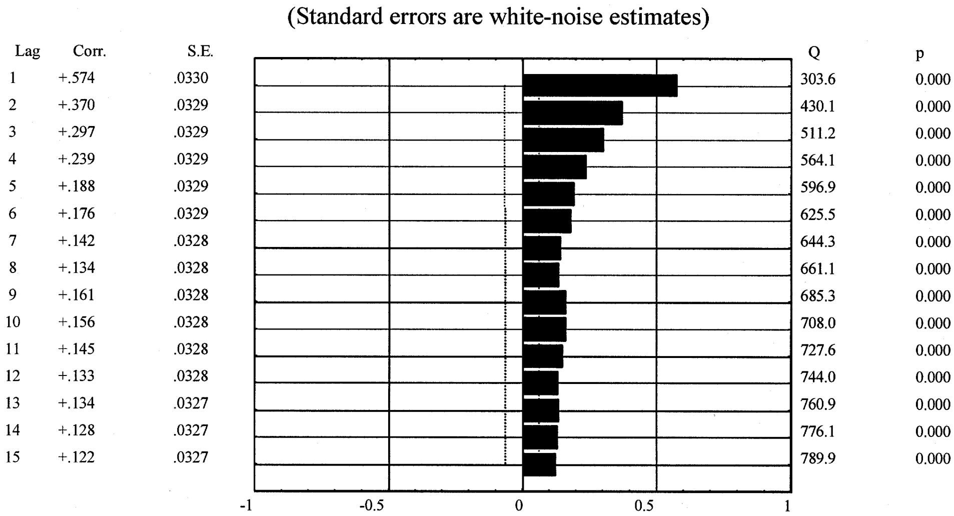

Figure 3. Autocorrelation function for O_3 time series, Liossion station, 1987–92.

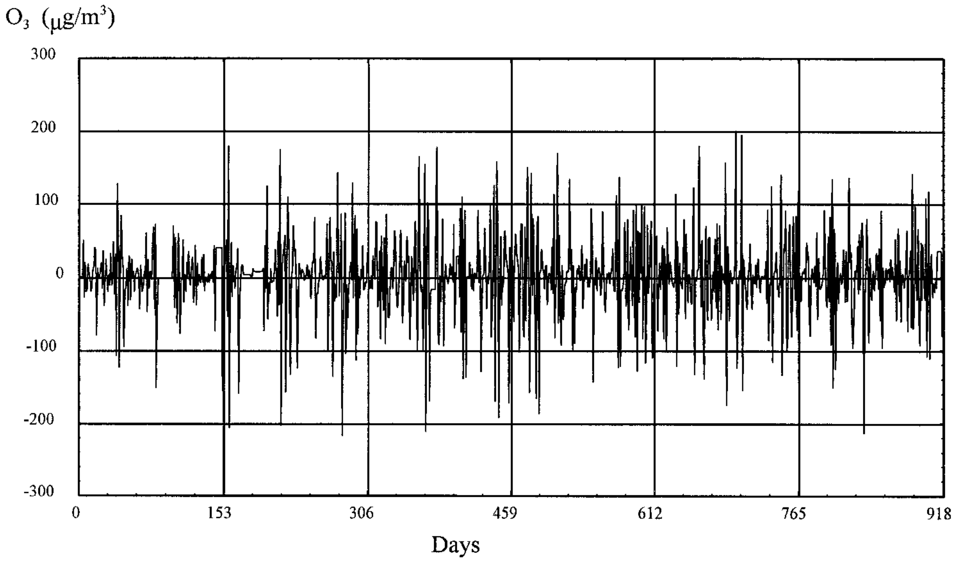

Figure 4. First-differenced O_3 time series, Liossion station, 1987–92.

appropriate. Parsimonious models are preferable to models with more parameters because, in practice, they generally produce better forecasts. Models with too many parameters often overfit the available data, thus reducing forecast accuracy (Pankratz, 1983). The form of this model and the values of estimated model parameters are given in Table II. The plot of ACF of the model residuals, shown in Figure 7, suggest an almost white noise behaviour and the proposed model could be accepted.

(Standard errors are white-noise estimates)

Lag	Corr.	S.E.	Q	p
1	-.261	.0330	62.55	.0000
2	-.152	.0330	83.85	.0000
3	-.020	.0329	84.21	.0000
4	-.007	.0329	84.25	.0000
5	-.045	.0329	86.16	.0000
6	+.024	.0329	86.71	.0000
7	-.031	.0329	87.57	.0000
8	-.041	.0328	89.15	.0000
9	+.038	.0328	90.51	.0000
10	+.008	.0328	90.56	.0000
11	+.001	.0328	90.56	.0000
12	-.017	.0328	90.83	.0000
13	+.010	.0328	90.93	.0000
14	-.001	.0327	90.93	.0000
15	-.000	.0327	90.93	.0000

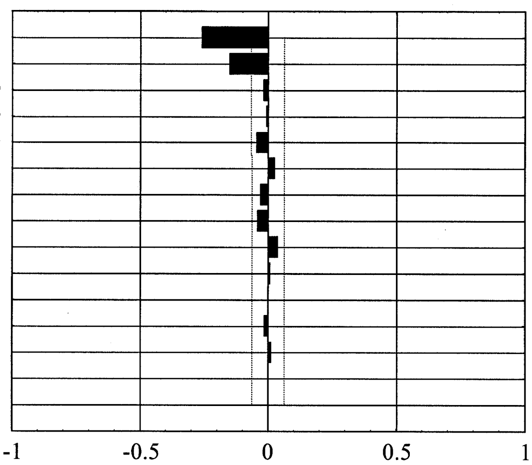

Figure 5. Autocorrelation function of the first-differenced O_3 time series, Liossion station, 1987–92.

Lag	Corr.	S.E.
1	-.261	.0330
2	-.236	.0330
3	-.148	.0330
4	-.112	.0330
5	-.132	.0330
6	-.071	.0330
7	-.102	.0330
8	-.129	.0330
9	-.070	.0330
10	-.066	.0330
11	-.051	.0330
12	-.070	.0330
13	-.051	.0330
14	-.049	.0330
15	-.048	.0330

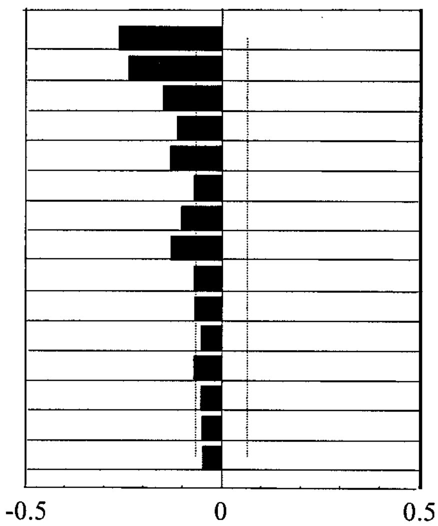

Figure 6. Partial autocorrelation function of the first-differenced O_3 time series, Liossion station, 1987-92.

4. Evaluation of the Models' Forecast Ability

In this section, ability of each model to predict maximum ozone concentration is tested using scatter plots of predicted versus observed ozone values for the 1993 (see Figures 8–11), selected statistics and estimates of the predicted episode days versus the real ones occurred the 1993.

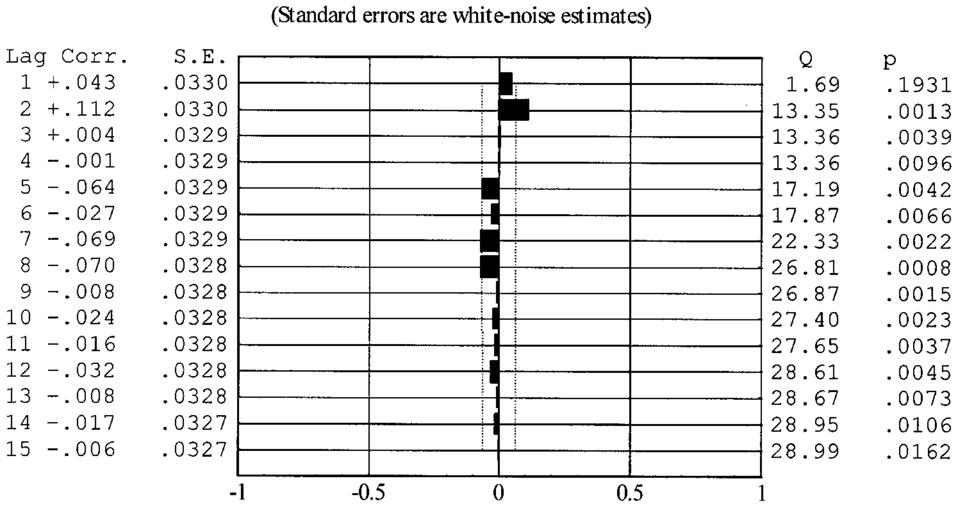

Figure 7. Autocorrelation function of the residuals of the ARIMA model.

TABLE III

Statistic estimates for the comparative assessment of models

1993	REGLIN6	WISPER	TEMPER	ARIMA	Persistence
Number of measurements	123	139	139	143	143
Observed mean	173.68	173.68	173.68	173.68	173.68
Predicted mean	168.59	179.30	166.00	167.37	173.45
Observed standard deviation	65.09	65.09	65.09	65.09	65.09
Predicted standard deviation	50.94	44.98	36.25	66.78	65.02
Regression line in scatter plots					
Slope	0.541	0.385	0.227	0.307	0.366
Intercept	72.84	112.46	127.01	114.34	109.81
Mean absolute error (MAE)	28.38	36.96	42.38	55.48	48.27
Mean percentage error (MPE)	–6.51	2.41	5.57	–5.27	–8.40
Root mean squared error (RMSE)	47.99	55.22	60.41	77.93	73.16
Root mean squared error systematic (RMSEs)	31.01	40.25	50.61	45.17	41.05
Root mean squared error unsystematic (RMSEu)	36.63	37.80	33.00	63.51	60.56
Index of agreement (d)	0.815	0.719	0.608	0.597	0.642

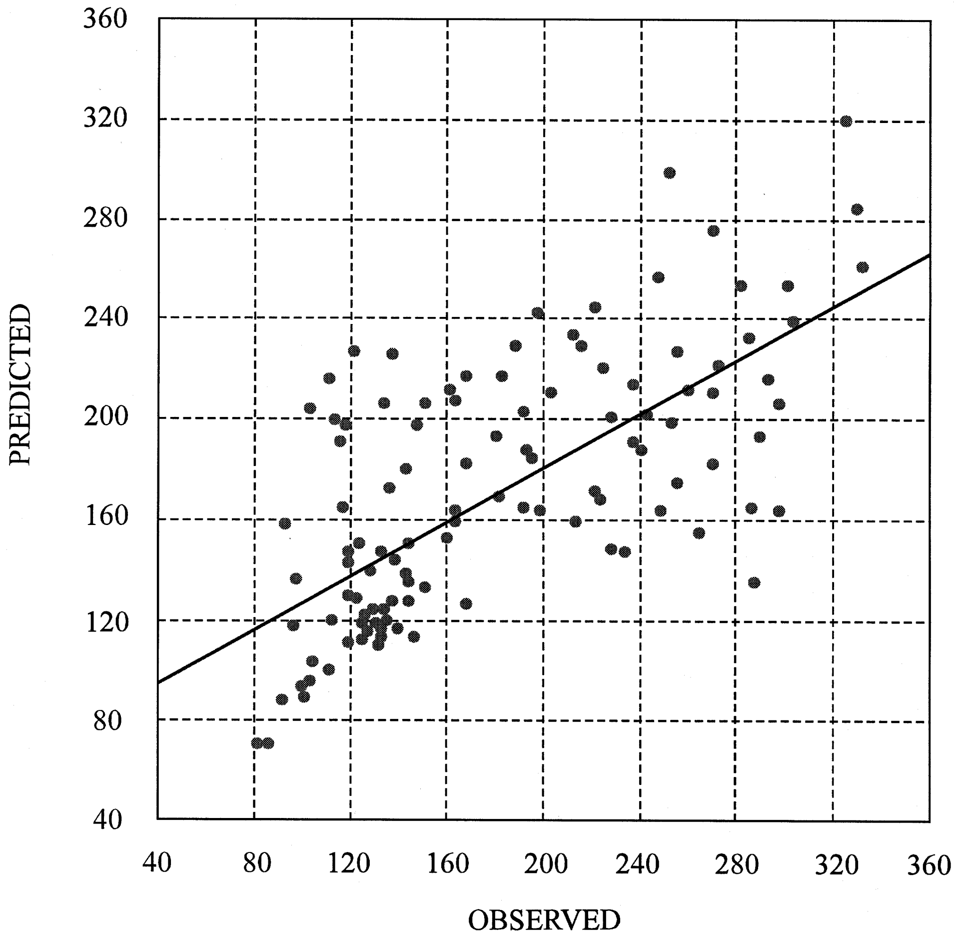

Figure 8. Plot of forecast versus observed daily 1-hour maximum ozone concentration for the 1993 high season at Liossion station using the REGLIN6 model. Solid line shows an ordinary least square regression fitting. Units are in μg m^{-3}.

In the first approach the slope and intercept of each regression line in Figures 8–11 are estimated and presented in Table III.

In the second approach a broad array of statistics, indicative of model forecast performance, have been reviewed and those finally adopted are estimated for each model, using the 1993 data and are presented in Table III for comparative purposes. For more details on the statistical meaning of these indices see (Willmott *et al.*, 1985; Rao and Visalli, 1981; Simpson and Layton, 1983; Wolf and Lioy, 1978; Robeson and Steyn, 1989). The performance of a simple persistence model ($[O_3]_{\text{predicted}} = [O_3]24_{\text{observed}}$) has been also estimated, used as a benchmark comparison for all models.

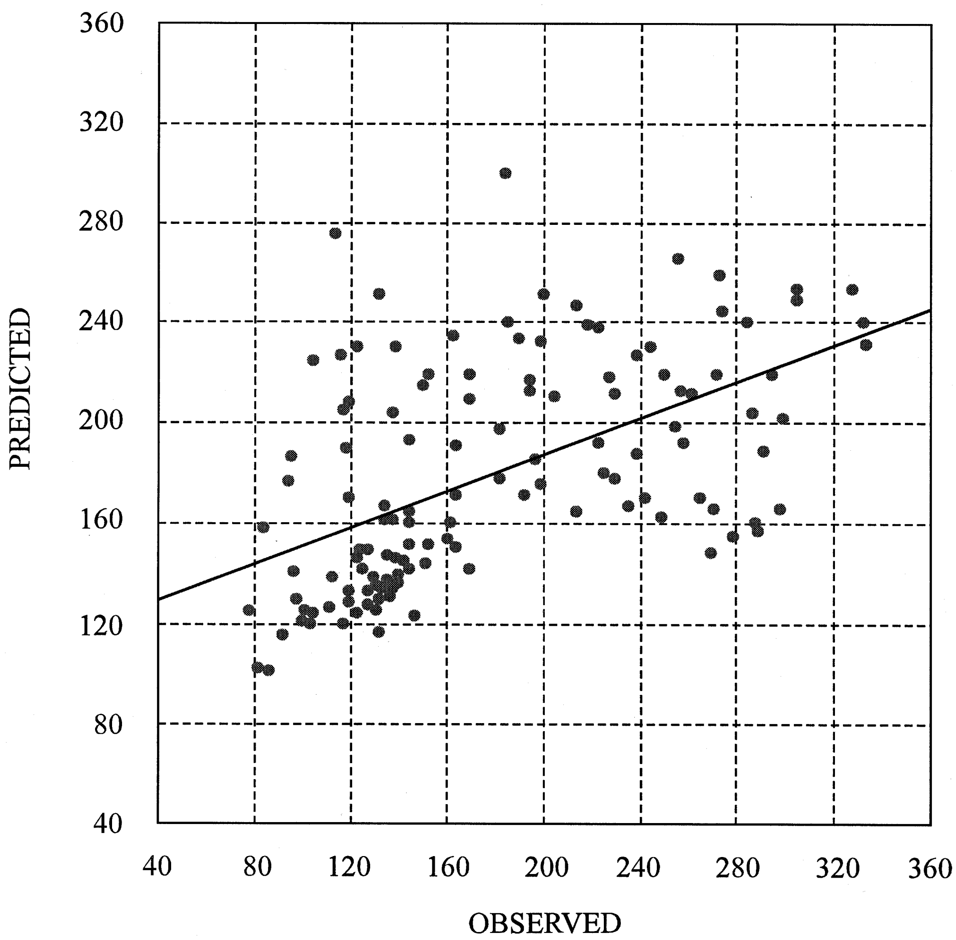

Figure 9. Plot of forecast versus observed daily 1-hour maximum ozone concentration for the 1993 high season at Liossion station using the WISPER model. Solid line shows an ordinary least square regression fitting. Units are in μg m^{-3}.

In the third approach two limit values (180 and 200 μg m^{-3}) for ozone maximum concentration are selected and used for the investigation of categorical results. The relative success of each model to forecast observed episode days for 1993 is presented in Tables IVa, IVb.

In Tables IVa and IVb the percentages of correct predicted alarms are calculated with respect to the observed alarms, whereas the false alarms are calculated with respect to the total number of days in the examined period.

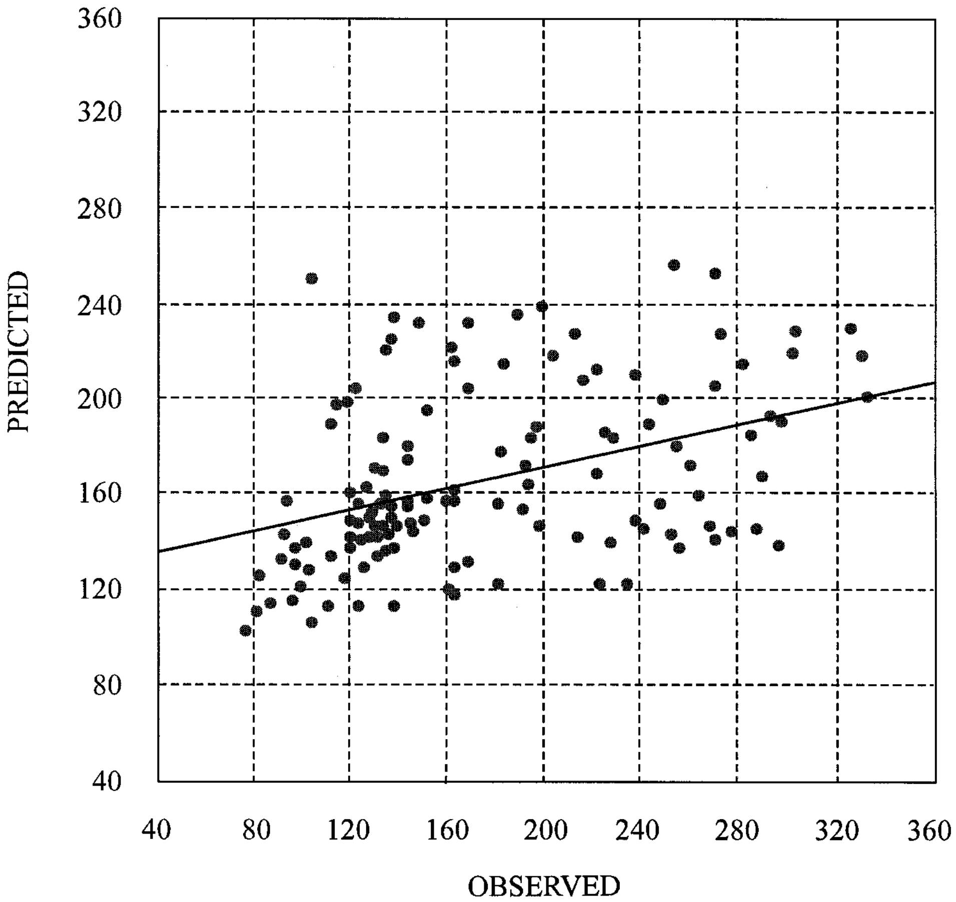

Figure 10. Plot of forecast versus observed daily 1-hour maximum ozone concentration for the 1993 high season at Liossion station using the TEMPER model. Solid line shows an ordinary least square regression fitting. Units are in μg m^{-3}.

5. Conclusions

To forecast daily maximum ozone concentrations in Athens, Greece, four statistical models and a persistence one were formulated and their parameters were estimated using seven years ozone data from the Liossion monitoring station. Considering the construction of multiple-linear models, it appears that the relative utility of each model has been assessed, using scatter plots of forecast versus observed daily maximum values for the high season of 1993, a representative series of statistics indicative of models' predictive accuracy, and specific forecast skill measures for high ozone events.

Of the three regression models, the one with six explanatory variables. REGLIN6, explains the greatest portion of ozone variance as indicated by the model evaluation

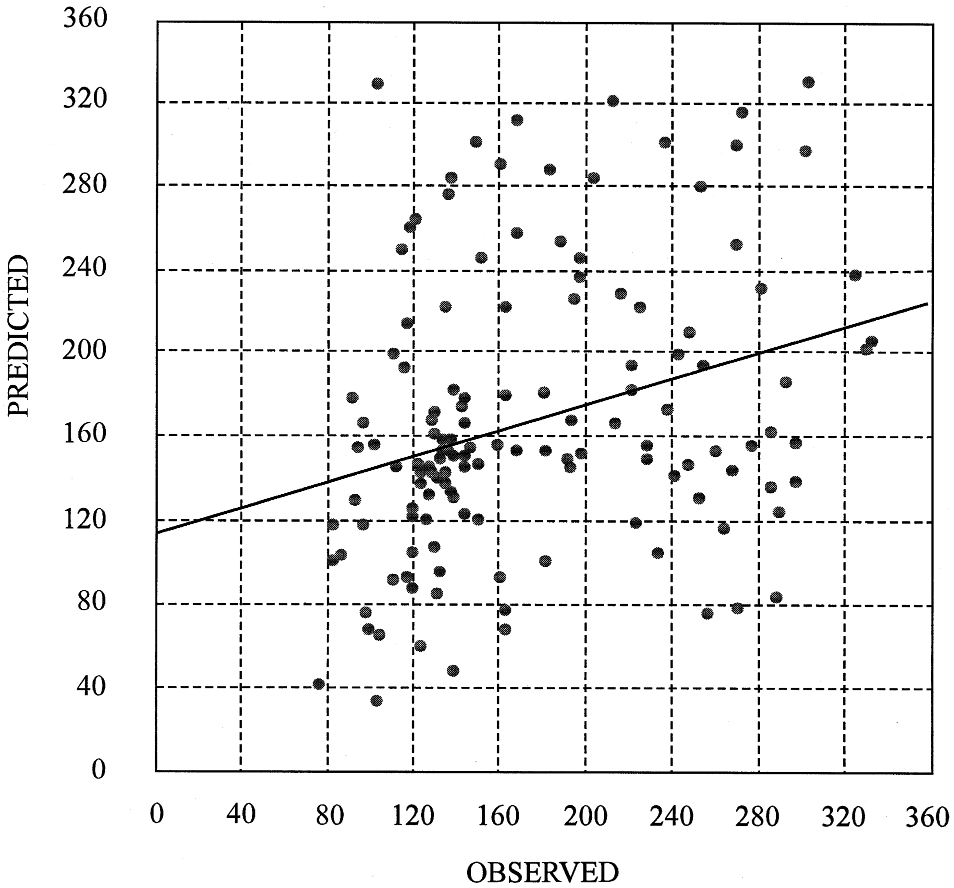

Figure 11. Plot of forecast versus observed daily 1-hour maximum ozone concentration for the 1993 high season at Liossion station using the ARIMA model. Solid line shows an ordinary least square regression fitting. Units are in μg m^{-3}.

statistics and gives the most reliable forecast. The WISPER model follows being very close to the multivariate REGLIN6 model.

For all models, the slope and intercept of the regression line indicates that low concentration values are over-predicted and high concentration values are under-predicted. The existing difficulty of the models to forecast high ozone values is not surprising since none of these models, because of their empirical nature, can handle extreme values successfully. A very interesting probabilistic approach concerning extreme value prediction is the application of extreme value theory which has already been applied successfully (Abatzoglou *et al.*, 1986; Surman *et al.*, 1987).

The ARIMA (0,1,2) model does not seem appropriate for ozone air-quality forecast. It performs no better than pure persistence a fact already pointed out by Robeson *et al.*, 1990. Generally, the forecast ability of tested models is, by category

TABLE IVa
Forecast skill for O_3 episodes. Occurrences of $[O_3] > 200\ \mu g\ m^{-3}$

	Observed	REGLIN6	WISPER	TEMPER	ARIMA	Persistence
Number of days with $[O_3] > 200\ \mu g\ m^{-3}$	42	38	48	30	38	42
Number of days of correct alarms		24	25	16	17	21
% correct alarms (POD)		*57%*	**60%**	*38%*	*40%*	*50%*
Number of days with false alarms		14	23	14	21	21
% false alarms		*10%*	*16%*	*10%*	*15%*	*15%*
SCI		*0.43*	*0.39*	*0.29*	*0.27*	*0.33*

TABLE IVb
Forecast skill for O_3 episodes. Occurrences of $[O_3] > 180\ \mu g\ m^{-3}$

	Observed	REGLIN62	WISPER	TEMPER	ARIMA	Persistence
Number of days with $[O_3] > 180\ \mu g\ m^{-3}$	55	51	61	46	46	55
Number of days of correct alarms		36	40	28	27	33
% correct alarms (POD)		*65%*	**73%**	*51%*	*49%*	*60%*
Number of days with false alarms		15	21	18	19	22
% false alarms		*10%*	*15%*	*13%*	*13%*	*15%*
SCI		*0.52*	*0.53*	*0.38*	*0.37*	*0.43*

and by estimated statistics, comparative and in some cases much better than those found in similar previous works (Robeson and Steyn, 1989; Wolff and Lioy, 1978).

As far as the ability of each model to forecast true episode-days is concerned, the WISPER model demonstrated the best performance (three times in four). It has forecasted 40 true episodes out of 55 observed during summer 1993 at the Liossion station (ozone concentration occurrences $>180\ \mu g\ m^{-3}$). Such a forecasting ability is superior to that achieved by Prior *et al*. for Saint Louis (1981), and by Lalas *et al*. (1983), for Athens with more complicated deterministic models. This is not surprising as the high pollution concentration in the area studied usually persists for some days and are associated with stationary anticyclonic conditions or with a counter balance between sea-breeze circulation and regional or synoptic circulation (Gusten *et al*., 1988; Lalas *et al*., 1985). Considering the simplicity of the WISPER model compared with the two regression models, it can be used on a daily basis as a predictive tool for photochemical air-pollution episodes in Athens Basin and as a useful element in planning strategies for ozone epiisodes abatement and prevention.

6. Appendix

Expressions of forecast skill (Ryan, 1995):

POD: The probability of detection, measures the percentage of ozone events that were correctly forecast:

$$POD = \frac{A}{A+B} .$$

CSI (or Threat score): The *C*ritical *Success* Index is a common skill score measure given by:

$$CSI = \frac{A}{A+B+C} .$$

The verification of the ozone forecast utilises a standard contingency table as:

	Forecast	
	yes	no
Observed yes	A	B
Observed no	C	D

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