3.3 **AIR-QUALITY MODELING USING OFF-LINE OR ON-LINE TECHNIQUES**

Gunilla Svensson*
Stockholm University, Stockholm, Sweden

1. INTRODUCTION

Meteorological fields are required inputs for Air-Quality Models (AQMs) and it is evident from many studies that the errors in these inputs may contribute considerably to uncertainties in the simulations of air-born chemical species. These errors may be caused by inadequate meteorological models, but also by the fact that these fields are considered as inputs and not as forecast variables in the AQMs. If the grids of the two models are incompatible, an interpolation step is necessary to project the meteorology onto the AQM's grid system. This may introduce major problems; see Byun (1999a,b) for an extensive discussion. Interpolation from one grid to another can lead to a change in mass and loss of detail. This is of course most important when there are large gradients in the meteorological and/or chemical fields. Another problem involves divergences in the horizontal wind field that may be used for diagnosing the vertical wind field. Small errors in the interpolated horizontal wind field may case large errors in the divergence field and as a consequence gives rise to very large errors in the vertical wind speed. This may in turn lead to serious problems in the air pollution calculations.

Commonly, the meteorological simulation is performed first and some of the fields are stored at certain times. Thus, an interpolation in time is also required. Some AQMs even hold the meteorology constant for an hour (or for whatever period is dictated by the input) and then update instantaneously at the end of that period. Clearly, this interpolation gives rise to sizeable errors as well.

From a scientific point of view, the most logical approach is to solve both the meteorology and chemistry at the same time on the same grid. The difference in computational time is not very large since the chemical species are normally many more than the meteorological forecast variables. This study investigates the influence of the interpolation time on the chemical calculations, from on-line to 6h interpolations. The day chosen for this study is 14 September 1994 and the location is the city of Athens in Greece (Figure 1). Observations for this area is available from the experimental part of the project MEDCAPHOT–TRACE (Mediterranean Campaign of Photochemical Tracers – Transport and Chemical Evolution; Ziomas et al., 1995).

* Corresponding address: Gunilla Svensson, Department of Meteorology, Stockholm University, S-106 91 Stockholm, Sweden; e-mail: gunilla@misu.su.se

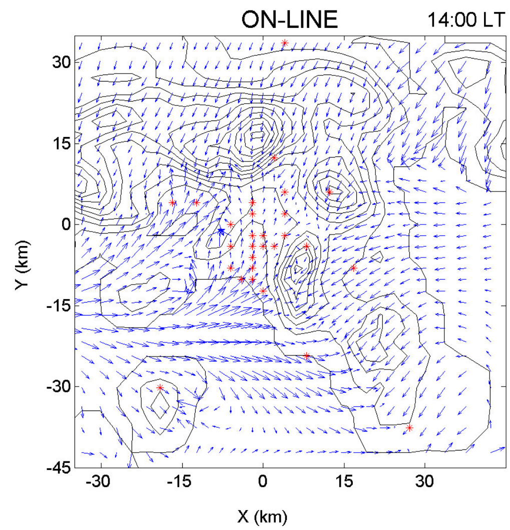

Figure1. The Attika peninsula with the city of Athens in the center of the domain. The terrain is indicated with isolines every 100m. The red stars show the location of meteorological observations. Also shown is surface wind field (7m above ground) at 14 LT.

This data was previously successfully modeled (Svensson 1998; Svensson and Klemm, 1998) and the same model that is used in this study. The model is a three-dimensional time-dependent coupled photochemical and meteorological model (Svensson 1996).

2. SIMULATIONS

For this study, the model was run fully coupled and all fields were saved every half-hour (on-line simulation). This simulation is basically the same as that presented and discussed thoroughly in Svensson (1998); only small model changes gives slightly different results. Then, the chemical part of the model was run with interpolated meteorological fields. The time intervals used for the interpolation were 1, 3 and 6 hours. No interpolation in space was done and all variables, including the turbulent kinetic energy and vertical velocity were interpolated. Thus, no variables where diagnosed from the standard meteorological output as is often done in AQMs.

Table I. Statistical parameters for the observed (o) and modeled (p) wind speed (m s^{-1}) and direction (º). Data with wind speeds >0.2 ms^{-1} are included. The table includes the mean, mean difference, standard deviations, correlation coefficients, index of agreement and root mean square error for the wind speed and mean difference and root mean square error for the direction.

	Wind speed								Wind direction	
	$\overline{U_o}$	$\overline{U_p}$	MD	σ_o	σ_p	R	RMSE	IOA	MD	RMSE
On-line	1.7	1.7	0.05	1.0	0.8	0.43	1.14	0.62	2.3	73.5
1h-interp.		1.7	0.07		0.8	0.42	1.14	0.62	3.8	73.2
3h-interp.		1.5	0.2		0.7	0.39	1.13	0.60	4.4	74.8
6h-interp.		1.4	0.3		0.7	0.27	1.18	0.55	2.7	76.5

Table II. Statistical parameters for the observed (o) and modeled (p) ozone mixing ratio (μg m^{-3}). The table includes the mean, maximum, standard deviations, correlation coefficients, index of agreement and root mean square error.

	$\overline{O_{3_o}}$	$\overline{O_{3_p}}$	Max_o	Max_p	σ_o	σ_p	R	IoA	RMSE
On-line	84	55	200	200	18	8	0.64	0.69	63
1h-interp.		67		232		10	0.65	0.71	63
3h-interp.		67		200		10	0.68	0.72	57
6h-interp.		61		155		14	0.56	0.63	57

The model is run for two days with constant synoptic forcing and only results from the second day are considered. The synoptic situation was dominated by a high-pressure system with a geostrophic wind from N 6 m s^{-1} over the Attica peninsula. The SST was set to 21 ºC and the land temperature was always higher, even during the night; thus excellent conditions for sea breeze circulations to develop. The model was initiated with significant background concentrations of ozone and CO and very low levels of the other species (Svensson 1998).

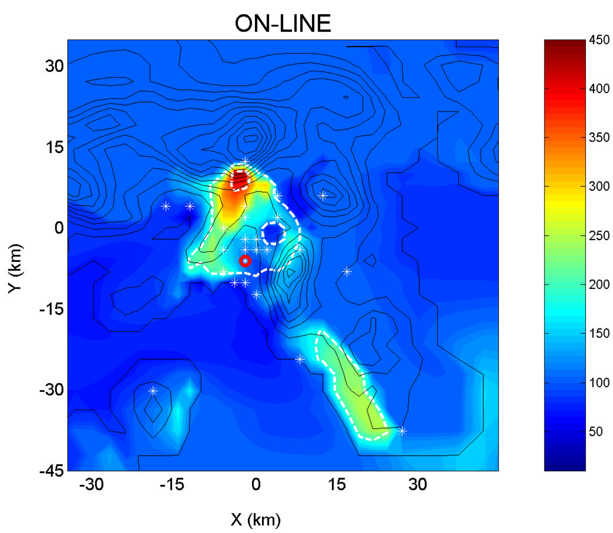

Figure 2. Near surface (7m above ground) mixing ration of ozone (μg m^{-3}) at 14 LT. The white stars show the location of chemical observations. The terrain is indicated with isolines every 100m.

3. RESULTS

The focus in this study is Athens, Greece. The city is located in a basin surrounded by mountains with tops around 1000 m. Figure 1 shows the central part of the model domain with the meteorological observational locations indicated with red stars. The horizontal resolution in this part of the domain was about 2 km, the same as for the emission database, Figure 1 also shows surface wind vectors at 14:00 LT. At this time the sea-breeze circulation is well developed. Figure 2 shows the near surface mixing ratios for ozone together with the locations for chemical observations. The sea breeze has transported the pollutions from downtown Athens towards north on the side of the mountainside. In total, there were 26 stations measuring ozone and 28 stations with basic meteorology; some of them coinciding and some separate.

Some statistical parameters for the wind field results are presented in Table I; all numbers are average over both the day and the stations. The wind speed is generally very low and the mean difference between the observed and modeled values is negligible, for both speed and direction. The wind fields obtained when interpolating data with 1, 3 and 6 hours interval, respectively, are also presented in the table. Generally, the correlation coefficient and total agreement is degrading with increasing interpolation time, as expected.

In Table II, similar statistical parameters are presented for the ozone concentration in μg m^{-3}. For the on-line simulation, the correlation coefficient as an average over the day for all stations is 0.65 and the Index of Agreement (IoA) is 0.69. The statistical numbers for the interpolated cases are not significantly different from the on-line case, some are even increasing somewhat

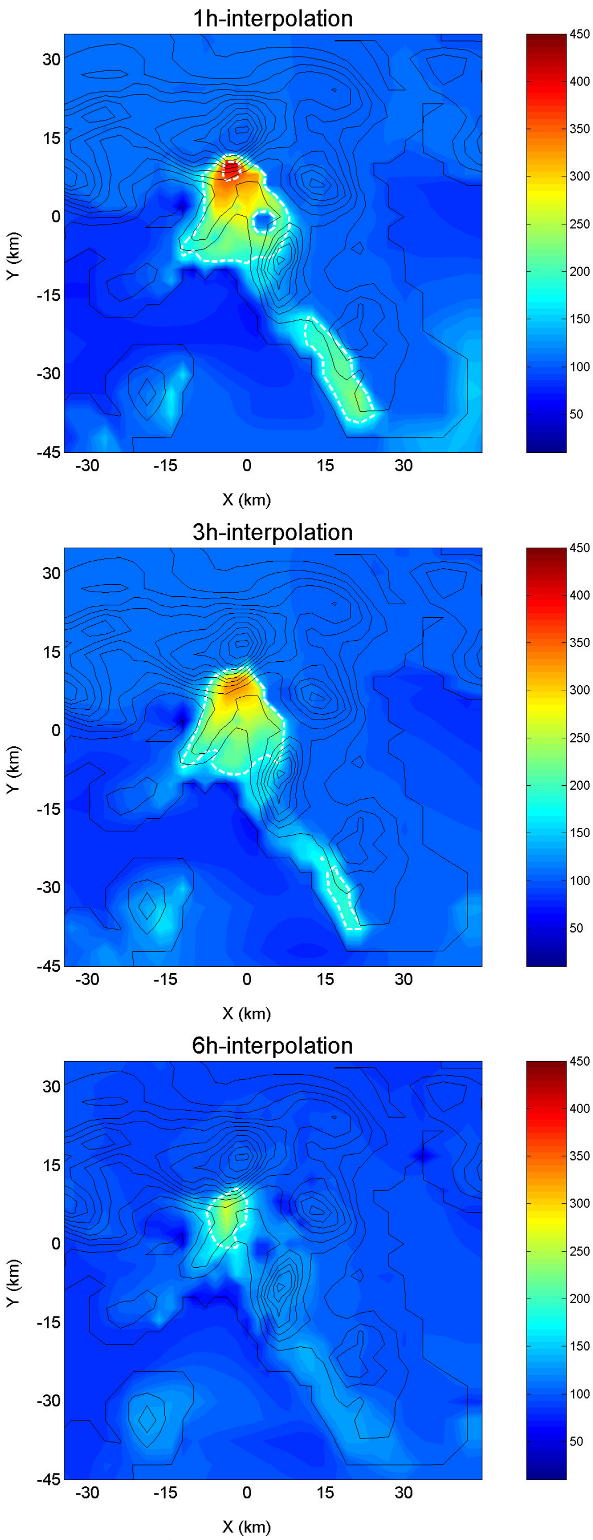

Figure 3. Near surface (7m above ground) mixing ration of ozone (μg m^{-3}) at 14 LT. The contourlines for 180 and 360 μg m^{-3} are plotted with white dashed lines. The terrain is indicated with isolines every 100m. Top figure: 1 hour interpolation, middle: 3 hour interpolation and bottom: 6 hours interpolation.

judging from these numbers the ideal seems to be to interpolate the meteorological fields from results saved every third hour. However, the further analysis will support the conclusion that even though we have a fair amount of observational material, it is not enough to fully determine the quality of the simulation.

Figure 3 shows the surface concentration of ozone for the three off-line simulations at 14:00 LT. When comparing with Figure 2, the conclusion is that even though the statistical result shows quite similar figures for all simulations, the concentration patterns are different. In the on-line simulation, the highest levels are concentrated to a rather small area outside the most populated parts of the basin. In the off-line simulations, the areas defined with 180 μg m^{-3} (dashed white line in Figures 2 and 3) are quite similar for the 1 and 3-h interpolation. The maximum concentration is decreasing with increasing interpolation time. When using the 6-h fields for interpolation, the area with concentrations above 180 μg m^{-3} is much smaller and the maximum concentration is less than 250 μg m^{-3}**.**

Table III. European Union directives for ozone.

European union directives for ground-levels of ozone	
Critical levels not to be exceeded causing vegetation damage	65 μg m^{-3} diurnal mean
	200 μg m^{-3} hourly mean
Critical levels not to be exceeded causing health problems	110 μg m^{-3} averaged over 8 hours
Information alert threshold	180 μg m^{-3} hourly mean
Warning alert threshold	360 μg m^{-3} hourly mean

Table IV. Number of hours with one-hour averages of ozone levels over thresholds, 180 and 360 μg m^{-3}, for September 14, 1994. Results from the inner domain (40 x 40 km^{-2}) and within the city-border.

	Number of hours > 180 μg m^{-3}		Number of hours > 360 μg m^{-3}	
	Inner domain	City	Inner domain	City
On-line	7	2	4	0
1h-interp.	9	2	6	0
3h-interp.	7	2	5	0
6h-interp.	3	0	2	0

The European Union has common directives for ozone mixing ratios for their member states, see Table III. (The Clean Air Act in US has similar levels: 0.08 ppm (~160 μg m^{-3}) 8 hours average, and 0.12 ppm (~235 μg m^{-3}) 1-hour average.) Further analysis using these criteria is summarized in Table IV and IV. The results in Table IV show that the number of hours that the mixing ratios exceed the information alert threshold varies between the simulations. It is interesting to note that the 1-h interpolation results give a longer time exceeding both thresholds within the inner domain. The longest interpolation time gives fewest hours over the criteria.

In Table V, the area with ozone levels above 110 μg m^{-3} is calculated for the simulated day divided to three 8-h periods according to the criteria presented in Table III. The area exceeding this threshold is larger for both the inner domain and within the city for all interpolation times for the first two time-periods. Especially the mid-day period shows a very large increase in the area for the 1-hour interpolation time. In addition, for this period, all results for the interpolation simulations have higher concentrations than the threshold within the city; this is not seen in the on-line simulation. For the evening period, the differences between the simulations are less pronounced.

Table V. Area (km^2) that has 8h-average ozone levels above 110 μg m^{-3} for three periods on September 14, 1994. Results from the inner domain (40 x 40 km^{-2}) and within the city-border.

	00-08		08-16		16-24	
	Inner	City	Inner	City	Inner	City
On-line	112	0	250	0	46	0
1h-interp.	135	0	419	89	66	0
3h-interp.	135	0	367	93	40	0
6h-interp.	135	0	156	20	0	0

3. CONCLUSIONS

Simulations for an air pollution episode in Athens Greece were performed both with on-line and interpolated meteorology using three interpolation times. Statistical measures are calculated for all simulations and no significant difference is found for these measures for the wind field. However, the simulated ozone concentrations changes when interpolated meteorological fields are used instead of the on-line simulation. Further analysis shows that for example the area that exceeds the critical level 110 μg m^{-3} increases with 65 % when interpolation using data every hour instead of on-line simulation. In addition, the number of hour increases from 4 to 6 for exceeding the warning alert threshold.

The amount of chemical and meteorological stations is not enough to make it possible to distinguish which simulation that is closest to the truth. However, this study shows that interpolation, only in time, gives quite a large impact on the chemical results. The simulated situation is complicated with local circulations – for a simpler meteorological setting, the sensitivity would be less. Interpolation will always introduce errors – to minimize this problem it is best to perform the calculations on-line, the additional calculation time is not very large.

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