A Screening Procedure for Monitoring Ozone and Nitrogen Dioxide in “Small- to Medium-sized” Cities:

Phase II – application of the procedure

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ABSTRACT

A screening procedure for determining the need for monitoring of nitrogen dioxide (NO_2) and ozone (O_3) in small to medium cities without large industry has been applied to generic coastal and inland towns. The procedure involves simulating a 12-month period with the air quality model TAPM, for towns of different population sizes, and determining the maximum concentration likely to be monitored in the town. Population sizes evaluated were 250 000, 150 000, 100 000, 50 000 and 25 000.

Maximum concentrations were compared to acceptance limits, specified as a percentage of the relevant NEPM standard in the NEPM Technical Paper No. 4 (Peer Review Committee, 2001). Screening would be considered acceptable only if the procedure yielded a prediction of maximum pollutant concentration that was below the acceptance limit for that procedure. For the category of screening procedure applied in this Study, the acceptance limit for hourly-averaged O_3 is 48 ppb, for 4-hourly averaged O_3 it is 41 ppb, and for NO_2 the limit is 42 ppb. A background O_3 concentration of 20 ppb was used in our simulations.

Our results indicate that coastal towns with populations of less than 100 000 do not produce hourly-averaged O_3 glcs exceeding the acceptance limit, while inland towns of 150 000 or less people do not exceed the limit. For 4-hourly averaged O_3 concentrations, the acceptance limit is only exceeded by coastal towns greater than 150 000 population and inland towns of greater than 100 000 (on only one day per year for a population of 150 000).

For hourly-averaged NO_2, emissions from coastal populations of less than 100 000 produce concentrations below the acceptance limit. Although a population of 150 000 exceeds the limit, this only happens on one day per year. For the inland town, exceedance of the acceptance limit is predicted for all population sizes.

Comparison of results from a simulation for the inland town of 50 000 population with monitoring data from Wagga (population 55 000) showed satisfactory agreement for NO_2 concentrations. However, modelled O_3 results at the higher end of the concentration distribution were about 15 ppb lower than the observations. This was attributed to background concentrations of O_3 on many days being considerably higher than the value of 20 ppb used in our modelling. On hot days, background values near 45 ppb were observed about 7 km upwind of Wagga town centre. These values were produced by reactions involving VOC emissions from vegetation and NO_x emissions from soil, and may also have been enhanced by O_3 produced from fire emissions. Examination of results from the Australian Air Quality Forecasting System suggested that long-range transport of O_3 associated with emissions from Melbourne and Sydney may also contribute to background levels. If a worst-case background O_3 concentration of 45 ppb is assumed, it is estimated that the acceptance limits are exceeded by smaller populations, with all evaluated population sizes for an inland town equalling or exceeding both O_3 limits.

1 Introduction

The NEPM for Ambient Air Quality requires monitoring to occur within regions that contain urban centres with a population greater than 25 000. A formula for the required number of monitoring stations is given in the NEPM Clause 14(1). Clause 14(3) says that fewer performance monitoring stations may be needed where it can be demonstrated that pollutant levels are reasonably expected to be consistently lower than the standards mentioned in this Measure. The Peer Review Committee (PRC), established by Environment Ministers, has as one of its key roles the development of procedures and criteria to ensure consistency of monitoring plans across jurisdictions. The PRC has been considering a range of suitable screening procedures that might be applied as per Clause 14(3) to confidently demonstrate that monitoring is not required in particular situations.

In Phase I of our Study, validation results were presented for a screening procedure for O_3 and NO_2 in non-industrial cities with populations greater than 25 000 but smaller than those capital cities in which these pollutants are known to be potential problems. The essence of the procedure, involving CSIRO's The Air Pollution Model (TAPM, Hurley, 2002), is the linking of emissions to population numbers in regions where emissions are unknown, then running TAPM for an extended period and examining ground-level concentrations. Within the procedure, a simple scheme is also used for biogenic emissions whereby a conservative emission flux is linked to the vegetation fraction in each grid square. The procedure was validated by applying it to Perth, where both emissions and population are known, and comparing model results for a 12-month period (1999) to monitoring data from three stations. The difference between results from the surrogate population plus the biogenics inventory and the DEPWA inventory was certainly small enough to give confidence in application of the procedure in Phase II of this Study, as described in this Report.

The aim of this phase of the Study is to apply the screening procedure to derive generic criteria, primarily involving population numbers, that can be used to determine the likelihood that any particular city's emissions will lead to exceedance of the NEPM standards. We consider two types of cities, coastal and inland.

2 Experiment details

2.1 Locations of the towns

It is now well-known that the most important mechanism leading to high photochemical smog concentrations in coastal regions is early morning transport of emissions offshore followed by a recirculation in the sea breeze. Data analysis and modelling work in various parts of Australia suggest that the coastal region from Sydney to Brisbane is a particularly suitable area for photochemical smog formation. Favourable factors include the high annual frequency of sunny skies and warm temperatures, the coastal plain and topography, and the synoptic meteorology. The location of a generic coastal town (31^o12'S, 152^o53'E) was chosen to be near Kempsey in northern New South Wales, about halfway between Sydney and the Queensland – New South Wales border. In this area, there is a relatively wide coastal plain with a straight north/south coastline.

In inland areas, a recirculation mechanism is unlikely to play any part in photochemical smog production. Rather, significant smog levels are likely to form in situ on warm and sunny days with light winds and relatively shallow mixed layers. It is proposed to model Wagga (35^o8'S, 147^o22'E), just west of the Great Dividing Range, for the inland generic city as there are available O_3 and NO_2 data for 1998 from a monitoring site about 7 km north-northeast from the Wagga town centre. These can be compared in a general way to the model results.

The 12-month period chosen for simulation was 1 July 1997 to 30 June 1998. Data from EPA Queensland's southeast Queensland regional monitoring network showed that photochemical activity during the 1997-98 summer was the highest (number of days with hourly-averaged O_3 values greater than 80 ppb) for any season from 1996 to 2001. However, higher peak values occurred in the summers of 1996/97 and 1998/99.

2.2 Model grid setup

2.2.1 TAPM

Three nested grids were run for each location, with the coastal grids centred at (31^o12'S, 152^o54'E) and the inland grids at (35^o8'S, 147^o22'E). For the meteorology component of TAPM, grid domains consisted of 35 x 35 x 20 gridpoints with grid spacings of 30, 10 and 3 km. Air quality simulations, centred on the same location, were undertaken with 33 x 33 x 20 gridpoints, using half the grid spacings (15, 5 and 1.5 km), so that the area covered (48 x 48 km^2 for the smallest domain) was slightly less than half that of the meteorology simulations. This was considered appropriate as pollutant concentrations are primarily of interest over the area covered by the towns. Deep soil moisture was set at 0.05 for months August through to April while a value of 0.15 was used for May, June and July.

2.2.2 Anthropogenic emissions

Emissions of nitrogen oxides (NO_x) and volatile organic compounds (VOCs) from the towns are directly related to population through the emission factors (kg day^{-1} $capita^{-1}$) that were derived for Perth in the Phase I study (Physick and Cope, 2001). These were calculated for commercial/domestic sources, petrol vehicles (tailpipe and evaporative emissions) and diesel vehicles (tailpipe). The Perth diurnal, weekday, Saturday and Sunday profiles were applied. Surface emissions were distributed evenly over the first two model layers. Comparison of the Perth emission factors with those for small- to medium-sized towns via National Pollutant Inventory (NPI) data is not feasible because the NPI does not log vehicle or domestic emissions.

Populations (emissions) were distributed about the town centre in a bi-Gaussian (coastal) and Gaussian (inland) manner. The coastal distribution was bi-Gaussian because populations tend to stretch further along the coastline than they do in the inland direction. The area covered by towns of different population sizes was determined by examining 28 Australian towns with populations ranging from 25,800 to 229 000. Population sizes were obtained from the 1996 census (http://www.abs.gov.au/). Areas were obtained from the shaded built-up area on Australian topographic survey maps (1:100000). Figure 2.1 is a plot of area against population for these towns, with the curve of best fit used as a guide to assigning an area value to the populations used in the Study. Model simulations were carried out for five populations ranging from 25 000 to 250 000. Dimensions of the towns are listed in Table 2.1.

The emissions were calculated on a 1-km spaced grid for all towns. Population at the town centre was assumed the same for all population sizes. This assumption was made to give each town a central business district with a similar emission flux. Naturally, the smaller the total population, the faster the population decreases with distance from the town centre.

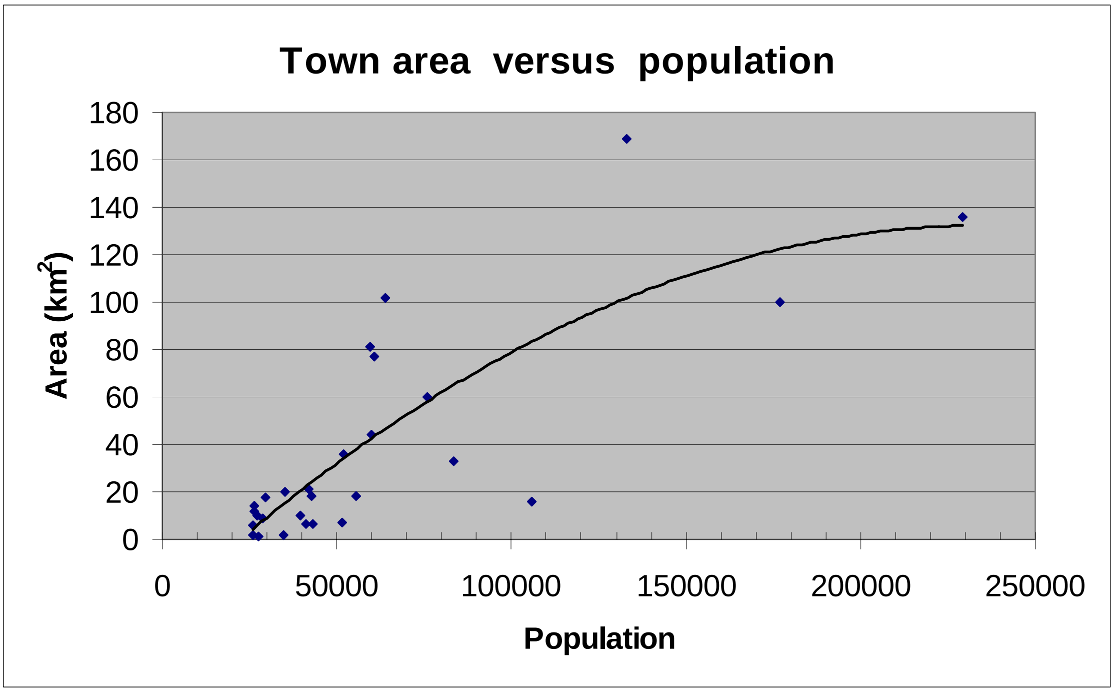


Figure 2.1 Area (km^2) of 28 Australian towns versus population. A curve of best fit is also shown.

Table 2.1 Area (km^2) assigned to towns of different populations for coastal and inland locations. Also shown are approximate east-west (E-W) and north-south (N-S) dimensions of the towns, with outer limits defined as where the population is 1% that of the town centre.

Population	*Coastal*			*Inland*		
	Area (km^2)	*E-W*	*N-S*	*Area (km^2)*	*E-W*	*N-S*
250 000	180	10.0	18.0	180	13.4	13.4
150 000	117	8.5	13.4	117	10.8	10.8
100 000	77	7.0	11.0	77	8.8	8.8
50 000	35	4.8	7.2	35	6.0	6.0
25 000	14	3.0	4.6	14	3.8	3.8

2.2.3 Biogenic emissions

For application of the screening procedure to generic small- to medium-sized cities in this Study, biogenic VOC emissions are modelled using an approach that does not include specific vegetation types. To create a generic biogenic inventory, we have chosen to assume that all vegetation at 30^{o}C and a photosynthetic active radiation level (PAR) of 1000 μmol m^{-2} s^{-1} emits at the relatively high rate of 0.11x10^{-5} g s^{-1} m^{-2} (typical of isoprene from eucalyptus), and to allocate emissions to a grid square according to the fraction of that square that is vegetated. This assumption may lead to a small bias in over-predicting ozone and under-predicting nitrogen dioxide, but this is the preferred bias as actual ozone levels in Australian towns and cities are expected to be more of a problem than nitrogen dioxide levels. Vegetation fractions are obtained from a 5-km spaced grid covering all of Australia, developed by Dean Graetz at CSIRO Office of Space Science Applications (COSSA) and included in the TAPM data set.

For coastal and inland simulations, the 5-km spaced biogenic emissions grid covers all modelling domains and is centred at the same location as the TAPM grid. VOC emissions are specified at 30^{o}C and a PAR level of 1000 μmol m^{-2} s^{-1}. When the emissions are input in this way, TAPM is able to calculate hourly VOC emissions that are a function of temperature and PAR.

3 Sensitivity to background VOCs

The photochemistry equations in TAPM are formulated in terms of the smog-producing reactivity R_{smog}, defined as VOC concentration multiplied by an activity coefficient for smog production. The value of the coefficient differs between VOC species, but an appropriate value for the VOC mix in an urban air mass is considered to be 0.0067 ppm/ppmC (Johnson et al., 1990). This value was used here to multiply emission rates for all VOC sources. It is also necessary to assign a background value for R_{smog}, partly to account for a general background concentration of VOCs (even though biogenic emissions are included separately) but also to compensate for the omission of some inorganic radical-producing reactions in the GRS photochemical mechanism. In order to examine the sensitivity of O_3 and NO_2 glcs to the background value of R_{smog}, TAPM simulations with R_{smog} varying between 0.25 and 1.0 were done for the generic coastal town for populations of 250 000 and 25 000.

Although the statistic of primary interest in this Study is the annual highest concentration, other statistics may also be of interest and so results throughout the Report are presented in terms of mean and maximum concentration, percentile concentrations, and robust highest concentration (RHC). The RHC approach (Cox and Tikvart, 1990) recognises that peak (maximum) concentrations are highly variable in both models and observations, and uses information contained in the upper end of the concentration distribution to calculate a robust statistic (RHC) for simulation and model comparison purposes. In this study, we have used the 11^{th} highest concentration (over 12-months), and the mean of the top-ten concentrations, to extrapolate to the RHC.

Annual concentration statistics for NO_2 and O_3 within the town boundaries are shown in Figure 3.1 for the population of 250 000. The hourly-averaged NO_2 maximum glcs range between 41 ppb and 54 ppb (Figure 3.1(a)), a 32% increase when R_{smog} ranges from 0.25 to 1.0. Over the same range, hourly-averaged O_3 glcs increase by 92% (33 ppb in Figure 3.1(b)) and 4-hourly averages of O_3 by 48% (Figure 3.1(c)). Percentage increases are smaller for a population of 25 000 (Figure 3.2). As discussed in Section 4.1, the higher O_3 glcs for the year occur around midday when the morning peak-hour emissions, having drifted offshore, return over the town in the sea breeze. As higher concentrations of VOCs (R_{smog}) enable the photochemistry to proceed at a faster rate, it is not surprising that O_3 glcs in the town are higher for the larger values of background R_{smog}. However, if the air mass becomes NO_x-limited later in the day at a location further inland, there may be less difference between the O_3 maxima at this site for different values of R_{smog}. This is confirmed by examining the total 1.5 km grid domain where the difference in maximum hourly-averaged O_3 between R_{smog} values of 0.25 and 1.0 is 26 ppb (down from 33 ppb).

In Phase I of this Study, preliminary simulations with various values of R_{smog} showed that a value of 1.0 was considered appropriate for the urban environment of Perth, a city of 1 million people and associated area sources. TAPM simulations for Brisbane (Ischtwan, 2002) found that a value of 0.8 gave the best results, and a value of 0.7 was used by Hurley et al. (2002) in their Melbourne simulations. In contrast, a value of 0.1 was found by Physick et al. (2002) to be most suitable for the Burrup Peninsula area in north-western Australia, where two point sources emit into an almost pristine background environment and anthropogenic area sources are associated with a few hundred people in two towns. These studies suggest that the appropriate value for background R_{smog} in a TAPM simulation is proportional to the population in the modelled region, and consequently a lower rather than higher value should be used for the experiments in this Study. However, given the uncertainty associated with this issue and given that it is better to err on the conservative side here, we have chosen a value of 0.75 for background R_{smog} for the coastal and inland simulations presented in Sections 4 and 5 respectively.

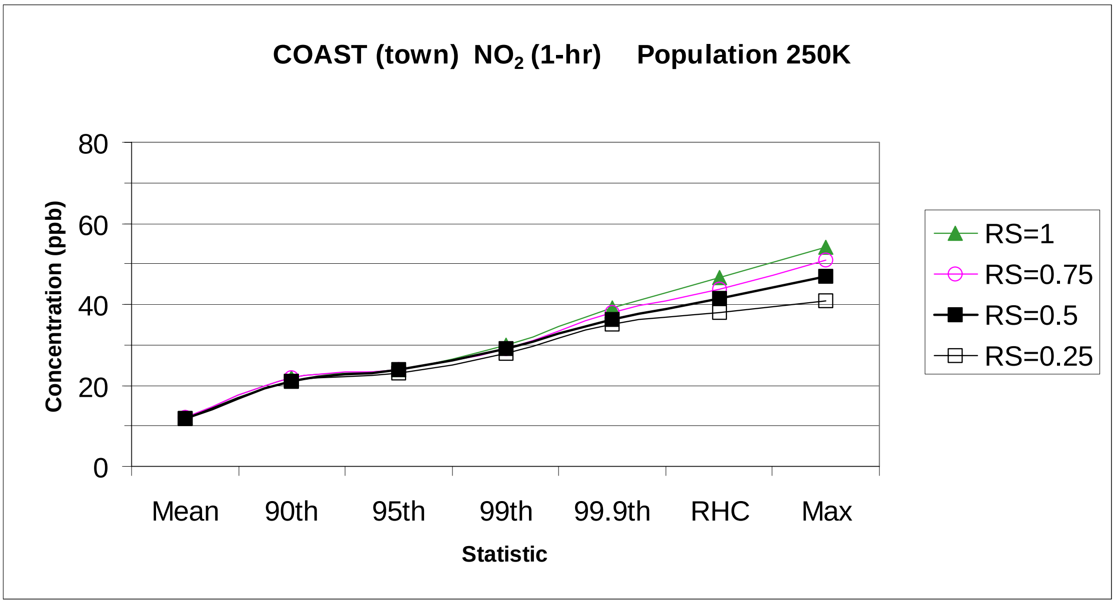


Figure 3.1(a) Annual glc statistics for hourly-averaged NO_2 for the *coastal* town with a population of 250 000. Curves are for different values of the background VOC concentration R_{smog} (RS). Statistics are calculated within the town's boundaries.

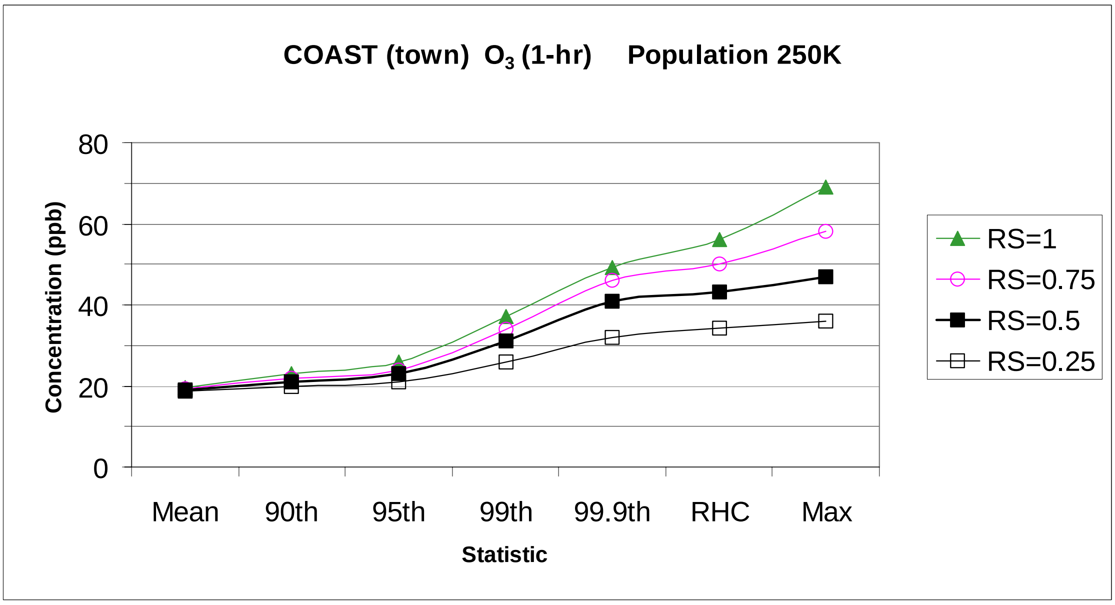


Figure 3.1(b) Annual glc statistics for hourly-averaged O_3 for the *coastal* town with a population of 250 000. Curves are for different values of the background VOC concentration R_{smog} (RS). Statistics are calculated within the town's boundaries.

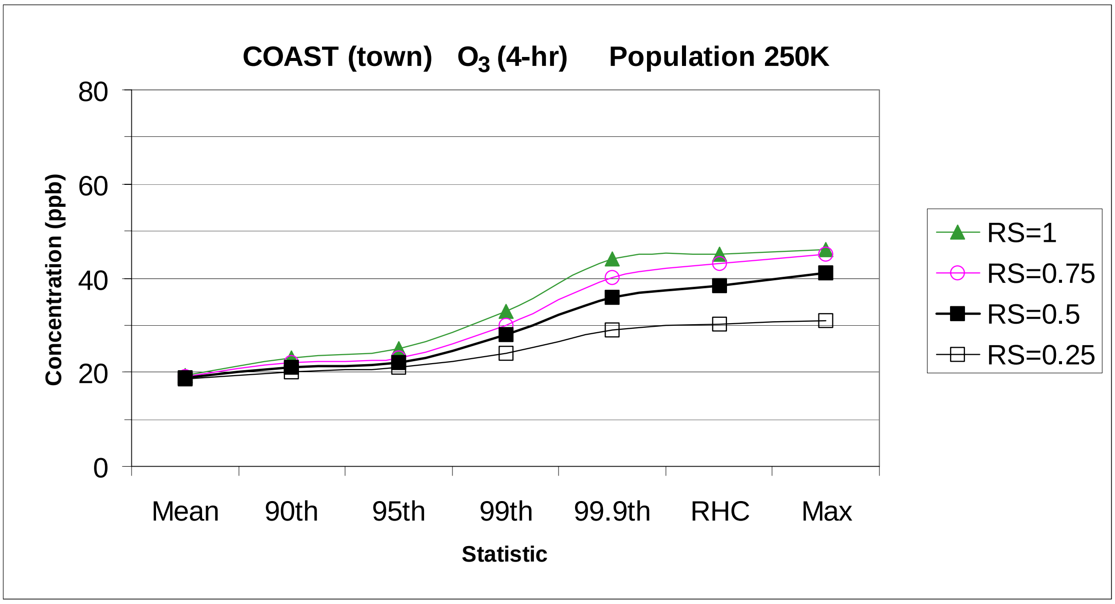


Figure 3.1(c) Annual glc statistics for 4-hourly averaged O_3 for the *coastal* town with a population of 250 000. Curves are for different values of the background VOC concentration R_{smog} (RS). Statistics are calculated within the town's boundaries.

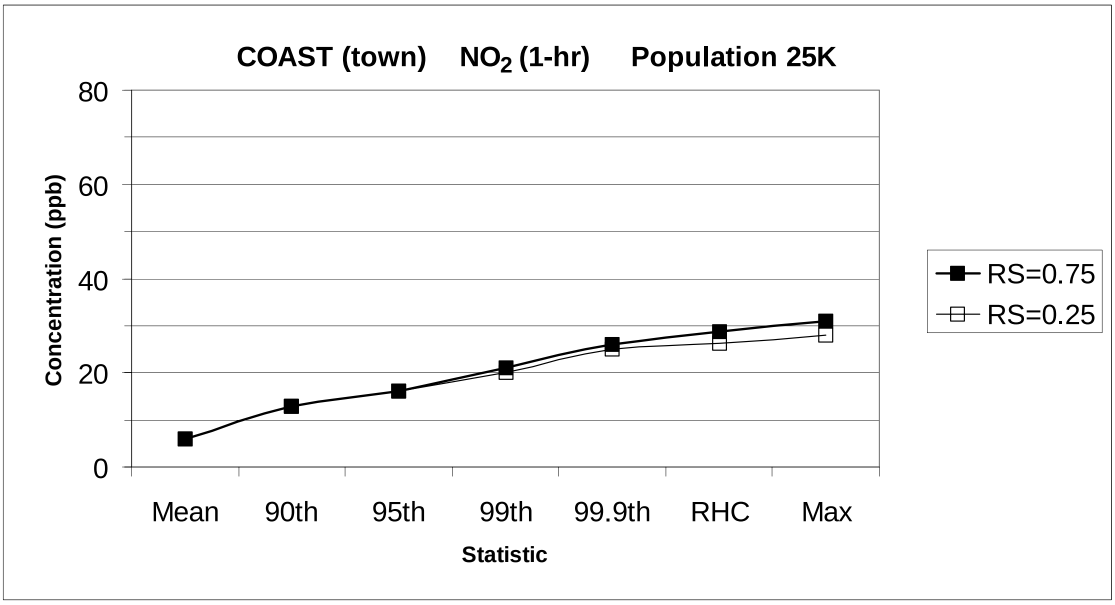


Figure 3.2(a) Annual glc statistics for hourly-averaged NO_2 for the *coastal* town with a population of 25 000. Curves are for different values of the background VOC concentration R_{smog} (RS). Statistics are calculated within the town's boundaries.

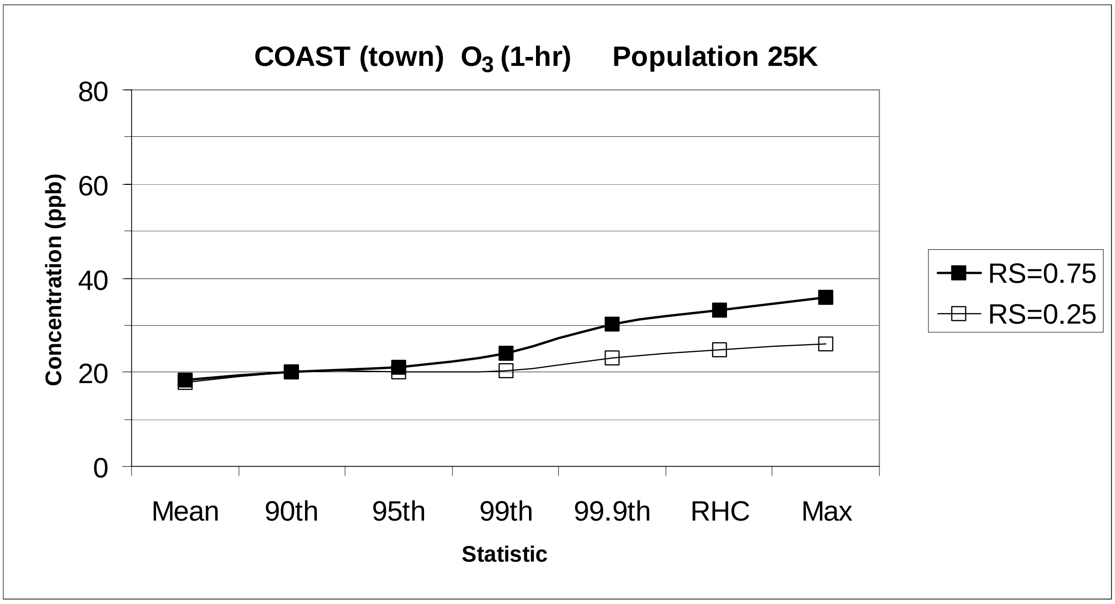


Figure 3.2(b) Annual glc statistics for hourly-averaged O_3 for the *coastal* town with a population of 25 000. Curves are for different values of the background VOC concentration R_{smog} (RS). Statistics are calculated within the town's boundaries.

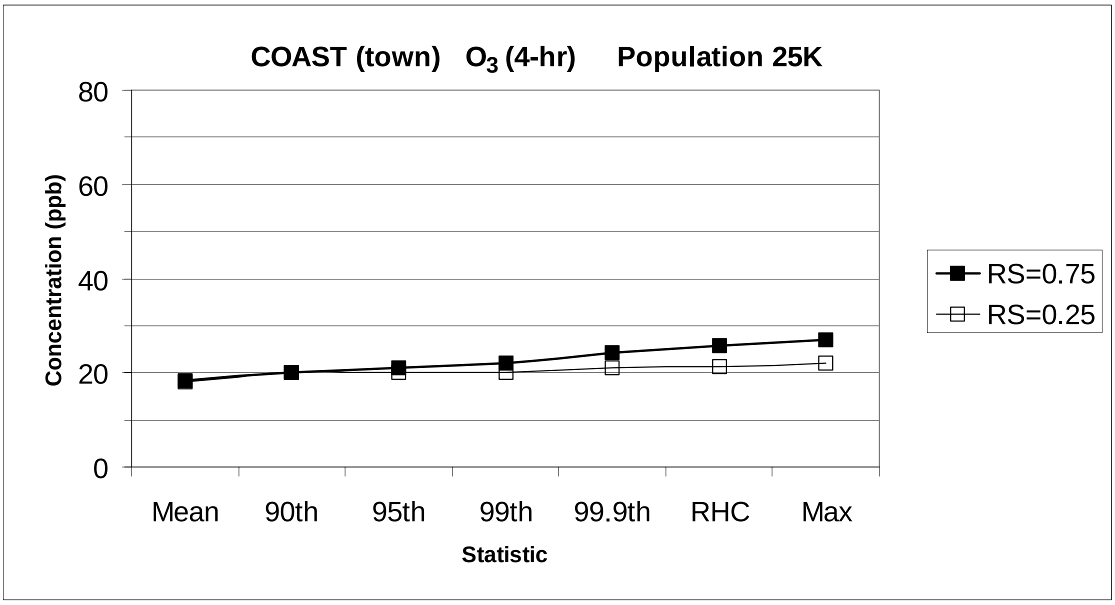


Figure 3.2(c) Annual glc statistics for 4-hourly averaged O_3 for the *coastal* town with a population of 25 000. Curves are for different values of the background VOC concentration R_{smog} (RS). Statistics are calculated within the town's boundaries.

4 Modelling results

4.1 Coastal town

TAPM was run for 12 months for populations of 250 000, 150 000, 100 000, 50 000 and 25 000. Annual ground-level concentration statistics for NO_2 and O_3 within the town boundaries are shown in Figure 4.1. The maximum values for NO_2 range from 51 ppb down to 31 ppb (Figure 4.1(a)), and occur throughout the year in the morning and evening peak traffic times when the mixed layer is shallow and winds are very light. The largest concentrations are predicted to occur at the actual or adjacent gridpoint where emission rates of NO_x are highest, suggesting that they are the result of the fast reaction involving titration of O_3 by NO. A small amount of NO_2 is also emitted directly (taken here to be 10% of NO_x).

Maximum values within the town boundaries for hourly-averaged O_3 range from 58 ppb down to 36 ppb (Figure 4.1(b)), and from 45 ppb down to 27 ppb for 4-hourly averaged values (Figure 4.1(c)). These typically occur in the summer months in the late morning/early afternoon period after the morning peak-hour emissions have drifted offshore and are transported back over the town in the sea breeze. These are not the highest O_3 concentrations that are produced by the town's emissions, as the urban air mass continues to produce more ozone as it moves further inland with the sea breeze. This is illustrated by the concentration statistics over the 1.5-km modelling domain (an area of 48 x 48 km^2) in Figure 4.2(b, c), which show higher values than are predicted for the town area in Figure 4.1(b, c). Note that there is no difference for the NO_2 statistics (Figure 4.2(a)) because the highest values occur within the town boundaries. Contours of the annual maximum O_3 concentration at each gridpoint in the 1.5-km domain are shown in Figure 4.3 for the 250 000 and 50 000 populations. This plot also illustrates that the highest O_3 concentrations occur away from the town. Corresponding plots for NO_2 in Figure 4.4 show that the highest concentrations occur within the town, although for the 250 000 population there is a secondary maximum (photochemically produced) of between 35 and 40 ppb over the sea. Similar values of NO_2, produced through photochemical reactions, occur west of the town's boundaries.

The number of days per year on which glcs exceed threshold concentrations are listed in Table 4.1 for various populations. For example, for towns with populations of 100 000 or less, TAPM predicts, for hourly-averaged NO_2 and for both averaging periods for O_3, that a concentration of 40 ppb will not be exceeded on more than one day a year.

Table 4.1 Number of days per year on which threshold modelled concentration values (listed) are exceeded within the boundaries of the coastal town. Values are shown for populations ranging between 250 000 and 25 000.

	NO_2 (1-hr)		*O_3 (1-hr)*		*O_3 (4-hr)*	
	>40 ppb	*>50 ppb*	*>40 ppb*	*>50 ppb*	*>35 ppb*	*>40 ppb*
250 000	4	1	11	3	11	4
150 000	1	0	10	1	6	0
100 000	1	0	1	1	0	0
50 000	0	0	1	0	0	0
25 000	0	0	0	0	0	0

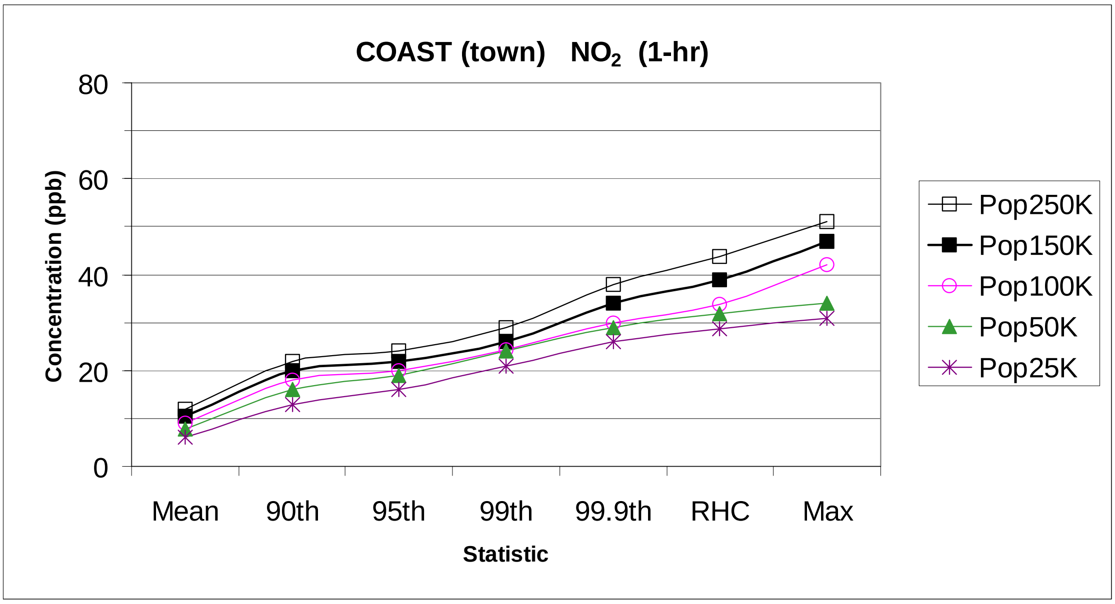


Figure 4.1(a) Annual glc statistics for hourly-averaged NO_2 for the *coastal* town. Curves are for different population sizes and statistics are calculated within each town's boundaries.

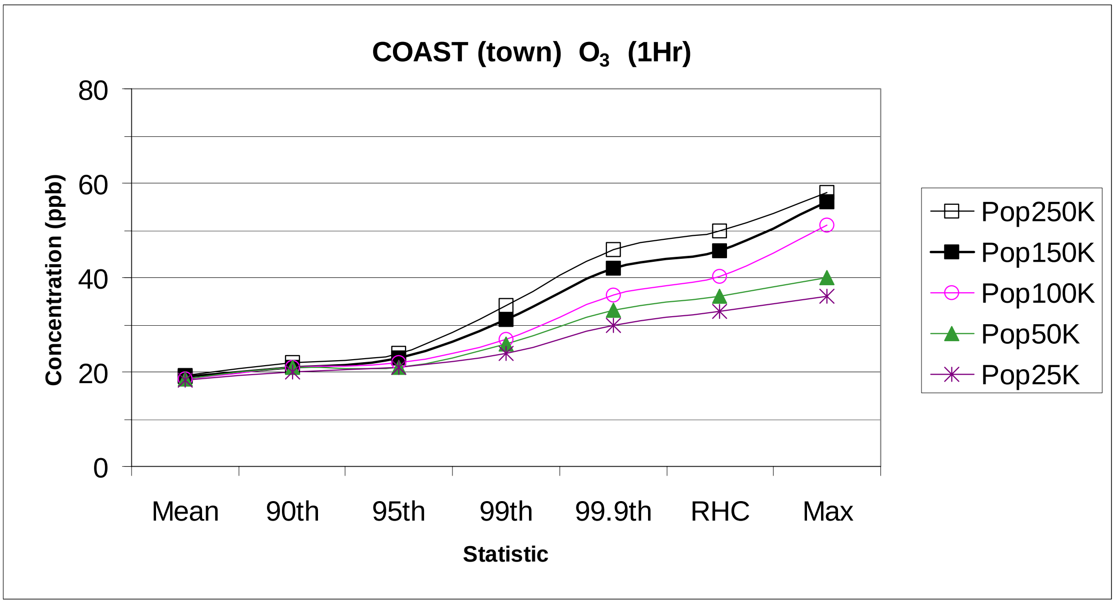


Figure 4.1(b) Annual glc statistics for hourly-averaged O_3 for the *coastal* town. Curves are for different population sizes and statistics are calculated within each town's boundaries.

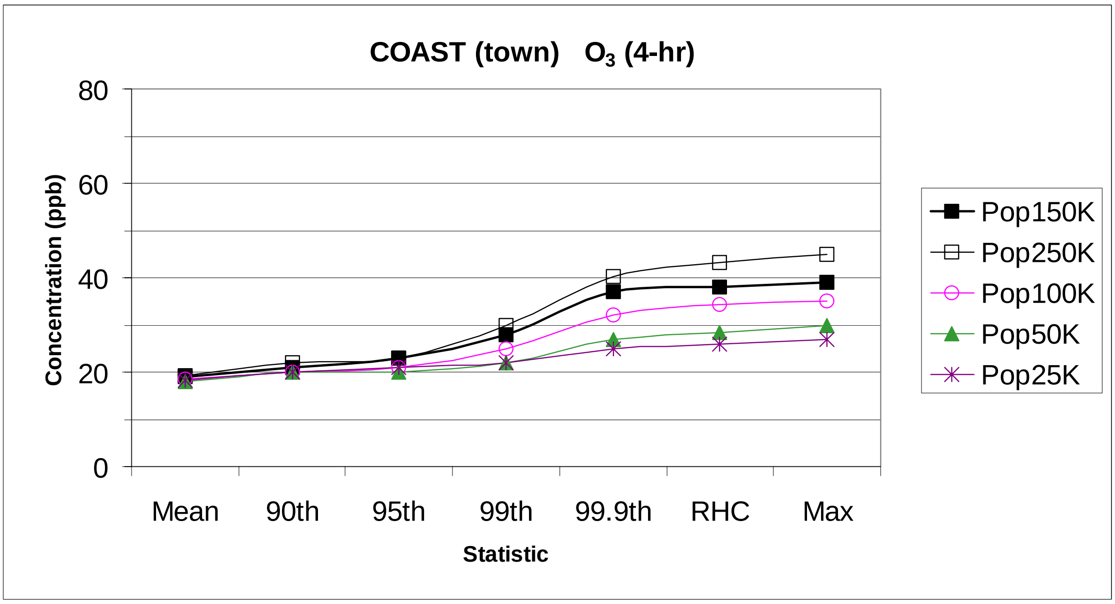


Figure 4.1(c) Annual glc statistics for 4-hourly-averaged O_3 for the *coastal* town. Curves are for different population sizes and statistics are calculated within each town's boundaries.

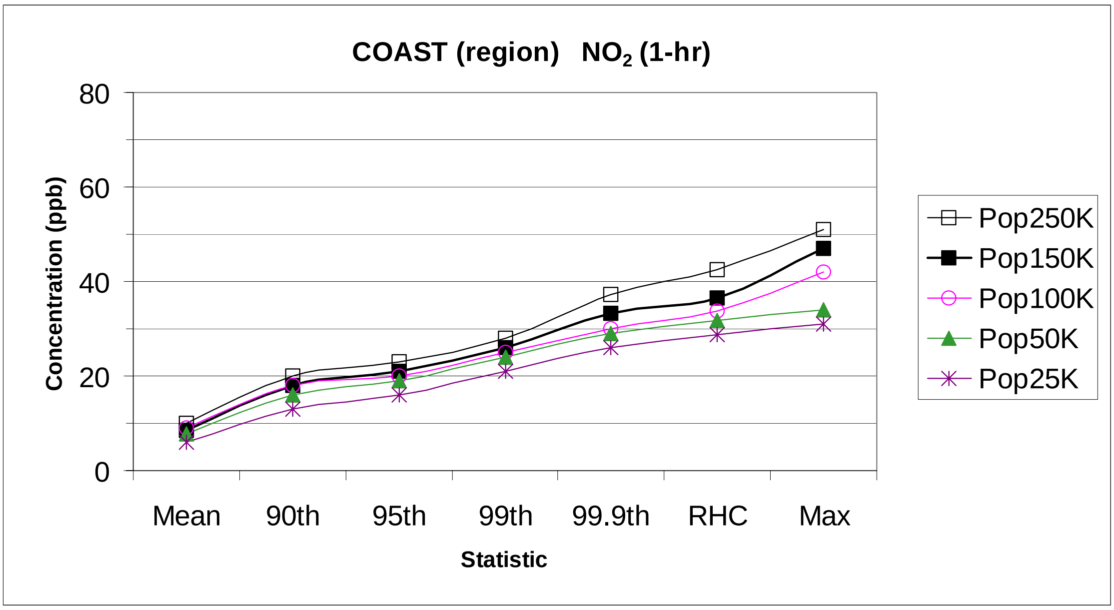


Figure 4.2(a) Annual glc statistics for hourly-averaged NO_2 for the *coastal* town. Curves are for different population sizes and statistics are calculated over the 1.5-km spacing modelling domain (48 x 48 km^2).

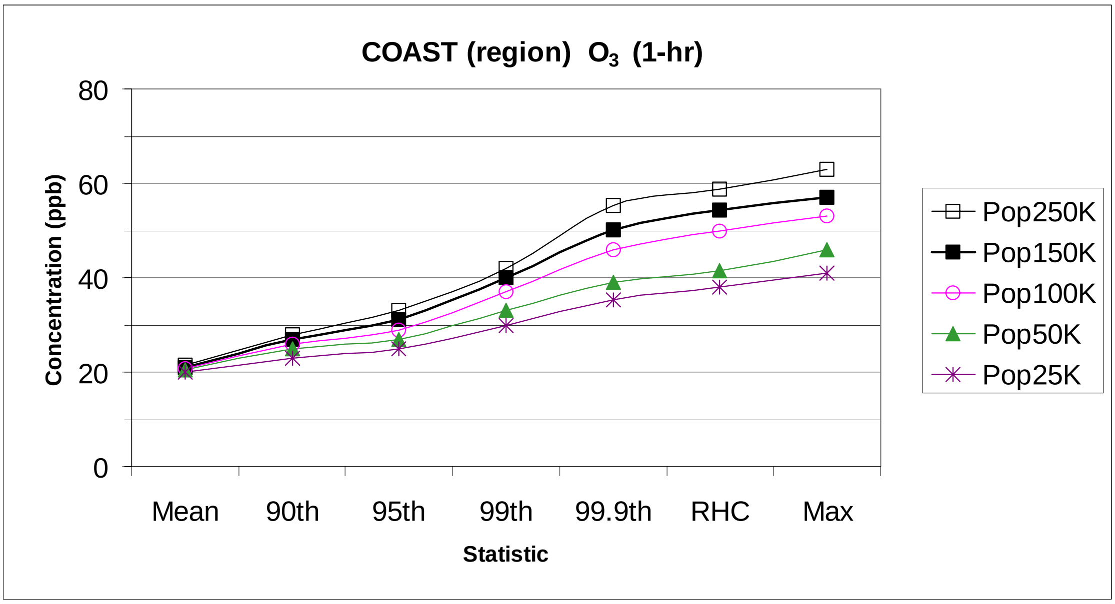


Figure 4.2(b) Annual glc statistics for hourly-averaged O_3 for the *coastal* town. Curves are for different population sizes and statistics are calculated over the 1.5-km spacing modelling domain (48 x 48 km^2).

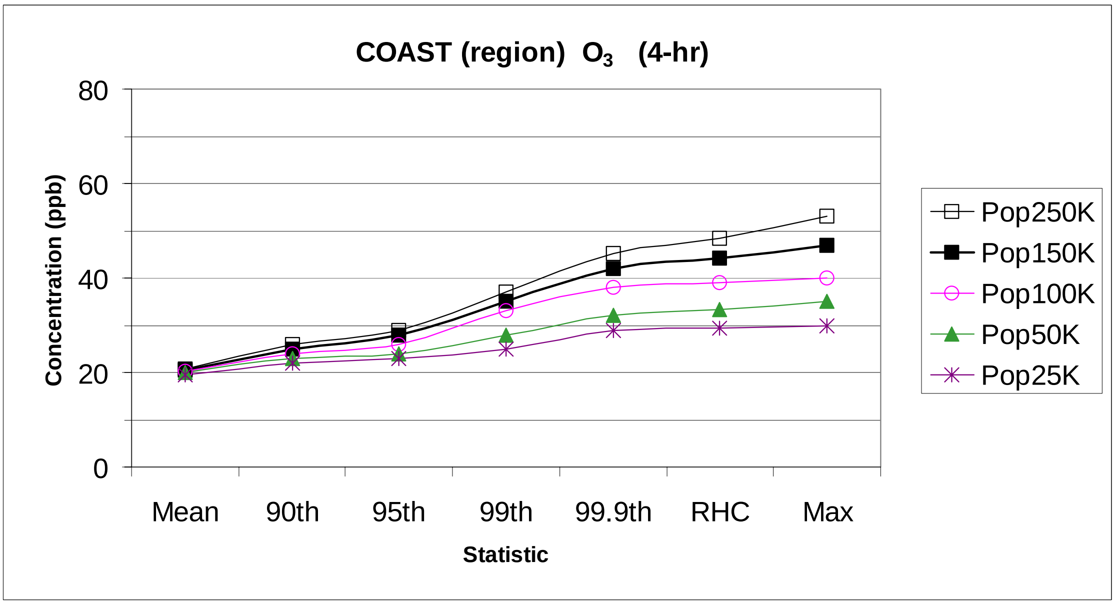


Figure 4.2(c) Annual glc statistics for 4-hourly-averaged O_3 for the *coastal* town. Curves are for different population sizes and statistics are calculated over the 1.5-km spacing modelling domain (48 x 48 km^2).

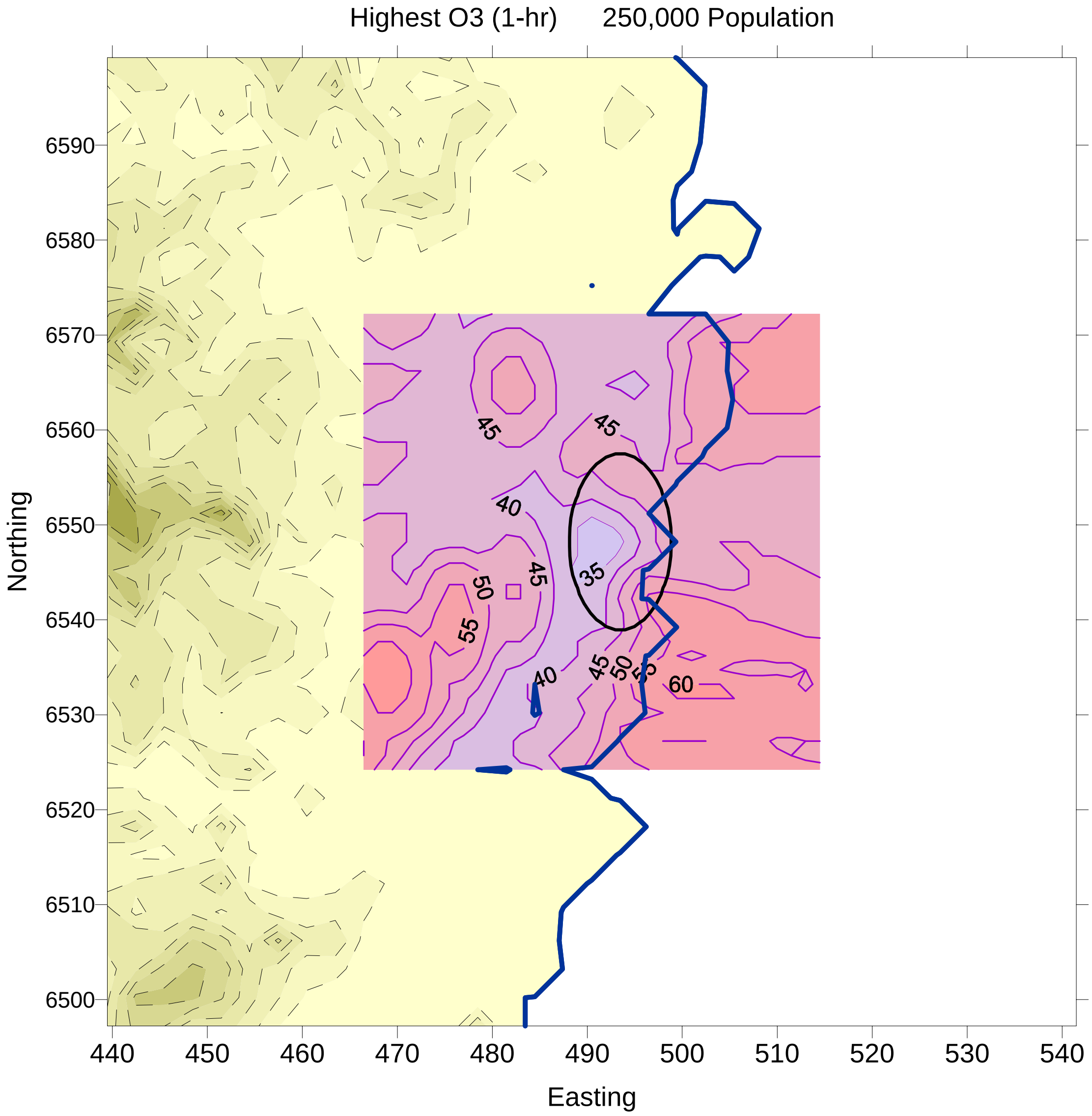


Figure 4.3(a) Contours at 5 ppb intervals of annual maximum O_3 concentration (hourly-averaged) for emissions from *coastal* towns with a population of 250 000. The air quality domain size is 48 x 48 km^2 and dashed contours indicate terrain height above sea level. The thick blue line is the coastline and the town area is indicated by the ellipsoid.

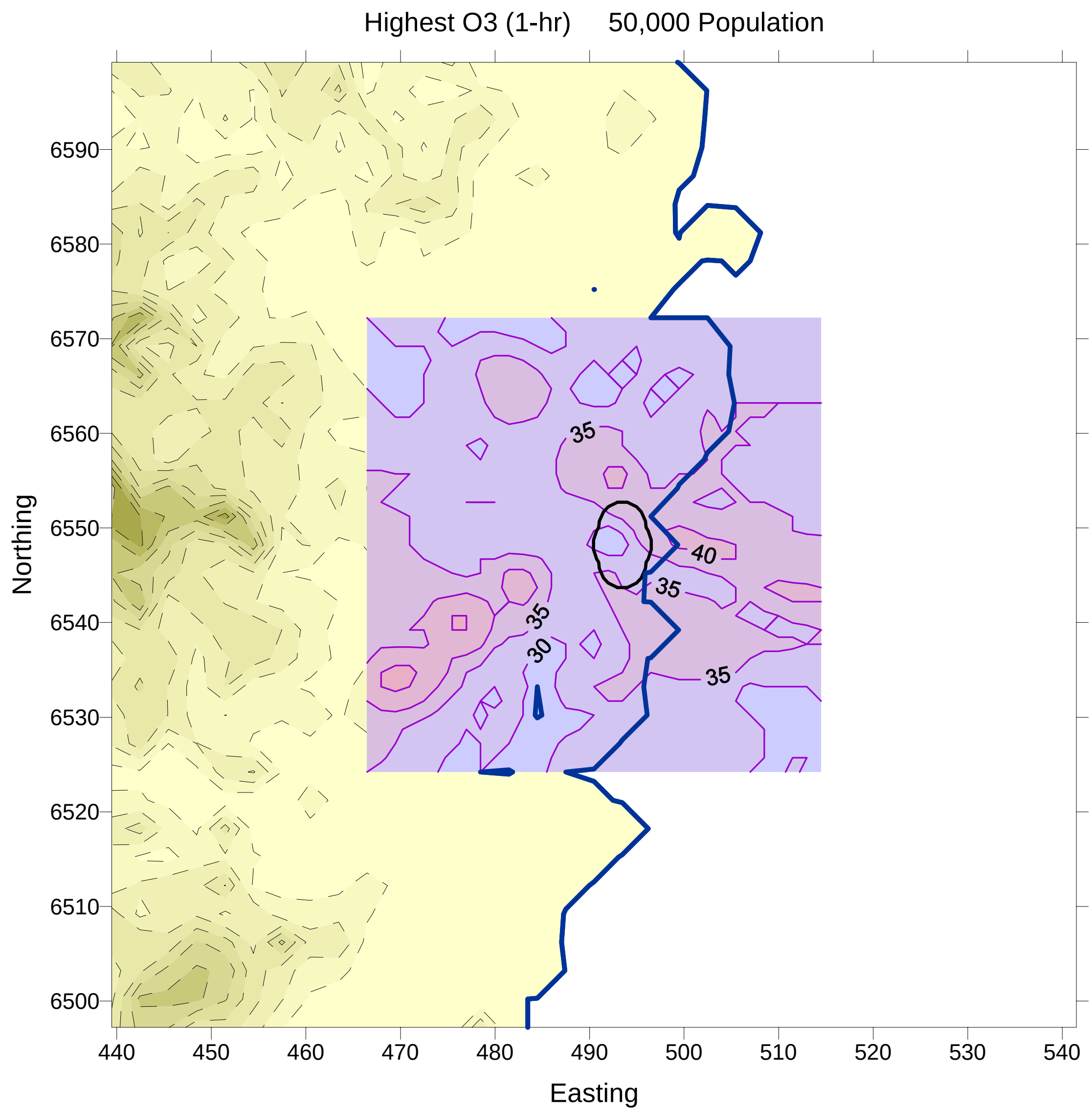


Figure 4.3(b) Contours at 5 ppb intervals of annual maximum O_3 concentration (hourly-averaged) for emissions from *coastal* towns with a population of 50 000. The air quality domain size is 48 x 48 km^2 and dashed contours indicate terrain height above sea level. The thick blue line is the coastline and the town area is indicated by the ellipsoid.

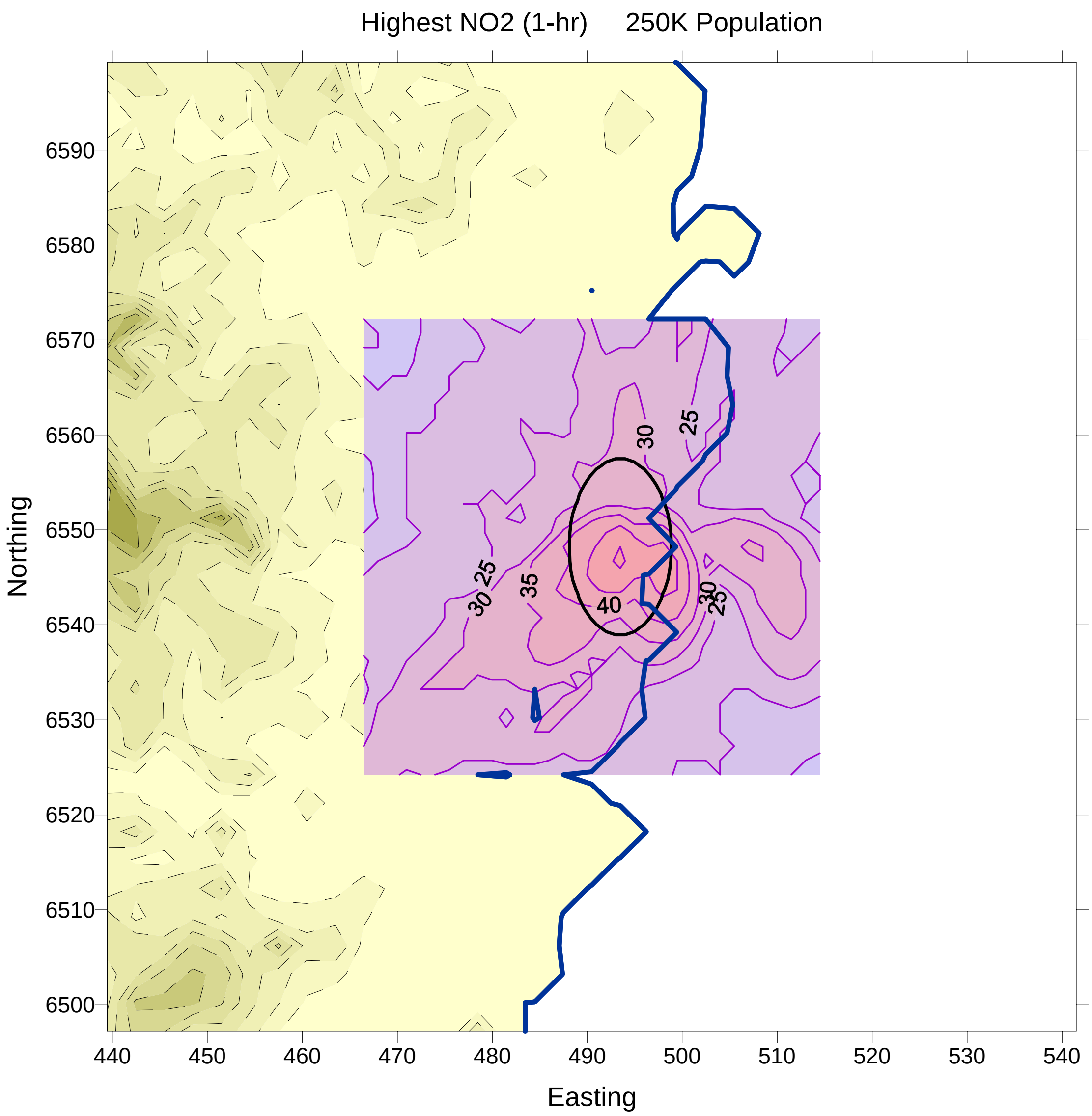


Figure 4.4(a) Contours at 5 ppb intervals of annual maximum NO_2 concentration (hourly-averaged) for emissions from *coastal* towns with a population of 250 000. The air quality domain size is 48 x 48 km^2 and dashed contours indicate terrain height above sea level. The thick blue line is the coastline and the town area is indicated by the ellipsoid.

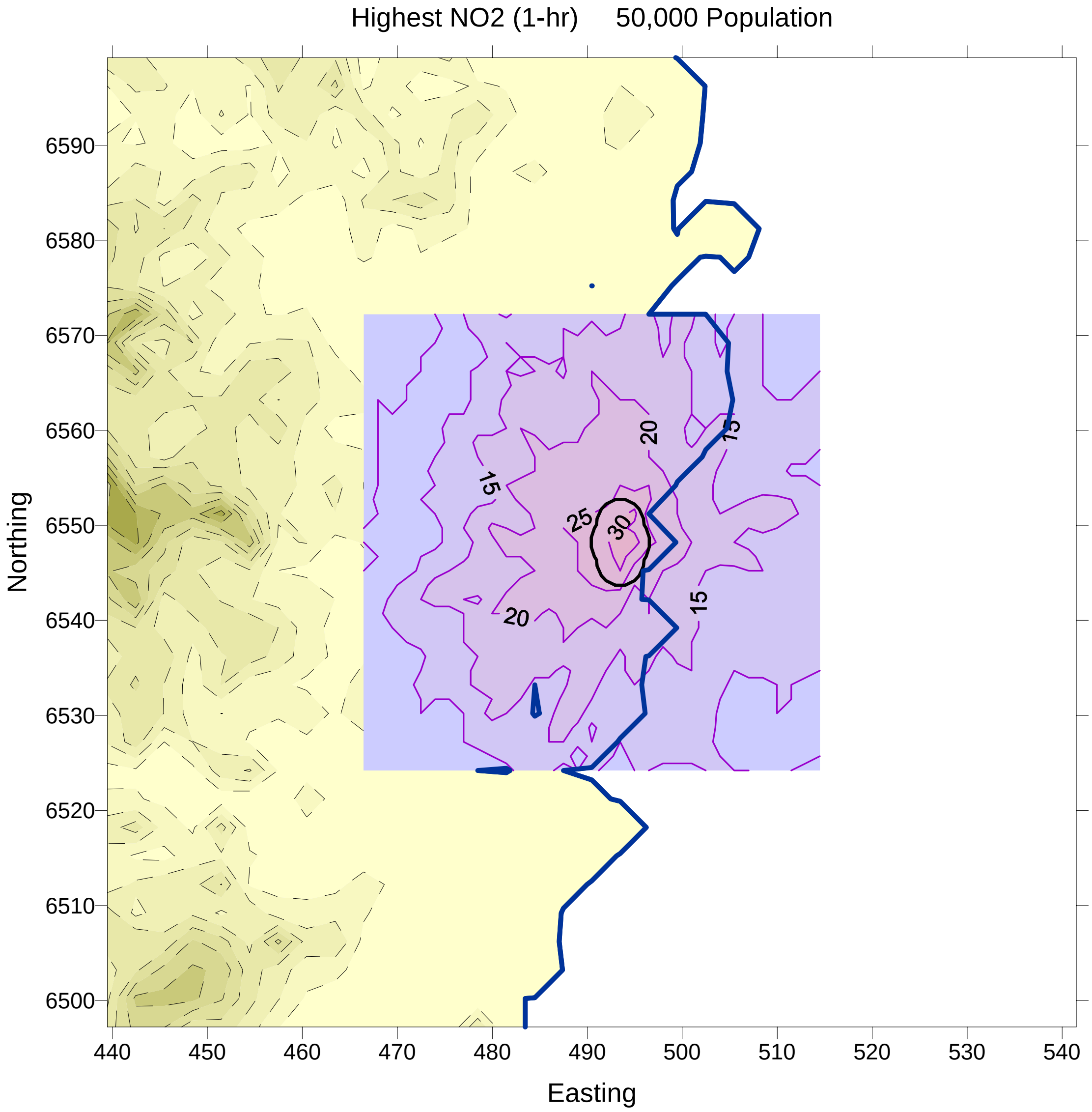


Figure 4.4(b) Contours at 5 ppb intervals of annual maximum NO_2 concentration (hourly-averaged) for emissions from *coastal* towns with a population of 50 000. The air quality domain size is 48 x 48 km^2 and dashed contours indicate terrain height above sea level. The thick blue line is the coastline and the town area is indicated by the ellipsoid.

4.2 Inland town

TAPM was run for 12 months for populations of 250 000, 150 000, 100 000, 50 000 and 25 000. Annual ground-level concentration statistics for O_3 and NO_2 within the town boundaries are shown in Figure 4.5. The maximum values for NO_2 range from 55 ppb down to 46 ppb, and occur in the cooler months in the morning and evening peak traffic times when the mixed layer is shallow and winds are very light. As was the case for the coastal town, the largest concentrations are predicted to occur at the actual or adjacent gridpoint where emission rates of NO_x are highest. Concentrations above the 99^{th} percentile are higher than the equivalent values for the coastal situation (Figure 4.1(a)). This is because well away from the coastline in the early morning and evening periods there are more calm/light wind situations and the low-level stability is stronger. Near a coastline, the land-sea temperature difference regularly leads to onshore/offshore winds and consequently a lot fewer calms and low wind speeds.

Maximum values for hourly-averaged O_3 (Figure 4.5(b)) range from 54 ppb down to 39 ppb, and from 48 ppb down to 34 ppb for 4-hourly averaged values. These typically occur in the summer months in mid to late afternoon on light-wind days. Morning peak-hour emissions drift slowly to the west or south-west and move back over the town later in the day. Usually the synoptic pressure gradients are slack in the region and sometimes the wind change is associated with the passage of a weak trough.

Higher O_3 concentrations occur outside the boundaries of the town. This is illustrated by the concentration statistics over the 1.5-km modelling domain (an area of 48 x 48 km^2) in Figure 4.6(b, c), which show higher values than are predicted for the town area in Figure 4.5(b, c). Note that there is no difference for the NO_2 statistics (Figures 4.5(a) and 4.6(a)) because the maxima occur within the town boundaries. Contours of the annual maximum O_3 concentration at each gridpoint in the 1.5-km domain are shown in Figure 4.7 for the 250 000 and 50 000 populations. This plot also illustrates that the highest O_3 concentrations occur away from the town. Corresponding plots for NO_2 in Figure 4.8 show that the highest concentrations occur within the town.

The number of days per year on which glcs exceed threshold concentrations are listed in Table 4.2 for various populations. For example, for towns with populations of 150 000 or less, TAPM predicts that hourly-averaged O_3 glcs will not exceed 50 ppb, and that 4-hourly-averaged ozone will exceed 40 ppb on only one day.

Table 4.2 Number of days per year on which threshold modelled concentration values (listed) are exceeded within the boundaries of the inland town. Values are shown for populations ranging between 250 000 and 25 000.

	NO_2 (1-hr)		*O_3 (1-hr)*		*O_3 (4-hr)*	
	>40 ppb	*>50 ppb*	*>40 ppb*	*>50 ppb*	*>35 ppb*	*>40 ppb*
250 000	12	2	11	1	9	2
150 000	3	1	2	0	3	1
100 000	2	1	2	0	2	0
50 000	1	0	0	0	0	0
25 000	1	0	0	0	0	0

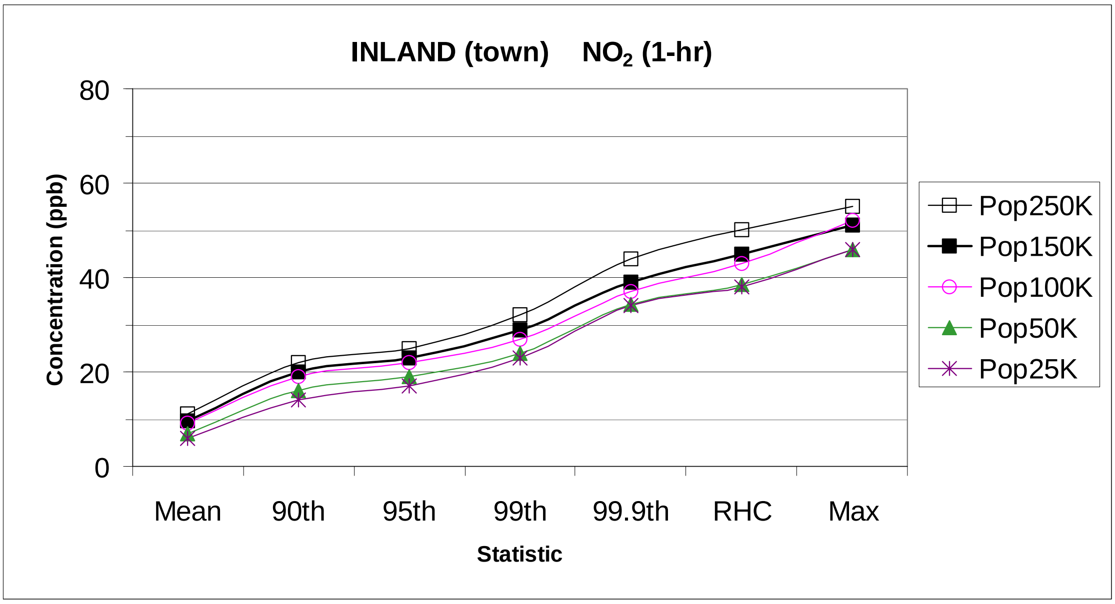


Figure 4.5(a) Annual glc statistics for hourly-averaged NO_2 for the *inland* town. Curves are for different population sizes and statistics are calculated within each town's boundaries.

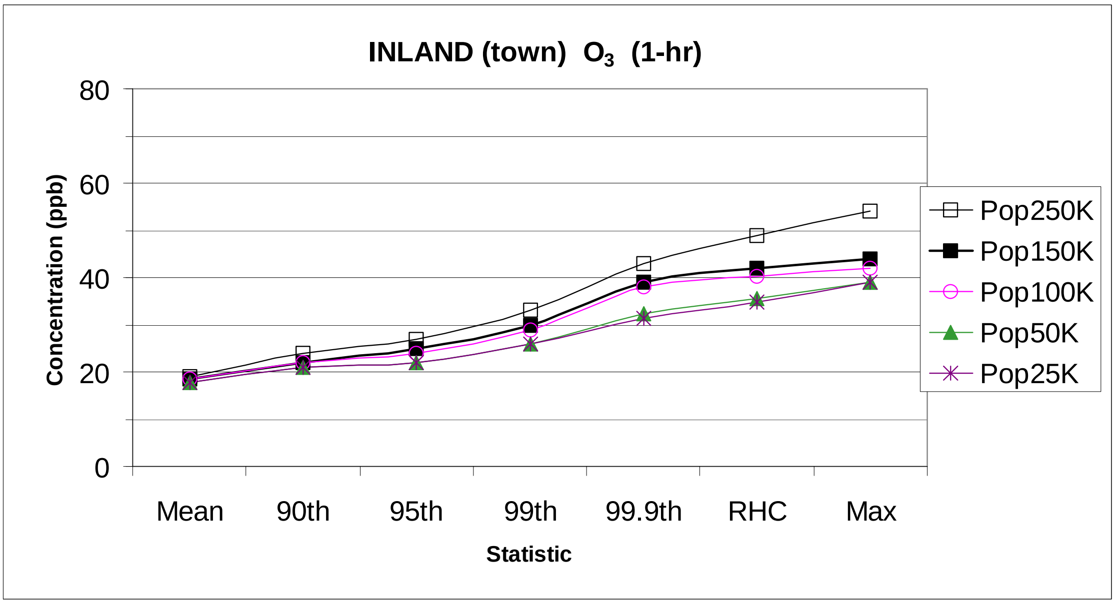


Figure 4.5(b) Annual glc statistics for hourly-averaged O_3 for the *inland* town. Curves are for different population sizes and statistics are calculated within each town's boundaries.

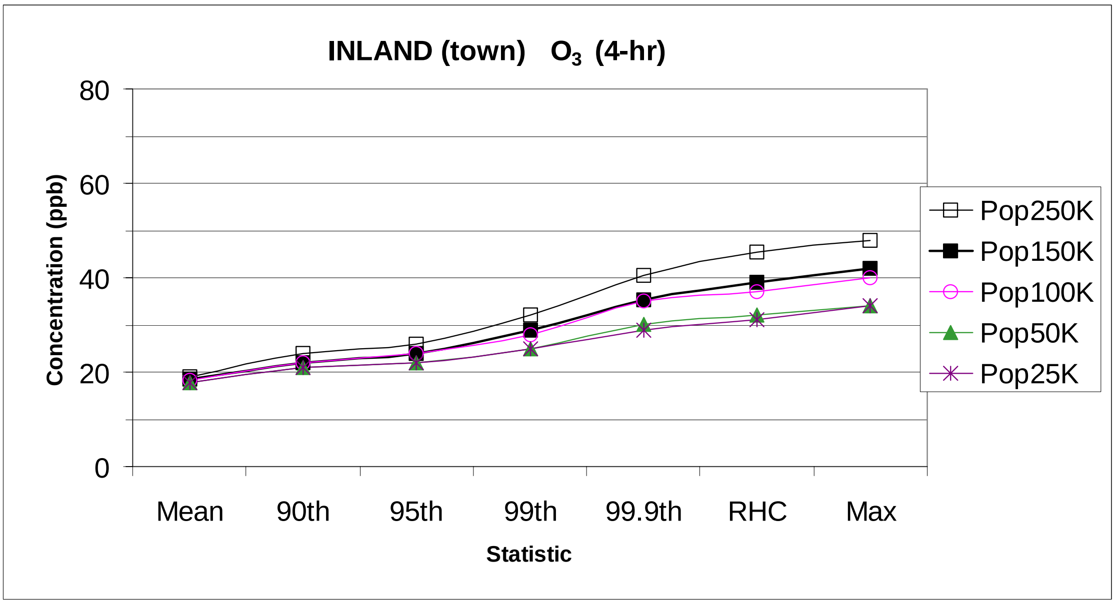


Figure 4.5(c) Annual glc statistics for 4-hourly-averaged O_3 for the *inland* town. Curves are for different population sizes and statistics are calculated within each town's boundaries.

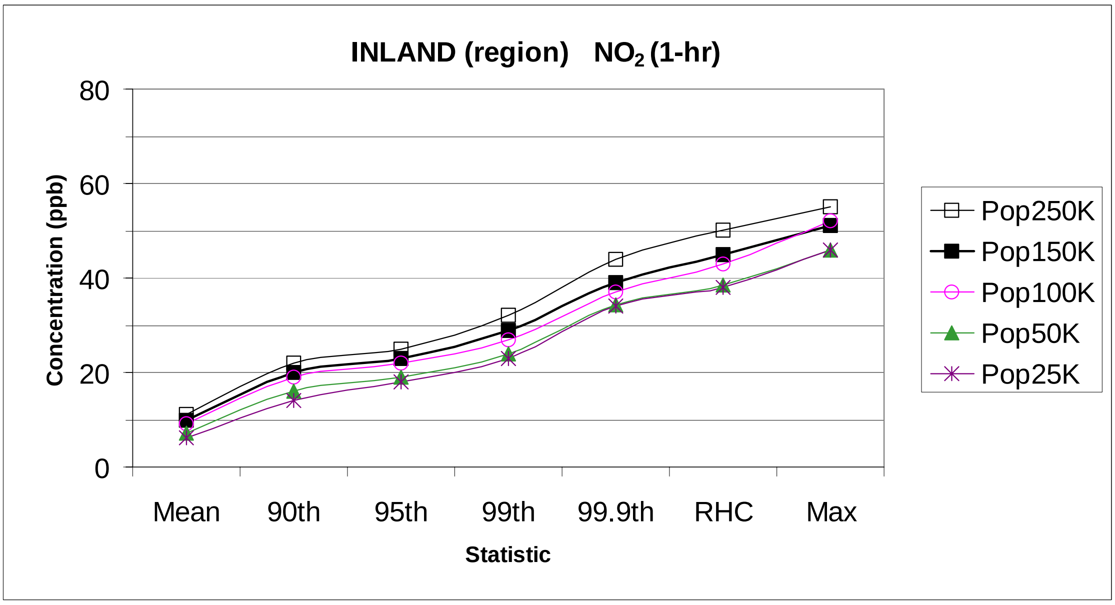


Figure 4.6(a) Annual glc statistics for hourly-averaged NO_2 for the *inland* town. Curves are for different population sizes and statistics are calculated over the 3-km spacing modelling domain (48 x 48 km^2) .

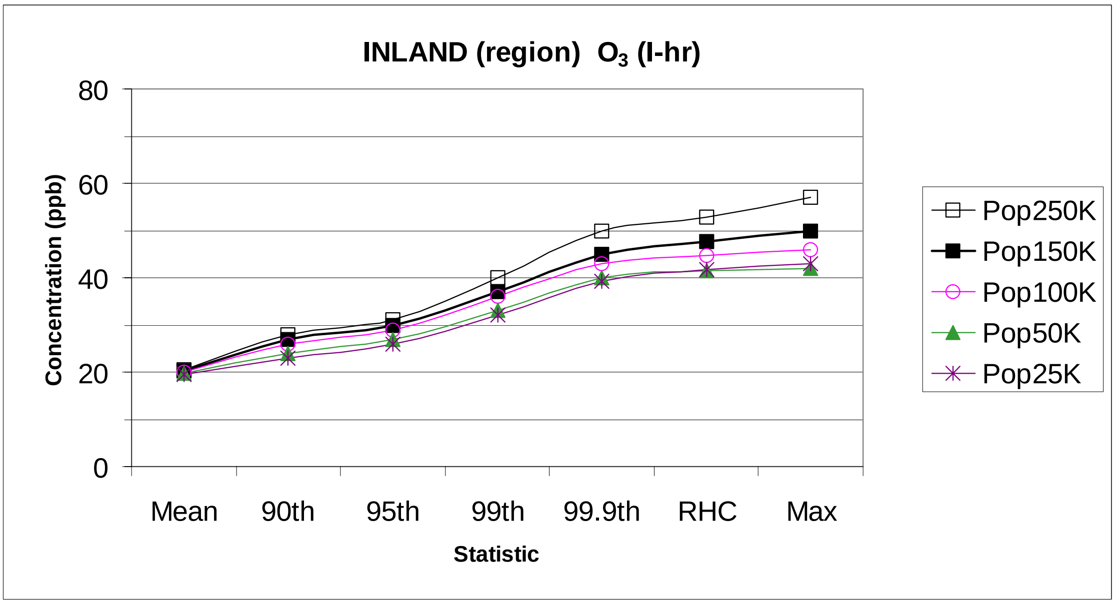


Figure 4.6(b) Annual glc statistics for hourly-averaged O_3 for the *inland* town. Curves are for different population sizes and statistics are calculated over the 3-km spacing modelling domain (48 x 48 km^2) .

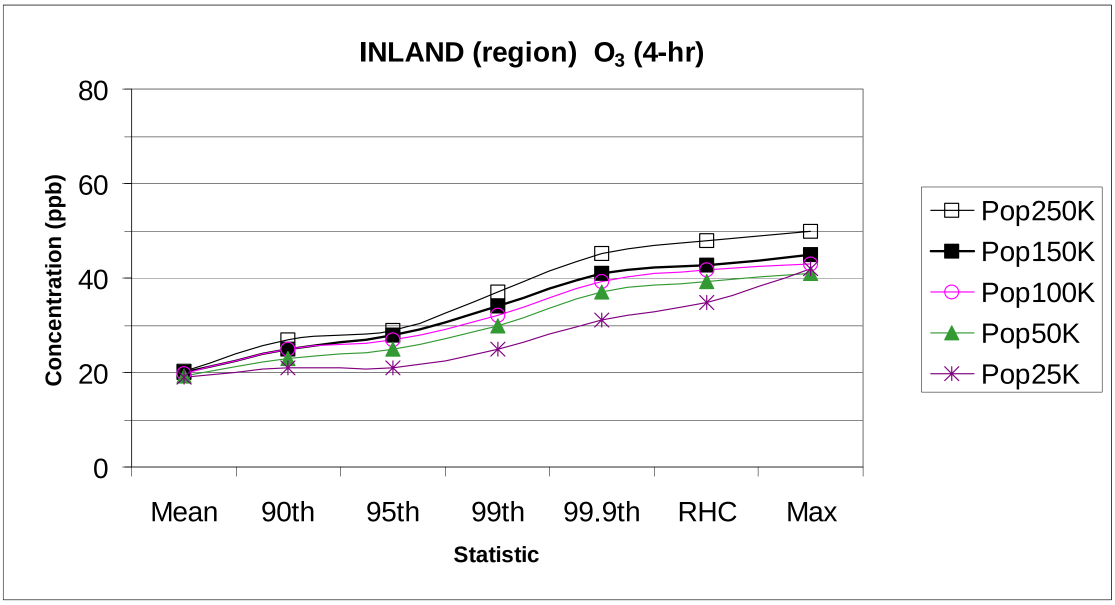


Figure 4.6(c) Annual glc statistics for 4-hourly-averaged O_3 for the *inland* town. Curves are for different population sizes and statistics are calculated over the 1.5-km spacing modelling domain (48 x 48 km^2) .

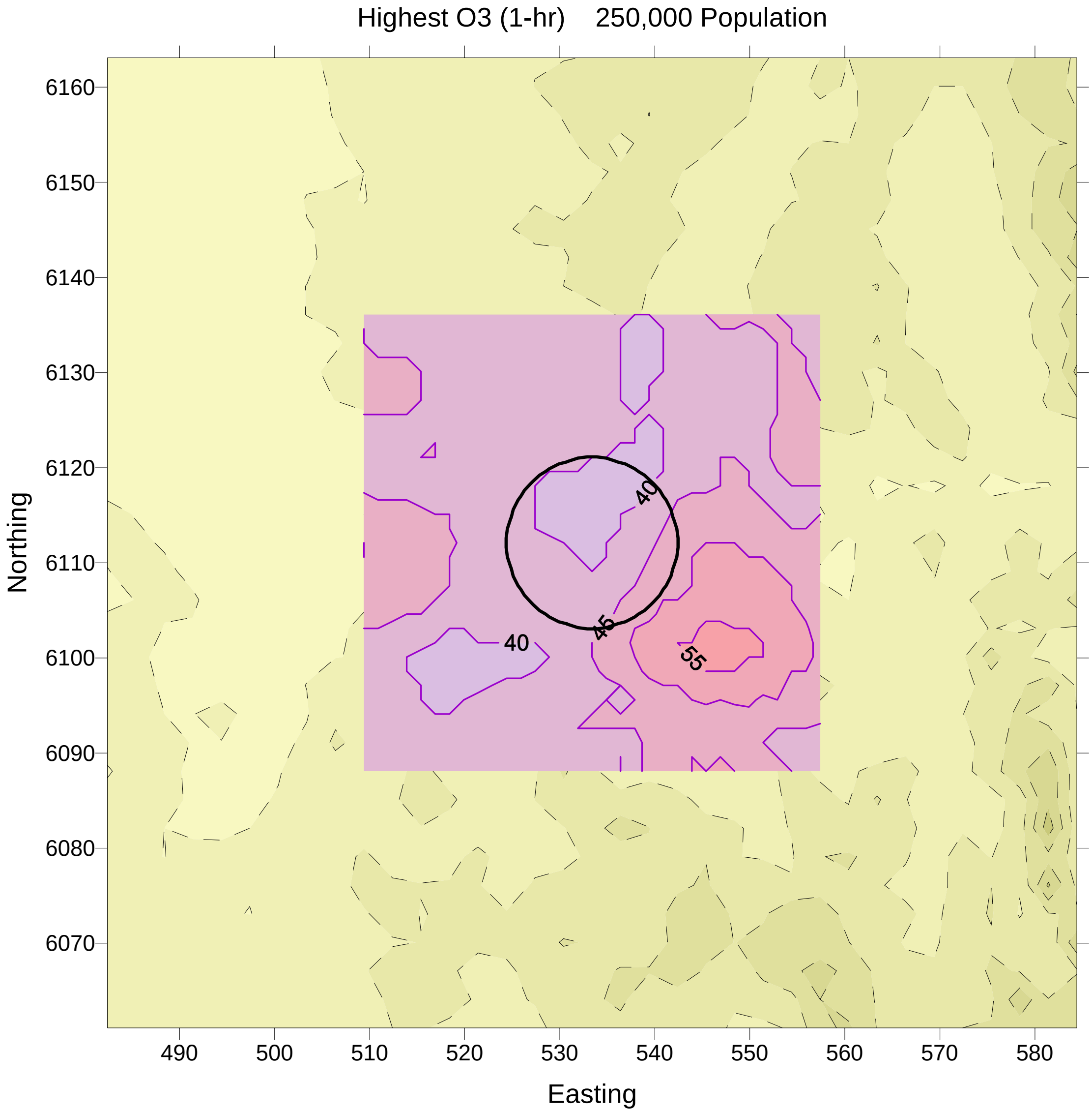


Figure 4.7(a) Contours at 5 ppb intervals of annual maximum O_3 concentration (hourly-averaged) for emissions from *inland* towns with populations of 250 000. The air quality domain size is 48 x 48 km^2 and dashed contours indicate terrain height above sea level. The town area is indicated by the ellipsoid.

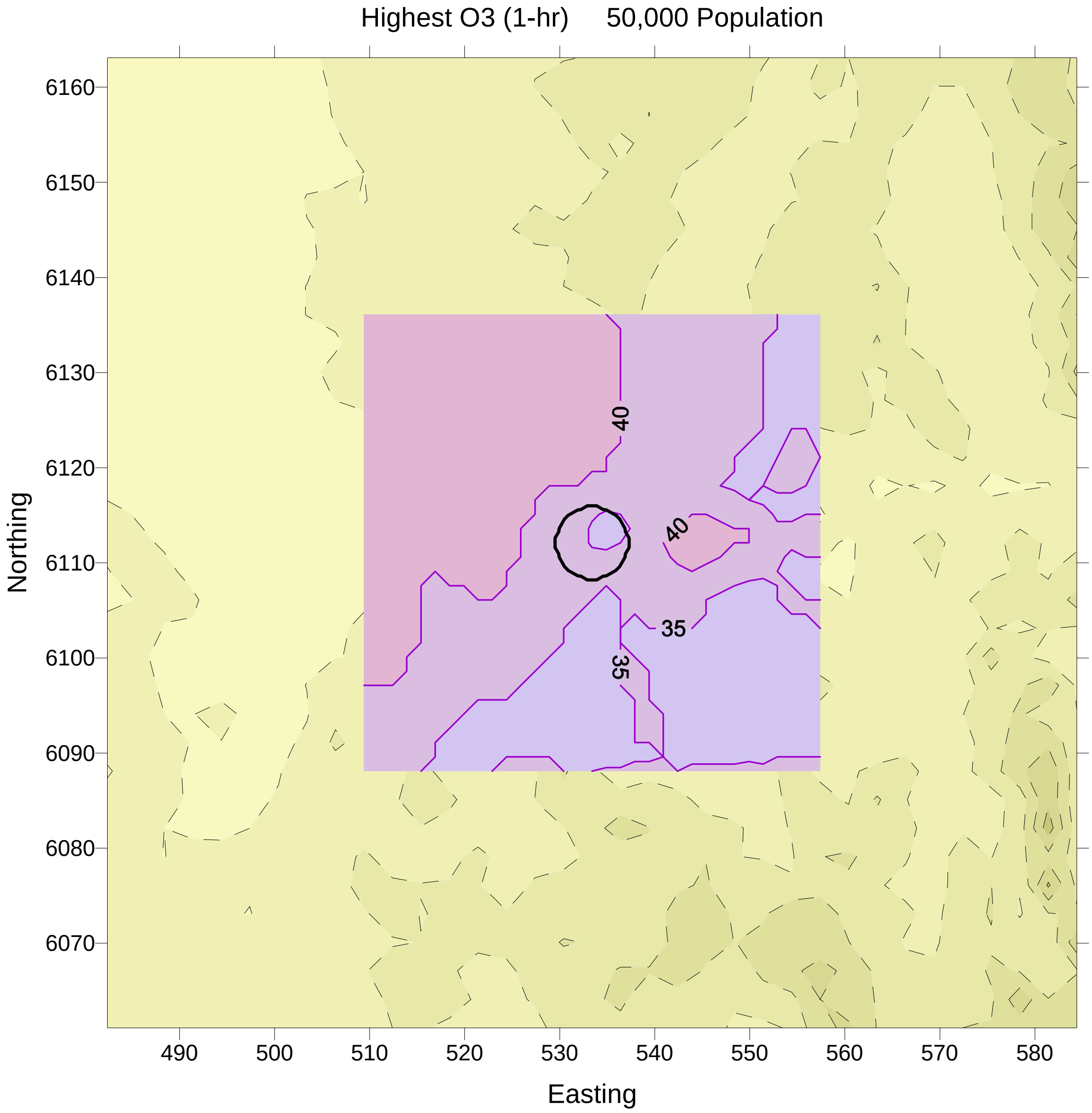


Figure 4.7(b) Contours at 5 ppb intervals of annual maximum O_3 concentration (ppb, hourly-averaged) for emissions from *inland* towns with a population of 50 000. The air quality domain size is 48 x 48 km^2 and dashed contours indicate terrain height above sea level. The town area is indicated by the ellipsoid.

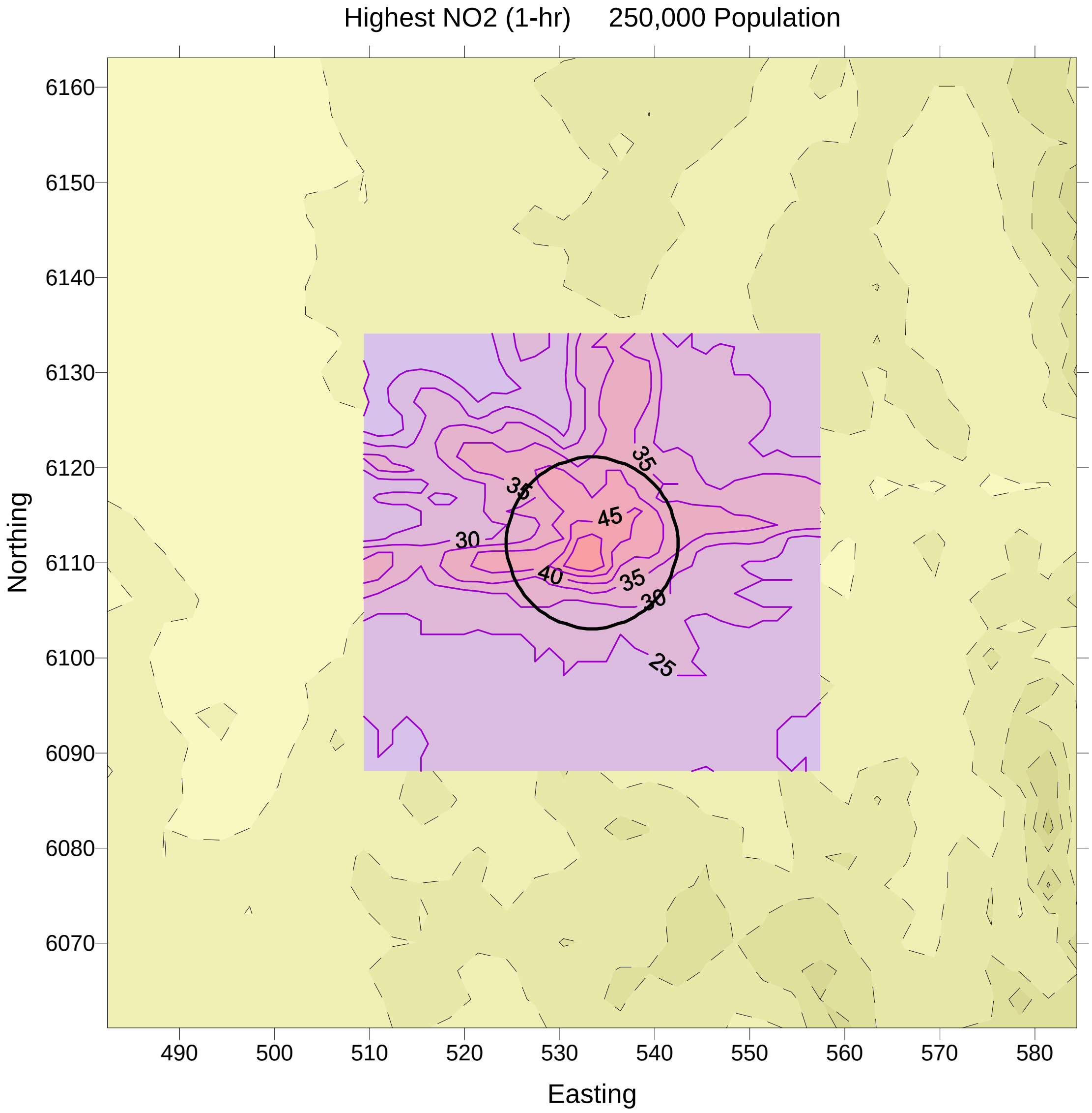


Figure 4.8(a) Contours at 5 ppb intervals of annual maximum NO_2 concentration (ppb, hourly-averaged) for emissions from *inland* towns with a population of 250 000. The air quality domain size is 48 x 48 km^2 and dashed contours indicate terrain height above sea level. The town area is indicated by the ellipsoid.

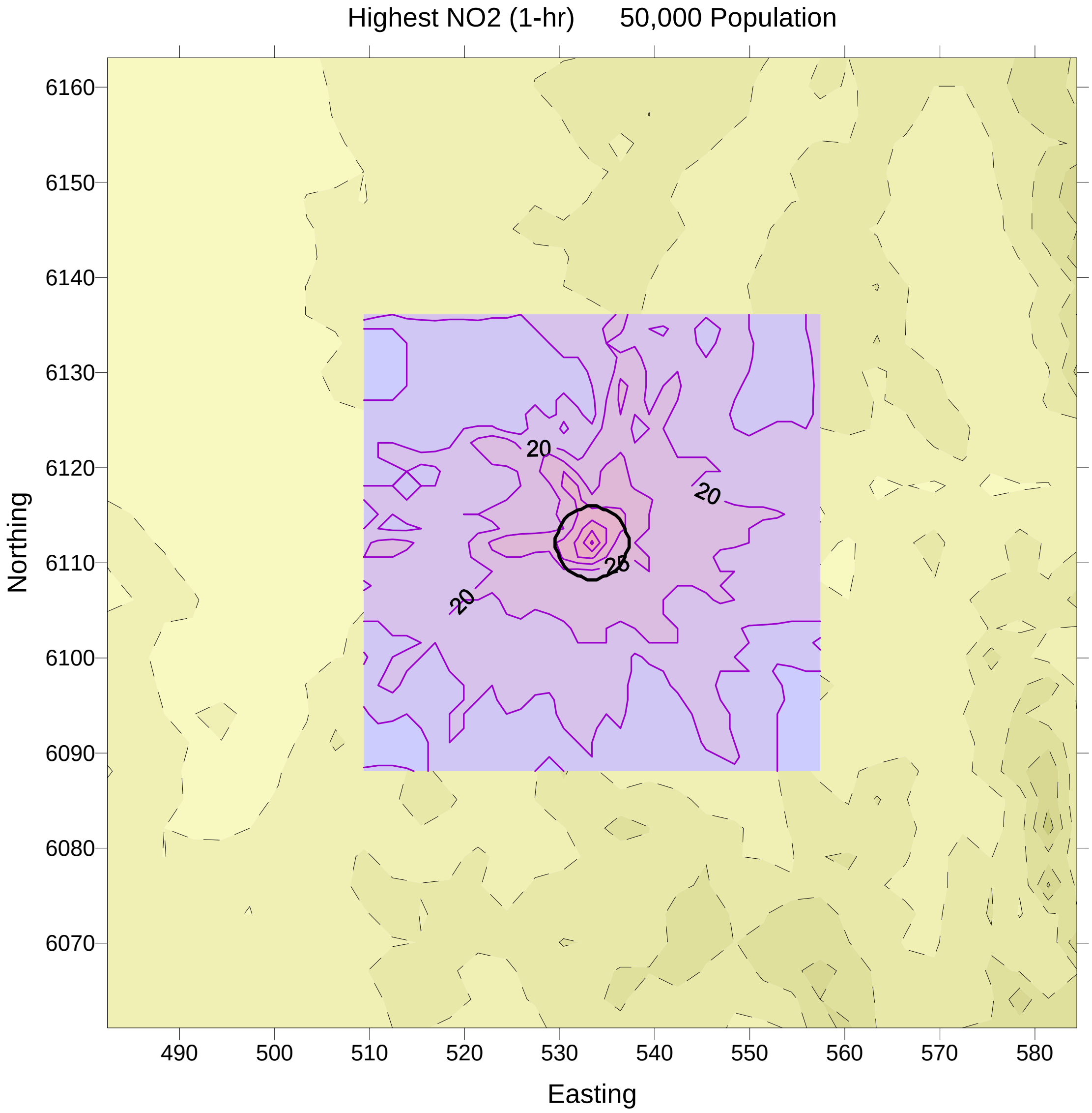


Figure 4.8(b) Contours at 5 ppb intervals of annual maximum NO_2 concentration (ppb, hourly-averaged) for emissions from *inland* towns with a population of 50 000. The air quality domain size is 48 x 48 km^2 and dashed contours indicate terrain height above sea level. The town area is indicated by the ellipsoid.

4.2.1 Comparison to Wagga data

Hourly-averaged O_3 and NO_2 concentrations were monitored over 12 months (1998) by Pacific Power at a rural site 7 km north-northeast of Wagga town centre, and outside the model's town boundaries as defined in Table 2.1. PPI believe that the data are of good quality. Although this period does not coincide with the simulation period (1/7/97 – 30/6/98), it is quite valid to compare glc frequency distributions over the two 12-month periods. Figure 4.9 shows the annual cumulative frequency distributions (CFDs) for the observed NO_2 and O_3 glcs from Wagga (population 55 000) and those for the inland simulation with a population of 50 000. Results are shown for the modelled town-maximum glcs and for the predicted glcs at the monitor gridpoint. The highest observed NO_2 concentration at this site was 33 ppb, compared with the model value of 27 ppb (Figure 4.9(a)). The observed CFD lies between those of the modelled gridpoint and the town-maximum, showing that TAPM has modelled the emission and dispersion of NO_2 satisfactorily.

However there is a greater discrepancy between observations and model results for O_3 (Figure 4.9(b)). Examination of the time series for O_3 reveals that on many days the observed concentrations are higher than the maximum modelled value for the whole year, yet on these days the observed wind direction is not from Wagga (between 180 and 250 degrees). In other words, the background O_3 concentration is significantly higher than the value of 20 ppb used in the simulations. As an example, Figure 4.10 shows the observed time-series for wind, temperature and O_3 during January. On days 1, 6, 12, 16, 17, 21 and 22, O_3 concentrations are higher than 45 ppb, but wind directions are not from within an arc containing Wagga. Time series of wind speed and temperature are also shown in Figure 4.10, and a strong relation between O_3 concentrations and temperature can easily be seen.

A scatter plot of O_3 concentrations greater than 35 ppb against wind direction for the warmer months of December through to March in Figure 4.11 shows that a value of 45 ppb could be inferred as an upper-bound value for background O_3. Although a large proportion of the higher glcs (i.e. above 45 ppb) occur when winds are from the direction of Wagga, it is also possible that there is a contribution from long-range transport of O_3 associated with emissions from Melbourne (350 km southwest of Wagga). Examination of O_3 glcs at a location about 110 km southwest of Wagga on the Victorian grid of the Australian Air Quality Forecasting System shows values as high as 49 ppb, and values exceeding 40 ppb on 42 occasions (hours) between 1 December 2001 and 31 March 2002. Over the same period, at a point 110 km east-northeast of Wagga on the New South Wales grid, and in a straight line from Sydney, hourly-averaged O_3 glcs were predicted to reach as high as 47 ppb and to exceed 40 ppb on 34 occasions. These findings suggest that emissions from Melbourne and Sydney may at times add to the general background concentration of O_3 in the Wagga area.

As well as long-range transport, a significant proportion of the O_3 background values can be attributed to reactions on hot days between VOC emissions from vegetation and NO_x emissions from soil and small towns and settlements. Note that at low NO_x concentrations, the production of O_3 is about 3 times more efficient than at higher concentrations. Higher background concentrations of O_3 also occur in smoky air masses when burnt vegetation releases VOC and NO_x. The Bureau of Meteorology's observer's reports from Wagga indicate that smoke or haze was present on 4 out of the 10 highest concentration days.

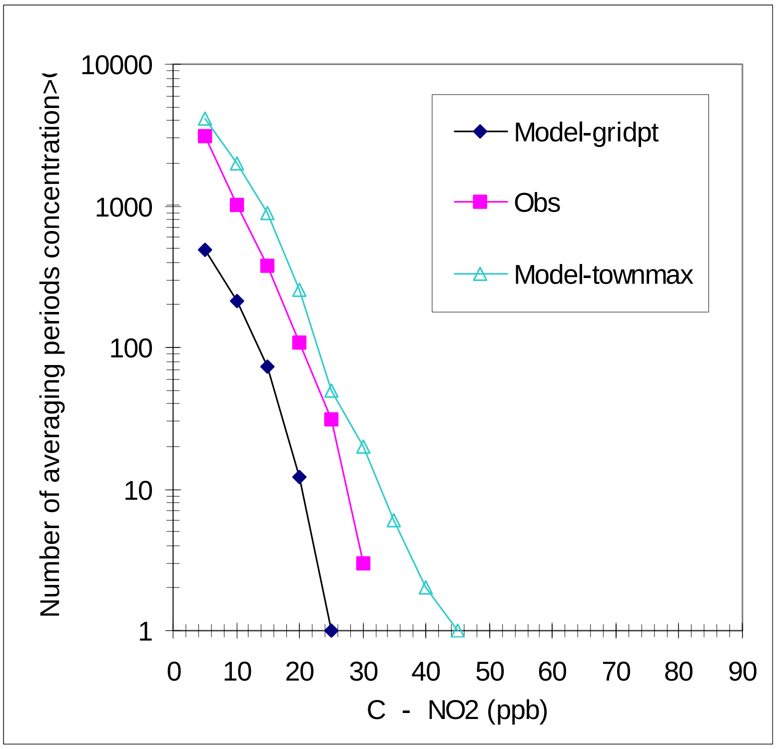


Figure 4.9(a) Observed (■), modelled (◆) and modelled town maximum (∆) annual cumulative frequency distributions for NO_2 ground-level concentrations (ppb) at Wagga.

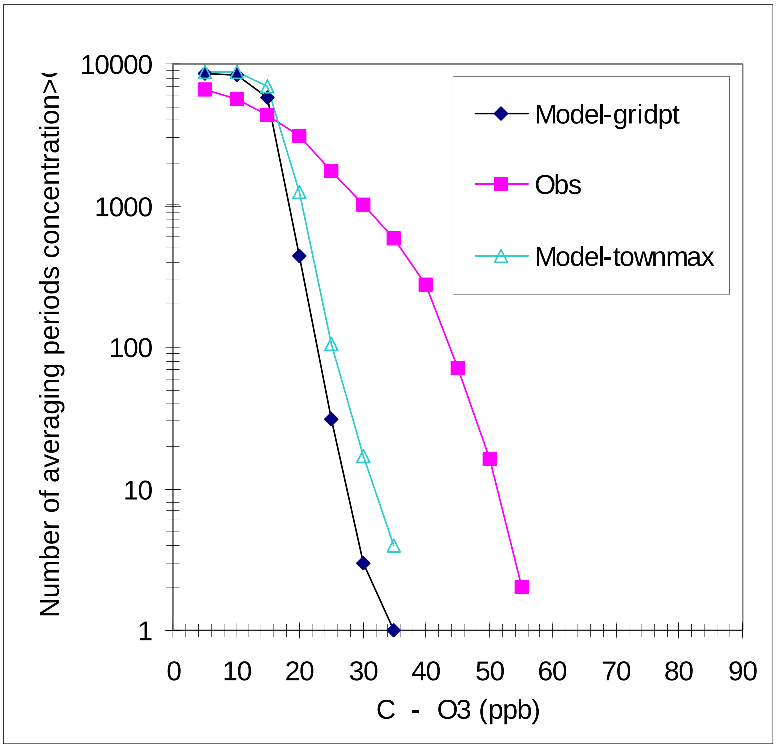
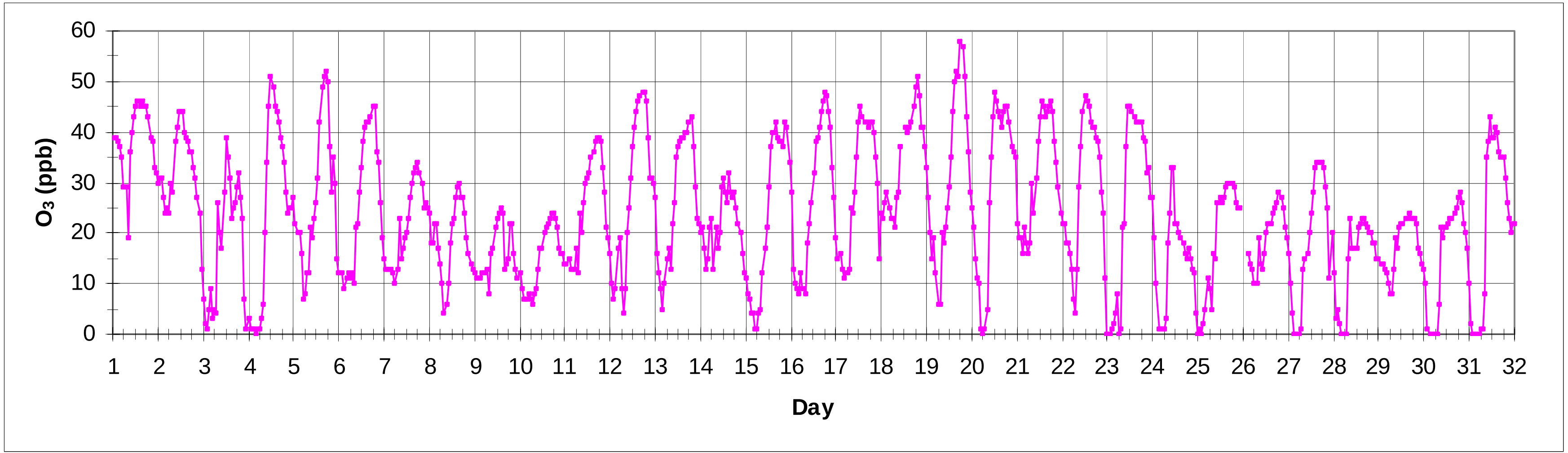


Figure 4.9(b) Observed (■), modelled (◆) and modelled town maximum (∆) annual cumulative frequency distributions for O_3 ground-level concentrations (ppb) at Wagga.



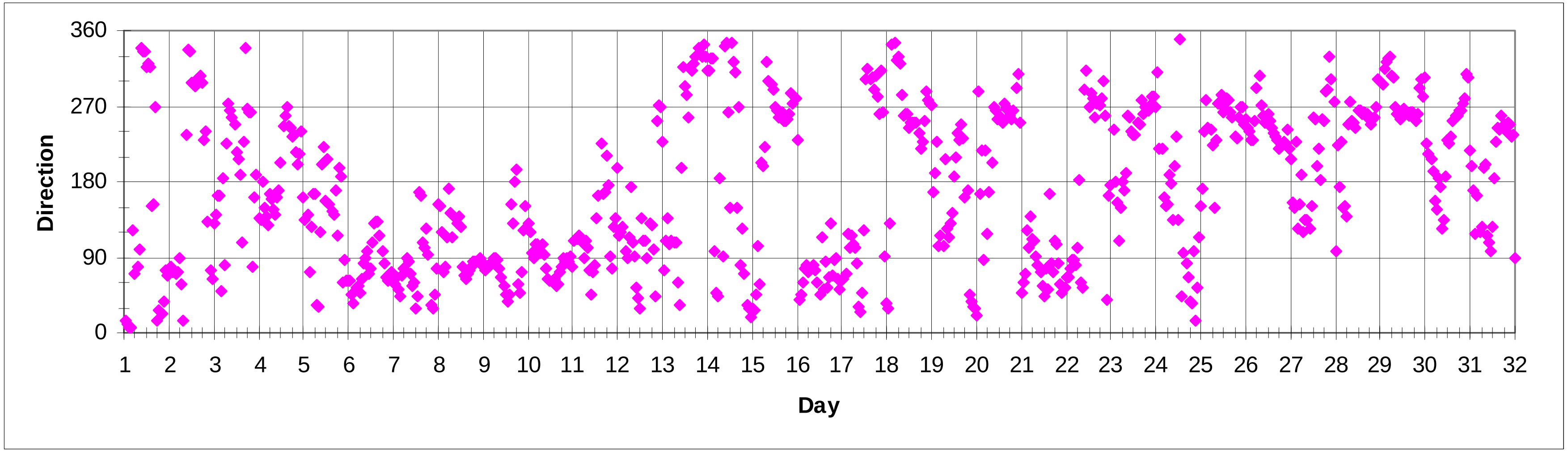
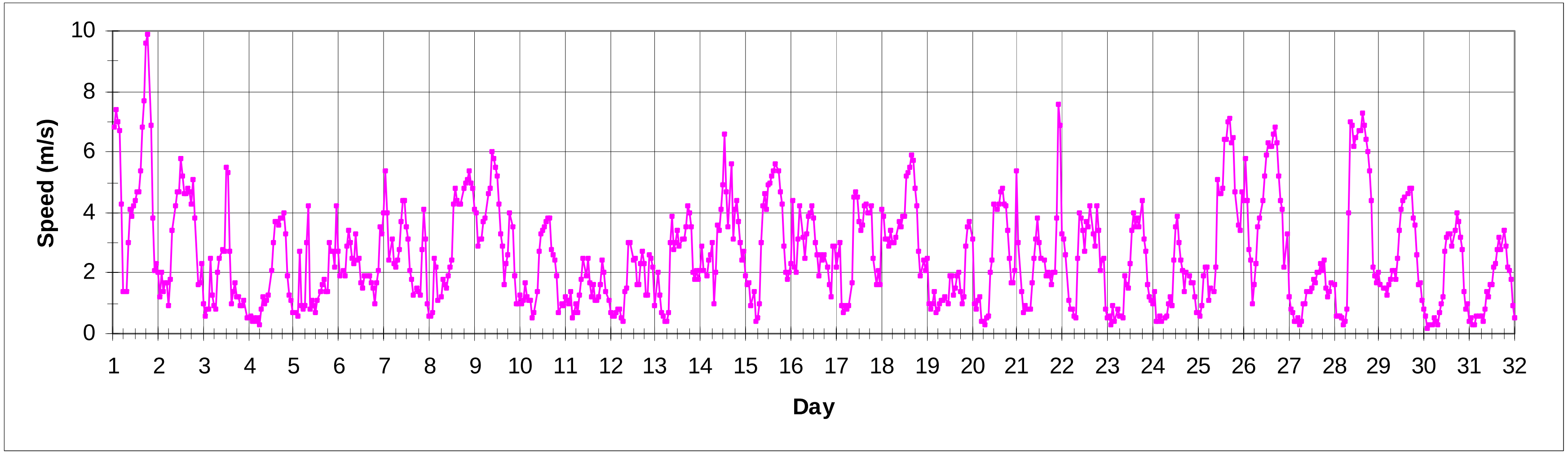


Figure 4.10 Observed hourly-averaged O_3 concentrations (top) and wind direction (below) at Wagga for January 1998.



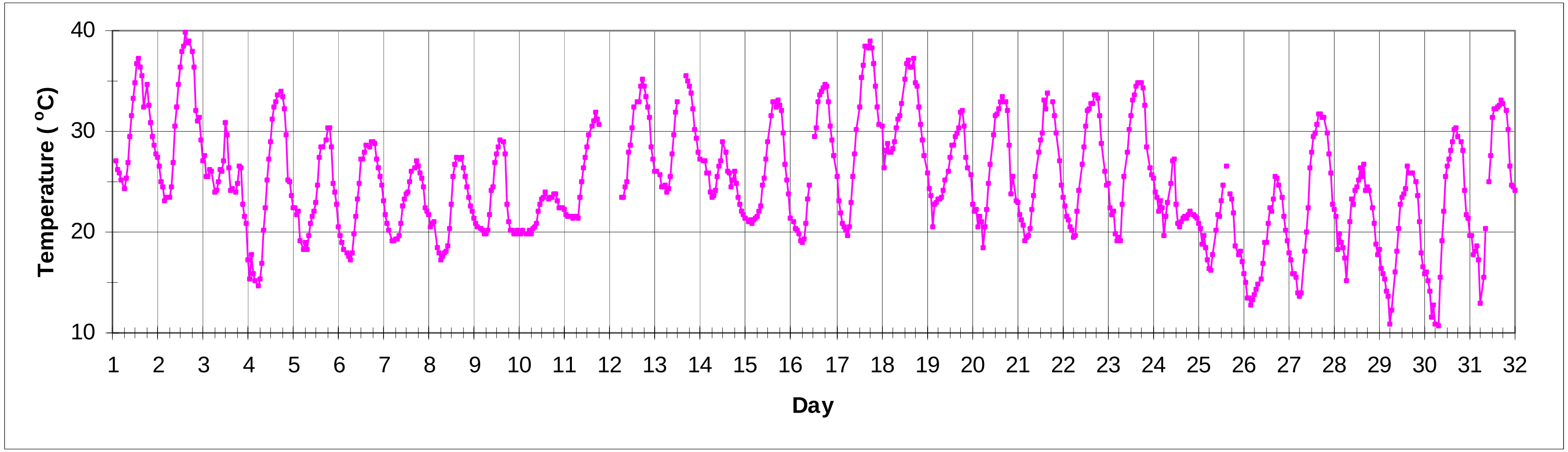


Figure 4.10 (continued) Observed wind speed (top) and temperature (below) at Wagga for January 1998.

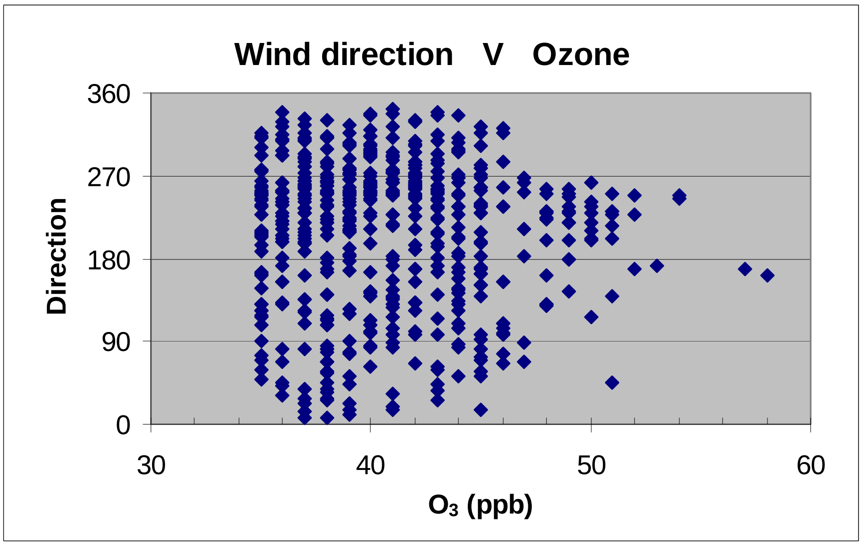


Figure 4.11 Scatter plot of observed hourly-averaged O_3 concentrations greater than 35 ppb and wind direction at Wagga for December, January, February and March 1998.

4.3 Biogenics contribution

The contribution of biogenic VOC emissions to the NO_2 and O_3 concentrations within the coastal town has been evaluated for populations of 250 000 (Figure 4.12) and 50 000 (Figure 4.13). No natural NO_x sources were specified, so that the biogenics contribution to O_3 concentrations comes about through reaction with NO_x from the town anthropogenic sources. Results are shown for simulations with and without the biogenic emissions. It is evident that, within the town, the biogenic VOCs contribute very little (of the order of 1 ppb) to the glcs at any concentration level. This most likely occurs because maximum glcs within the town arise from re-circulation of the early-morning urban emissions, as described in Section 4.1. The level of biogenic VOCs in this air mass is likely to be low because of the cool temperatures and low PAR levels at this time of day, and so the biogenic contribution to the photochemistry can be expected to be small. For the inland town and a population of 250 000, the biogenics contribution to the ozone maximum within the town is 3 ppb (not shown).

For the coastal simulation, when the area over which the O_3 concentration statistics are calculated is expanded to include all the inner air-quality modelling domain (48 x 48 km^2), the contribution of biogenic emissions to the higher concentrations of ozone is greater, i.e. 4 ppb for a 250 000 population (Figure 4.14(a)) and 3 ppb for a population of 50 000 (Figure 4.14(b)).

The contribution of biogenic VOC emissions to ozone concentrations is smaller than might be expected because of the omission of natural (e.g. soil) NO_x sources.

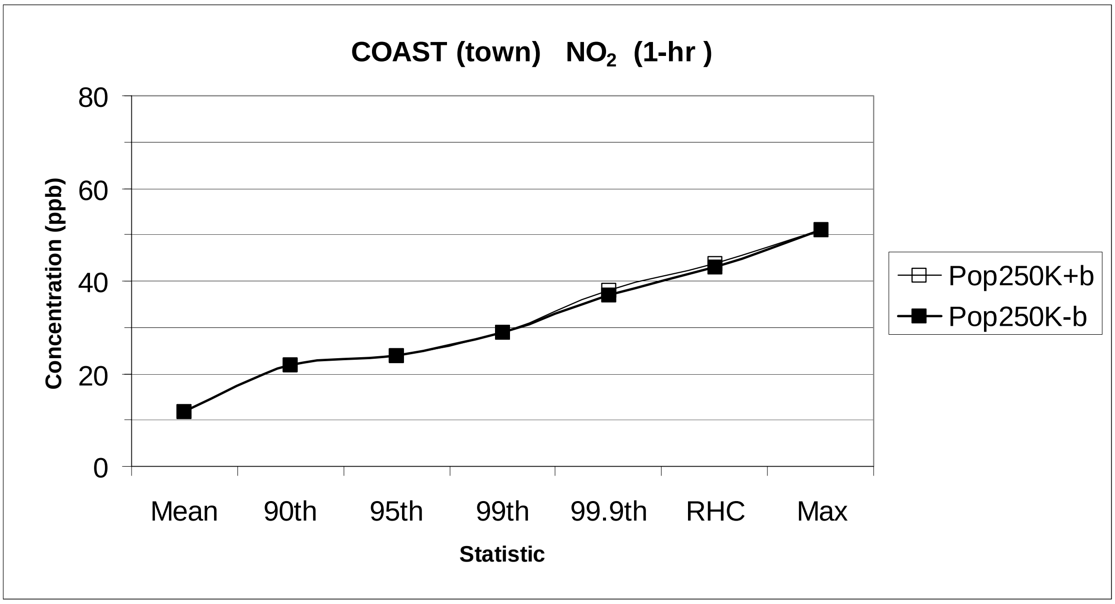


Figure 4.12(a) Annual glc statistics for hourly-averaged NO_2 for emissions from the *coastal* town with a population of 250 000. Curves are for simulations with (+b) and without (-b) biogenic emissions. Statistics are calculated within the town's boundaries.

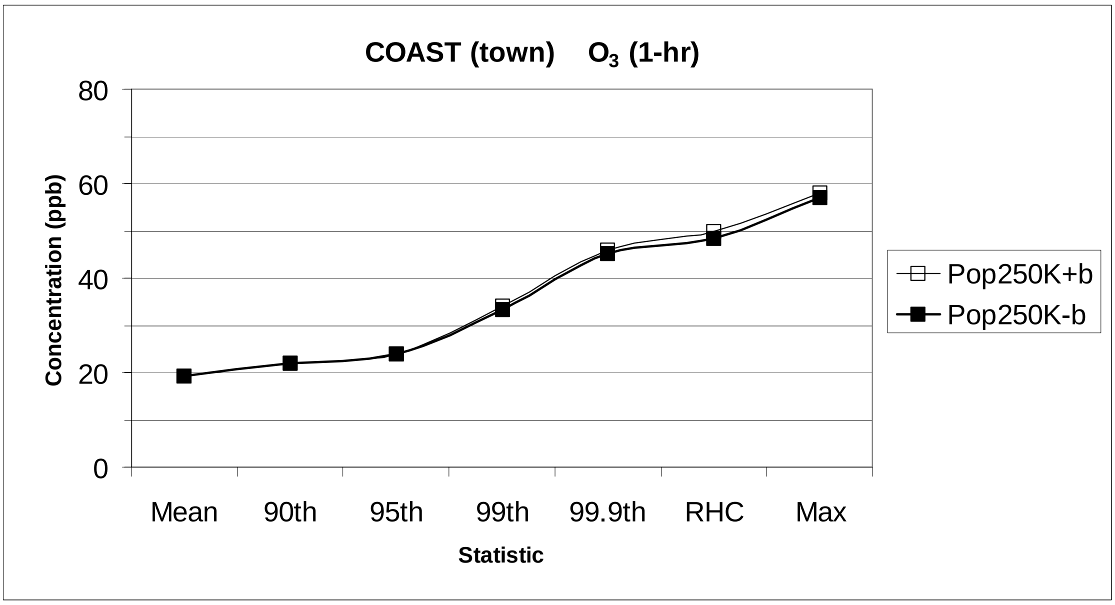


Figure 4.12(b) Annual glc statistics for hourly-averaged O_3 for emissions from the *coastal* town with a population of 250 000. Curves are for simulations with (+b) and without (-b) biogenic emissions. Statistics are calculated within the town's boundaries.

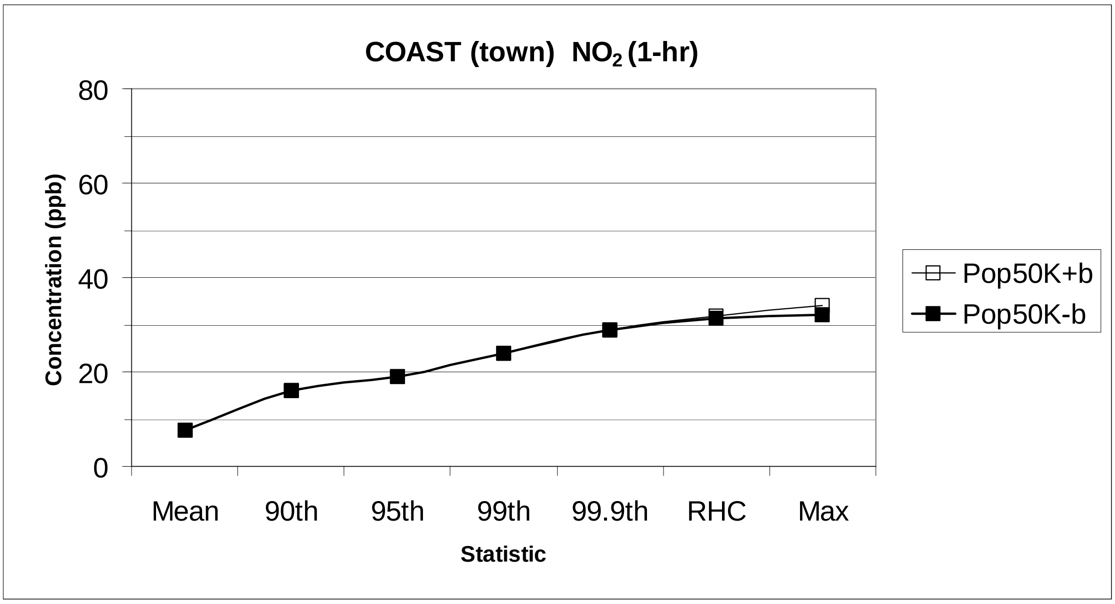


Figure 4.13(a) Annual glc statistics for hourly-averaged NO_2 for emissions from the *coastal* town with a population of 50 000. Curves are for simulations with (+b) and without (-b) biogenic emissions. Statistics are calculated within the town's boundaries.

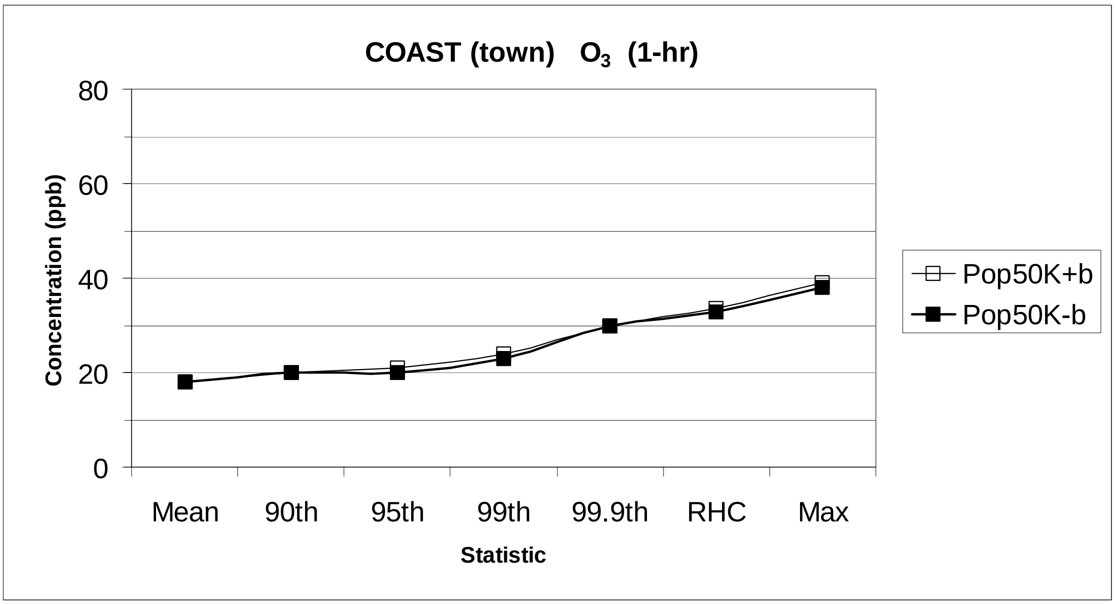


Figure 4.13(b) Annual glc statistics for hourly-averaged O_3 for emissions from the *coastal* town with a population of 50 000. Curves are for simulations with (+b) and without (-b) biogenic emissions. Statistics are calculated within the town's boundaries.

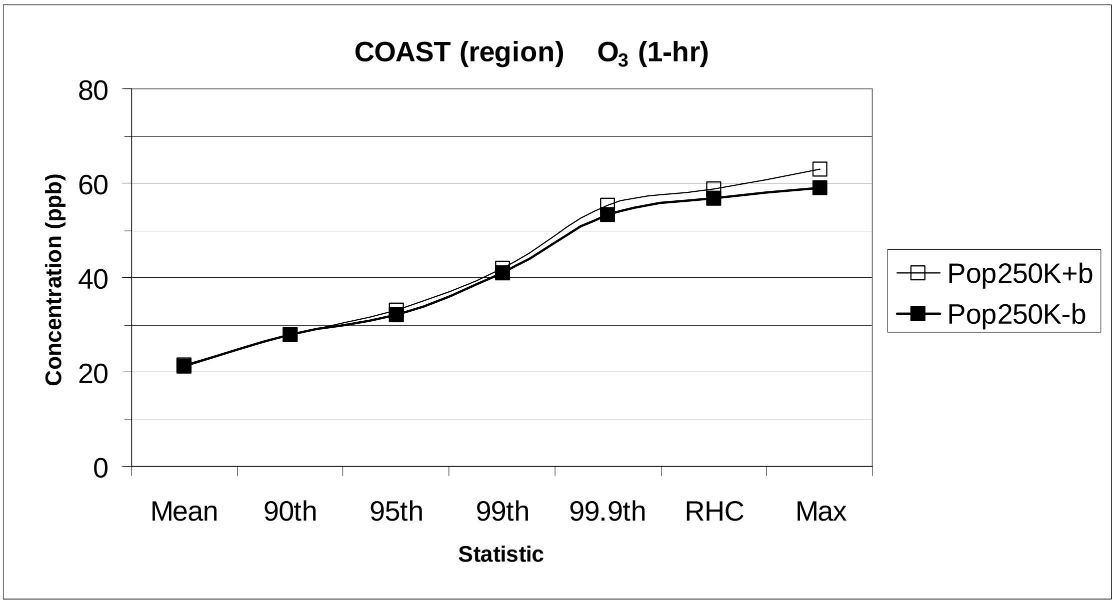


Figure 4.14(a) Annual glc statistics for hourly-averaged O_3 for emissions from the *coastal* town with a population of 250 000. Curves are for simulations with (+b) and without (-b) biogenic emissions. Statistics are calculated over the 1.5-km spacing modelling domain (48 x 48 km^2).

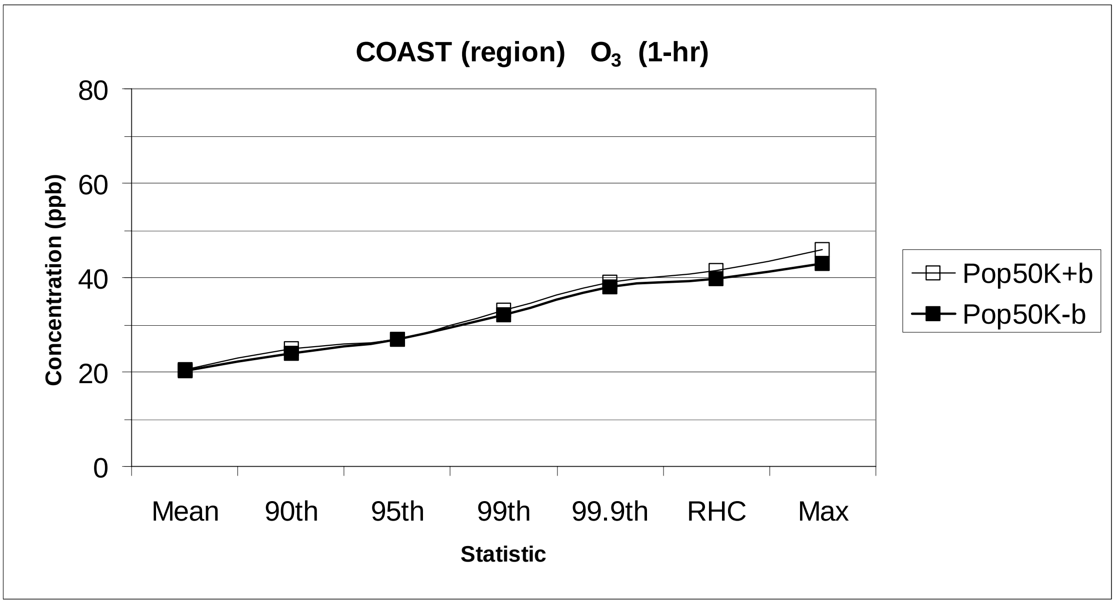


Figure 4.14(b) Annual glc statistics for hourly-averaged O_3 for emissions from the *coastal* town with a population of 50 000. Curves are for simulations with (+b) and without (-b) biogenic emissions. Statistics are calculated over the 1.5-km spacing modelling domain (48 x 48 km^2).

5 Discussion and summary

In NEPM Technical Paper No. 4 (Peer Review Committee, 2001), the Peer Review Committee has considered and documented a range of screening procedures for individual pollutants. They have ranked these in terms of the confidence that can be attached to the respective screening determinations, and have formalised their use by setting acceptance limits, generally expressed as percentages of the NEPM Standards for air quality. These acceptance limits take account of the confidence attached to the associated screening procedures. Screening would be considered acceptable only if the procedure yielded a prediction of maximum pollutant concentration that was below the acceptance limit for that procedure. Here the results of Section 4 are discussed with reference to the acceptance limits.

The screening procedure applied in this Report is a category E procedure, defined in NEPM Technical Paper 4 as

> In a region with no performance monitoring, and in the absence of emissions and detailed meteorological data, use of generic model results based on gross emissions estimates, "worst case" meteorology estimates and other conservative assumptions.

5.1 NO_2 concentration

For NO_2, the acceptance limit for screening procedure E is 35% of the NEPM standard (120 ppb for hourly-averaged concentrations), i.e. a value of 42 ppb. From Table 5.1, in which are listed the maximum glcs predicted by TAPM over a 12-month period for the generic coastal and inland towns, it can be seen that emissions from coastal populations of less than 100 000 produce glcs below the acceptance limit. Although a population of 150 000 exceeds the limit, this only happens on one day per year. For the inland town, exceedance of the acceptance limit is predicted for all population sizes. The maximum glc does not decrease for the smaller populations, as it does for the coastal town, and may be due to the assumption of the same population density at the town centre for all populations, in combination with a stable almost-calm meteorological situation. For populations of 25 000 and 50 000, the acceptance limit is exceeded on only one day per year, and for 100 000 it is exceeded two days per year.

Table 5.1 Maximum modelled hourly-averaged glcs of NO_2 (ppb) within the town boundaries for different population sizes. The number of days on which the acceptance limit (42 ppb) is exceeded is shown in parentheses.

	Coastal	*Inland*
250 000	51 (3)	55 (7)
150 000	47 (1)	51 (3)
100 000	42 (-)	52 (2)
50 000	34 (-)	46 (1)
25 000	31 (-)	46 (1)

5.2 O_3 concentration

The acceptance limit for O_3, outlined in NEPM Technical Paper No. 4, is calculated by applying the screening percentage of 35% for pollutants with negligible backgrounds (e.g. NO_2) to the anthropogenic component of the O_3 standard, and then adding the result to the non-anthropogenic (background) value. In our simulations, we assumed a background concentration of 20 ppb, so the acceptance limit for hourly-averaged O_3 is 0.35*(100 - 20) + 20, i.e. 48 ppb. Table 5.2 shows that coastal towns with populations of less than 100 000 do not produce glcs exceeding the acceptance limit, while inland towns of 150 000 or fewer people do not exceed the limit.

For 4-hourly averaged O_3 concentrations, the NEPM standard is 80 ppb, so the acceptance limit becomes 41 ppb. This value is only exceeded by coastal towns greater than 150 000 population and inland towns of greater than 100 000 (on only one day per year for a population of 150 000).

Table 5.2 Maximum modelled hourly-averaged glcs of O_3 (ppb) within the town boundaries for different population sizes. Assumed background concentration is 20 ppb. The number of days on which the acceptance limit (48 ppb) is exceeded is shown in parentheses.

	Coastal	*Inland*
250 000	58 (3)	54 (2)
150 000	56 (1)	44 (-)
100 000	51 (1)	42 (-)
50 000	40 (-)	39 (-)
25 000	36 (-)	39 (-)

Table 5.3 Maximum modelled 4-hourly-averaged glcs of O_3 (ppb) within the town boundaries for different population sizes. Assumed background concentration is 20 ppb. The number of days on which the acceptance limit (41 ppb) is exceeded is shown in parentheses.

	Coastal	*Inland*
250 000	45 (3)	48 (2)
150 000	39 (-)	42 (1)
100 000	36 (-)	40 (-)
50 000	30 (-)	34 (-)
25 000	27 (-)	34 (-)

5.3 Background O_3

Background concentrations of O_3 in the lower troposphere arise from the intrusion of ozone-rich air from the stratosphere and the in-situ photochemical production and destruction of O_3. Important precursors for O_3 formation include VOCs from vegetation, and NO_x from lightning, soil and the oceans. Background O_3 values can be significant, and vary according to location and season. VOC emissions from vegetation were modelled in TAPM, although no natural NO_x sources were specified, so that the biogenics contribution to O_3 concentrations came about through reaction with NO_x from the town anthropogenic sources. Ideally, we would like a model to simulate explicitly the diurnal and seasonal variation in background O_3 concentrations, but the current knowledge of natural sources and the simplified photochemistry of the GRS mechanism in TAPM do not allow this.

Comparison of model results from the inland town with O_3 glcs from Wagga suggested that the model's background concentration of 20 ppb was too low and that a value as high as 45 ppb (in the middle of the day) may be more appropriate, certainly on very warm and perhaps smoky days. A similar value was also found to be appropriate on hot days in the Latrobe Valley region by Galbally et al. (1986). A background value of this magnitude was also modelled for the Latrobe Valley by Cope et al. (1988) using measured biogenic VOC emissions and soil NO_x emissions. In a modelling and data analysis study of air quality in the Pilbara's Burrup Peninsula region, where vegetation is sparse, Physick and Blockley (2001) found that 25 ppb was an appropriate background value for O_3 concentrations. However, on days of smoky air (a total of 31 days from September through to November), they found that O_3 concentrations were enhanced by about 20 ppb. Examination of results from the Australian Air Quality Forecasting System suggested that long-range transport of O_3 associated with emissions from Melbourne and Sydney may also contribute to background levels at Wagga.

If a background O_3 value of 45 ppb (instead of 20 ppb) had been used in our Study, at least for the summer months, a close approximation to the maximum values would be the addition of 25 ppb to those values in Tables 5.2 and 5.3. These amended concentrations are tabulated in Tables 5.4 and 5.5. The acceptance limits for hourly-averaged and four-hourly-averaged O_3 would be 64 ppb and 57 ppb respectively. Results in the Tables show that under a background value of 45 ppb, the hourly-averaged O_3 acceptance limit would be exceeded by inland towns with populations of 100 000 or greater. For coastal towns, the limit would be exceeded by towns of 50 000 (on one day) and greater population. For four-hourly averaged O_3, the acceptance limit is exceeded by inland towns of 25 000 or more population while for a coastal town it is exceeded by towns with population of 100 000 or more.

Table 5.4 Maximum modelled hourly-averaged glcs of O_3 (ppb) within the town boundaries for different population sizes. Assumed background concentration is 45 ppb. The number of days on which the acceptance limit (64 ppb) is exceeded is shown in parentheses.

	Coastal	*Inland*
250 000	83 (12)	79 (12)
150 000	81 (10)	69 (3)
100 000	76 (2)	67 (2)
50 000	65 (1)	64 (-)
25 000	61 (-)	64 (-)

Table 5.5 Maximum modelled 4-hourly-averaged glcs of O_3 (ppb) within the town boundaries for different population sizes. Assumed background concentration is 45 ppb. The number of days on which the acceptance limit (57 ppb) is exceeded is shown in parentheses.

	Coastal	*Inland*
250 000	70 (18)	73 (19)
150 000	64 (13)	67 (7)
100 000	61 (3)	65 (5)
50 000	55 (-)	59 (2)
25 000	52 (-)	59 (1)

5.4 Summary

The modelling experiments in this Study have evaluated the likely maximum concentrations of NO_2 and O_3 to be produced within towns of populations ranging from 25 000 to 250 000. In sections 5.1 and 5.2, we have discussed these results in terms of acceptance concentration limits for screening procedures detailed in NEPM Technical Paper No. 4 (Peer Review Committee, 2001). The value of a 'threshold' population in terms of the expected maximum concentration relative to an acceptance limit varies with pollutant, averaging period and town location (inland and generic), as outlined in Tables 5.1–5.3.

Comparison of simulation results to monitoring data from Wagga showed satisfactory agreement for NO_2, but revealed that on many days the observed background O_3 concentrations were considerably higher than the chosen background value of 20 ppb. An estimate of modelled maximum concentrations for a worst-case background O_3 concentration of 45 ppb was made in section 5.3, with 'threshold' populations decreasing for both hourly- and four-hourly-averaged O_3 concentrations, i.e. smaller populations produced maximum glcs over the acceptance limit than with a 20 ppb O_3 background value.

When assessing the results in this Report, it should be noted that the use of a background VOC concentration of R_{smog} = 0.75 is conservative, and could increase hourly-averaged O_3 glcs by 10 ppb and NO_2 glcs by 5 ppb over those obtained from a more likely value of 0.5. It should also be mentioned that, although there was terrain in the vicinity of the generic inland town, it was of a gently-sloping nature. Emissions from towns in regions of steeper terrain may be strongly influenced by terrain-induced meteorology and it is recommended that a simulation similar to those in this Report should be carried out for the particular town of interest.

Acknowledgements

We are grateful to Pacific Power for provision of the Wagga monitoring data, and to Peter Hurley for discussions on the experimental design.

References

Azzi, M., Johnson, G. J., and Cope, M.E. (1992). An introduction to the Generic Reaction Set photochemical smog mechanism. *Proc. 11th International Clean Air Environment Conf., 5-9 July 1992, Brisbane, Clean Air Society of Australia and New Zealand, 451-462.*

Cope, M.E., Carnovale, F., Galbally, I.E., Cook, B. and Hearn, D. (1988). Modelling photochemical smog in the Latrobe Valley. *Clean Air*, **22**, 185-191.

Cox W. and Tikvart J. (1990). A statistical procedure for determining the best performing air quality simulation. *Atmos. Environ*., **24A**, 2387-2395.

Galbally, I.E., Miller, A.J., Hoy, R.D., Ahmet, S., Joynt, R.C. and Attwood, D. (1986). Surface ozone at rural sites in the Latrobe Valley and Cape Grim, Australia. *Atmos. Environ.*, **20**, 2403-2422.

Hurley, P.J. (1999). The Air Pollution Model (TAPM) Version 1 : Technical description and examples. CSIRO Atmospheric Research Technical Report No. 43.

Hurley P.J. (2000a). Verification of TAPM meteorological predictions in the Melbourne region for a winter and summer month. *Australian Meteorol. Mag.*, **49**, 97-107.

Hurley, P.J. (2000b). The air pollution model (TAPM): Summary of some recent verification work in Australia. *Proc. 15th International* Clean *Air Environment Conf., November 2000, Sydney, Clean Air Society of Australia and New Zealand.*

Hurley. P., Manins, P, Lee, S., Boyle, R, Ng, Y.L., and Dewundege, P. (2002). Year-long urban airshed modelling in Melbourne: verification of TAPM for photochemical smog and particles. *Proceedings of the 16th International* Conference *of the Clean Air Society of Australia and New Zealand, Christchurch, New Zealand, August 2002.*

Ischtwan, J. (2002). Prognostic modelling of a summer period of photochemical smog in south-east Queensland. *Proceedings of the 16th International Conference of the Clean Air Society of Australia and New Zealand, Christchurch, New Zealand, August 2002.*

Johnson, G.M., Quigley, S.M. and Smith, J.G. (1990). Management of photochemical smog using the airtrak approach. *Proceedings of the 10th* International *Conference of the Clean Air Society of Australia and New Zealand, Auckland, New Zealand, March 1990*

Peer Review Committee, (2001). Screening procedures. *National Environment Protection (ambient air quality) Measure, Technical Paper No. 4*, May 2001, 9pp.

Physick, W.L. and Blockley, A. (2001). An evaluation of air quality models for the Pilbara region. *CSIRO Division of Atmospheric Research. A Report to the Department of Environmental Protection, Western Australia, 98pp, June 2001.*

Physick, W., Blockley, A., Farrar, D, Rayner, K. and Mountford, P. (2002). Application of three air quality models to the Pilbara region. *Proceedings of the 16th International Conference of the Clean Air Society of Australia and New Zealand, Christchurch, New Zealand, August 2002*.

Rye, P. (1996). Meteorological and source analysis of smog events during the Perth Photochemical Smog Study. *Technical Series 83,* Department *of Environmental Protection, Perth, Western Australia, May 1996.*