



Department of Planning, Industry and Environment

Vales Point Power Station photochemical modelling for EPA

Application for group 5 exemption



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Introduction

The EPA has requested photochemical modelling in response to an application for group 5 exemption license condition from Vales Point Power Station (VPPS). The current 99th percentile limit of NO_x emission rate of 1651 g/s is proposed to be reduced to 1276 g/s 99th percentile limit. For the Group 5 limit, the NO_x emission rate is 1201 g/s.

The implication of these new proposed emission limits on the air quality in the local area and the Greater Metropolitan Region (GMR) of Sydney needs to be investigated. The following report describes the setup and results of the photochemical modelling of the proposed changes to the VPPS operations.

Methodology

Emission from coal-fired power stations contribute significantly to emissions of GHGs and air pollutants such as SO_x, NO_x and PM. These emissions play key roles in local and regional air quality. In the presence of sunlight, NO_x can undergo complex non-linear chemical reactions to produce ozone and secondary organic aerosols. NO_x can also react with NH₃ and SO₂ to form secondary inorganic aerosols.

Vales Point Power Station (VPPS) is one of many anthropogenic sources in the GMR. To study the impact of change in emissions from a source, usually a photochemical dispersion model is used and run under two scenarios, one for base case emission condition with all sources and one with the proposed emissions changes of one source. The difference in predicted air pollutant concentrations across the modelling domain will be used to assess the impact of the proposed emission change of the source at the VPPS.

For this study, we used the latest EPA 2013 emission inventory (EI) covering all anthropogenic and biogenic sources within the GMR. It is important to highlight that the VPPS source characteristics as specified in the EPA EI are different from the current characteristics shown in Table 1.

Table 1 **Stack parameters of the VPPS**

Stack Parameters	Value	units
Latitude	-33.161	degrees
Longitude	151.541	degrees
Stack height	178.0	m
Stack diameter	10.3	m
Exit Velocity	26.0	m/s
Exit temperature	369.0	K
Exit temperature	95.9	C
Flow Rate (Normalised)	1,501.0	Nm ³ /s
Flow Rate Actual	2166	m ³ /s

The emission concentrations for each proposed scenario are presented in Table 2.

Table 2 Emission concentrations and rates at VPPS for each proposed scenario

Scenario	NO _x Emission Concentration (mg/Nm ³)	NO _x Emission rate (g/s)
1. Current 99 th percentile limit and proposed 100 th percentile limit – new base case	1100	1,651.0
2. Proposed 99 th percentile limit	850	1276
3. Group 5 limit	800	1201

Table 3 shows the following emission rates for SO₂ and total solid particles (TSP) that are used in all three scenarios.

Table 3 Emission concentration and rate for SO₂ and TSP

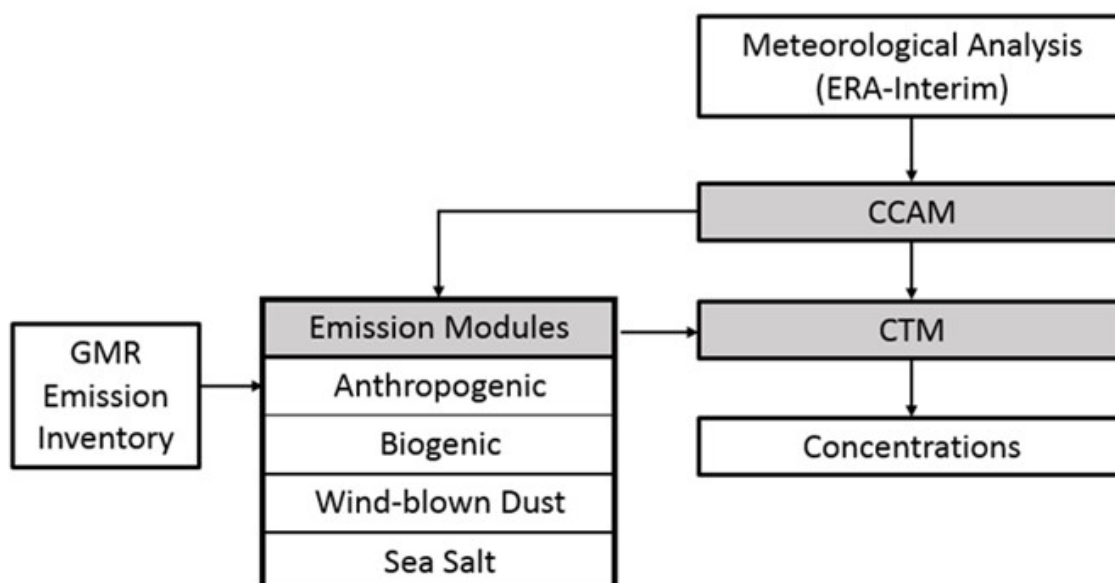
Pollutant	Emission Concentration (mg/Nm ³)	Emission rate (g/s)
Sulfur Dioxide	1700	2,551.7
Total Solid Particles	50	75.1

The photochemical air quality model used in this study is CCAM-CTM developed by CSIRO. The model is run for one calendar year from 1 January to 31 December 2013. It is assumed that the VPPS source is running the whole 2013 period with constant emission. The results will be presented as annual average and annual average of daily maximum of four main pollutants: NO, NO₂, Ozone (O₃) and PM_{2.5}.

Model description

The coupled Conformal Cubic Atmospheric Model (CCAM) and Chemical Transport Model (CTM; hereafter, the CCAM-CTM modelling system) was used to generate spatial and temporal concentrations of air pollutants of interest. Meteorological fields including wind velocity, turbulence, temperature, radiation and the water vapour mixing ratios are produced by CCAM. CTM uses the extended Carbon Bond 5 mechanism (CB05) that consists of 65 gas phase species, 19 aerosol species and 172 reactions.

The components of the modelling system (meteorology, emissions and CTM) are presented in Figure 1.

**Figure 1 Schematic diagram of the CCAM-CTM modelling system**

The updated PM_{2.5}/PM₁₀ ratios that were used to create the emission files for CTM are presented in Table 4.

Table 4 PM_{2.5}/PM₁₀ ratios used in the generation of emissions from the emission inventory.

Source	EDMS	CTM	PM _{2.5} /PM ₁₀ ratios
<i>Inventory Sources</i>	<i>CIT</i>	<i>CTM</i>	<i>2013 Inventory</i>
Aircraft	aems	gse	0.983
Commercial Vehicles and Equipment	aems	gse	0.970
Industrial Vehicles and Equipment	aems	gse	0.970
Locomotives	aems	gse	0.970
Ships	aems	gse	0.920
Industrial fugitives (excl wind erosion)	aems	gse	0.150
Domestic-Commercial (total exc. solid fuel burning)	aems	gse	0.940
All - Non-Exhaust PM	aems	gse	0.532
Diesel - Exhaust	mvems	vdx	0.970
Others - Exhaust	mvems	vlx	0.953
Petrol - Exhaust	mvems	vpx	0.953
Solid Fuel Burning (Domestic)	aems	whe	0.963
Generation of electrical power from coal	pems	pse	0.408
Generation of electrical power from gas	pems	pse	0.998
Industrial point sources (except for coal and gas)	pems	pse	0.680

Emission preparation

As the CCAM-CTM model requires emission of 17 species from a source such as NO, NO₂, CO, SO₂, PM₁₀ or PM_{2.5}, NH₃, Toluene. The emission inventory only specifies the total NO_x emission rate. We partitioned the total NO_x emission into NO and NO₂ emission according to the ratio we obtain from the EDMS which is about 92.5% NO and 7.5% NO₂

The NO_x base case of 1651 g/s is therefore split into 1527 g/s NO and 124 g/s NO₂. These values are then converted to corresponding values in the point source emission (pems) file (in ppm/min) for each boiler using the following formula:

$$Pollutant_{ppm/min} = \frac{Pollutant_{g/s}}{factor \times mol\ weight}$$

The emissions rates are divided by 2 to get the value for 1 boiler (boiler 3 and 4 are ignored as they are startup). The factor is 0.68194 and is calculated from the ideal gas equation as outlined in Appendix 1..

Table 5 Gas emission rate conversions

Source	Emission rate (g/s)	Factor	Molar weight	Base case emission rate per boiler	Scenario 1 emission rate per boiler	Scenario 2 emission rate per boiler
Units	g/s			ppm/min	ppm/min	ppm/min
NO	1527		30	37.32	28.84	27.13
NO ₂	124	0.68194	46	1.98	1.53	1.43
SO ₂	2551.7		64.1	29.19	29.19	29.19

Table 6 Particulate emission rate conversion

Source	Emission rate (g/s)	Base case emission rate (g/s) per boiler	Scenario 1 emission rate (g/s) per boiler	Scenario 2 emission rate (g/s) per boiler
Units	g/s	g/s	g/s	g/s
PM ₁₀	75.1	37.55 (g/s)	37.55	37.55

We used the emission rate for all other species as given by the EPA 2013 EI for VPPS source. For scenarios (S1 and S2) emission, we use similar approach to obtain the emission rate values as described above for the base case.

Results

The base case for the whole 2013 calendar year was simulated using CCAM-CTM air quality model with all anthropogenic source emission (including Vale Point PS base case emission). The 2 scenarios (S1 and S2) were also simulated with all anthropogenic source emission as in the base case but Vales Point PS emission were reduced according to the specified emission scenarios described above. The results of base case simulation, base case minus scenario 1 and base case minus scenario 2 will be analysed.

Base case

Annual average

Figure 2 shows the 2013 annual average of NO, NO₂, O₃ and PM_{2.5} concentration over the GMR as predicted by CCAM-CTM air quality model. It can be seen that high NO and NO₂ concentration occurred in the so-called "NO_x-rich" areas of the Upper Hunter, the Central Coast and Sydney where power station emission and mobile sources emission dominate. For ozone, these NO_x-rich regions have less ozone as compared to the high ozone concentration mostly occurring in north west and western Sydney where NO_x-limited photochemical regime frequently happens during summertime. Western Sydney is also downwind from central Sydney where most emission occurs during sea breeze period from early morning to late afternoon. The ozone pattern is a classic representation of interaction between NO_x and VOC emission with meteorology in urban settings with various anthropogenic sources such as the GMR.

For PM_{2.5}, high concentration mostly occurs in the Upper Hunter and Sydney regions where wood heating and mining activities (Upper Hunter) caused elevated concentration of PM_{2.5}, especially during wintertime. Emission from point sources (such as power station in the Central

Coast and Lower Hunter) does not cause high concentration of particles which composed of primary emitted particles, secondary organic aerosols and secondary inorganic aerosols formed from complex aerosol chemical processes.

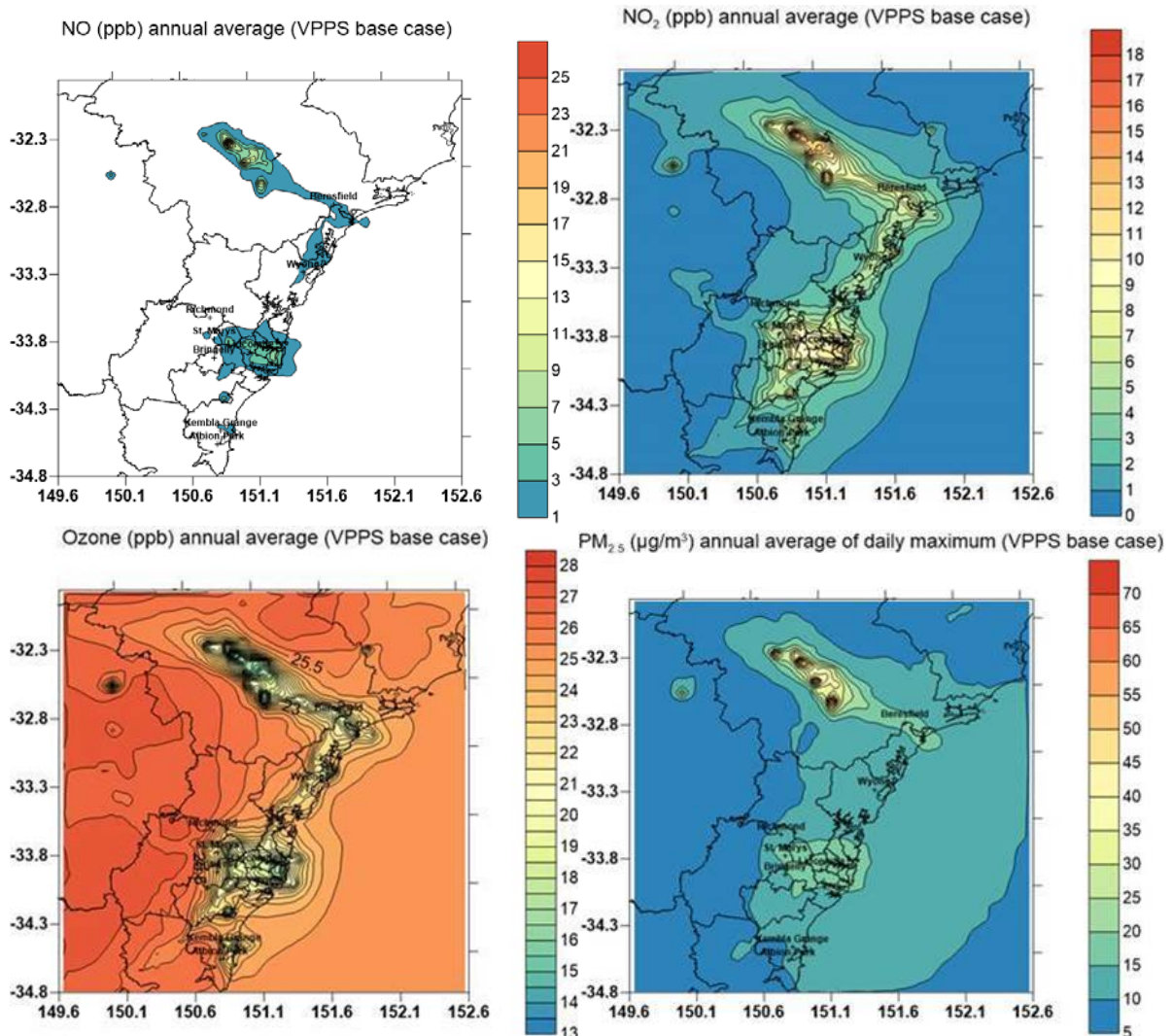


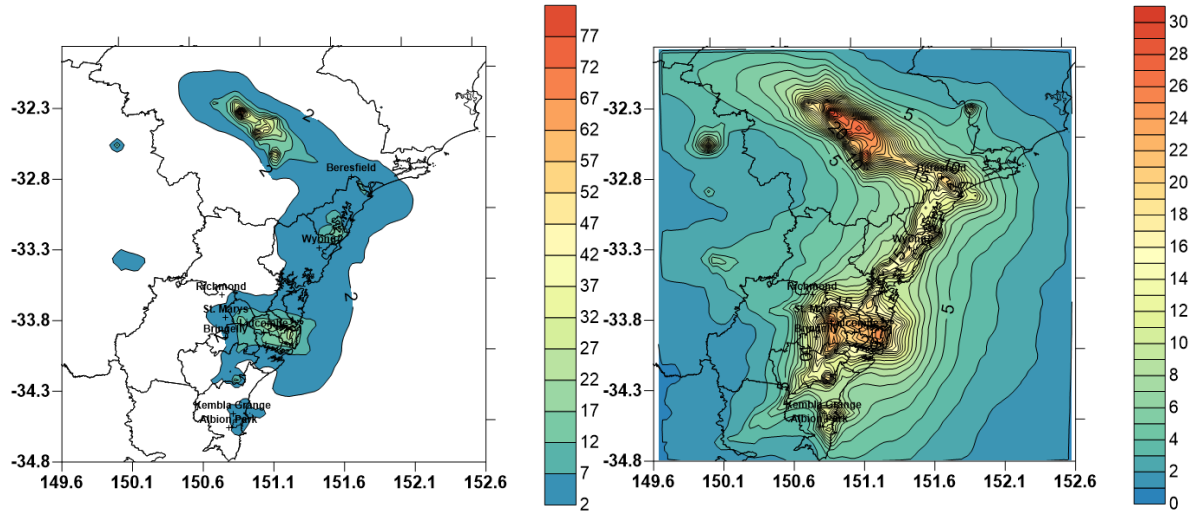
Figure 2 Annual average of NO, NO₂, O₃ and PM_{2.5} as predicted from CCAM-CTM over the GMR in 2013.

The above results are what we expected regarding NO_x and O₃, PM_{2.5} concentration distribution pattern in Sydney as shown in previous studies.

Annual average of daily maximum

The annual average of daily maximum patterns of NO, NO₂, O₃ and PM_{2.5} (Figure 3) are similar to those of annual average. However, for ozone, the high concentration in north west and west of Sydney is more pronounced in north west and west of Sydney. Meteorology pattern (sea breeze) in the Sydney basin plays an important role in high ozone in western Sydney.

NO (ppb) annual average of daily maximum (VPPS base case) NO₂ (ppb) annual average of daily maximum (VPPS base case)



Ozone annual average of daily maximum (VPPS base case) PM_{2.5} (µg/m³) annual average of daily maximum (VPPS base case)

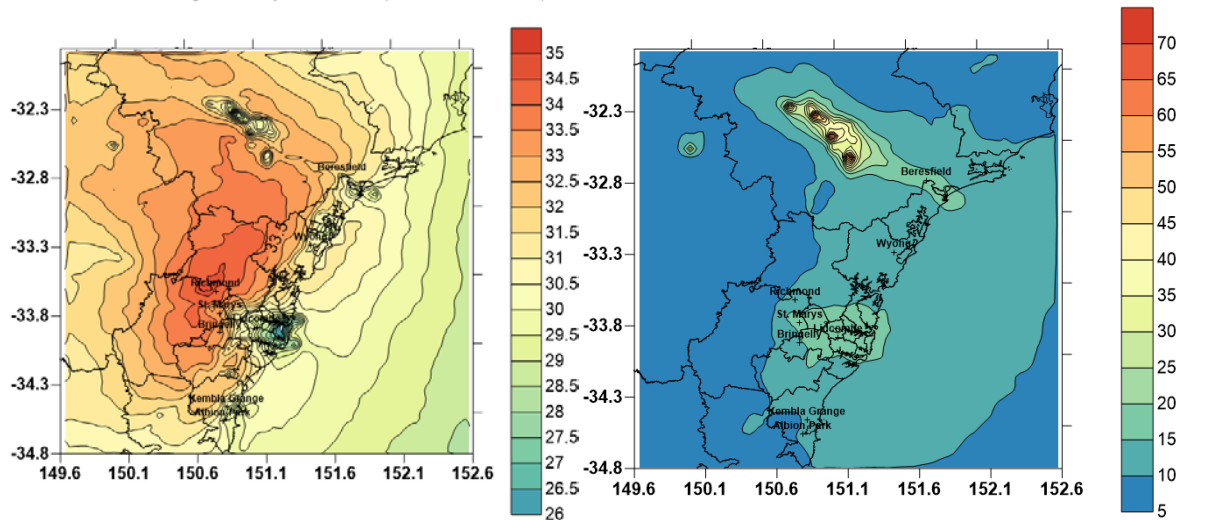


Figure 3 Annual average of daily maximum of NO, NO₂, O₃ (ppb) and PM_{2.5} (µg/m³) as predicted by CCAM-CTM model over the GMR in 2013.

Difference between base case and S1 scenario

Annual average

Figure 4 shows the difference between the base case and S1 of annual average for NO, NO₂, O₃ and PM_{2.5}. As expected, the difference is very small. For NO, the maximum difference is 0.52 ppb, while for NO₂ the value is 0.36 ppb. The results show that annual averages of NO, NO₂ concentrations decrease with Scenario 1 as compared to the base case.

For ozone, the reduction of NO_x emissions from VPPS resulted in an increase of ozone near the facility but this increase is gradually decreasing further away from the facility. The increase in O₃ is small with a maximum of 0.3 ppb around VPPS and most of the GMR.

PM_{2.5} annual average decreases in most of the domain but the maximum change is around 0.012 µg/m³.

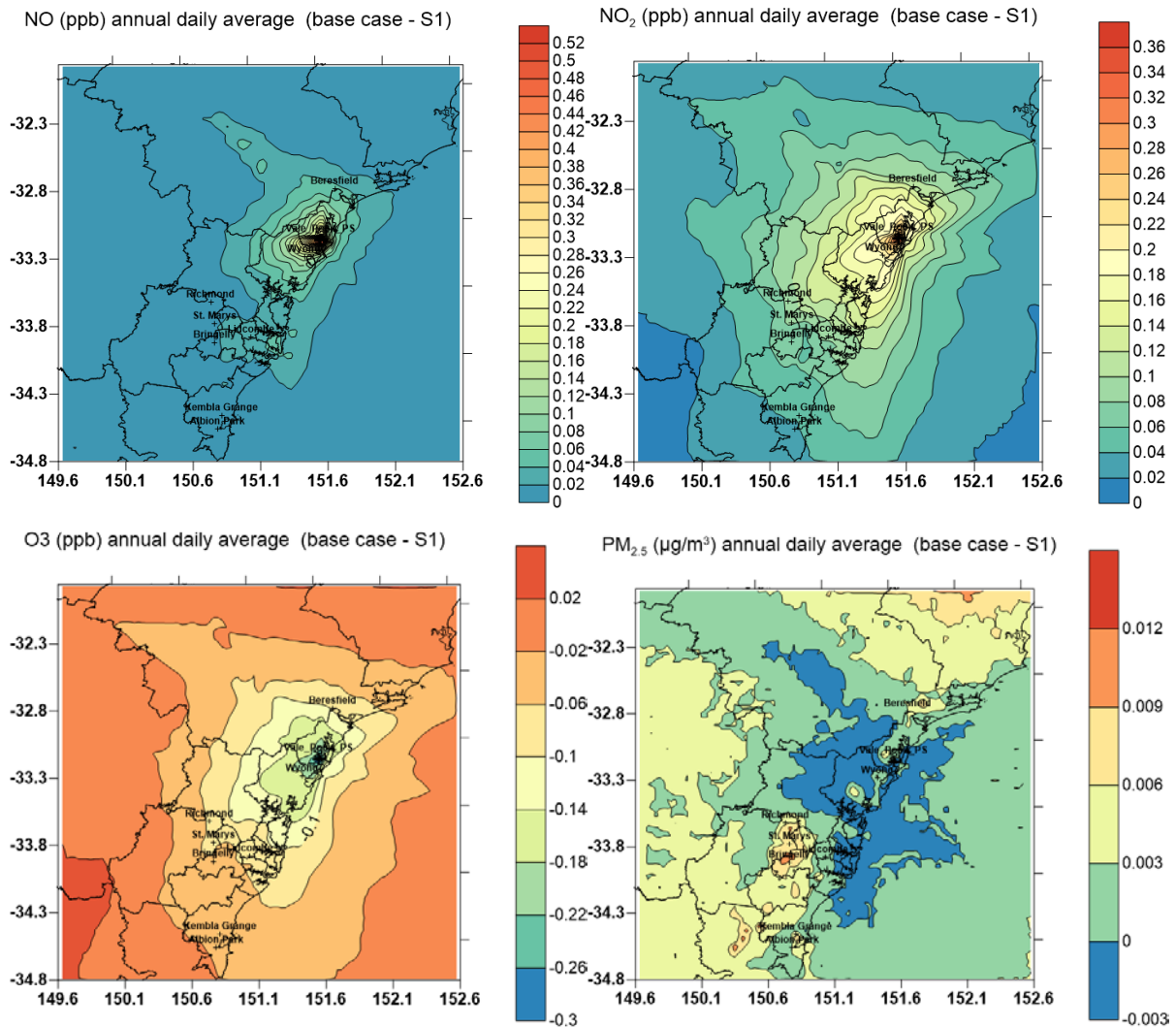


Figure 4 Difference in annual average of NO, NO₂, O₃ and PM_{2.5} between base case and S1 scenario emission as predicted by CCAM-CTM model over the GMR in 2013

Annual average of daily maximum

As for annual average, the difference is small except for maximum ozone as shown in Figure 5. For annual average of daily maximum, the results for NO and NO₂ are similar as in the annual average analysis but the scale of difference is higher (4.1 ppb max for NO and 1.25 ppb max for NO₂) in the modelling domain.

The difference in annual of daily maximum of ozone shows an increase of ozone around the VPPS and in most of the GMR when NO_x emission is reduced as in Scenario 1. Maximum increase is 0.2 ppb.

For PM_{2.5}, the values of difference are too small (0.024 or 0.028 µg/m³ max differences) to have any meaningful conclusion.

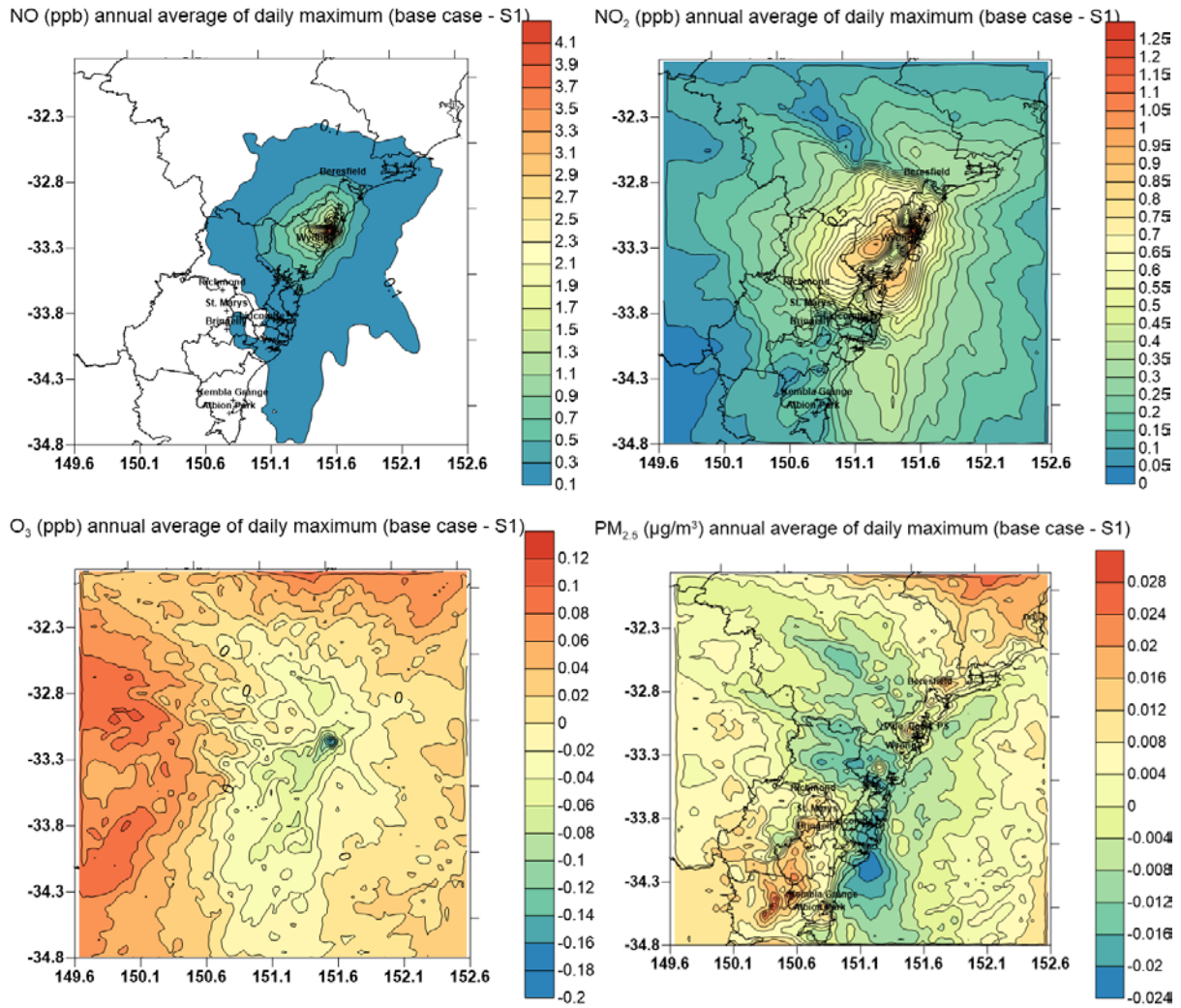


Figure 5 Difference in annual average of daily maximum of NO, NO₂, O₃ and PM_{2.5} between base case and S1 scenario emission as predicted by CCAM-CTM model over the GMR in 2013

Difference between base case and S2

The results as compared to base case are similar to S1 analysis above. There are decreases of NO and NO₂ concentration as compared with those in S1 scenario.

Annual average

As compared to the base case, the maximum decrease in annual average of NO concentration is about 0.6 ppb while for NO₂ the figure is 0.44 ppb as shown in Figure 6.

The increase in O₃ occurred in most of the GMR and reached 0.4 ppb around VPPS.

PM_{2.5} annual average decreases in most of the domain but the maximum change is of 0.014 µg/m³.

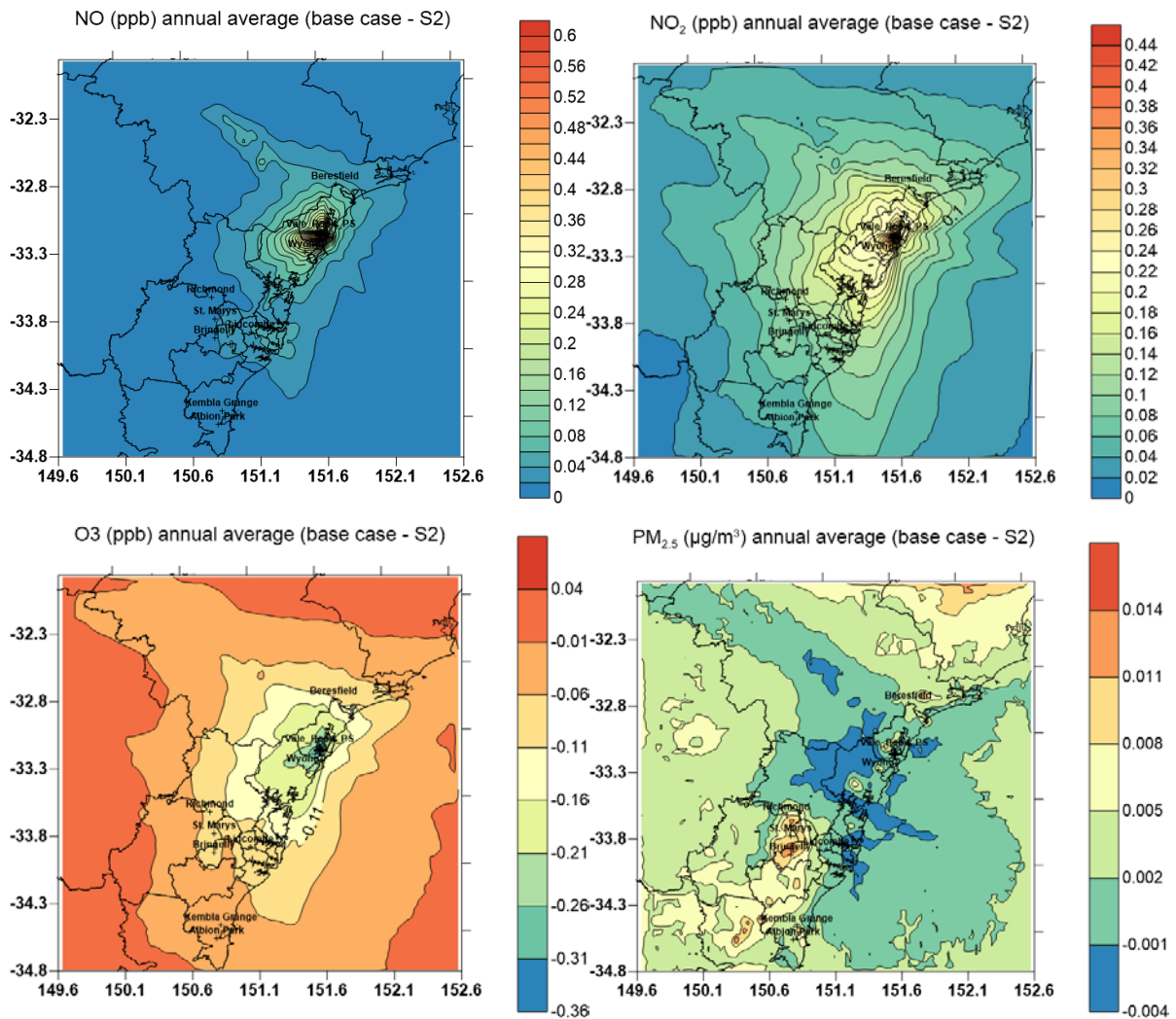


Figure 6 Difference in annual average of NO, NO₂, O₃ and PM_{2.5} between base case and S2 scenario emission as predicted by CCAM-CTM model over the GMR in 2013

Annual average of daily maximum

The changes (difference between base case and S2) of annual average of daily maximum, as shown in Figure 7 for NO, NO₂, O₃ and PM_{2.5}, are small as expected. For NO the maximum difference is 4.9 ppb in the modelling domain, near Vales Point PS, while the value for NO₂ is 1.5 ppb.

Similar to S1 emission scenario, the difference in annual of daily maximum of ozone shows an increase of ozone around the VPPS and most of the GMR when NO_x emission is reduced. Maximum increase is 0.16 ppb. And for PM_{2.5}, the values of difference are too small (0.03 or 0.04 µg/m³ maximum differences) to have any meaningful conclusion.

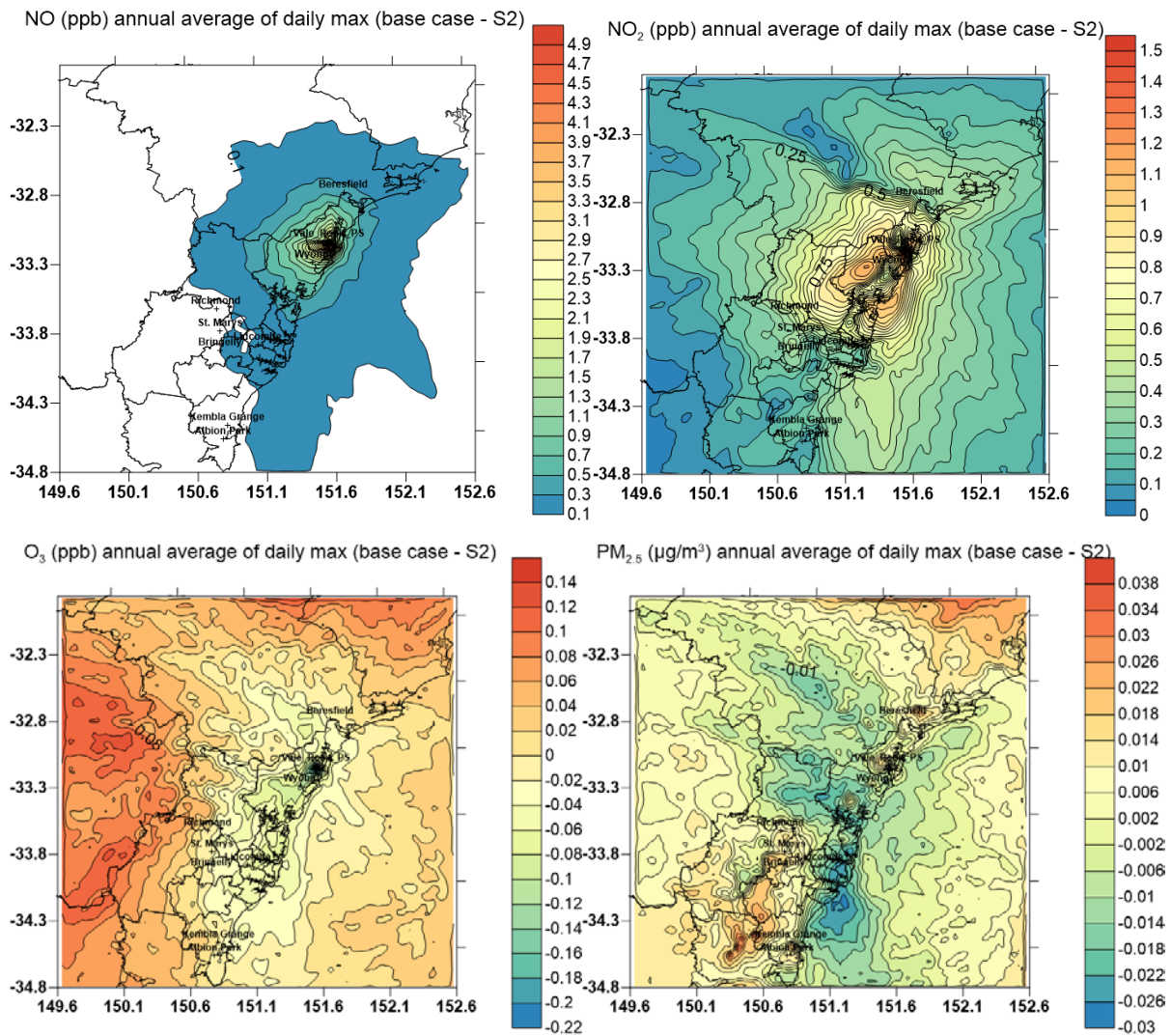


Figure 7 Difference in annual average of daily maximum of NO, NO₂, O₃ and PM_{2.5} between base case and S2 scenario emission as predicted by CCAM-CTM model over the GMR in 2013

Summary statistics of predicted annual average concentration over domain grid

The CCAM-CTM air quality model predicts the concentration of many pollutants in the hourly basis at each grid point in the domain GMR at 1km by 1km resolution. These daily gridded data files are then aggregated over the 2013 modelling period into yearly files: annual average and annual average of daily maxima for each of the pollutants.

The contour graphs as shown in Figure 2 to Figure 7 are interpolated from the grids to show the contours of equal concentration over the domain.

Another way to summarise the difference between the base case and S1, S2 scenarios is to plot the boxplots of concentration difference of all grid cells in the GMR modelling domain. Using this method, we can visualise the whole distribution of concentration difference in each grid cell. Figure 8 shows the box plots of annual average difference in the GMR domain

between base case and S1 and S2 scenarios for NO, NO₂, O₃ and PM_{2.5}. Over the whole domain, the S1 and S2 scenarios reduce the NO and NO₂ annual average of daily maximum as compared to the base case, with S2 having higher reduction as compared to S1. The median value of the distribution of concentration differences of NO, NO₂, O₃ and PM_{2.5} between base case and S2 are higher than that between base case and S1. However, all the differences between base case and S1 and S2 are very small (~0.8 ppb for NO, ~0.5 ppb for NO₂, ~0.4 ppb for O₃ and 0.015 µg/m³ for PM_{2.5}). Both S1 and S2 cause higher ozone concentration as compared to the base case in some areas

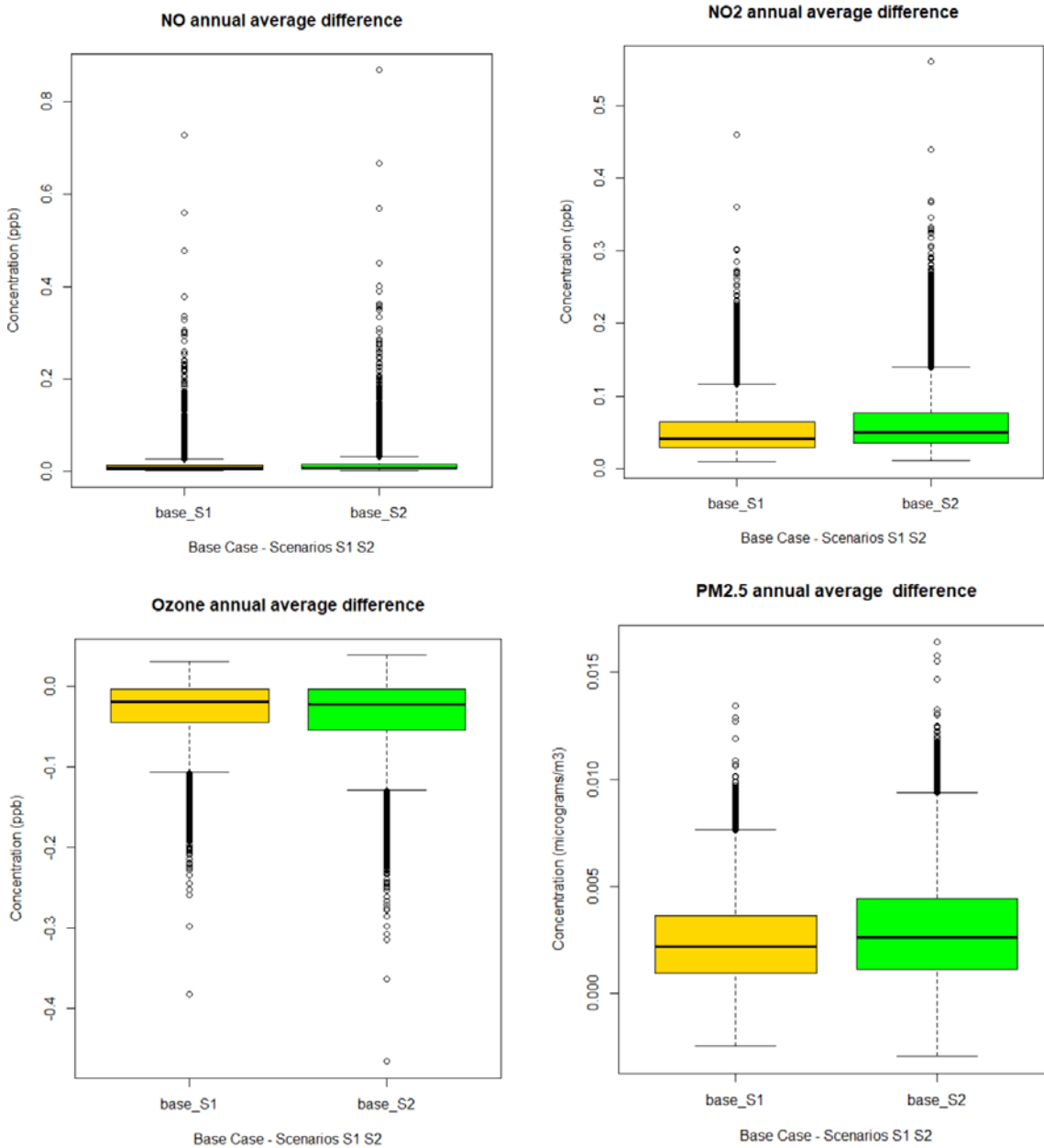


Figure 8 - Box plots of annual average difference in the GMR domain between base case and S1 and S2 scenario for NO, NO₂, O₃ and PM_{2.5}.

And Figure 9 shows the box plots of annual average of daily maximum difference in the GMR modelling domain between base case and S1 and S2 scenarios for NO, NO₂, O₃ and PM_{2.5}. Over the whole domain, the S1 and S2 scenarios reduce the NO and NO₂ annual average of daily maximum as compared to the base case, with S2 having higher reduction as compared to S1. The median value of the distribution of concentration difference between base case and S2 is higher than that between base case and S1. Similar results are also obtained for O₃ and

PM_{2.5}. However, both S1 and S2 cause higher ozone concentration in some areas of the domain. These results are similar to those based on annual average as described above but the magnitude scales is higher

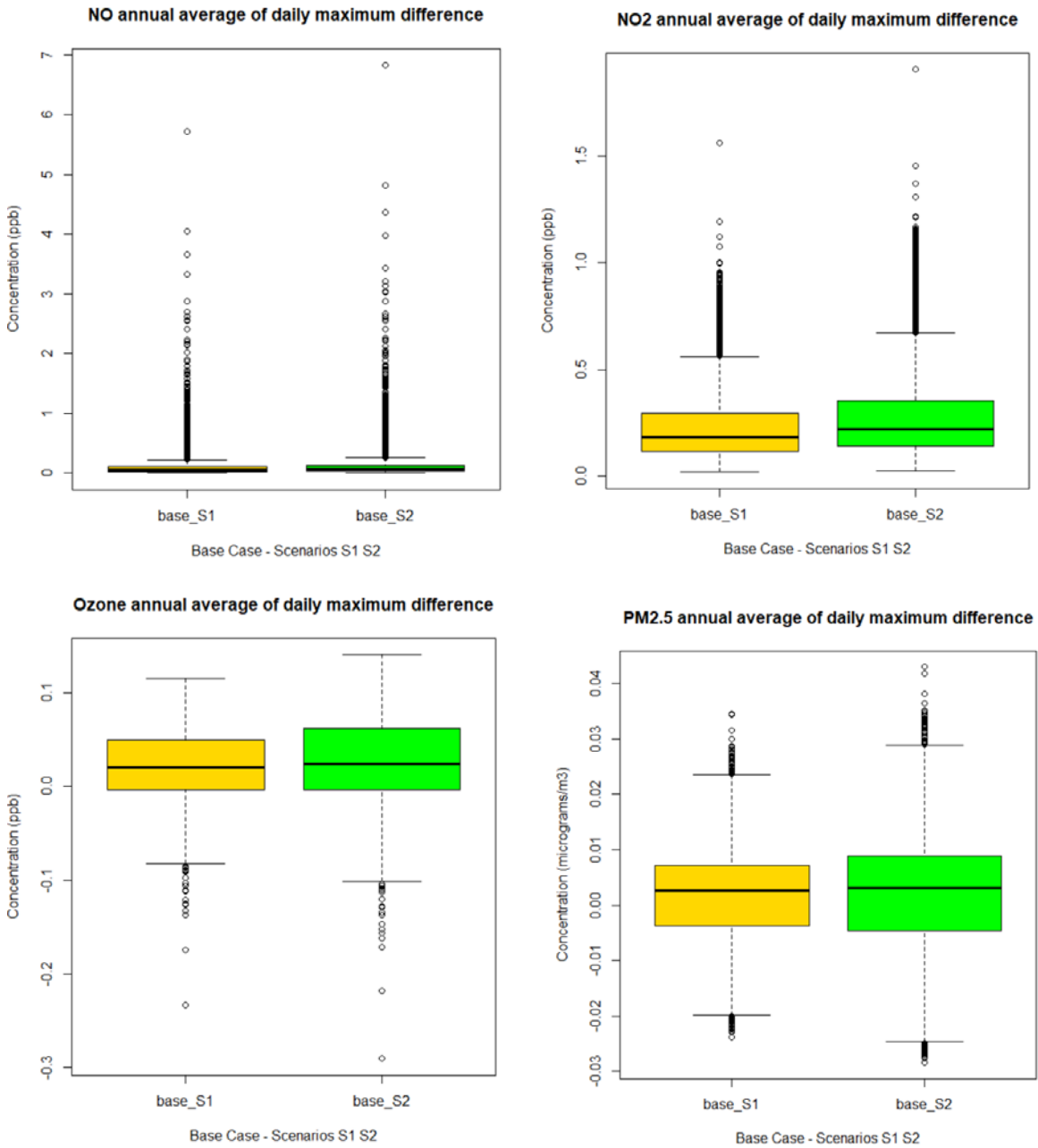


Figure 9 - Box plots of annual average of daily maximum difference in the GMR domain between base case and S1 and S2 scenario for NO, NO₂, O₃ and PM_{2.5}.

Table 6 summarises the statistics of base case, S1 and S2 scenarios regarding the predicted NO, NO₂, O₃ and PM_{2.5} annual average and annual average of daily maximum concentration in the GMR domain. The changes in NO, NO, O₃ and PM_{2.5} concentration (annual average and annual average of daily maximum) from base case to S1 or S2 scenario are very small or below the detection limit.

			Min	Mean	1 st quartile	Median	3 rd quartile	Max
Base case - S1	Annual average	NO	0.00063	0.0134	0.0037	0.0068	0.013	0.728
		NO ₂	0.0093	0.0535	0.029	0.041	0.064	0.459
		O ₃	-0.382	-0.03	-0.045	-0.019	-0.0037	0.031
		PM _{2.5}	-0.0025	0.0023	0.0009	0.0022	0.0036	0.0135
	Annual average of daily max	NO	0	0.104	0.027	0.057	0.105	5.72
		NO ₂	0.021	0.234	0.12	0.186	0.30	1.56
		O ₃	-0.23	0.022	-0.003	0.02	0.05	0.115
		PM _{2.5}	-0.0238	0.0018	-0.037	0.0026	0.0072	0.0345
Base case - S2	Annual average	NO	0.00075	0.0158	0.0045	0.0081	0.0156	0.868
		NO ₂	0.011	0.0644	0.035	0.049	0.077	0.56
		O ₃	-0.466	-0.036	-0.054	-0.023	-0.004	0.038
		PM _{2.5}	-0.0029	0.0028	0.0011	0.0026	0.0044	0.0164
	Annual Average of daily max	NO	0	0.124	0.0323	0.068	0.125	6.824
		NO ₂	0.025	0.28	0.143	0.222	0.356	1.90
		O ₃	-0.29	0.027	-0.0039	0.0245	0.0617	0.14
		PM _{2.5}	-0.028	0.00216	-0.0046	0.0031	0.0088	0.0429

Table 6 – Summary statistics of base case, S1, S2 annual average and annual average of daily maximum for NO, NO₂, O₃ and PM_{2.5} in the GMR domain. Negative values in the Table above indicate that the base case values are less than the scenario values. Unit for NO, NO₂ and O₃ is in ppb and PM_{2.5} is in µg/m³.

Conclusion

The air quality model CCAM-CTM is used to determine the impact of change in NO_x emission from Vales Point power station on air quality in the GMR. Four pollutants are considered, namely nitrogen monoxide (NO), nitrogen dioxide (NO₂), Ozone (O₃) and particulate matter less than 2.5 µm in diameter (PM_{2.5}).

Three emission scenarios are considered: the current limit of 99th percentile NO_x emission rate of 1651 g/s (base case), the proposed 99th percentile limit of NO_x emission rate of 1276 g/s (S1 scenario) and the Group 5 limit NO_x emission rate of 1201 g/s

The simulations using CCAM-CTM show that the changes in NO_x emission from base case to S1 or S2 resulted in a decrease of annual average and annual average of daily maximum of NO and NO₂ in the GMR. Higher decrease mostly occurred near Vales Point. But ozone increases near the power station. However, the change in NO, NO₂ and Ozone are very small across the GMR domain. For PM_{2.5}, there are no change in annual average and annual average of daily maximum over the GMR domain.

Appendix 1

Conversion of emission rate of a species from g/s to ppm/min

The CCAM-CTM air quality model uses the input file containing the emission rate of various species from a source in ppm/min. The emission rate given is in g/s. A conversion is required to run the model.

The factor is determined by using the ideal gas equation

$P * V = n * R * T$, where

P = pressure [Pa]

V = volume [m³]

T = temp [K]

n = number [mol]

R is the Boltzmann constant and is equal to 8.31446261815324 [m³ * Pa ^ K⁻¹ * mol⁻¹]

Hence the number of moles of air at standard pressure and temperature (25oC Or 298oK) in 1 m³ is

$$n = P*V/R*T = 101325/8.31/298$$

The concentration rate in ppm/min of a species is convert to part per second by dividing by 60 and multiplied by 10⁻⁶ and then multiplying by the above equation to obtain the number of moles of the species at standard pressure and temperature. That is

$$\text{Emission rate in ppm/min} / 60 \times e^{-6} \times 101325/8.31/298 = \text{emission rate in g/s}$$

Or

$$\text{Emission rate (ppm/min)} \times 6.8194 \times e^{-7} = \text{emission rate (g/s)}.$$

In summary, to convert from ppm-m/min to g/sec, multiply the emission rate of the species by a factor (6.81943e-7). Then the result is multiplied with molecular weight of the species. This is the emission rate in grams per sec per m². The EDMS CIT grid cell is 1 km by 1km. So the rate over the grid cell volume at 1m high is 6.8194e-7 x 1e6 or 0.68194.

To convert from g/sec to ppm-m/min, multiply the emission rate (in g/sec per m²) by 1/(6.81943e-7) and (1/molecular weight). This is the emission rate in ppm-m/min per m²