

In contrast to Zamdela, AJ Jacobs and Leitrim, where the peak concentration was definitely shown to be from SO and Natref, only about 26%, 30% and 38% of the observed concentration was simulated at Eco Park, Three Rivers and Sharpeville respectively. Although this may still have resulted from SO and Natref, there is also a strong likelihood that more localised sources may have added to the observed peak. Other sources of NO<sub>2</sub> concentrations are also observed at these sites in the polar plots (Figure 5-60 for Eco Park, Figure 5-61 for Three Rivers and Figure 5-62 for Sharpeville). This is also illustrated by the 99<sup>th</sup> percentile that indicates a notable fraction of unaccounted for concentrations.

Subsequently, fractional biases (i.e. using the 99<sup>th</sup> percentile simulated concentrations and the estimated background concentration) were calculated for the monitoring stations within the study area. The results are summarised in Figure 5-71. The fractional bias of the means and standard deviations for AJ Jacobs indicated an over-prediction of the simulated NO<sub>2</sub> concentrations. The fractional bias of the means and standard deviations for Leitrim and AJ Jacobs were within -0.67 to +0.67, clearly showing good model performance. The model's simulations are shown to within the acceptable model performance range (-2.0 to +2.0) at Three Rivers, Sharpeville, Eco Park and Zamdela.

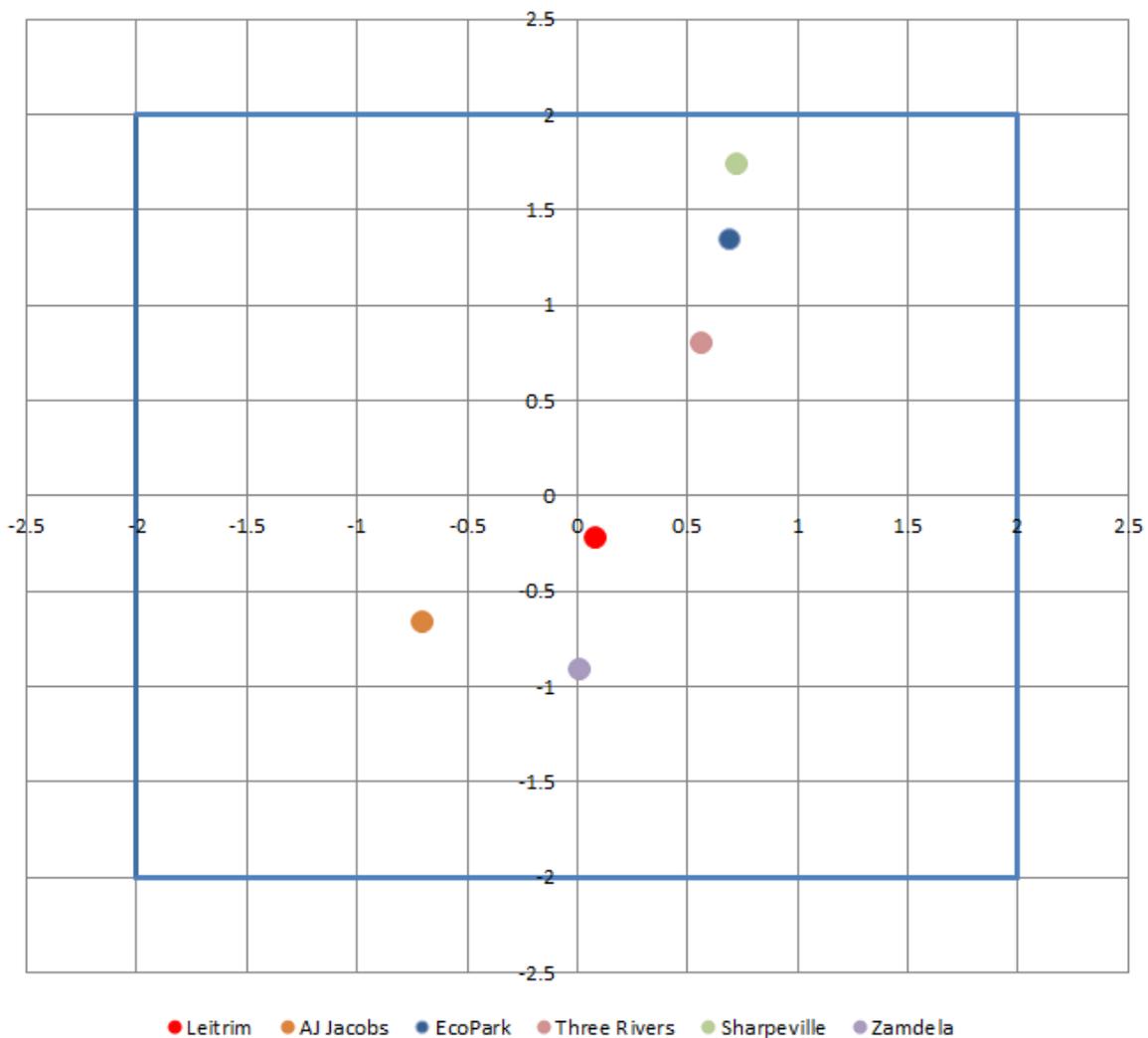


Figure 5-71: Fractional bias of means and standard deviation for NO<sub>2</sub>

### 5.1.7 Scenario Emission Inventory

Dispersion modelling included all Natref stack emission sources in all scenarios. The source parameters and emissions for Scenario 1 operations, as provided by Natref, is given in Table 5-19. The SO<sub>2</sub> emissions with and without SRU as well as the SRU availability per scenario are given in Table 5-20.

**Table 5-19: Source emissions for baseline conditions provided for Natref (units: g/s)**

Source name	Height of Release Above Ground (m)	Diameter at Stack Tip / Vent Exit (m)	Actual Gas Exit Temperature (°C)	Actual Gas Exit Velocity (m/s)	Emission rate (g/s)			
					SO <sub>2</sub>	NO <sub>x</sub> as NO <sub>2</sub>	Particulates	CO
Main Stack	145.0	5.5	267	16.96	286.11	46.39	30.56	32.94
B14001	26.5	1.37	373	4.89	0.13	0.28	0.04	0.32
B14002	24.56	0.99	264	3.57	0.13	0.05	0.03	0.43
B14005	62.0	1.87	205	5.86	2.08	0.70	0.24	0.00
B14006	27.42	1.60	276	2.63	0.58	0.27	0.09	0.09
B17004	20.02	0.91	307	4.84	0.53	0.14	0.05	4.0 x 10 <sup>-3</sup>
B25001	19.15	1.52	302	27.45	5.60	3.19	0.57	0.77

**Table 5-20: SO<sub>2</sub> emissions with and without SRU and the SRU availability per scenario for Natref**

Source name	SO <sub>2</sub> emissions <u>with</u> SRU (g/s)	SO <sub>2</sub> emissions <u>without</u> SRU (g/s)	SRU availability (annual percentage (%))
<b>Scenario 1</b>			
Main Stack	286.11	1 307.39	100
<b>Scenario 2 (At New Plant Emission Standards)</b>			
Main Stack	286.11	1 307.39	99
<b>Scenario 3</b>			
Main Stack	286.11	1 307.39	95

### 5.1.8 Model Results

Air quality standards are fundamental tools to assist in air quality management. The NAAQS (Section 5.1.2.2) are intended to reduce harmful effects on health of the majority of the population, including the very young and the elderly. In this section, predicted ambient concentrations of criteria pollutants at specific sensitive receptors are compared against the promulgated local NAAQS (Table 5-2).

Prior to dispersion modelling, 42 receptors were identified in the vicinity of Natref (within the 57-by-57 km modelling domain). Sensitive receptors included residential areas, schools, hospitals and clinics, monitoring stations (Figure 5-72 and Table 5-21). Ambient air quality monitoring stations (AQMS) were the first receptors identified because comparison of the predicted concentrations could be compared with measured concentrations for model validation. Schools, hospitals and clinics within the domain were identified and included as sensitive receptors in the dispersion model (full list provided in Appendix J). All receptors are presented in the isopleth plots, where the AQMS are included in results figures and the 20 closest receptors are included in the results tables at increasing distance from the centre of Natref.

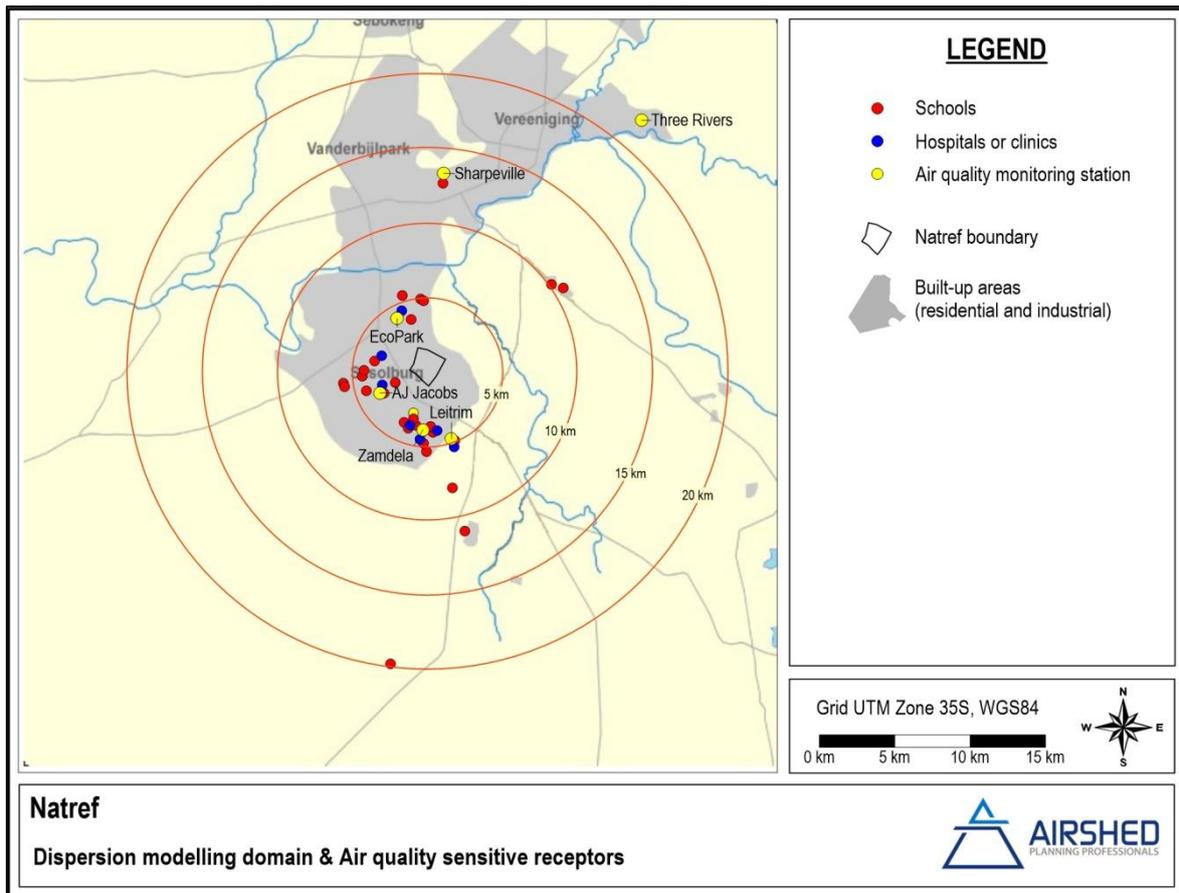


Figure 5-72: Sensitive receptors identified for assessment of impact as a result of Natref Operations

Table 5-21: Receptors identified for assessment of impact as a result of Natref emissions

Receptor code name <sup>(a)</sup>	Receptor details	Distance from centre of operations (km) <sup>(b)</sup>
Zamdela	VTAPA Zamdela monitoring station	4.2
Leitrim	Sasol Leitrim monitoring station	5.1
AJ Jacobs	Sasol AJ Jacobs monitoring station	3.5
EcoPark	Sasol EcoPark monitoring station	3.8
Sharpeville	VTAPA Sharpeville monitoring station	13.0
Three Rivers	VTAPA Three Rivers monitoring station	21.8
34	HTS Secondary School	2.3
43	Sasolburg Provincial Hospital	3.0
52	Sasolburg Clinic	3.2
24	Lumiere Primary School	3.3
14	AJ Jacobs Primary School	3.3
19	Fonteine Primary School	3.4
25	Malakabeng Primary School	3.6
15	Bofula-Tshepe Primary School	4.0
29	Tsatsi Primary School	4.0
32	Cedar Secondary School	4.0
51	Zamdela Hospital Zumayear	4.1
42	Vaalpark Hospital	4.1

Receptor code name <sup>(a)</sup>	Receptor details	Distance from centre of operations (km) <sup>(b)</sup>
38	Sasolburg High School	4.1
49	Clinic A Zamdela	4.2
33	Fakkel Secondary School	4.3
37	Nkopoleng Secondary School	4.3
36	Kahobotjha-sakubusha Secondary School	4.3
35	Iketsetseng Secondary School	4.3
48	Clinic B Zamdela	4.3
39	Vaalpark Articon Secondary School	4.4

Since the focus of the study is to illustrate the relative changes in ambient concentrations of pollutants theoretically arising from different point source emission scenarios, the predicted concentration differences from scenario to scenario were provided as percentage increase or decrease over the modelled Scenario 1 ( $C_{Scenario 1}$ ).

$$\frac{C_{S, scenario 2/3} - C_{S, scenario 1}}{C_{Scenario 1}}$$

Equation 1

#### 5.1.8.1 Criteria pollutants

The findings for each of the criteria pollutants (SO<sub>2</sub>, NO<sub>2</sub>, CO and PM) are presented for Natref in three forms. The first figure presents the predicted pollutant concentration (99<sup>th</sup> percentile) at the AQMS (Table 5-21) for each of the emission scenarios relative to the appropriate NAAQS. A table then presents the percentage change in ground-level concentrations between the emission scenarios and Scenario 1 at the AQMS and 20 closest sensitive receptors (Table 5-21). Finally, isopleth plots have been included for the all relevant emission scenarios and pollutants.

##### 5.1.8.1.1 Sulfur dioxide (SO<sub>2</sub>)

Ambient concentrations of SO<sub>2</sub> as a result of Natref scenarios are predicted to fall below the NAAQS at the AQMS (Figure 5-73 to Figure 5-75) and receptors (Table 5-22 to Table 5-24). An increase in ambient hourly SO<sub>2</sub> concentrations are evident from Scenario 1 to Scenario 2 and Scenario 3, by more than 100% (Table 5-22 to Table 5-24). Ambient hourly SO<sub>2</sub> concentrations are within NAAQS for all scenarios.

It should be noted that the results are provided at the 99<sup>th</sup> percentile for comparison to NAAQS. With the SRU availability for Scenario 2 and Scenario 3 being 99% and 95% respectively, the hourly SO<sub>2</sub> ground level concentrations for these two scenarios are the same, effectively representing impacts for when the SRU is not on. For Scenario 1 (100% SRU availability) the SO<sub>2</sub> hourly impacts reflect ground level concentrations for when the SRU is on.

Isopleth plots are presented for all averaging periods ground-level SO<sub>2</sub> concentrations as a result of all emission scenarios for Natref, as per the figure numbers below:

Scenario	Hourly	Daily	Annual
Scenario 1 (100% SRU availability)	Figure 5-76	Figure 5-79	Figure 5-82
Scenario 2 (99% SRU availability)	Figure 5-77	Figure 5-80	Figure 5-83
Scenario 3 (95% SRU availability)	Figure 5-78	Figure 5-81	Figure 5-84

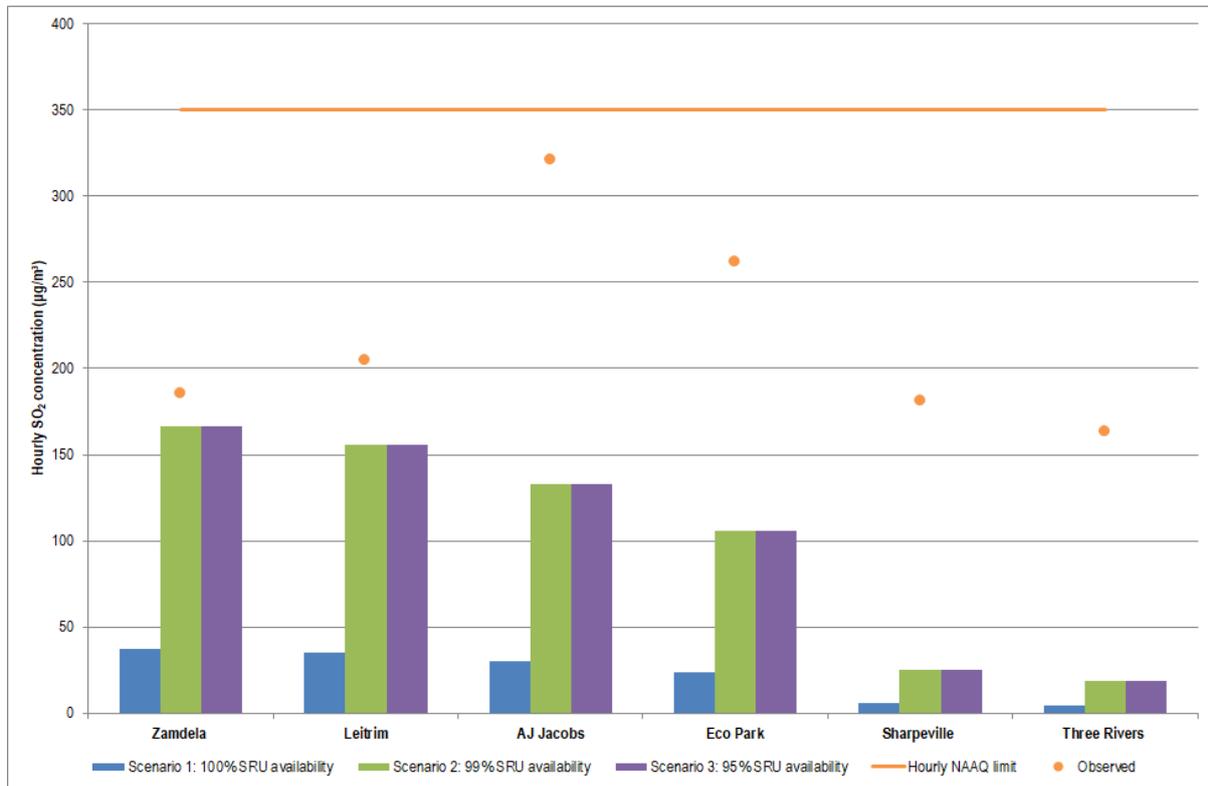


Figure 5-73: Simulated hourly SO<sub>2</sub> concentrations (99th percentile) at AQMS for Natref

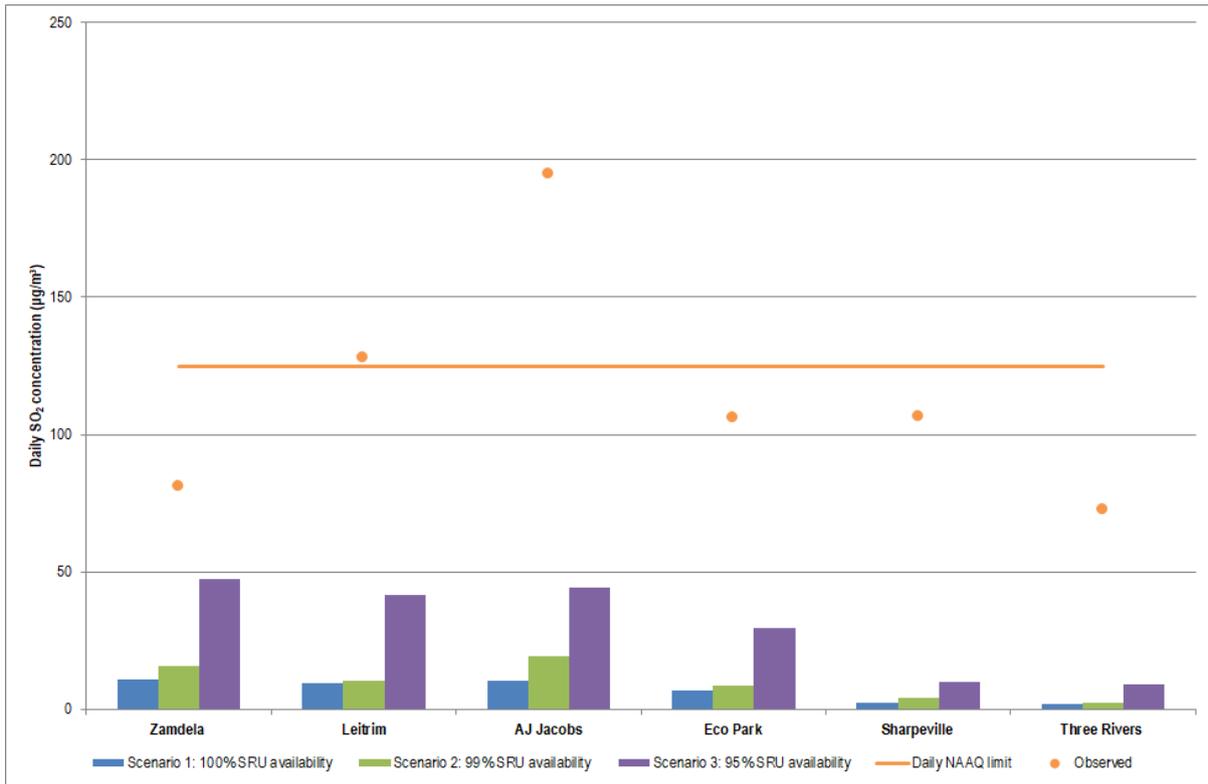


Figure 5-74: Simulated daily SO<sub>2</sub> concentrations (99th percentile) at AQMS for Natref

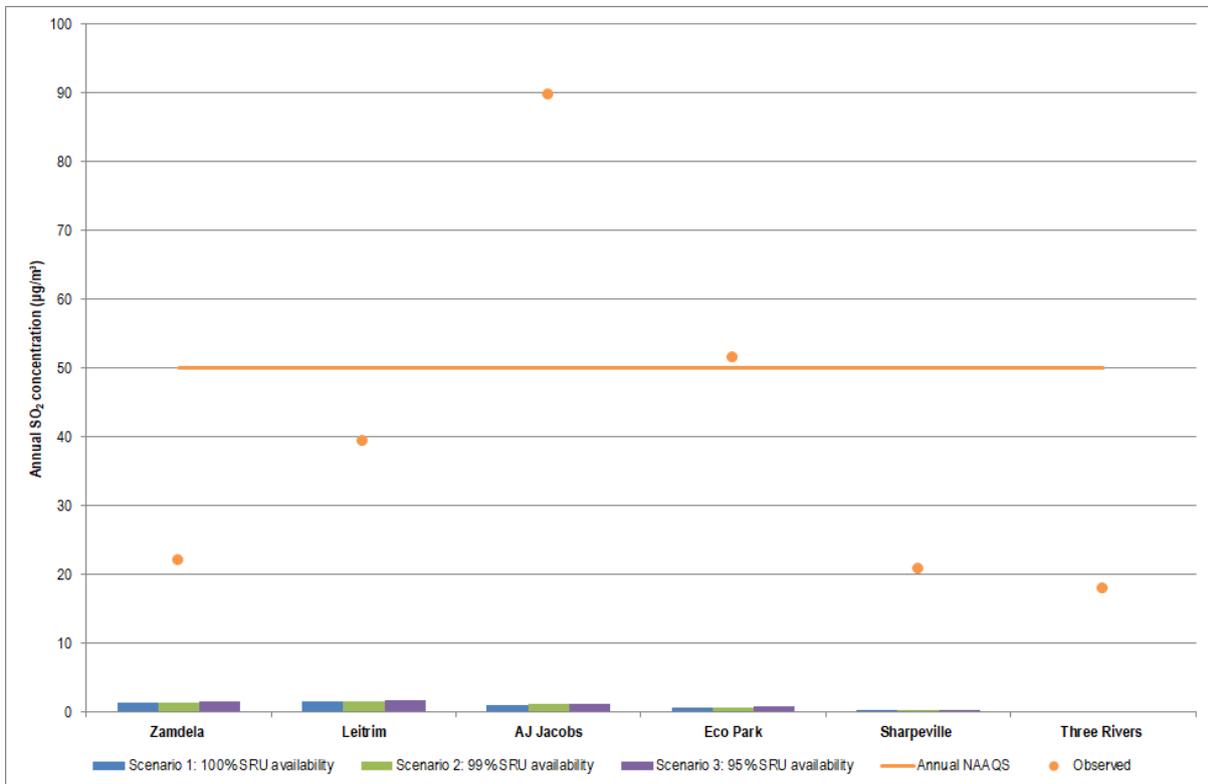


Figure 5-75: Simulated annual SO<sub>2</sub> concentrations at AQMS for Natref

**Table 5-22: Simulated baseline hourly SO<sub>2</sub> concentrations and the theoretical change in concentrations relative to Scenario 1 at the AQMs and 20 closest receptors**

Receptor	Hourly SO <sub>2</sub> (99 <sup>th</sup> percentile)				
	Scenario 1 (100% SRU availability)	Scenario 2 (99% SRU availability)		Scenario 3 (95% SRU availability)	
	Concentration (µg/m <sup>3</sup> )	Concentration (µg/m <sup>3</sup> )	Relative change	Concentration (µg/m <sup>3</sup> )	Relative change
Zamdela AQMS	35.4	158.5	347.5%	158.5	347.5%
Leitrim AQMS	34.3	153.2	346.9%	153.2	346.9%
AJ Jacobs AQMS	26.0	113.3	335.8%	113.3	335.8%
Eco Park AQMS	19.4	86.2	344.1%	86.2	344.1%
Sharpeville AQMS	5.1	22.7	343.8%	22.7	343.8%
Three Rivers AQMS	4.1	18.2	343.9%	18.2	343.9%
Malakabeng Primary School	35.3	155.6	341.4%	155.6	341.4%
Cedar Secondary School	39.6	176.1	345.3%	176.1	345.3%
Bofula- Tshepe Primary School	35.0	155.6	344.9%	155.6	344.9%
Clinic A Zamdela	36.1	160.8	345.9%	160.8	345.9%
Zamdela Hospital Zumayear	31.4	140.6	347.3%	140.6	347.3%
Iketsetseng Secondary School	35.0	155.6	344.9%	155.6	344.9%
Clinic B Zamdela	38.8	172.9	346.1%	172.9	346.1%
Tsatsi Primary School	30.3	134.5	344.6%	134.5	344.6%
Isaac Mhlabi Primary School	35.8	159.7	345.5%	159.7	345.5%
Nkopoleng Secondary School	29.2	131.0	348.4%	131.0	348.4%
HTS Secondary School	34.1	146.0	327.7%	146.0	327.7%
Szamdela Community Clinic	29.5	131.1	345.2%	131.1	345.2%
AJ Jacobs Primary School	25.8	114.6	345.0%	114.6	345.0%
Theha Setjhaba Primary School	29.3	131.5	348.7%	131.5	348.7%
Sasolburg Clinic	32.3	140.9	336.5%	140.9	336.5%
Credo Primary School	32.3	144.5	346.9%	144.5	346.9%
Lehutso Primary School	26.1	116.7	346.9%	116.7	346.9%
Harry Gwala Clinic   Creche	29.8	132.5	345.5%	132.5	345.5%
Kahobotjha-sakubusha Secondary School	26.3	113.9	333.6%	113.9	333.6%
Sasolburg Provincial Hospital	35.0	153.1	337.8%	153.1	337.8%

**Table 5-23: Simulated baseline daily SO<sub>2</sub> concentrations and the theoretical change in concentrations relative Scenario 1 at the AQMs and 20 closest receptors**

Receptor	Daily SO <sub>2</sub> (99 <sup>th</sup> percentile)				
	Scenario 1 (100% SRU availability)	Scenario 2 (99% SRU availability)		Scenario 3 (95% SRU availability)	
	Concentration (µg/m <sup>3</sup> )	Concentration (µg/m <sup>3</sup> )	Relative change	Concentration (µg/m <sup>3</sup> )	Relative change
Zamdela AQMS	10.5	15.8	49.8%	45.2	328.4%
Leitrim AQMS	9.3	10.6	14.4%	41.3	345.0%
AJ Jacobs AQMS	10.0	19.4	92.6%	43.1	329.3%
Eco Park AQMS	6.4	8.9	37.8%	28.4	341.5%
Sharpeville AQMS	2.2	4.2	94.7%	9.4	333.7%
Three Rivers AQMS	1.7	2.6	57.7%	7.5	354.8%
Malakabeng Primary School	9.9	19.2	93.1%	42.8	330.8%
Cedar Secondary School	11.2	17.4	55.5%	47.4	324.0%
Bofula- Tshepe Primary School	10.4	15.7	50.0%	44.8	328.8%
Clinic A Zamdela	10.7	16.3	51.6%	46.6	334.4%
Zamdela Hospital Zumayear	8.4	17.5	108.2%	36.7	336.5%
Iketsetseng Secondary School	10.4	15.7	50.0%	44.8	328.8%
Clinic B Zamdela	9.9	15.0	51.7%	44.2	345.4%
Tsatsi Primary School	7.9	15.2	92.5%	35.4	348.1%
Isaac Mhlabi Primary School	10.4	16.0	53.4%	45.4	336.6%
Nkopoleng Secondary School	7.9	16.3	106.0%	33.9	327.2%
HTS Secondary School	12.3	24.1	96.6%	49.1	300.0%
Szamdela Community Clinic	8.5	12.2	43.8%	37.2	337.1%
AJ Jacobs Primary School	10.0	19.0	90.5%	42.1	323.1%
Theha Setjhaba Primary School	8.4	13.1	56.1%	36.5	333.2%
Sasolburg Clinic	10.8	17.2	59.3%	44.3	309.6%
Credo Primary School	8.6	10.5	21.8%	38.6	346.8%
Lehutso Primary School	7.2	12.0	66.8%	31.3	335.5%
Harry Gwala Clinic   Creche	7.7	10.8	40.8%	34.5	349.2%
Kahobotjha-sakubusha Secondary School	9.0	13.7	51.4%	39.4	336.8%
Sasolburg Provincial Hospital	12.3	18.0	45.9%	54.2	339.6%

**Table 5-24: Simulated baseline annual SO<sub>2</sub> concentrations and the theoretical change in concentrations relative to Scenario 1 at the AQMs and 20 closest receptors**

Receptor	Annual SO <sub>2</sub>				
	Scenario 1 (100% SRU availability)	Scenario 2 (99% SRU availability)		Scenario 3 (95% SRU availability)	
	Concentration (µg/m <sup>3</sup> )	Concentration (µg/m <sup>3</sup> )	Relative change	Concentration (µg/m <sup>3</sup> )	Relative change
Zamdela AQMS	1.3	1.4	3.1%	1.6	15.4%
Leitrim AQMS	1.5	1.5	3.2%	1.7	16.2%
AJ Jacobs AQMS	1.0	1.0	2.8%	1.1	14.0%
Eco Park AQMS	0.6	0.6	3.2%	0.7	16.2%
Sharpeville AQMS	0.2	0.2	3.1%	0.2	15.3%
Three Rivers AQMS	0.2	0.2	3.3%	0.2	16.3%
Malakabeng Primary School	1.3	1.4	2.9%	1.5	14.4%
Cedar Secondary School	1.6	1.6	3.1%	1.8	15.6%
Bofula- Tshepe Primary School	1.3	1.4	3.1%	1.5	15.3%
Clinic A Zamdela	1.4	1.4	3.1%	1.6	15.3%
Zamdela Hospital Zumayear	1.2	1.2	2.9%	1.3	14.6%
Iketsetseng Secondary School	1.3	1.4	3.1%	1.5	15.3%
Clinic B Zamdela	1.6	1.6	3.2%	1.8	15.8%
Tsatsi Primary School	1.1	1.1	2.9%	1.2	14.5%
Isaac Mhlabi Primary School	1.5	1.5	3.1%	1.7	15.7%
Nkopoleng Secondary School	1.1	1.1	3.0%	1.2	14.8%
HTS Secondary School	1.4	1.4	2.4%	1.6	12.1%
Szamdela Community Clinic	1.1	1.2	3.1%	1.3	15.4%
AJ Jacobs Primary School	1.0	1.0	2.8%	1.1	13.8%
Theha Setjhaba Primary School	1.1	1.2	3.1%	1.3	15.4%
Sasolburg Clinic	1.1	1.2	2.7%	1.3	13.6%
Credo Primary School	1.4	1.4	3.2%	1.6	16.2%
Lehutso Primary School	1.1	1.1	3.1%	1.2	15.3%
Harry Gwala Clinic   Creche	1.3	1.3	3.2%	1.5	16.1%
Kahobotjha-sakubusha Secondary School	0.9	0.9	2.9%	1.0	14.7%
Sasolburg Provincial Hospital	1.1	1.1	3.0%	1.3	15.2%

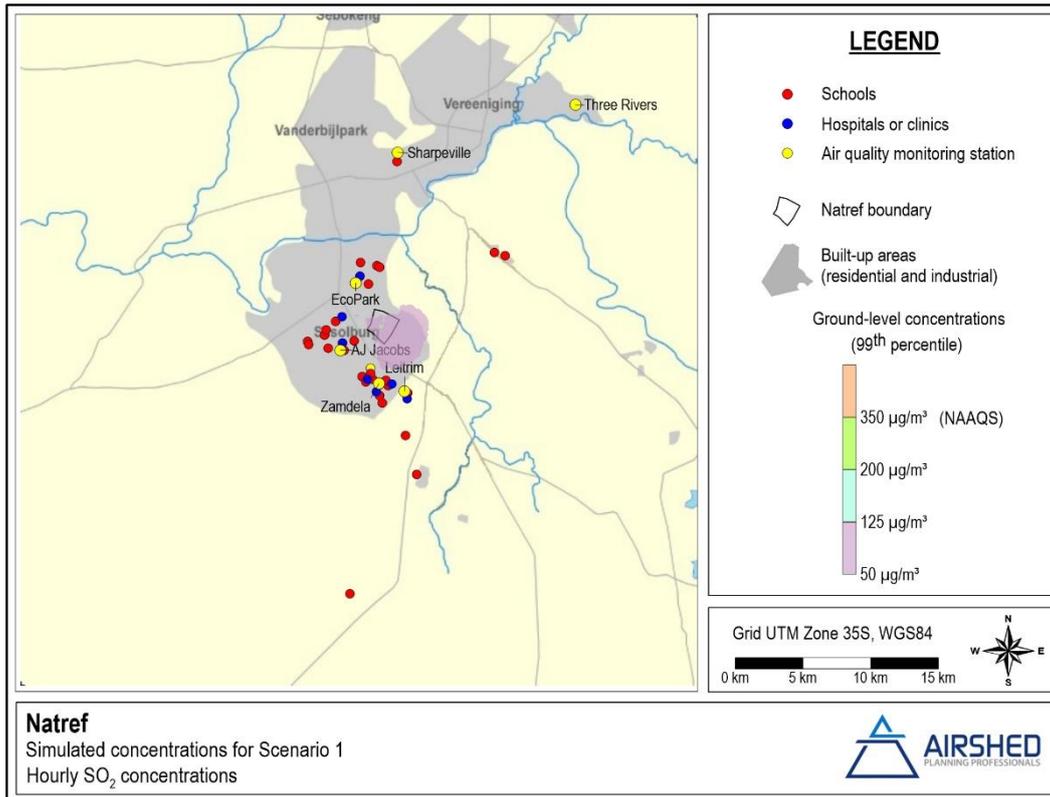


Figure 5-76: Simulated hourly SO<sub>2</sub> concentrations (99<sup>th</sup> percentile) as a result of Scenario 1 (100% SRU availability)

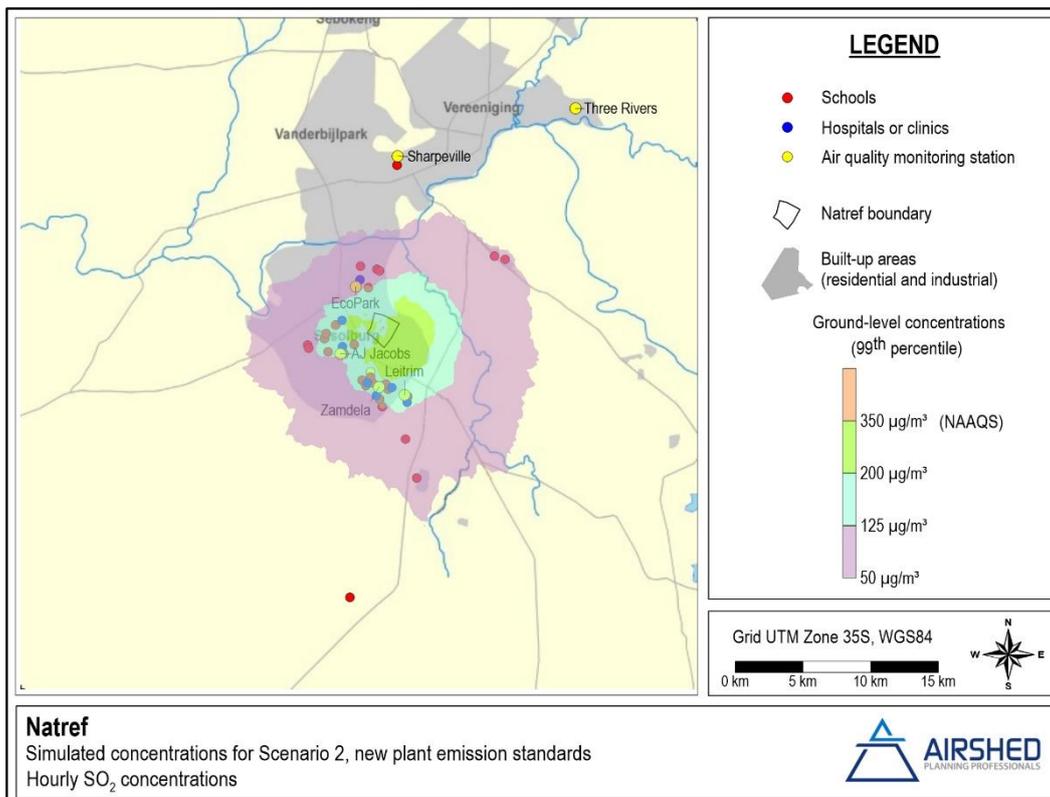


Figure 5-77: Simulated hourly SO<sub>2</sub> concentrations (99<sup>th</sup> percentile) as a result of theoretical compliance with new plant emission standards, Scenario 2 (99% SRU availability)

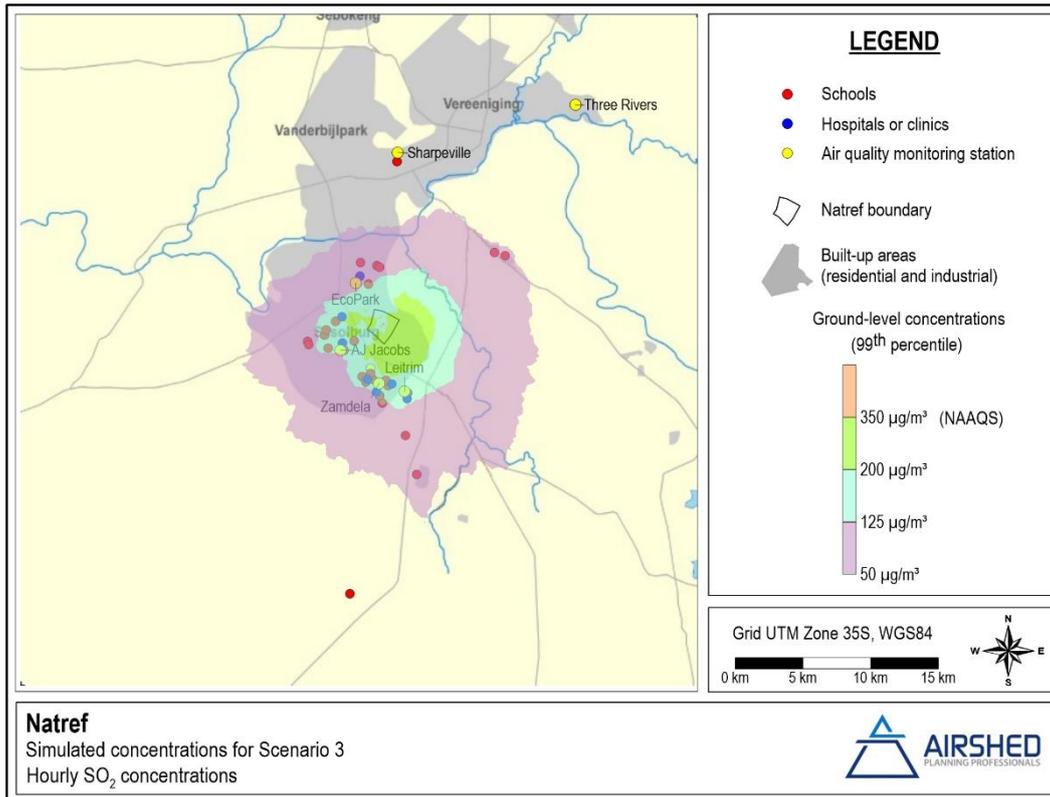


Figure 5-78: Simulated hourly SO<sub>2</sub> concentrations (99<sup>th</sup> percentile) as a result of Scenario 3 (95% SRU availability)

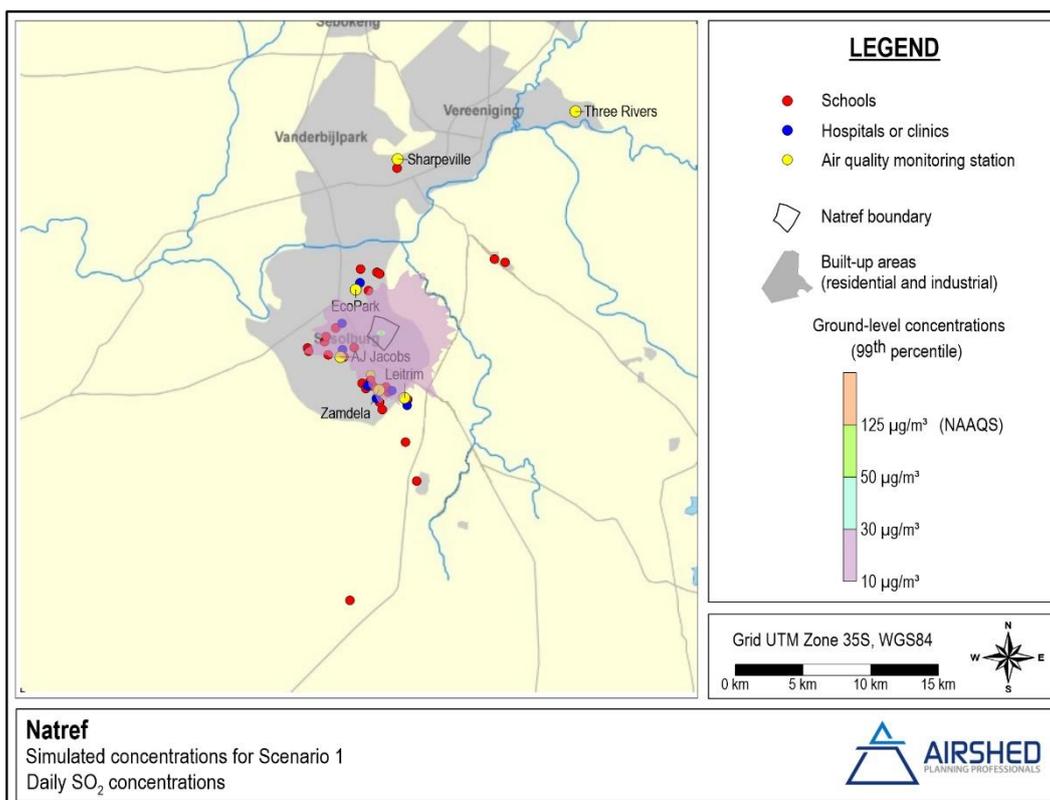


Figure 5-79: Simulated daily SO<sub>2</sub> concentrations (99<sup>th</sup> percentile) as a result of Scenario 1 (100% SRU availability)

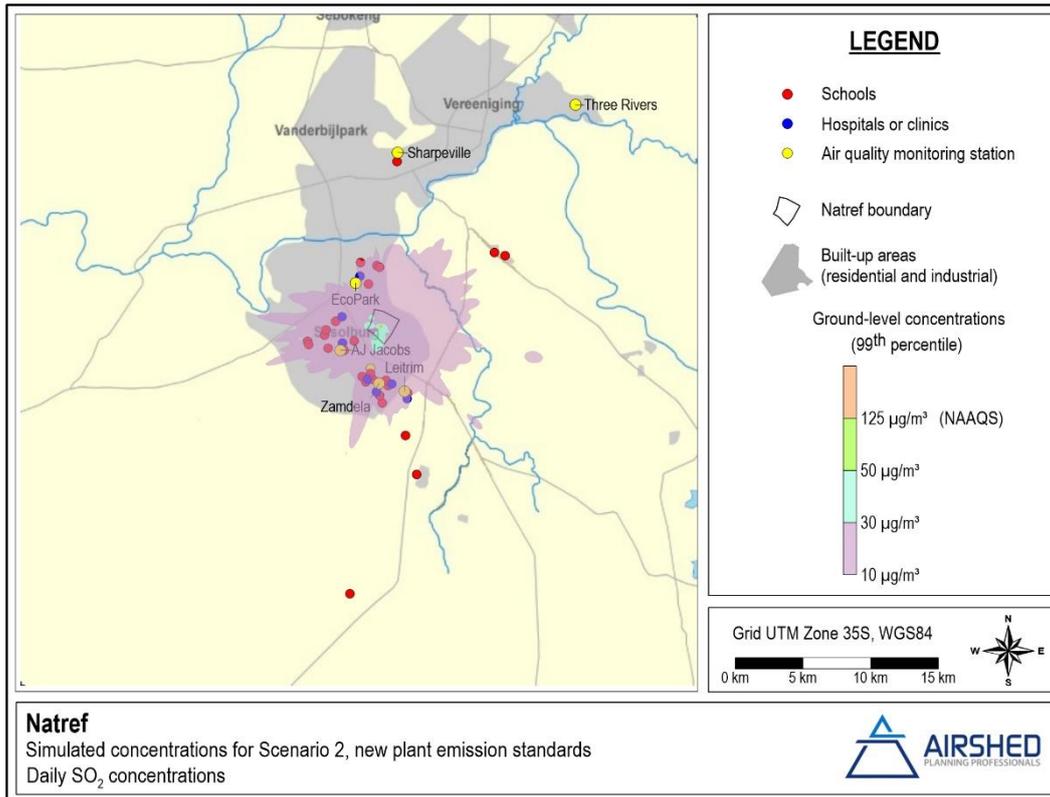


Figure 5-80: Simulated daily SO<sub>2</sub> concentrations (99<sup>th</sup> percentile) as a result of theoretical compliance with new plant emission standards, Scenario 2 (99% SRU availability)

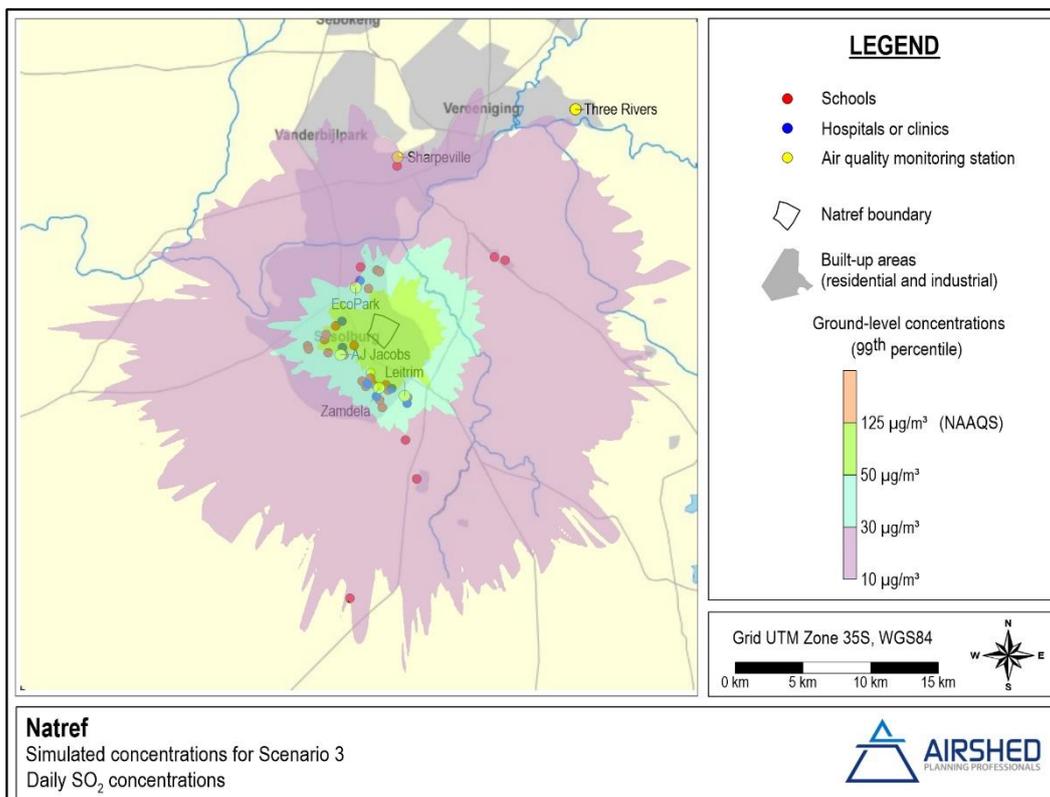


Figure 5-81: Simulated daily SO<sub>2</sub> concentrations (99<sup>th</sup> percentile) as a result of Scenario 3 (95% SRU availability)

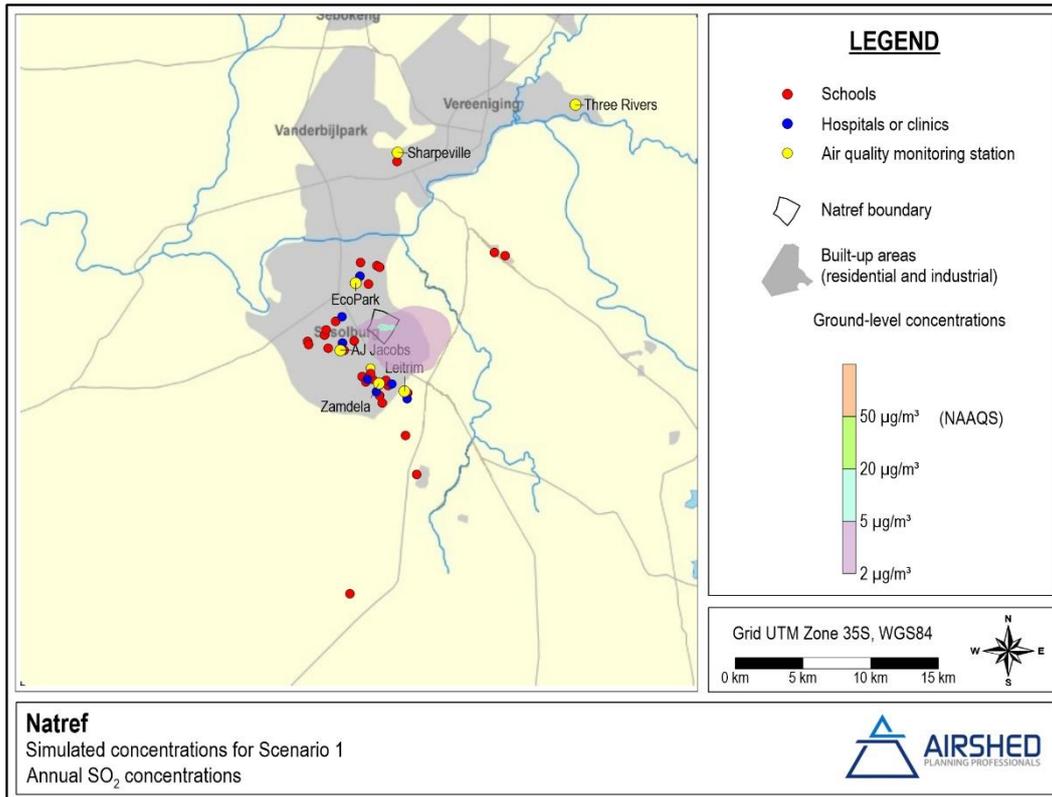


Figure 5-82: Simulated annual SO<sub>2</sub> concentrations as a result of Scenario 1 (100% SRU availability)

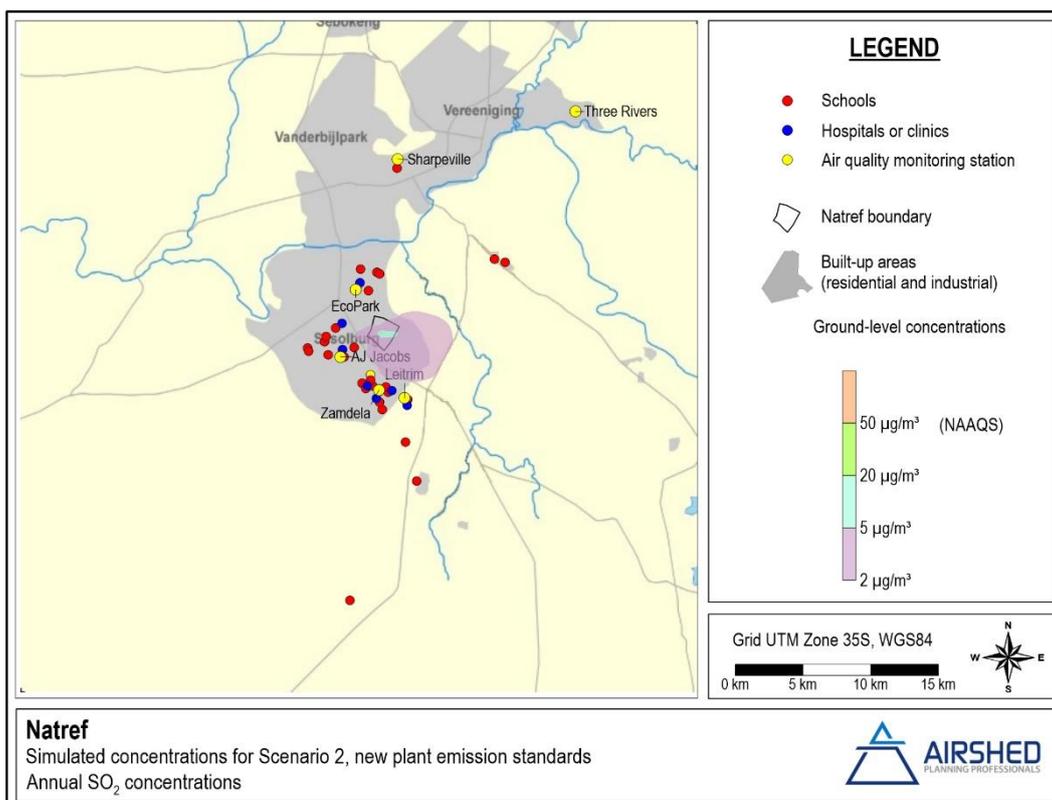


Figure 5-83: Simulated annual SO<sub>2</sub> concentrations as a result of theoretical compliance with new plant emission standards, Scenario 2 (99% SRU availability)

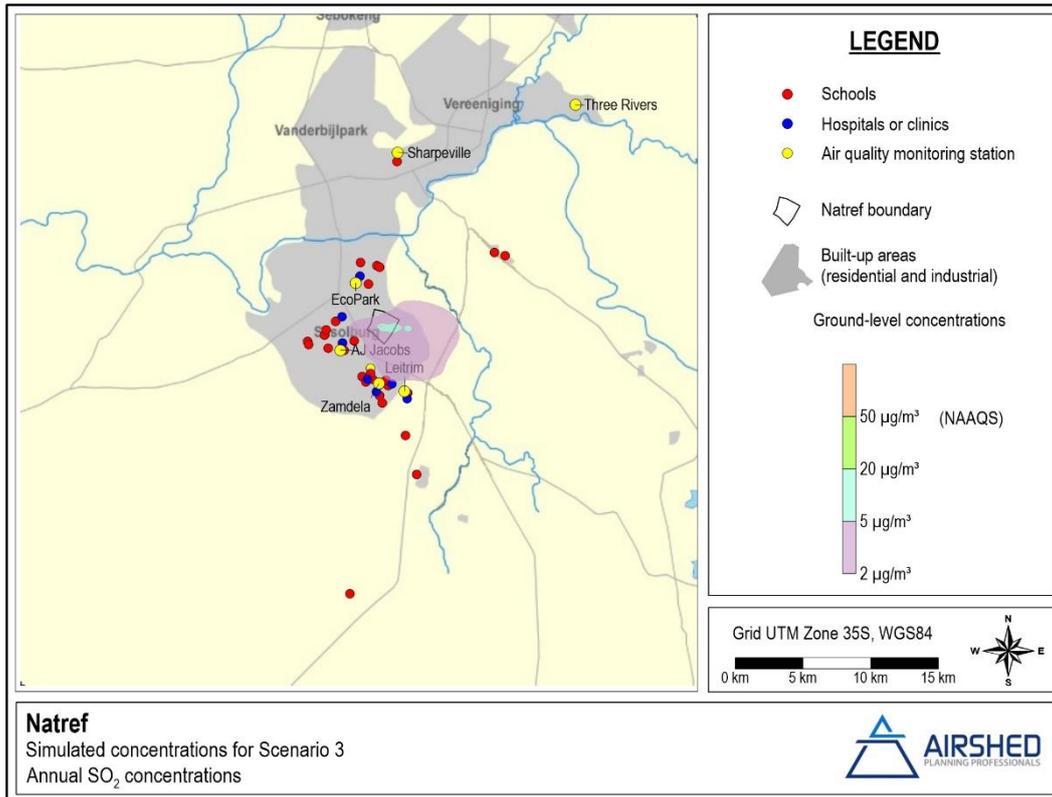


Figure 5-84: Simulated annual SO<sub>2</sub> concentrations as a result of Scenario 3 (95% SRU availability)

5.1.8.1.2 Nitrogen dioxide (NO<sub>2</sub>)

Emission rates for NO<sub>2</sub> does not differ for the three scenarios. Only simulated baseline conditions were therefore provided in this section (Figure 5-85 and Figure 5-86). The ambient NO<sub>2</sub> concentrations due to baseline conditions Natref operations is within hourly and annual NAAQS (Figure 5-87 and Figure 5-88).

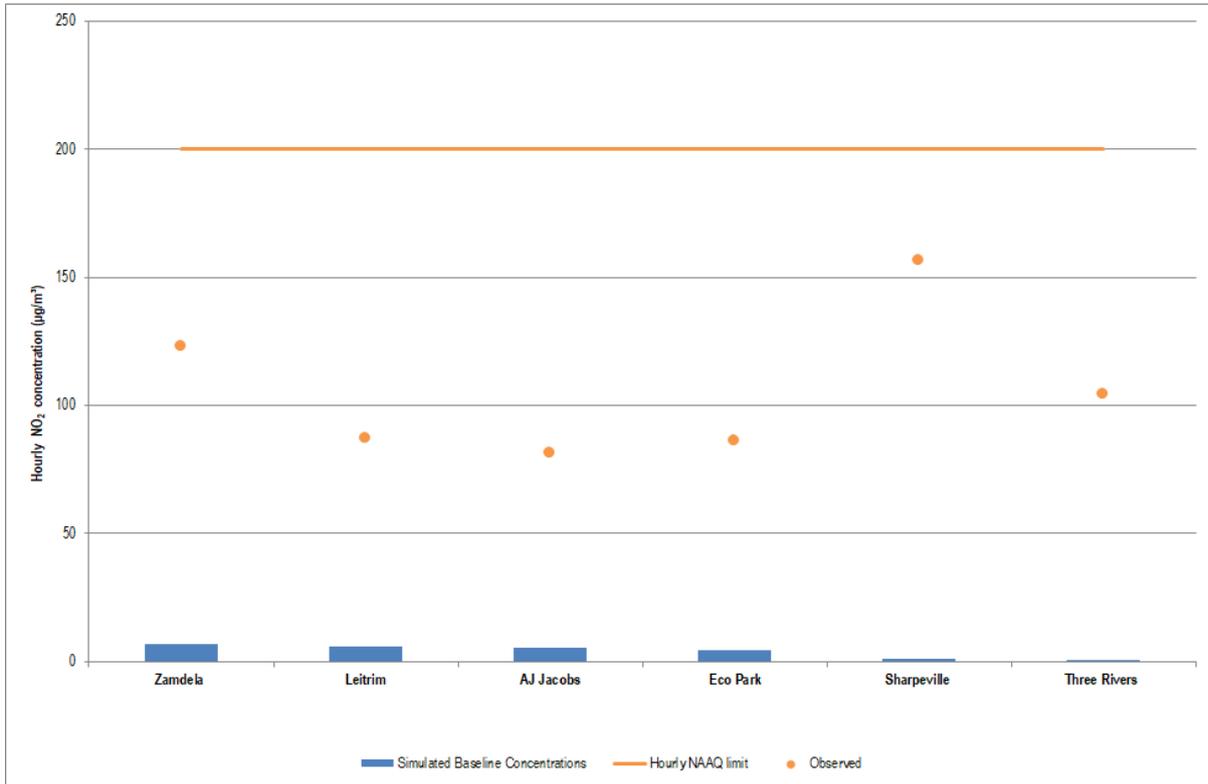


Figure 5-85: Simulated hourly NO<sub>2</sub> concentrations at AQMS for Natref

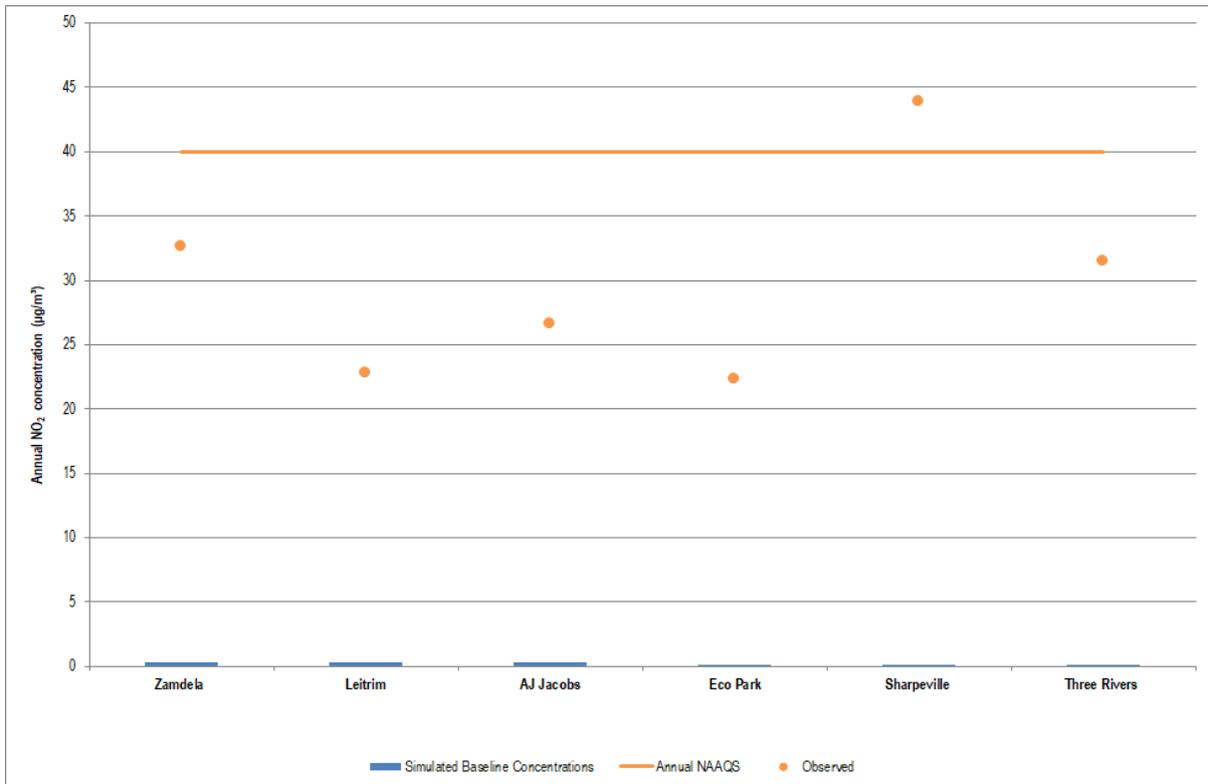


Figure 5-86: Simulated annual NO<sub>2</sub> concentrations at AQMS for Natref

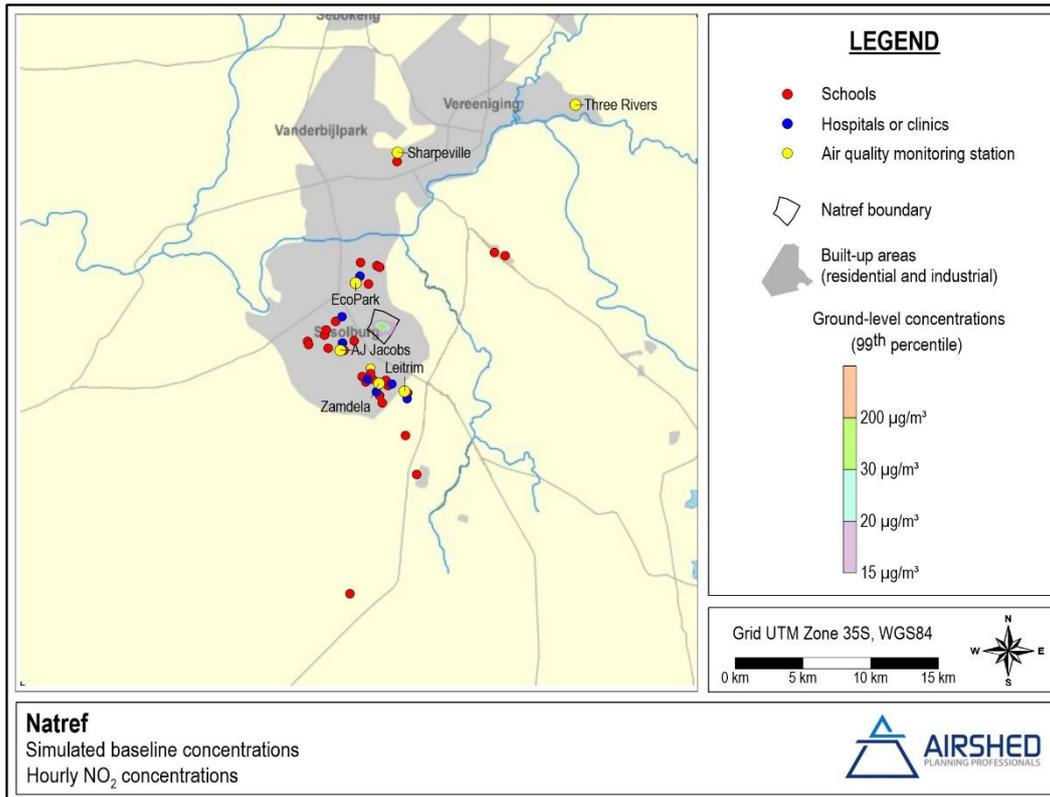


Figure 5-87: Simulated hourly NO<sub>2</sub> concentrations (99<sup>th</sup> percentile) as a result of baseline emissions

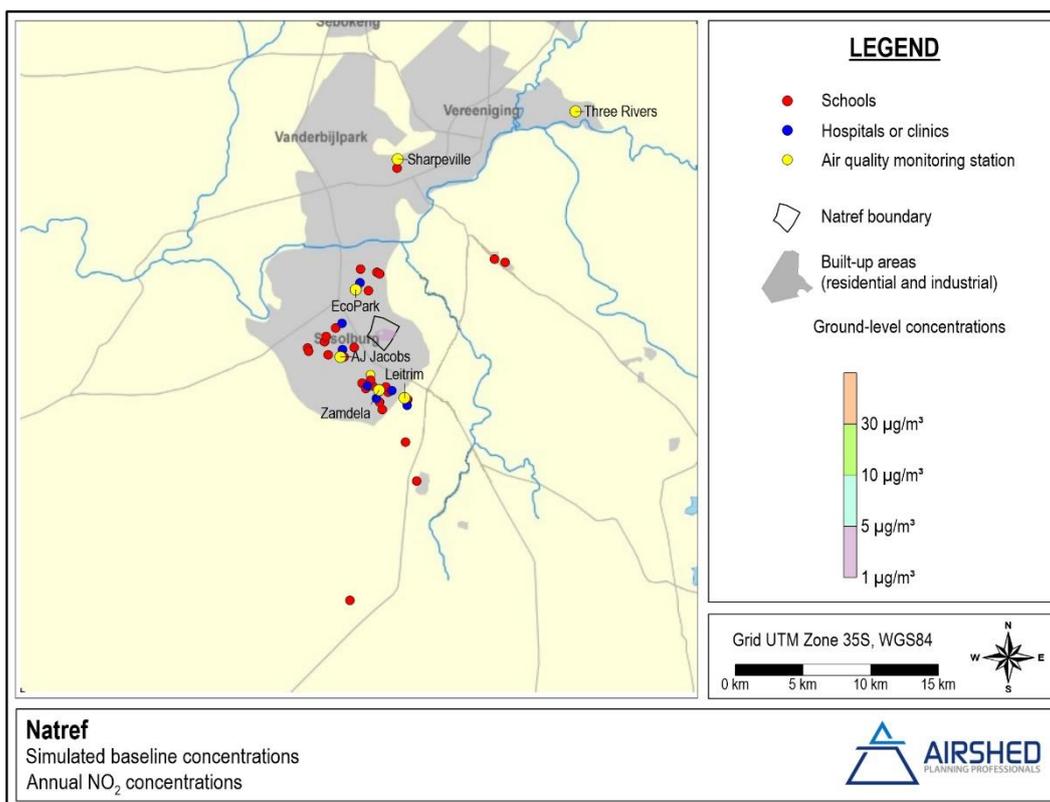


Figure 5-88: Simulated annual NO<sub>2</sub> concentrations as a result of baseline emissions

### 5.1.8.1.3 Particulate Matter (PM<sub>10</sub> and PM<sub>2.5</sub>)

Although the PM emissions from Natref do not change for the three scenario's, the contribution of sulphates (secondary particulates) differ (due to the SRU availability). The impacts for Scenario 1 result in low ground-level concentrations of PM; less than 2 µg/m<sup>3</sup> at all AQMS (Figure 5-89). Simulated annual PM concentrations are less than 0.25 µg/m<sup>3</sup> at all AQMS (Figure 5-90). Scenario 2 results in an increase of daily ground-level PM concentrations by up to 114%, while Scenario 3 result in an increase in daily ground-level PM concentrations by more than 400% (Table 5-25 and Table 5-26).

For particulate matter, NAAQS are available for PM<sub>10</sub> and PM<sub>2.5</sub>. Ambient air quality impacts for both particulate fractions (i.e. PM<sub>10</sub> and PM<sub>2.5</sub>) thus need to be considered. Simulated concentrations of particulate matter (PM) are conservatively assumed to be PM<sub>2.5</sub> since it is not possible to establish the PM<sub>2.5</sub>/PM<sub>10</sub> split of emissions from Natref only. Figure 5-89 and Figure 5-90 present predicted PM concentrations at the AQMS relative to both the PM<sub>10</sub> and PM<sub>2.5</sub> NAAQS.

PM<sub>10</sub> and PM<sub>2.5</sub> measurements at the AQMS suggest a 50% contribution of PM<sub>2.5</sub> to PM<sub>10</sub>; however, the sources contributing to the PM signature at the AQMS are varied, including the Natref sources, other industrial sources, windblown particulates, vehicles, domestic fuel burning, mining, agriculture, and power generation. The range of the 2015 – 2017 PM<sub>2.5</sub>:PM<sub>10</sub> ratios at the AQMS in the Sasolburg domain ranged between 0.31 and 0.59 (Section 5.1.5.4); while the urban population-weighted average across South Africa in 2000 - reported by Norman *et al.* (2007) - was 0.57. A study in the Vaal Triangle used the PM<sub>2.5</sub>:PM<sub>10</sub> ratio of 0.59 based on the concentrated industrial activity in the area (Witi, 2005). This value (0.59) is slightly more conservative than the measured ambient data and the population-weighted country average.

Based on the conservative assumption that all PM is in the PM<sub>2.5</sub> fraction, the simulated daily PM<sub>2.5</sub> concentrations comply with the current daily (40 µg/m<sup>3</sup>) and annual (20 µg/m<sup>3</sup>) PM<sub>2.5</sub> NAAQS, for all scenarios (Table 5-25 and Table 5-26).

Isopleth plots are presented for all averaging periods ground-level PM concentrations as a result of all scenarios for Natref, as per the figure numbers below:

<b>Scenario</b>	<b>Daily</b>	<b>Annual</b>
Scenario 1 (100% SRU availability)	Figure 5-92	Figure 5-95
Scenario 2 (99% SRU availability)	Figure 5-93	Figure 5-96
Scenario 3 (95% SRU availability)	Figure 5-94	Figure 5-97

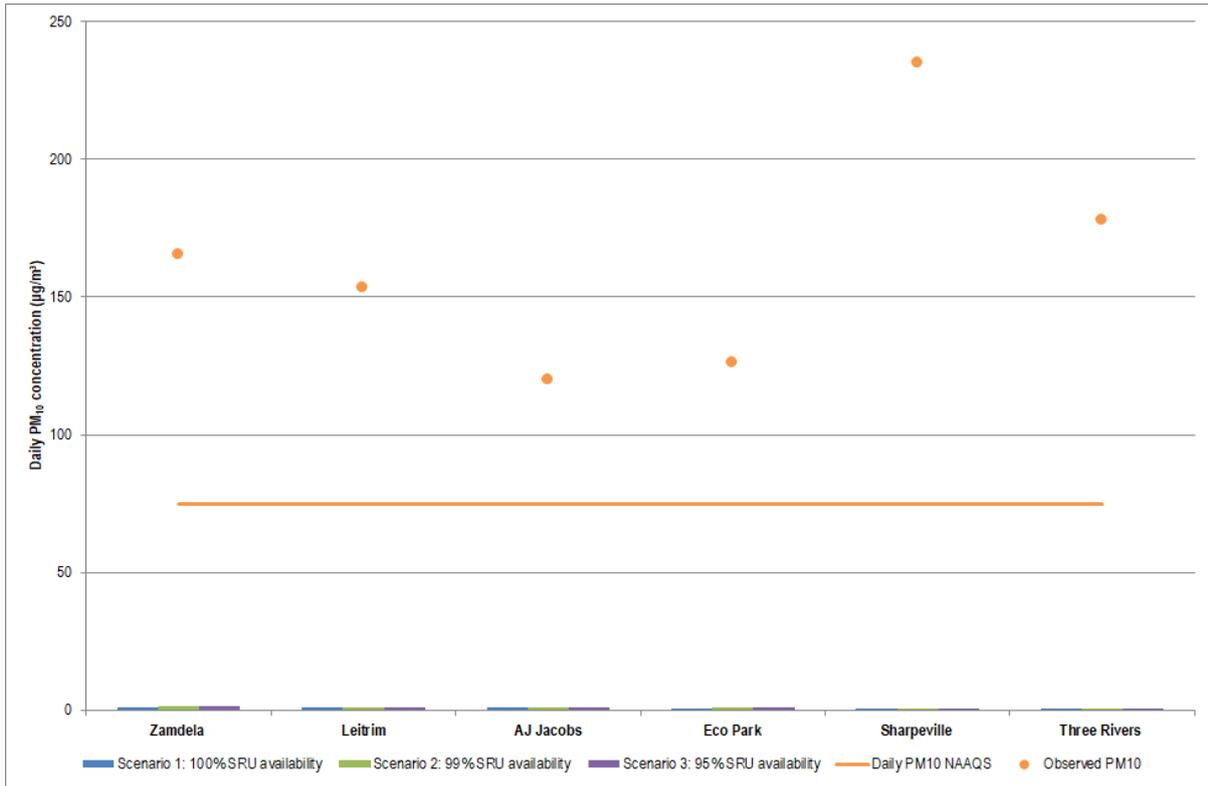


Figure 5-89: Simulated daily PM concentrations (99<sup>th</sup> percentile) at AQMS for Natref Operations with observed ambient levels

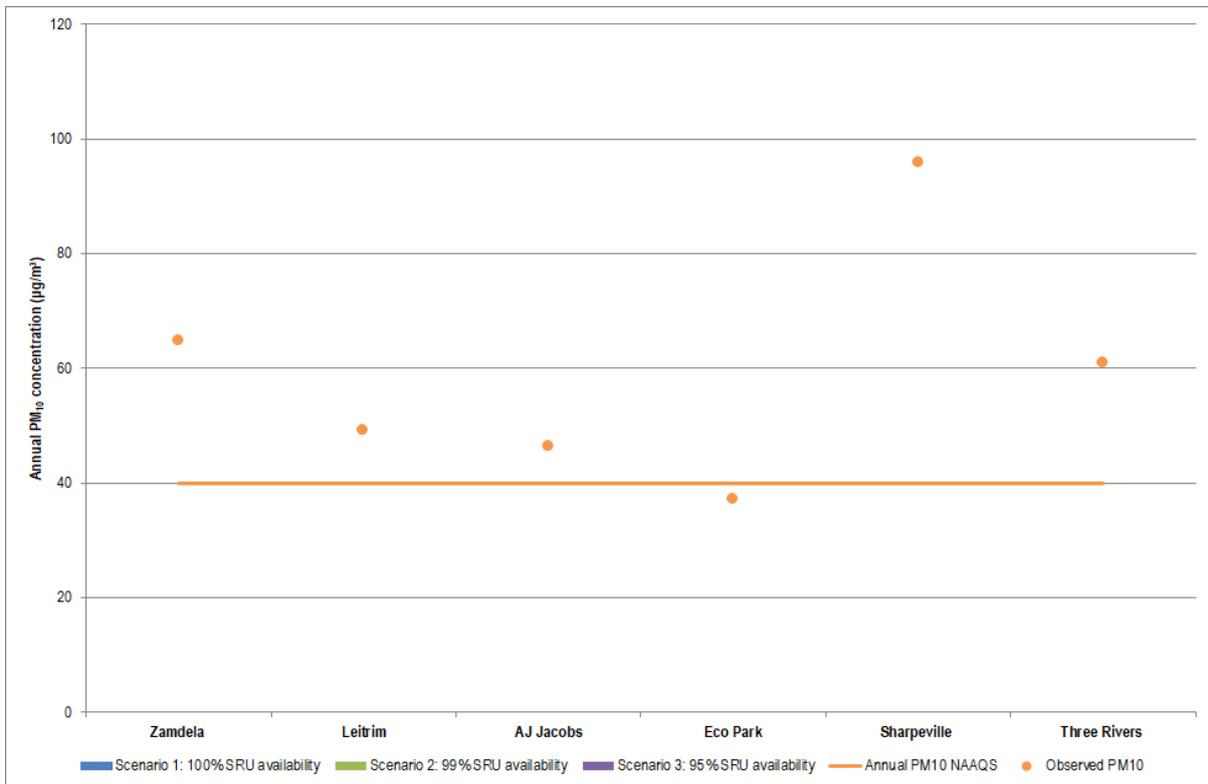


Figure 5-90: Simulated annual PM concentrations at AQMS for Natref Operations with observed ambient levels

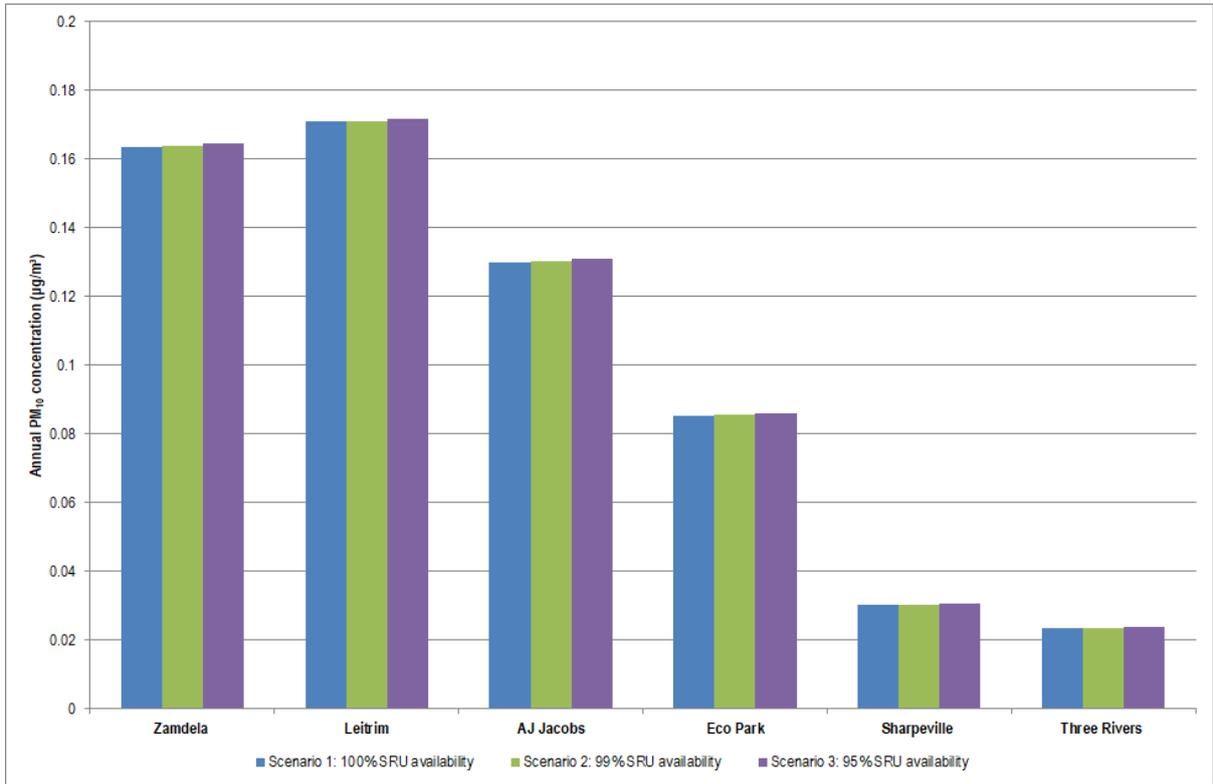


Figure 5-91: Simulated annual PM concentrations at AQMS for Natref Operations

**Table 5-25: Simulated baseline daily PM concentrations and the theoretical change in concentrations relative to the baseline at the AQMs and 20 closest receptors**

Receptor (a)	Daily PM (99th percentile)				
	Scenario 1 (100% SRU availability)	Scenario 2 (99% SRU availability)		Scenario 3 (95% SRU availability)	
	Concentration (µg/m³)	Concentration (µg/m³)	Relative change	Concentration (µg/m³)	Relative change
Zamdela AQMS	1.1	1.2	8.8%	1.2	8.8%
Leitrim AQMS	1.0	1.1	8.0%	1.1	8.0%
AJ Jacobs AQMS	1.1	1.2	11.7%	1.2	11.7%
Eco Park AQMS	0.7	0.9	26.3%	0.9	26.3%
Sharpeville AQMS	0.3	0.4	33.6%	0.4	33.6%
Three Rivers AQMS	0.2	0.3	34.7%	0.3	34.7%
Malakabeng Primary School	1.1	1.2	11.4%	1.2	11.4%
Cedar Secondary School	1.2	1.3	8.9%	1.3	8.9%
Bofula- Tshepe Primary School	1.1	1.2	5.2%	1.2	5.2%
Clinic A Zamdela	1.2	1.3	5.7%	1.3	5.7%
Zamdela Hospital Zumayear	1.0	1.1	19.4%	1.1	19.4%
Iketsetseng Secondary School	1.1	1.2	5.2%	1.2	5.2%
Clinic B Zamdela	1.1	1.3	15.3%	1.3	15.3%
Tsatsi Primary School	0.9	1.0	17.7%	1.0	17.7%
Isaac Mhambi Primary School	1.1	1.2	8.5%	1.2	8.5%
Nkopoleng Secondary School	0.9	1.0	17.4%	1.0	17.4%
HTS Secondary School	1.3	1.5	12.0%	1.5	12.0%
Szamdela Community Clinic	0.9	1.1	13.8%	1.1	13.8%
AJ Jacobs Primary School	1.1	1.2	6.1%	1.2	6.1%
Theha Setjhaba Primary School	0.9	1.0	11.6%	1.0	11.6%
Sasolburg Clinic	1.3	1.4	10.0%	1.4	10.0%
Credo Primary School	1.0	1.0	7.4%	1.0	7.4%
Lehutso Primary School	0.8	0.9	15.6%	0.9	15.6%
Harry Gwala Clinic   Creche	0.9	1.0	10.8%	1.0	10.8%
Kahobotjha-sakubusha Secondary School	1.0	1.2	20.0%	1.2	20.0%
Sasolburg Provincial Hospital	1.3	1.3	0.2%	1.3	0.2%
<b>Note:</b>					
(a) Conservatively assumes all PM is either PM <sub>10</sub> or PM <sub>2.5</sub> .					

**Table 5-26: Simulated baseline annual PM concentrations and the theoretical change in concentrations relative to the baseline at the AQMs and 20 closest receptors**

Receptor (a)	Annual PM				
	Scenario 1 (100% SRU availability)	Scenario 2 (99% SRU availability)		Scenario 3 (95% SRU availability)	
	Concentration (µg/m³)	Concentration (µg/m³)	Relative change	Concentration (µg/m³)	Relative change
Zamdela AQMS	0.2	0.2	0.1%	0.2	0.6%
Leitrim AQMS	0.2	0.2	0.1%	0.2	0.5%
AJ Jacobs AQMS	0.1	0.1	0.1%	0.1	0.7%
Eco Park AQMS	0.1	0.1	0.2%	0.1	1.0%
Sharpeville AQMS	0.0	0.0	0.3%	0.0	1.5%
Three Rivers AQMS	0.0	0.0	0.4%	0.0	1.8%
Malakabeng Primary School	0.2	0.2	0.1%	0.2	0.5%
Cedar Secondary School	0.2	0.2	0.1%	0.2	0.5%
Bofula- Tshepe Primary School	0.2	0.2	0.1%	0.2	0.6%
Clinic A Zamdela	0.2	0.2	0.1%	0.2	0.5%
Zamdela Hospital Zumayear	0.1	0.1	0.1%	0.1	0.6%
Iketsetseng Secondary School	0.2	0.2	0.1%	0.2	0.6%
Clinic B Zamdela	0.2	0.2	0.1%	0.2	0.5%
Tsatsi Primary School	0.1	0.1	0.1%	0.1	0.6%
Isaac Mhiambi Primary School	0.2	0.2	0.1%	0.2	0.5%
Nkopoleng Secondary School	0.1	0.1	0.1%	0.1	0.6%
HTS Secondary School	0.2	0.2	0.1%	0.2	0.5%
Szamdela Community Clinic	0.1	0.1	0.1%	0.1	0.6%
AJ Jacobs Primary School	0.1	0.1	0.1%	0.1	0.6%
Theha Setjhaba Primary School	0.1	0.1	0.1%	0.1	0.6%
Sasolburg Clinic	0.1	0.1	0.1%	0.1	0.6%
Credo Primary School	0.2	0.2	0.1%	0.2	0.6%
Lehutso Primary School	0.1	0.1	0.1%	0.1	0.7%
Harry Gwala Clinic   Creche	0.1	0.1	0.1%	0.1	0.6%
Kahobotjha-sakubusha Secondary School	0.1	0.1	0.2%	0.1	0.8%
Sasolburg Provincial Hospital	0.1	0.1	0.1%	0.1	0.6%
<b>Note:</b>					
(a) Conservatively assumes all PM is either PM <sub>10</sub> or PM <sub>2.5</sub> .					

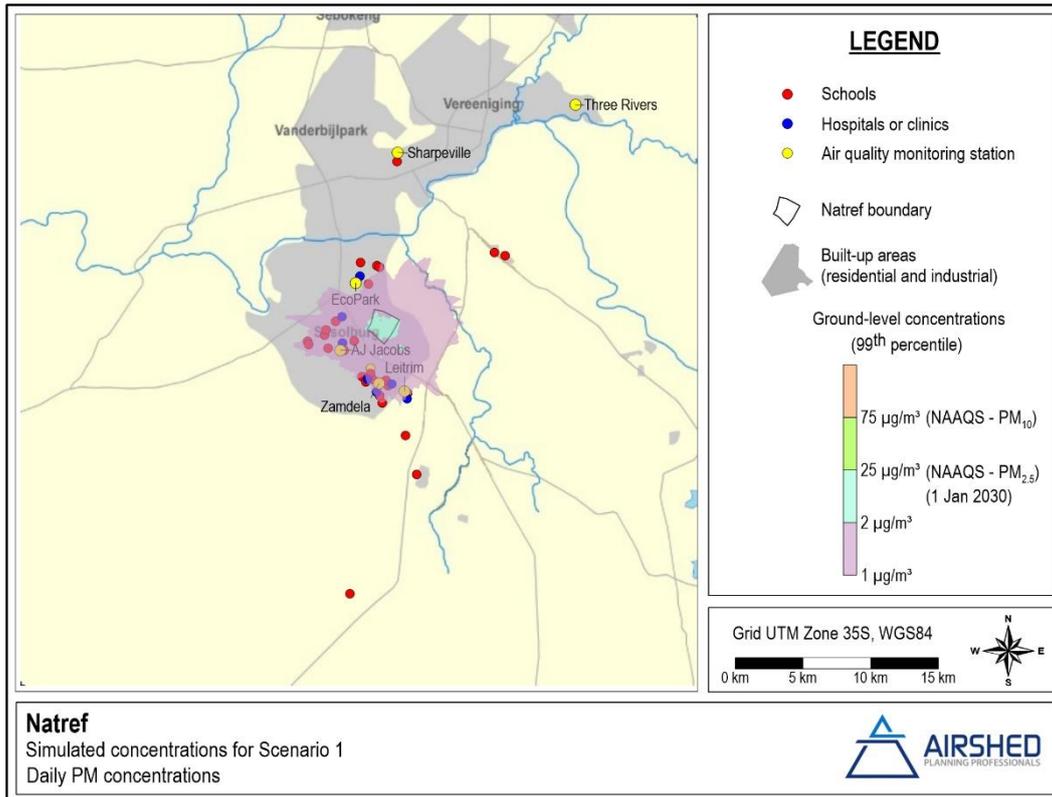


Figure 5-92: Simulated daily PM concentrations (99<sup>th</sup> percentile) for Scenario 1 (100% SRU availability)

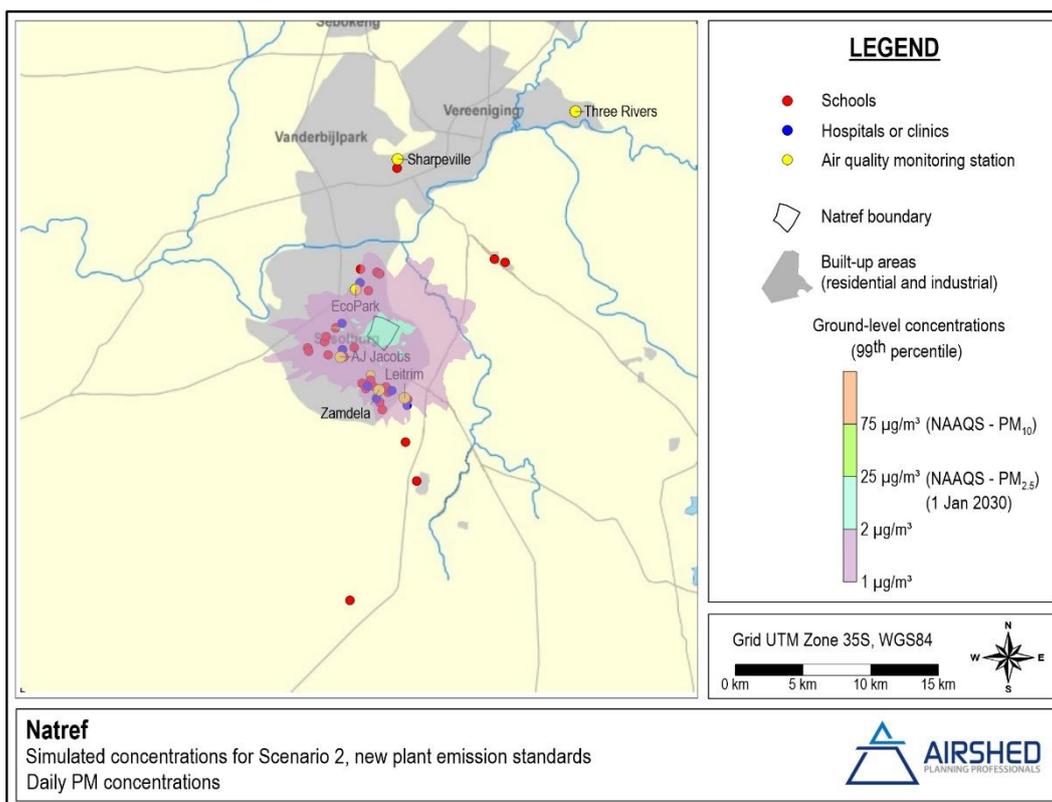


Figure 5-93: Simulated daily PM concentrations (99<sup>th</sup> percentile) as a result of theoretical compliance with new plant emission standards, Scenario 2 (99% SRU availability)

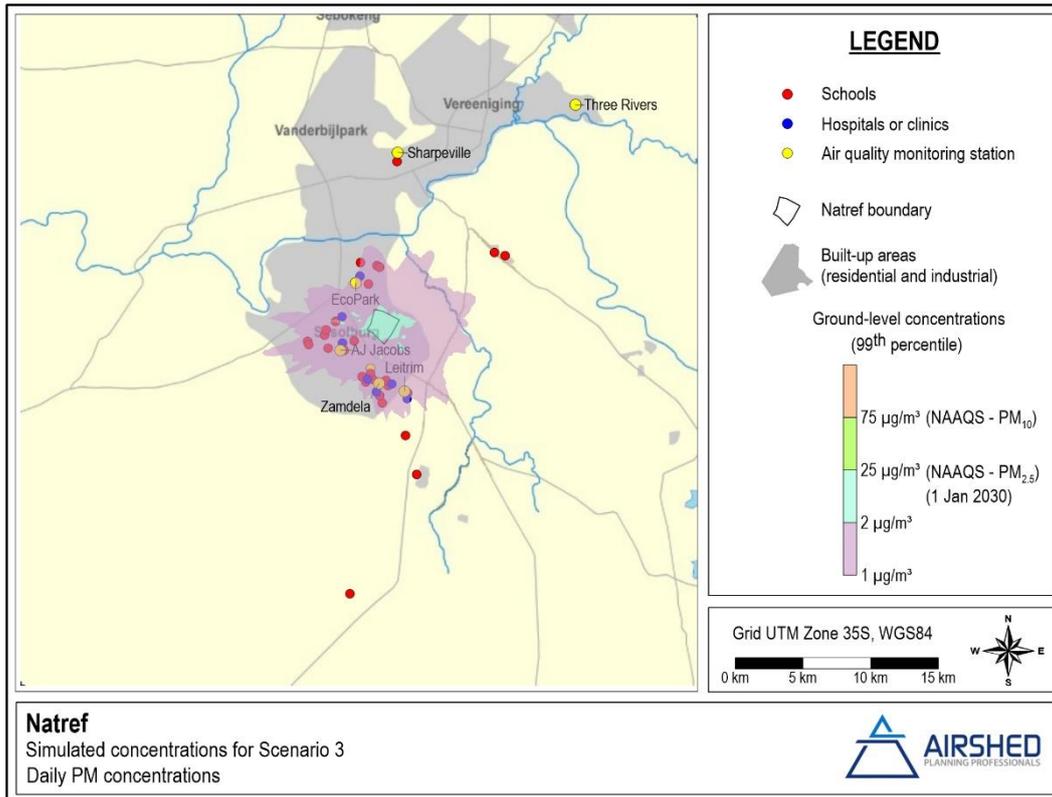


Figure 5-94: Simulated daily PM concentrations (99<sup>th</sup> percentile) for Scenario 3 (95% SRU availability)

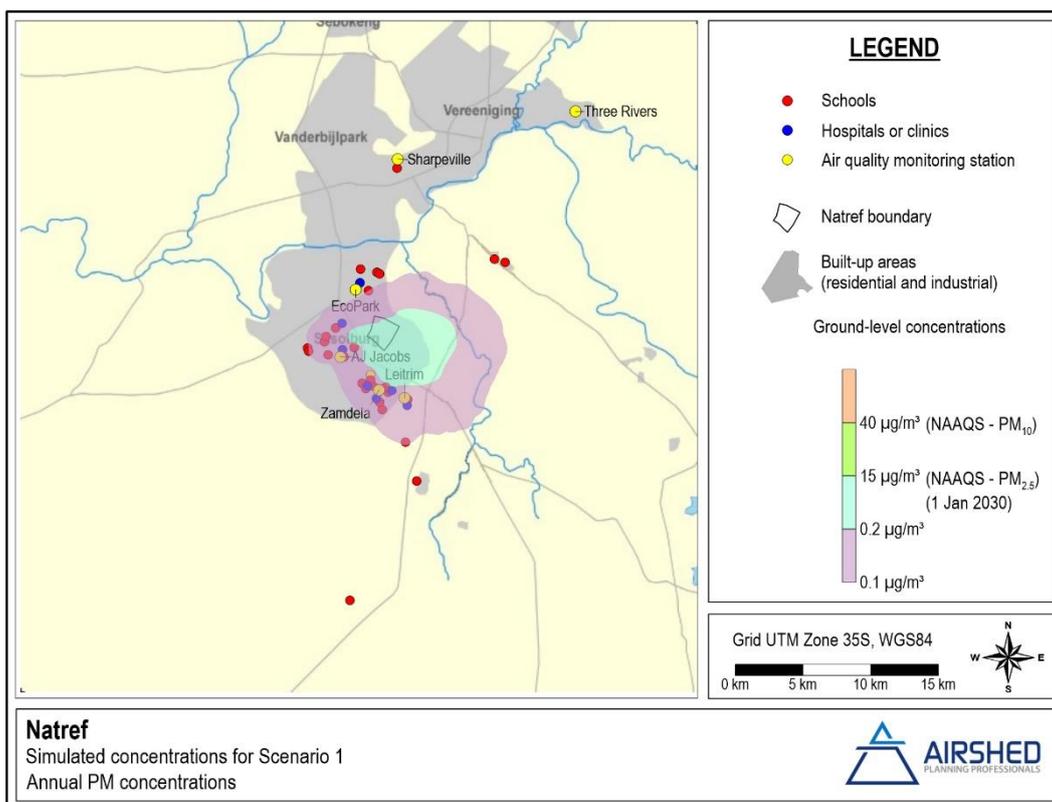


Figure 5-95: Simulated annual PM concentrations for Scenario 1 (100% SRU availability)

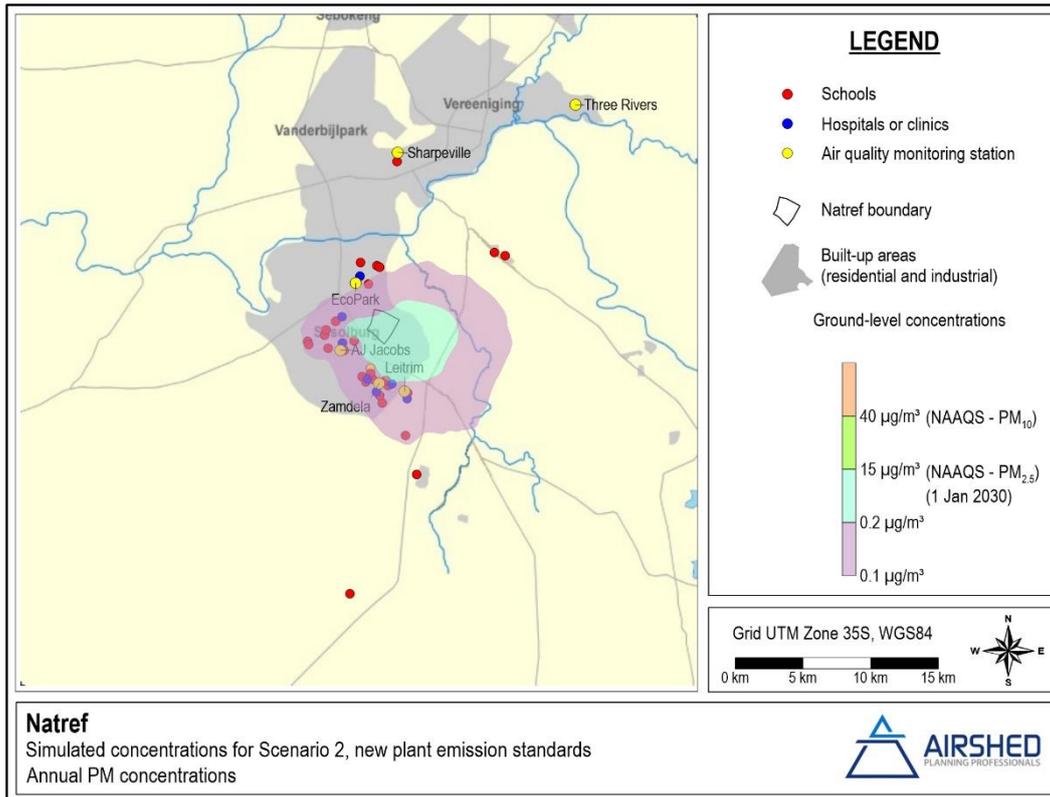


Figure 5-96: Simulated annual PM concentrations as a result of theoretical compliance with new plant emission standards, Scenario 2 (99% SRU availability)

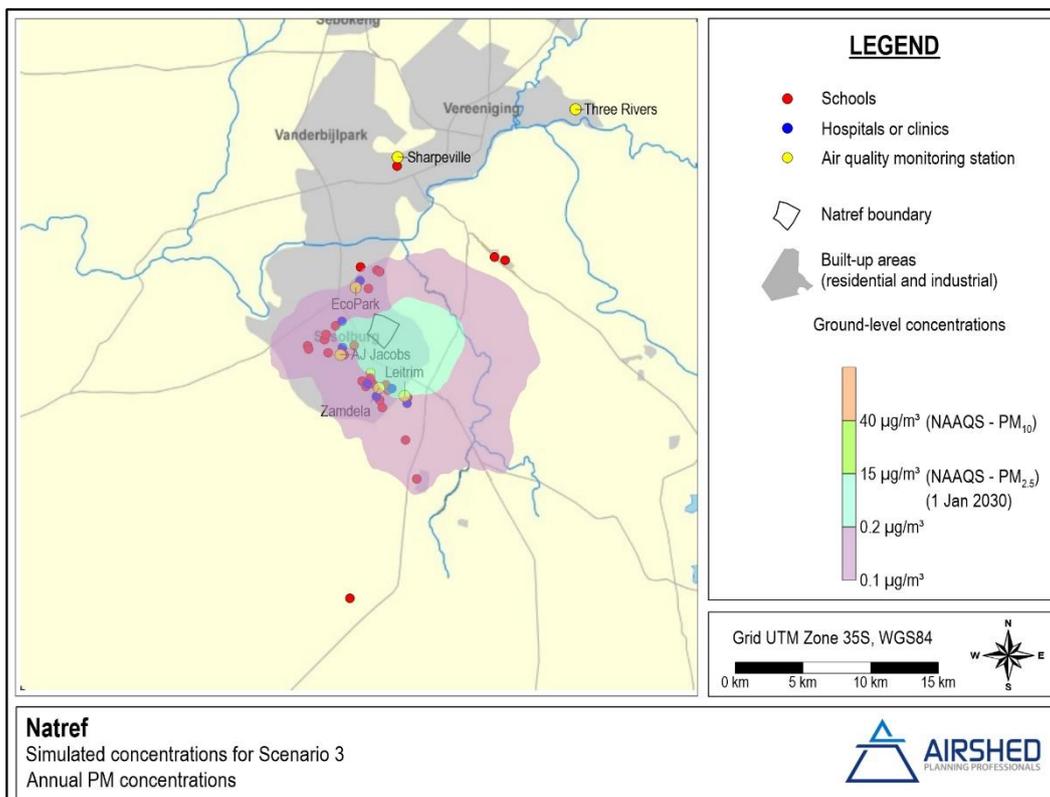


Figure 5-97: Simulated annual PM concentrations for Scenario 3 (95% SRU availability)

#### 5.1.8.1.4 Carbon Monoxide (CO)

Emission rates for CO does not differ for the three scenarios. Only simulated baseline conditions was therefore provided in this section (Figure 5-97 and Figure 5-98). The ambient CO concentrations due to baseline Natref operations is within hourly NAAQS (Figure 5-99).

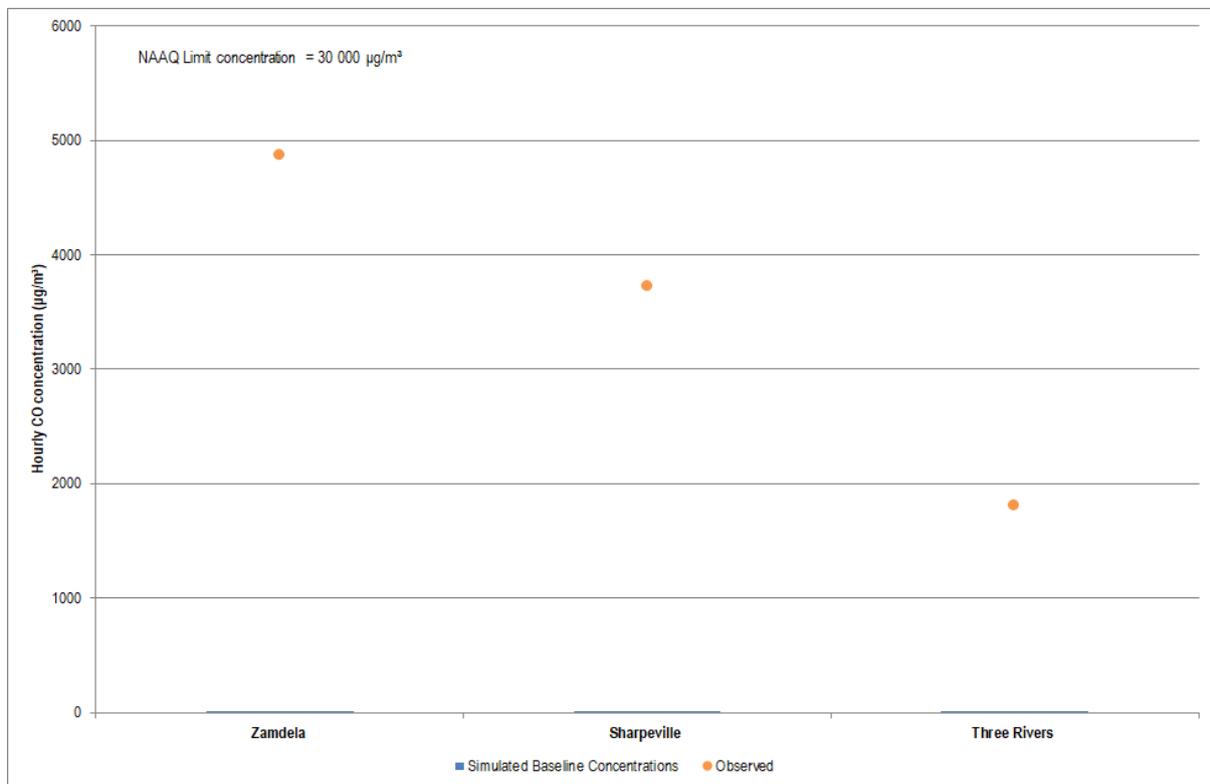


Figure 5-98: Simulated hourly CO concentrations at AQMS for Natref with observed ambient levels

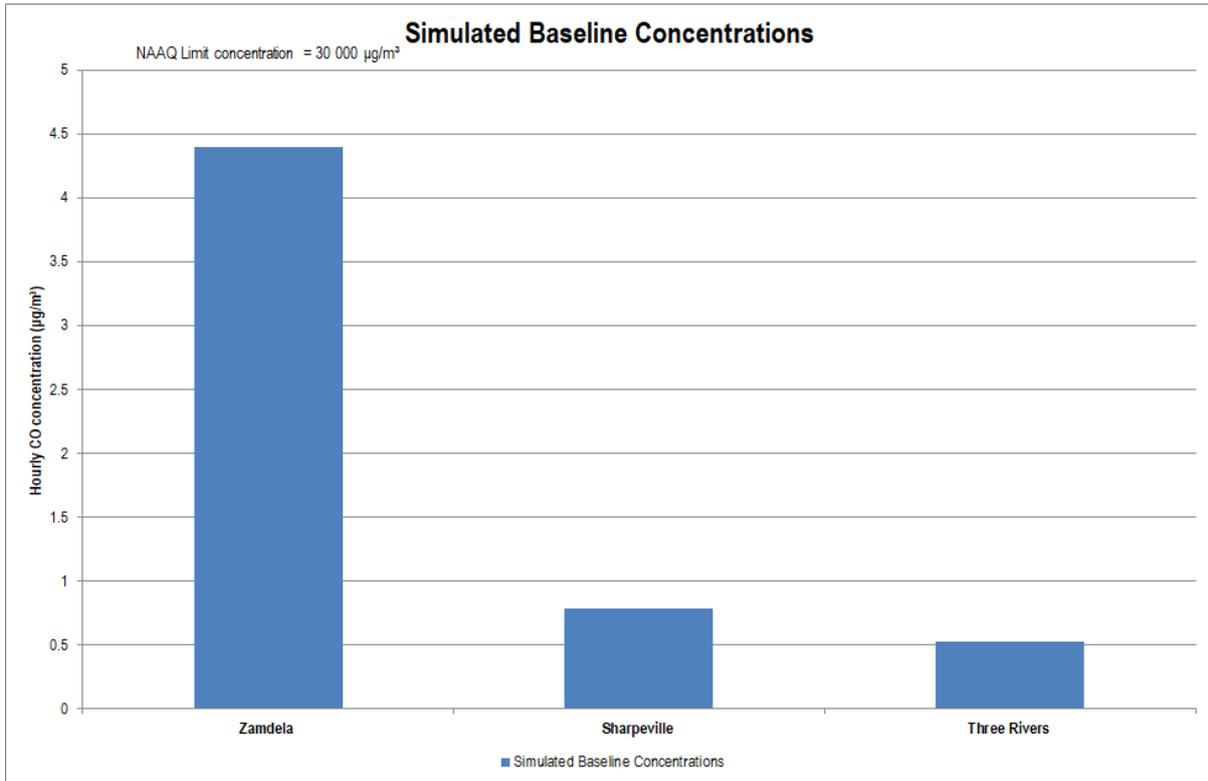


Figure 5-99: Simulated hourly CO concentrations at AQMS for Natref

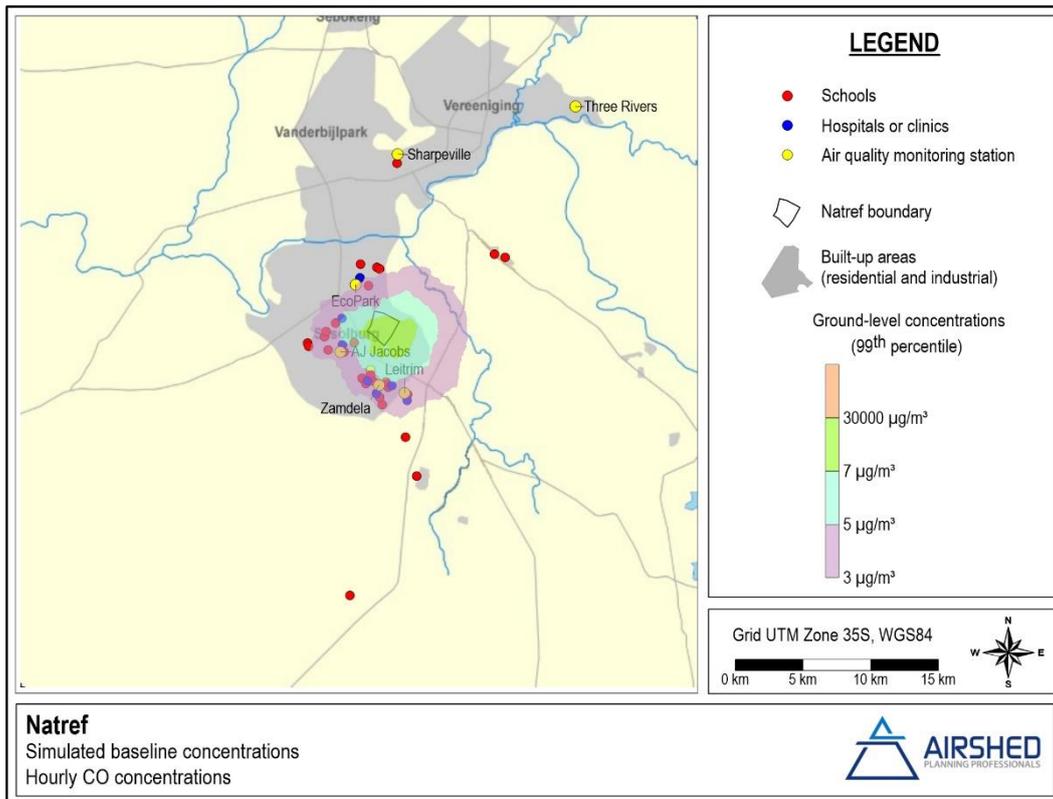


Figure 5-100: Simulated hourly CO concentrations (99<sup>th</sup> percentile) as a result of baseline emissions

### 5.1.9 *Uncertainty of Modelled Results*

The main steps of uncertainty management are to:

- identify and understand uncertainties;
- understand whether uncertainties matter for decisions being made at the time;
- if they do matter, decide what to do about them; and,
- recommend a way forward.

Managing uncertainties attempts to eliminate the source of technical disagreements and failure to understand them often leads to a conclusion that all uncertainties need to be eliminated before project decisions can be made. The first decision about how to manage uncertainties relates to their significance given the decision being addressed. In the current context, the different parts of the investigation were grouped into similar uncertainty regimes, namely:

- dispersion model uncertainties;
- input data uncertainties;
- the methodology of validating model results; and,
- the methodology of expressing the modelled scenarios.

A comprehensive discussion on uncertainties is provided in Appendix H.

As discussed in Section 5.1.6, the baseline predictions with the inclusion of estimated background concentrations performed well within the generally accepted (U.S. EPA 2005) “factor of two” accuracy of dispersion models. Unless greater general experience is gained, or some further formal validation studies are conducted, it is not possible to say how much more confidence can be given to well-executed plume and puff models.

As discussed in Appendix I, it is estimated that the ambient monitoring has an uncertainty of 5% with a 95% confidence interval and the emissions monitoring an uncertainty of 10% with a 95% confidence interval. Based on these uncertainties, it is estimated that the concentration ratios of the different emission scenarios have an uncertainty of -36% and +58%, i.e. potential under-prediction of 36% and over-prediction of 58%.

The Intergovernmental Panel on Climate Change (IPCC) produced a qualitative method for consistent communication of uncertainties in the IPCC Fifth Assessment Report. This Guidance Note has been summarised in Appendix I. On application of this guide, the results from this investigation is considered to be of “high confidence” based on a “high agreement” of the baseline predictions with observations, based on “medium evidence”.

## 5.2 **Analysis of Emissions’ Impact on the Environment**

### 5.2.1 *Critical Levels for Vegetation*

The impact of Natref emissions on surrounding vegetation was assessed by comparing the simulated annual SO<sub>2</sub> and NO<sub>2</sub> concentrations for each of the emission scenarios against the critical levels for vegetation as defined by the United Nations Economic Commission for Europe (UNECE) Convention on Long Range Trans-boundary Air Pollution Limits (CLRTAP, 2015) (Table 5-27).

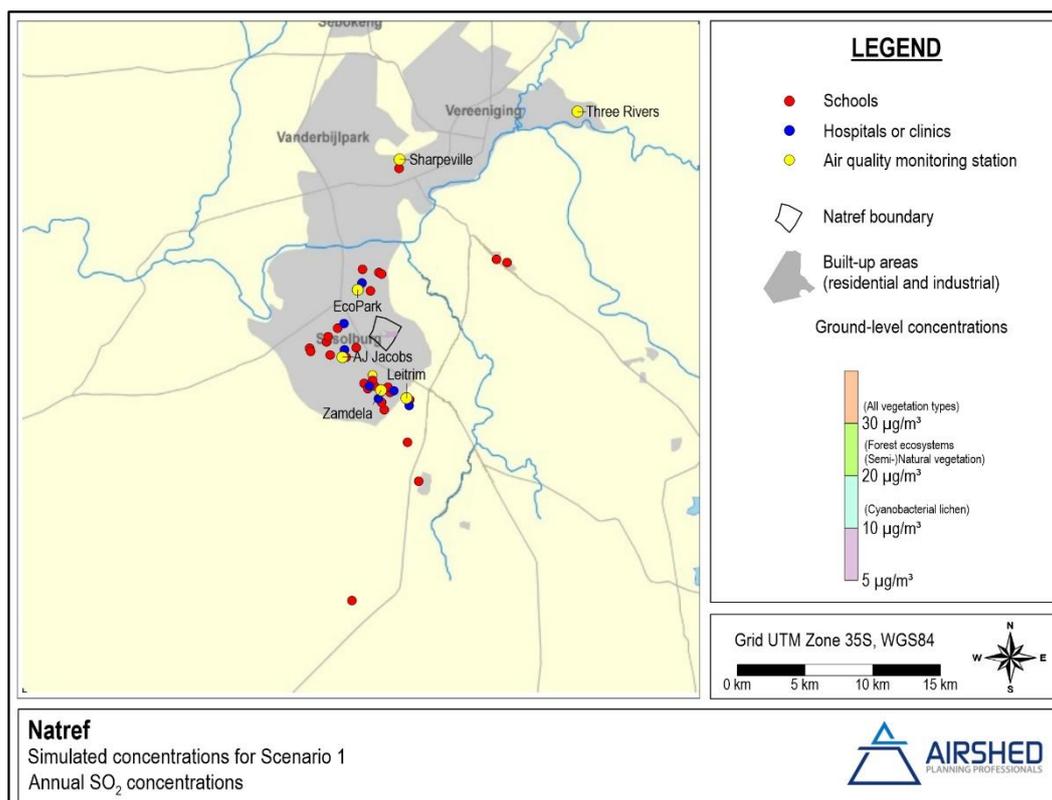
**Table 5-27: Critical levels for SO<sub>2</sub> and NO<sub>2</sub> by vegetation type (CLRTAP, 2015)**

Pollutant	Vegetation type	Critical Level (µg/m <sup>3</sup> )	Time Period <sup>(a)</sup>
SO <sub>2</sub>	Cyanobacterial lichens	10	Annual average
	Forest ecosystems (including understorey vegetation)	20	Annual average and Half-year mean (winter)
	(Semi-)natural vegetation	20	Annual average and Half-year mean (winter)
	Agricultural crops	30	Annual average and Half-year mean (winter)
NO <sub>2</sub>	All	30	Annual average and Half-year mean (winter)
		75	Daily average

**Notes:**

(a) For the purposes of mapping of critical levels and exceedances CLRTAP recommend using only the annual average, due to increased reliability of mapped and simulated data for the longer time period. It is also noted that long-term effects of NO<sub>x</sub> are considered to be more significant than short-term effects (CLRTAP, 2015).

The simulated off-site annual concentrations of SO<sub>2</sub> do not exceed the critical levels for all vegetation types for all scenarios (Figure 5-101, Figure 5-102 and Figure 5-103). Similarly, NO<sub>2</sub> concentrations are likely to be below the critical levels for all vegetation types for baseline operations (Figure 5-104).



**Figure 5-101: Annual SO<sub>2</sub> concentrations for Scenario 1 compared with CLRTAP critical levels**

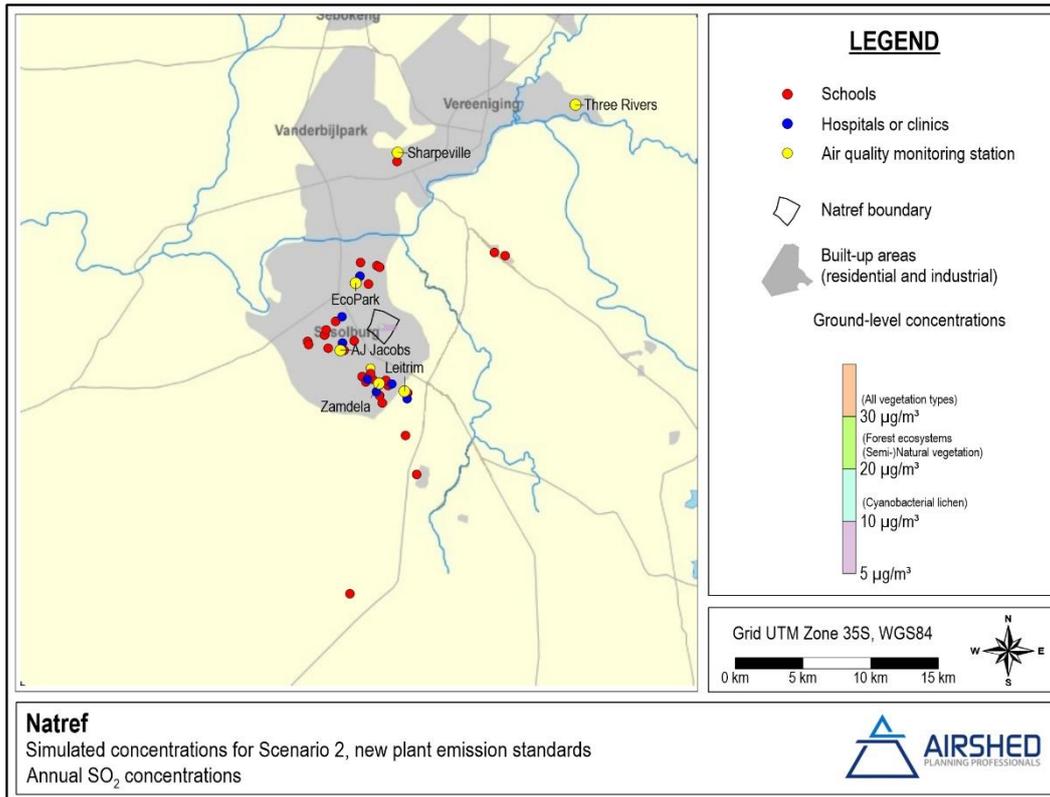


Figure 5-102: Annual SO<sub>2</sub> concentrations as a result of theoretical compliance with new plant emission standards compared, Scenario 2, with CLRTAP critical levels

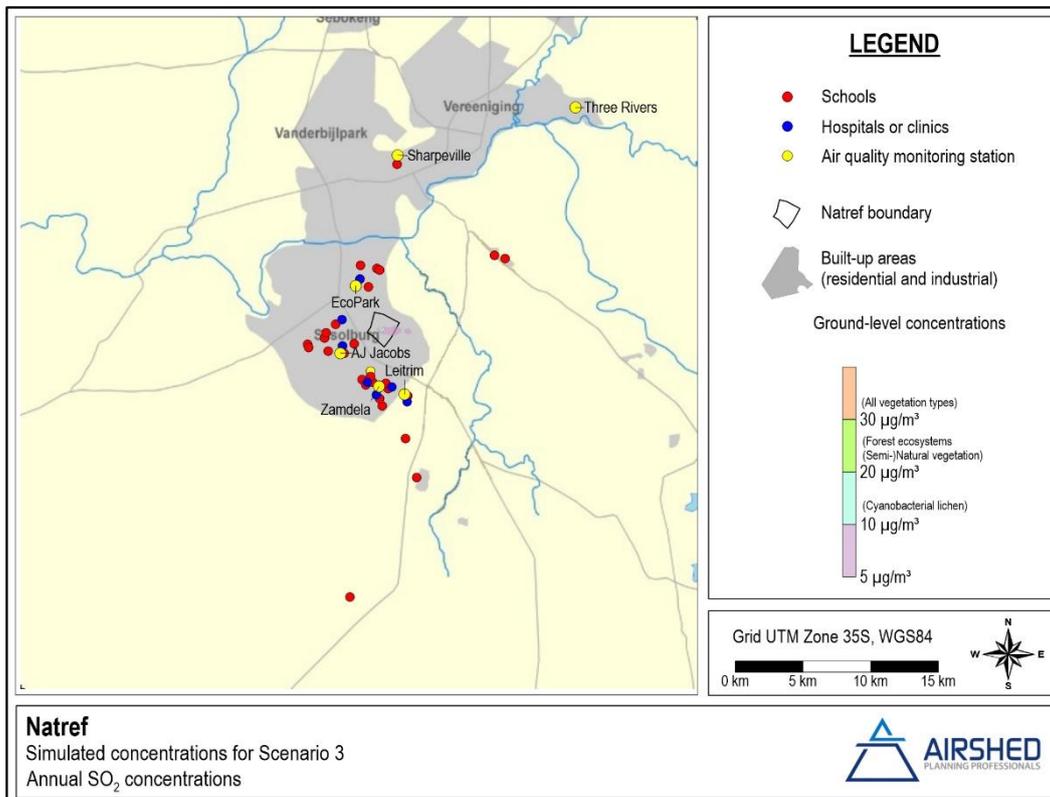


Figure 5-103: Annual SO<sub>2</sub> concentrations for Scenario 3 compared with CLRTAP critical levels

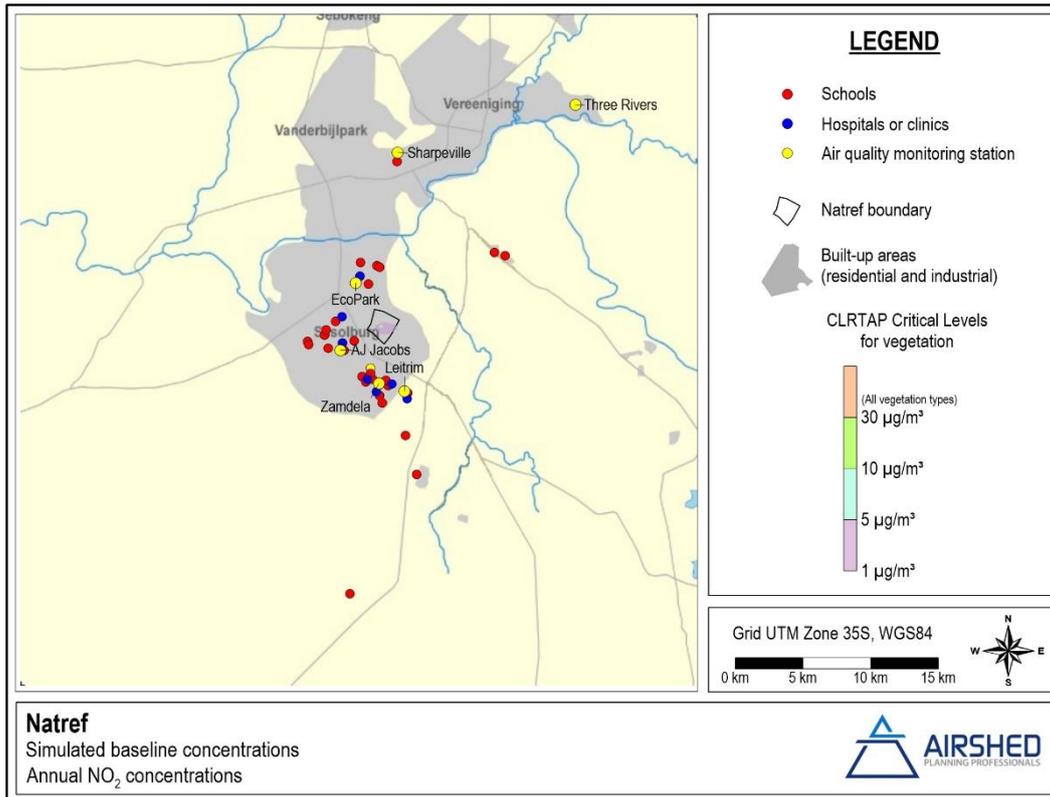


Figure 5-104: Annual NO<sub>2</sub> concentrations as a result of baseline emissions compared with CLRTAP critical levels

### 5.2.2 Dustfall

Dustfall deposition rates were estimated as a result of particulate emissions from the Natref point sources. The simulated PM concentrations (Section 5.1.8.1.3) were converted to deposition rates by assuming a settling velocity of  $6.43 \times 10^{-3}$  m/s (based on a 10 µm particle with a density of 2.1 g/m<sup>3</sup>). Estimated dustfall rates for the simulation scenarios ranged between 0.03 and 8.3 mg/m<sup>2</sup>.day (Table 5-28). No exceedances of the NDCR residential standard were simulated off-site. Isoleth plots are presented for dustfall deposition rates for the three scenarios in Figure 5-105 to Figure 5-107. Simulated dustfall rates have been compared to the acceptable dustfall rate applicable to residential areas as defined by the NDCR (Table 5-3).

Table 5-28: Summary of dustfall deposition rates as a result of operations at Natref

Criteria	Daily dustfall rate (mg/m <sup>2</sup> .day)		
	Scenario 1 (100% SRU availability)	Scenario 2 (99% SRU availability)	Scenario 3 (95% SRU availability)
Min	0.03	0.06	0.06
Max	8.33	8.33	8.33

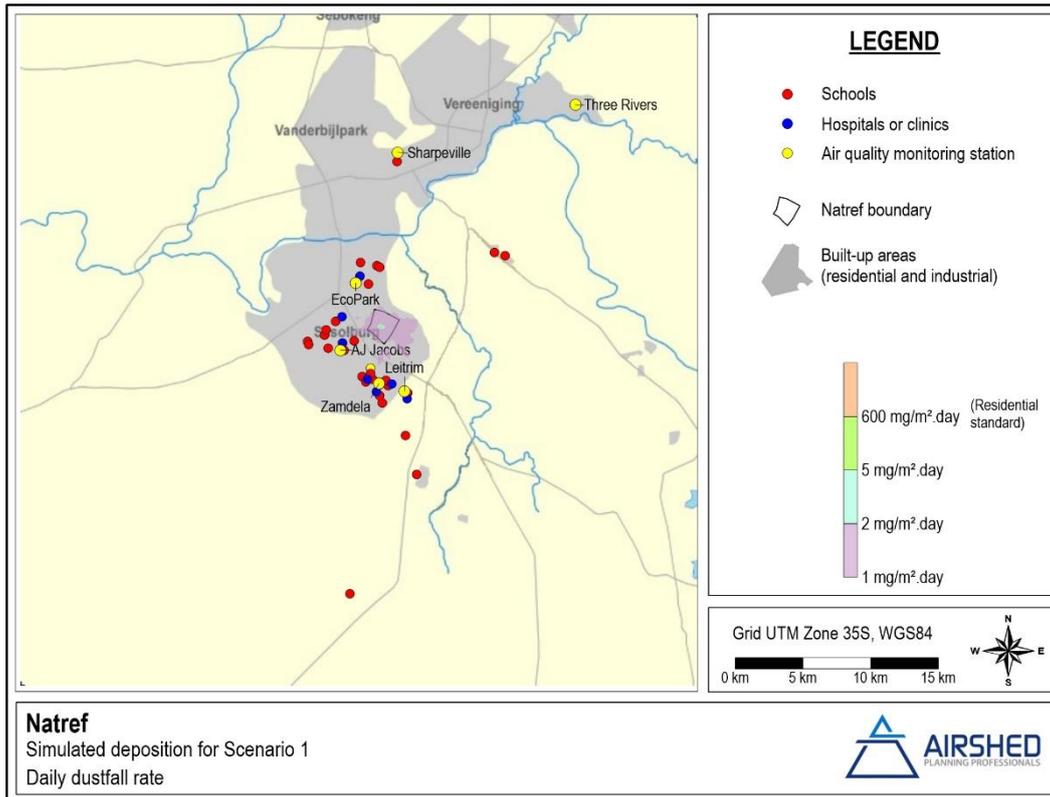


Figure 5-105: Simulated daily dustfall for Scenario 1 (100% SRU availability)

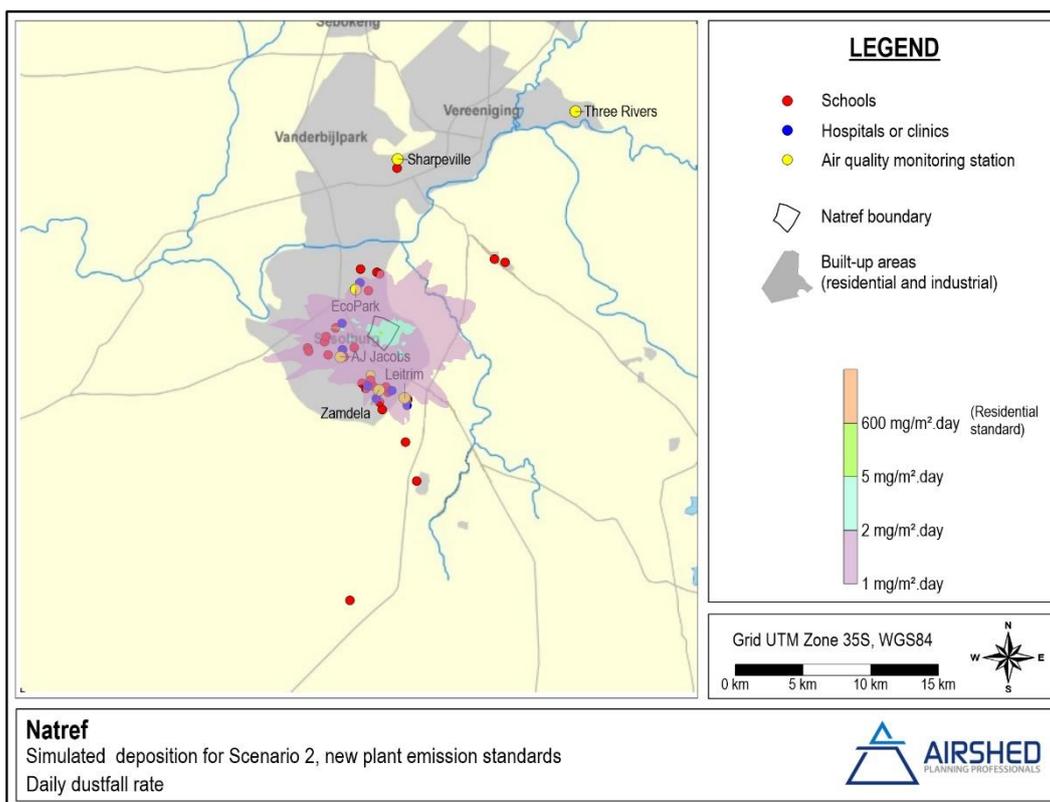


Figure 5-106: Simulated daily dustfall as a result of theoretical compliance with new plant standards, Scenario 2 (99% SRU availability)

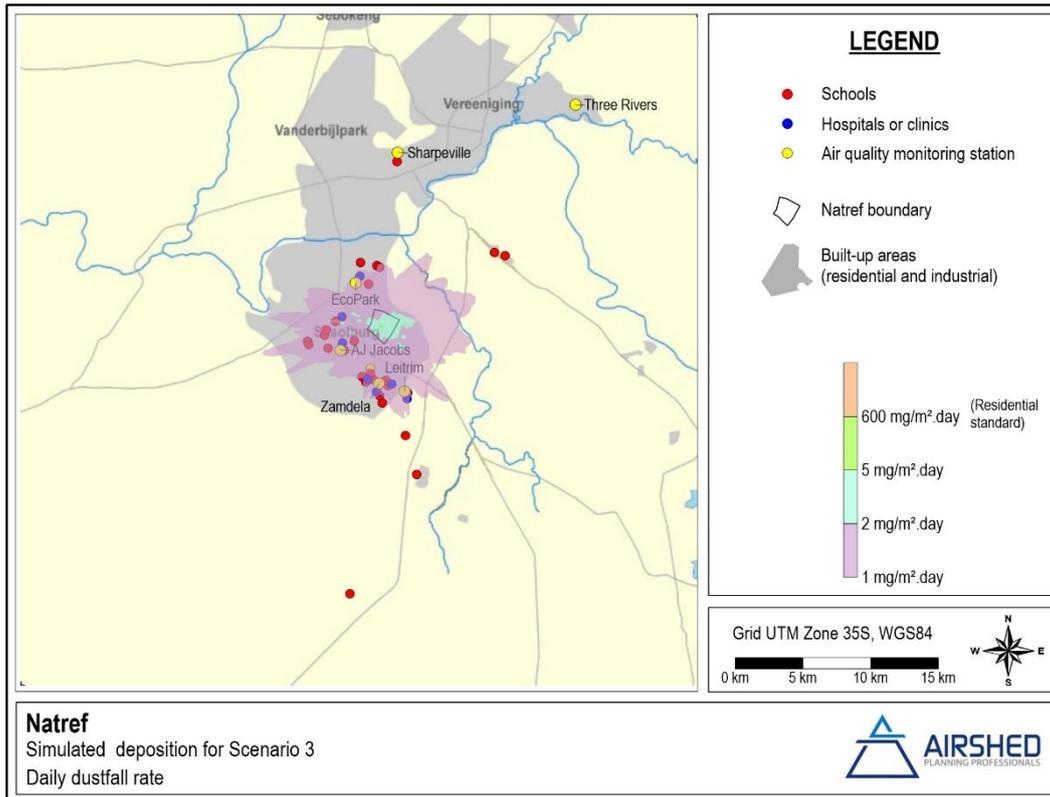


Figure 5-107: Simulated daily dustfall for Scenario 3 (95% SRU availability)

## 5.2.3 Corrosion

### 5.2.3.1 Factors Affecting Corrosion

The most important corrosion stimulators are water (humidity) and air pollutants, such as  $\text{SO}_2$ ,  $\text{NH}_3$ , and acids such as HCl and formic acid ( $\text{HCOOH}$ ), as well as aerosols and particles containing chlorides ( $\text{Cl}^-$ ), nitrates ( $\text{NO}_3^-$ ), and sulfates ( $\text{SO}_4^{2-}$ ). The presence of a moisture film on the surface allows these pollutants to dissolve and dissociate into its respective positive and negative ions, and therefore constitutes the electrolyte for corrosion to take place. The thickness of this aqueous layer depends on the relative humidity and surface properties, and is typically a few to a few tens of nanometres (nm) at room temperature (Phipps and Rice 1979).

Dry deposition near emission sources in urban and industrial areas consists largely of the adsorption of criteria pollutants such as  $\text{SO}_2$  and  $\text{NO}_x$  on surfaces, with the deposited amount proportional to the content in air. The deposition rate is high at elevated humidity, especially on some metals; e.g., steel and zinc (Sydberger and Vannerberg, 1972). Corrosion due to  $\text{SO}_2$  exposure is perhaps the most significant. Although  $\text{NO}_x$  may also contribute to corrosion of metals, it is considerably less significant. Like  $\text{SO}_2$ , this pollutant is mainly emitted from combustion processes such as boilers, power stations, motor vehicle exhausts, etc. It is predominantly emitted as nitrogen oxide ( $\text{NO}$ ) and oxidised in the atmosphere to nitrogen dioxide ( $\text{NO}_2$ ). This oxidation process is a relatively fast process, but further oxidation of  $\text{NO}_2$  to nitric acid ( $\text{HNO}_3$ ), i.e. the form conducive for corrosion, occurs at a slow rate and therefore exposure is normally at comparatively low concentrations.

Very little work has been reported on the effect of HCl on the degradation of materials in the environment. This is probably because HCl, which is present outdoors in markedly reduced concentrations when compared with  $\text{SO}_2$ , has not been considered to contribute to significant degradation of materials. The first major study of atmospheric degradation of metals by

HCl was carried out by Feitnecht (1952) who exposed zinc, iron and copper to HCl vapours at varying humidity's between 50% and 95%. Feitnecht found that HCl reacted with metals only when a critical relative humidity was exceeded, which he linked to the vapour pressure of a saturated solution of the metal chloride formed during corrosion. He regards the mechanism as electrochemical, with the oxide-film as cathodes and small areas of metal exposed at breaks as anodes; the interaction between the hydroxide ions ( $\text{OH}^-$  ions), formed by the cathodic reduction of oxygen, and the metal ions, formed by the anodic reaction, leads to hydroxide or basic chloride. Barton and Bartonova (1969) carried out an extensive investigation of the corrosive effect of HCl gas at concentrations between 7 and 10 ppm on zinc, mild steel, and copper at temperatures between 20°C and 50°C and at relative humidity's of 70% and 95%. Two distinct stages were seen in the behaviour:

- Stage 1 was characterized by a non-linear increase in mass loss with time; termed the "indication period for steady-state corrosion".
- Stage 2, after about 16 days' exposure, showed steady-state corrosion with a linear increase in mass-loss with time.

The primary corrosion products found on iron were  $\text{FeO}(\text{OH})$ ,  $\text{Fe}_3\text{O}_4$  and  $\text{FeCl}_2$ , whilst those found on zinc were  $4\text{Zn}(\text{OH})_2$ ,  $\text{ZnCl}_2$ ,  $\text{Zn}(\text{OH})_2$  and  $\text{ZnO}$ . The amount of chloride in the corrosion product tended to decrease slowly with time. After the steady state corrosion stage had been reached, the composition of the corrosion product remained unchanged.

Barton and Bartonova (1969) measured the corrosion rate at different temperatures in the steady state region. For zinc, the corrosion rate decreased as the temperature increased; for iron, the corrosion rate increased with temperatures up to 40°C, but decreased at 50°C. The rate of the reactions did not appear to depend on the diffusion of HCl to the surface since the corrosion rate was similar in flowing and stationery atmospheres. The implication is that the corrosion rate is dependent on chemical reaction rate. The kinetics of corrosion is controlled by the transfer of HCl to the corrosion product atmosphere interface, its adsorption and the subsequent production of soluble  $\text{ZnCl}_2$ . The corrosion rate also depends on the hydroxide / chloride ratio in the corrosion product as the hydroxides are more protective than the chlorides.

No literature could be obtained on the combined corrosive effects of gaseous  $\text{SO}_2$  and HCl pollutant. Furthermore, no dose-response relationships between hydrochloric acid concentrating or deposition rates and corrosion rates could be obtained. Most literature on chloride exposures discusses the corrosion rates associated with marine environments. Whilst the chemical reactions may be similar, it is not clear whether an assumption of equivalence may be made between hydrochloric acid and sodium chloride. Whilst both are donors of chloride ions, the former would also reduce the pH of the moisture layer on the metal surface. Given these limitations, and in an attempt to provide an indication of the corrosion potential that the proposed facility may have on the surrounding environment, it was decided to make reference to the International Standard Organisation (ISO) corrosion classification which considers  $\text{SO}_2$  and chloride deposition rates to establish the rate of corrosion of a number of different metal types.

#### 5.2.3.2 *International Standard Organisation*

The ISO provides a classification scheme that can directly be used for technical and economic analyses of corrosion damage due to atmospheric  $\text{SO}_2$  and chlorides, and for the rational choice of protection measures. As such, the corrosivity of the atmosphere is divided into five categories (C1 to C5), ranging from very low to very high corrosivity. These corrosivity categories are estimated using a combination of the meteorological parameters, sulfate deposition and airborne salinity (chloride ion). These are discussed below.

### 5.2.3.2.1 Time of Wetness

Relative humidity, rain, dew, and temperature are determinants of the so-called *time of wetness* (TOW), defined (ISO 9223) as the fraction of time with relative humidity in excess of 80%, at temperatures above freezing ( $>0^{\circ}\text{C}$ ). The TOW of a corroding surface is a key parameter, directly determining the duration of the electrochemical corrosion processes. This is a complex variable, since all the means of formation and evaporation of the surface electrolyte solution must be considered. The TOW refers to the period of time during which the atmospheric conditions are favourable for the formation of a surface layer of moisture on a metal or alloy. As pointed in the previous section, this moisture film is extremely important from the point of view of the chemical mechanisms of the corrosion process.

Meteorological data from the Eco Park and Leitrim AQMS were used to calculate the TOW. The average TOW at is 16% and 18% per year at Eco Park and Leitrim respectively. According to the ISO 9233 classification (Table 5-29), the TOW class represented by these weather conditions is **T3**.

**Table 5-29: ISO 9223 Classification of the Time of Wetness**

Category	Time of Wetness	Example of Occurrence	Comment
	Hours per Year	Percentage	
T1	$T \leq 10$	$T \leq 0.1$	Indoor
T2	$10 < T \leq 250$	$0.1 < T \leq 3$	Indoor without climate control
<b>T3</b>	<b><math>250 &lt; T \leq 2500</math></b>	<b><math>3 &lt; T \leq 30</math></b>	<b>Outdoor atmospheres in dry, cold climates and part of temperate climates</b>
T4	$2\ 500 < T \leq 5\ 500$	$30 < T \leq 60$	Outdoor atmospheres in all climates except for dry and cold climates
T5	$5\ 500 < T$	$60 < T$	Tropical outdoor or surf

### 5.2.3.2.2 Atmospheric pollutants

As indicated by the ISO standard, corrosion due to atmospheric pollution is dominated by sulfur dioxide (urban environments) and chlorides (marine environments). This is also evident from open literature where the focus of atmospheric corrosion of metals has predominantly been described through the impact of these two pollutants.

#### *Sulfur Dioxide*

Sulfate ions are formed in the surface moisture layer by the oxidation of sulfur dioxide and their formation is considered to be the main corrosion accelerating effect from sulfur dioxide. Sulfur dioxide may be expressed either in terms of a deposition rate or an airborne concentration. The method of determining the deposition rate in this instance followed the ISO 9223 Method, where the corrosion potential due to  $\text{SO}_2$  is classified according to the long-term (annual) deposition rate or air concentration of  $\text{SO}_2$ , as summarised in Table 5-29. Any concentration of  $\text{SO}_2$  within category  $P_0$  is considered to be the background concentration and is insignificant from the point of view of corrosive attack. Pollution by  $\text{SO}_2$  within category  $P_3$  is considered extreme and is typical of operational microclimates beyond the scope of the International Standard. The ground-level  $\text{SO}_2$  concentrations, as a result of emissions from Natref, fall into the  $P_2$  category for all three scenarios (Table 5-31).

**Table 5-30: ISO 9223 classification of pollution by sulfur-containing substances represented by SO<sub>2</sub>**

Category	Concentration of SO <sub>2</sub>	Deposition Rate of SO <sub>2</sub>
	µg/m <sup>3</sup>	mg/(m <sup>2</sup> .day)
P0	$P_c \leq 12$	$P_d \leq 10$
P1	$12 < P_c \leq 40$	$10 < P_d \leq 35$
P2	$40 < P_c \leq 90$	$35 < P_d \leq 80$
P3	$90 < P_c \leq 250$	$80 < P_d \leq 200$

**Table 5-31: ISO 9223 classification of pollution by sulfur-containing substances represented by SO<sub>2</sub> as a result of Natref**

Criterion	Scenario		
	Scenario 1 (100% SRU availability)	Scenario 2 (99% SRU availability)	Scenario 3 (95% SRU availability)
Maximum annual SO <sub>2</sub> concentration (µg/m <sup>3</sup> )	32.92	32.95	33.04
ISO corrosivity category for SO <sub>2</sub>	P1	P1	P1

#### *Airborne Chloride*

The ISO 9223 classification of pollution by chloride containing substances is provided in Table 5-32. Chloride deposition rates were estimated based HCl emissions from as a result of processes at the Sasol Sasolburg facility (Table 5-33). Although maritime chloride contributions are likely to be insignificant, other industrial sources in the vicinity may also contribute to the HCl deposition load however the contribution is unknown.

**Table 5-32: ISO 9223 classification of pollution by airborne chloride containing substances**

Category	Deposition Rate of Chloride (mg/m <sup>2</sup> .day)
S0	$S \leq 3$
S1	$3 < S \leq 60$
S2	$60 < S \leq 300$
S3	$300 < S \leq 1500$

**Table 5-33: ISO 9223 classification of pollution by airborne chloride containing substances for SO**

Criterion	Scenario		
	Scenario 1 (100% SRU availability)	Scenario 2 (99% SRU availability)	Scenario 3 (95% SRU availability)
Chloride deposition (mg/m <sup>2</sup> .day)	0.05		
ISO corrosivity category for Cl	S0		

#### 5.2.3.2.3 Corrosivity Potential

Having calculated the TOW, the classification of pollution by sulfate and chloride containing substances, the corrosivity category (C1 to C5) for individual metals can be estimated according to ISO 9223, as shown in Table 5-34, and specific corrosivity categories associated with Natref are summarised for the three scenarios in Table 5-35. Once the corrosivity category has been determined, the corrosion rate for carbon and weathered steel, zinc, copper and aluminium can be estimated using the rates given in Table 5-36.

**Table 5-34: Estimated corrosivity categories of the atmosphere**

Unalloyed carbon steel															
	T1			T2			T3			T4			T5		
	S <sub>0</sub> -S <sub>1</sub>	S <sub>2</sub>	S <sub>3</sub>	S <sub>0</sub> -S <sub>1</sub>	S <sub>2</sub>	S <sub>3</sub>	S <sub>0</sub> -S <sub>1</sub>	S <sub>2</sub>	S <sub>3</sub>	S <sub>0</sub> -S <sub>1</sub>	S <sub>2</sub>	S <sub>3</sub>	S <sub>0</sub> -S <sub>1</sub>	S <sub>2</sub>	S <sub>3</sub>
P <sub>0</sub> -P <sub>1</sub>	1	1	1/2	1	2	3/4	2/3	3/4	4	3	4	5	3/4	5	5
P <sub>2</sub>	1	1	1/2	1/2	2/3	3/4	3/4	3/4	4/5	4	4	5	4/5	5	5
P <sub>3</sub>	1/2	1/2	2	2	3	4	4	4/	5	5	5	5	5	5	5
Zinc and copper															
	T1			T2			T3			T4			T5		
	S <sub>0</sub> -S <sub>1</sub>	S <sub>2</sub>	S <sub>3</sub>	S <sub>0</sub> -S <sub>1</sub>	S <sub>2</sub>	S <sub>3</sub>	S <sub>0</sub> -S <sub>1</sub>	S <sub>2</sub>	S <sub>3</sub>	S <sub>0</sub> -S <sub>1</sub>	S <sub>2</sub>	S <sub>3</sub>	S <sub>0</sub> -S <sub>1</sub>	S <sub>2</sub>	S <sub>3</sub>
P <sub>0</sub> -P <sub>1</sub>	1	1	1	1	1/2	3	3	3	3/4	3	4	5	3/4	5	5
P <sub>2</sub>	1	1	1/2	1/2	2	3	3	3/4	4	3/4	4	5	4/5	5	5
P <sub>3</sub>	1	1/2	2	2	3	3/4	3	3/4	4	4/5	5	5	5	5	5
Aluminium															
	T1			T2			T3			T4			T5		
	S <sub>0</sub> -S <sub>1</sub>	S <sub>2</sub>	S <sub>3</sub>	S <sub>0</sub> -S <sub>1</sub>	S <sub>2</sub>	S <sub>3</sub>	S <sub>0</sub> -S <sub>1</sub>	S <sub>2</sub>	S <sub>3</sub>	S <sub>0</sub> -S <sub>1</sub>	S <sub>2</sub>	S <sub>3</sub>	S <sub>0</sub> -S <sub>1</sub>	S <sub>2</sub>	S <sub>3</sub>
P <sub>0</sub> -P <sub>1</sub>	1	2	2	1	2/3	4	3	3/4	4	3	3/4	5	4	5	5
P <sub>2</sub>	1	2	2/3	1/2	3/4	4	3	4	4/5	3/4	4	5	4/5	5	5
P <sub>3</sub>	1	2/3	3	3/4	4	4	3/4	4/5	5	4/5	5	5	5	5	5

Note: Corrosivity is expressed as the numerical part of the corrosivity category code (for example: 1 instead of C1).

**Table 5-35: Estimated corrosivity categories of the atmosphere associated with Natref**

Metal type	Scenario		
	Scenario 1 (100% SRU availability)	Scenario 2 (99% SRU availability)	Scenario 3 (95% SRU availability)
Unalloyed carbon steel	C2/3		
Zinc and copper	C3		
Aluminium	C3		

**Table 5-36: Average and steady state corrosion rates for Different Metals and Corrosivity Categories**

Metal	Average corrosion rate ( $r_{av}$ ) during the first 10 years for the following corrosivity categories ( $\mu\text{m/annum}$ )				
	C1	C2	C3	C4	C5
Carbon steel	$r_{av} \leq 0.5$	$0.5 < r_{av} \leq 5$	$5 < r_{av} \leq 12$	$12 < r_{av} \leq 30$	$30 < r_{av} \leq 100$
Weathering steel	$r_{av} \leq 0.1$	$0.1 < r_{av} \leq 2$	$2 < r_{av} \leq 8$	$8 < r_{av} \leq 15$	$15 < r_{av} \leq 80$
Zinc	$r_{av} \leq 0.1$	$0.1 < r_{av} \leq 0.5$	$0.5 < r_{av} \leq 2$	$2 < r_{av} \leq 4$	$4 < r_{av} \leq 10$
Copper	$r_{av} \leq 0.01$	$0.01 < r_{av} \leq 0.1$	$0.1 < r_{av} \leq 1.5$	$1.5 < r_{av} \leq 3$	$3 < r_{av} \leq 5$
Aluminium	$r_{av} \approx 0.01$	$r_{av} \leq 0.025$	$0.01 < r_{av} \leq 0.1$	(5)	(5)
Metal	Steady state corrosion rate ( $r_{lin}$ ) for the following corrosivity categories ( $\mu\text{m/annum}$ )				
	C1	C2	C3	C4	C5
Carbon steel	$r_{av} \leq 0.1$	$0.1 < r_{av} \leq 1.5$	$1.5 < r_{av} \leq 8$	$8 < r_{av} \leq 20$	$20 < r_{av} \leq 90$
Weathering steel	$r_{av} \leq 0.1$	$0.1 < r_{av} \leq 1$	$1 < r_{av} \leq 5$	$5 < r_{av} \leq 10$	$10 < r_{av} \leq 80$
Zinc	$r_{av} \leq 0.05$	$0.1 < r_{av} \leq 0.5$	$0.5 < r_{av} \leq 2$	$2 < r_{av} \leq 4$	$4 < r_{av} \leq 10$
Copper	$r_{av} \leq 0.01$	$0.01 < r_{av} \leq 0.1$	$0.1 < r_{av} \leq 1$	$1 < r_{av} \leq 3$	$3 < r_{av} \leq 5$
Aluminium	negligible	$0.01 < r_{av} \leq 0.02$	$0.02 < r_{av} \leq 0.2$	(5)	(5)
<b>Notes</b>					
1) The corrosion rate of carbon steel is not constant during the first 10 years.					

Metal	Average corrosion rate ( $r_{av}$ ) during the first 10 years for the following corrosivity categories ( $\mu\text{m/annum}$ )				
	C1	C2	C3	C4	C5
2)	The corrosion rate of weathering steel is strongly dependent on the combination of various influencing factors (alternation between wet and dry periods). In atmospheres with sulfur dioxide (SO <sub>2</sub> ) pollution, a more protective rust layer is formed. Rain protected surfaces in marine atmospheres heavily polluted with chlorides may have much higher corrosion rates than freely exposed surfaces.				
3)	Applies also to the copper-zinc, copper-tin and similar alloys with a copper content of at least 60 %.				
4)	The rates shown are based on commercially pure aluminium (purity > 99.5%) which, like most aluminium alloys, corrodes in the atmosphere at a rate that decreases with time. However, these rates are based on average mass loss results while the corrosion attack is usually manifested as pitting. Consequently, the rates shown do not represent rates of penetration. Penetration rates for pitting also decrease with exposure time. Commercially pure aluminium, aluminium alloys containing magnesium, manganese and/or silicon as the major alloying elements, and Alclad products generally have better corrosion resistance than aluminium alloys containing significant quantities of copper, zinc and/or iron. Alloys with significant quantities of magnesium, zinc, copper and/or iron may also be subject to other forms of localized corrosion such as stress corrosion cracking, exfoliation and intergranular attack.				
5)	In atmospheres defined by corrosivity categories C4 and C5, a marked increase in corrosion rate may be expected and local corrosion effects become important. For these two corrosivity categories, the data concerning general corrosion may be misleading.				

### 5.2.3.3 ISOCORRAG Atmospheric Corrosion Model

The ISOCORRAG equation was developed to predict the annual corrosion rate resulting from atmospheric corrosion for several metals. The equation was created by the multiple linear regressions of corrosion data from several sites around the globe. With ISOCORRAG, the annual corrosion rate is expressed as (Knotkova *et al.*, 1995):

$$K = a + b_1[SO_2] + b_2[Cl^-] + b_3[TOW]$$

**Equation 2**

Where the constants  $a$ ,  $b_1$ ,  $b_2$ , and  $b_3$ , differ according to the type of metal, shape of the specimen, and exposure conditions. Table 5-37 is a summary of constants for flat metal specimens. The deposition of SO<sub>2</sub> is expressed as an equivalent concentration, i.e.  $\mu\text{g}/\text{m}^3$ ; the deposition of chloride pollutants [Cl<sup>-</sup>] is expressed in  $\text{mg}/\text{m}^2\cdot\text{day}$ , and time of wetness [TOW] in hours per year.

**Table 5-37: ISOCORRAG regression model constants (Knotkova *et al.*, 1995)**

Metal	Regression Constants for ISOCORRAG model			
	a	b <sub>1</sub>	b <sub>2</sub>	b <sub>3</sub>
Steel	1.3269	0.4313	0.1384	0.0057
Zinc	0.2098	0.0232	0.0059	0.00027
Copper	0.9556	0.0065	0.00393	0.0000538
Aluminium	0.0069	0.00638	0.000558	0.0000650

Using simulated concentrations of SO<sub>2</sub> as a result of Natref operations and wet deposition rates of chloride (HCl emissions and simulated concentrations) (as in Section 5.2.3.2.2. above) the rate of corrosion (K) was calculated (using Equation 2) across the dispersion modelling domain. TOW from Section 5.2.3.2.1 was used. A summary of the findings is presented in Table 5-38. There is some agreement between the two methods for corrosion rate estimation for aluminium, however corrosion rates calculated using the ISOCORRAG method are in higher than corrosion rates presented for the ISO method for steel, zinc and copper (Table 5-36 compared with Table 5-38).

**Table 5-38: Corrosion rate of metals associated with Natref calculated according to the ISOCORRAG method**

Scenario	Criteria	Corrosion rate (K) [µm/annum]			
		Steel	Zinc	Copper	Aluminium
<b>Time of wetness at Eco Park AQMS [1377 hours]</b>					
Scenario 1 (100% SRU availability)	Min	9.19	32.16	1.03	0.10
	Max	23.38	32.92	1.24	0.31
Scenario 2 (99% SRU availability)	Min	9.19	32.16	1.03	0.10
	Max	23.39	32.93	1.24	0.31
Scenario 3 (95% SRU availability)	Min	9.19	32.16	1.03	0.10
	Max	23.43	32.93	1.24	0.31
<b>Time of wetness at Leitrim AQMS [1559 hours]</b>					
Scenario 1 (100% SRU availability)	Min	10.23	36.39	1.04	0.11
	Max	24.42	37.15	1.25	0.32
Scenario 2 (99% SRU availability)	Min	10.23	36.39	1.04	0.11
	Max	24.43	37.15	1.25	0.32
Scenario 3 (95% SRU availability)	Min	10.23	36.39	1.04	0.11
	Max	24.47	37.16	1.25	0.32

#### 5.2.4 Sulfur and Nitrogen Deposition Impacts

Understanding the impact of deposition of atmospheric sulfur (S) and nitrogen (N) on South African ecosystems has been ongoing since the late 1980's (Tyson *et al.* 1988), with much of the earlier work focussing on the circulation over the sub-continent (Tyson *et al.* 1996). More recent research has focussed on quantifying S and N deposition (Galpin and Turner 1999, Zunckel *et al.* 1996, Scorgie and Kornelius 2009, Josipovic *et al.* 2010) and the subsequent impacts on ecosystems (Fey and Guy 1993, Van Tienhoven *et al.* 1995, Reid 2007, Bird 2011, Josipovic *et al.* 2011).

These studies estimating deposition of S and or N compounds to ecosystems present ranges of deposition rates where the differences are related to the distance from major industrial sources; the method of estimation (field work and/or calculation based on deposition velocities or dispersion modelling). As an indication, total S deposition over the industrialised Highveld of South Africa was modelled to range between 8 and 35 kg/ha/year with background levels of approximately 1 kg/ha/year (Scorgie and Kornelius 2009). In contrast, using ambient SO<sub>2</sub> concentrations and an inferential deposition model to calculate S deposition, Zunckel *et al.* (1996) estimated total S deposition of 13.9 kg/ha/year as maximum deposition rate on the Highveld. Estimates of nitrogen deposition range between 6.7 kg/ha/year (Collett *et al.* 2010) and 15 kg/ha/year (Scorgie and Kornelius 2009). Considering total acidic input from atmospheric sources, Josipovic and colleagues (2011) calculated a range of deposition rates between 15.8 and 23.2 kg/ha/year. All estimates are within the range of deposition rates for S and N as for some of the industrialised regions of Europe and North America (compared in Scorgie and Kornelius 2009, and Bird 2011) raising concern that the acidic loading of sulfur and nitrogen on the ecosystems of the Highveld – South Africa's most heavily industrialised region – could have implications for ecosystem functioning.

Establishing clear cause-effect relationships in complex ecosystem studies can be difficult, especially where the extent of visible damage is large and local emissions are low (Matzner and Murach 1995). Reasons include: time lags between stressor (high concentration of atmospheric pollutants) and visible symptomatic response of biota; interaction of natural factors (e.g. climate, soil and pests) and human activities (such as management, site history and air pollution); local ecosystem uniqueness and difficulty of extrapolating to larger scales; or, symptomatic responses that are not unique to the cause (e.g. defoliation) (Matzner and Murach 1995). The synergistic effect of pollutant cocktails can also add complexity to identifying causative pollutants (Emberson 2003).

Mobilisation of active forms of S and N into the atmosphere, and later as deposition onto ecosystems, can result in acidification of soils and freshwater systems, soil nutrient depletion, fertilization of naturally (usually nitrogen) limited systems and increased availability of metal ions (e.g. Al) disrupting ecosystem functioning (Rodhe *et al.* 1995) and changing plant and/or freshwater species diversity (Stevens *et al.* 2004). Many of these impacts occur over a decade or longer where attributing source contributions can be complex within a regional setting. Sasol have, however, supported the long-term deposition quantification studies in South African under the DEBITS (Deposition of Biogeochemically Important Trace Species) programme, as part of the International Global Atmospheric Chemistry Project. Three DEBITS sites are maintained within South Africa, one located near Amersfoort, on the Mpumalanga Highveld, downwind from major industrial sources, including Natref. Investigating deposition and its impacts on the Highveld grasslands as a result of Natref operations was beyond the time-frame of the accompanying postponement application especially since long-term impact studies are not yet available for South Africa.

## 6 COMPLAINTS

Year	Nature of complaints	Actions taken to investigate complaints	Causes of complaints identified	Measures taken to avoid reoccurrences in instances where the plant's operations were found to be the cause
October 2016 – September 2018	<ul style="list-style-type: none"> <li>• A total of 5 complaints were received for the period of October 2016 – September 2018 that were relevant to Natref.</li> <li>• The complaints were received on the following dates:               <ul style="list-style-type: none"> <li>○ 31 August 2017;</li> <li>○ 18 September 2017;</li> <li>○ 24 November 2017;</li> <li>○ 20 January 2018; and</li> <li>○ 28 August 2018.</li> </ul> </li> <li>• All 5 complaints were related to odours.</li> </ul>	<p>Natref operates a complaints line where any environmental complaint can be registered. The Shift Superintendent and the environmental standby will investigate the complaint and ensure that the necessary steps are taken to reduce and manage the impact and to reduce the duration of the incident.</p>	<p>Process upsets, equipment failure</p>	<p>Measures are implemented to prevent a similar incident from recurring.</p>

## 7 CURRENT OR PLANNED AIR QUALITY MANAGEMENT INTERVENTIONS

An overview of approved air quality management improvement interventions, currently implemented and scheduled over the next 5 to 10 years, is detailed in the accompanying Motivation Report.

## 8 COMPLIANCE AND ENFORCEMENT ACTIONS

No compliance notices were received since 2015.

## 9 ADDITIONAL INFORMATION

Beyond the requirements stipulated in the AIR Regulations and Dispersion Modelling Regulations, the following additional information is considered useful for better understanding the impacts of Natref's activities and the implications of the requested postponements on ambient air quality. A brief description of each of these analyses is provided below, and referenced to where in the applications the information may be found.

### a) Polar plots

Polar plots have been provided in Section 5.1.6.1 to visually demonstrate directional contribution as well as the dependence of concentrations on wind speed, in much the same way as a pollution rose does. The polar plots identify major contributing emissions sources impacting on a monitoring station and the direction of the impact. These polar plots do not replace isopleth plots, but rather provide additional information on the measured air quality in the region of the facility.

### b) Delta approach to assessing implications of postponements for ambient air quality

In assessing the impacts of Natref's postponement applications on ambient air quality, a fit-for-purpose approach, as requested for by the Dispersion modelling Regulations, was taken to assess the results from the dispersion modelling, which we have referred to as the "delta approach". The delta approach is premised on recognising that the difference between the current or "before additional compliance is implemented" emission scenario (i.e. the baseline scenario) and "after additional compliance is implemented" scenario (i.e. the 2020 MES compliance scenario) relates to the change in emissions from the point sources in question.

Therefore, the delta approach focuses on demonstrating the change in predicted ambient impacts of the various compliance scenarios, to guide decision makers toward better understanding the implications of the approval of postponements on air quality, and how compliance with the existing and new plant standards would impact on prevailing ambient air quality.

A detailed explanation of the scenarios modelled to highlight the delta changes in ambient air quality arising from retrofit of abatement technology is provided in Section 5.1.1.2. In summary, the three scenarios modelled include:

- Scenario 1 – 100% SRU availability;
- Scenario 2 – 99% SRU availability (theoretically complying with New Plant Standards);
- Scenario 3 – 95% SRU availability.

### c) Estimating background ambient air pollutant concentrations

A background air concentration is normally defined as that concentration which would result from air emission sources outside the chosen modelling domain. This concentration can, for instance, be estimated by analysing observed air concentrations for those wind directions when it is blowing towards the sources included in the modelling domain. In other words, the observation point would be upwind from the sources being simulated by the dispersion modelling.

However, as used in the current investigation, background concentrations could also incorporate the contributions from air emission sources present in the modelling domain, but which were not included in the dispersion simulations. For example, air emissions from vehicle tailpipes can significantly contribute to the local ambient NO<sub>2</sub> concentrations. Although most of the sources of air emissions within the Sasol operations were included in the simulations, there remains some that were excluded, for instance fugitive emissions, but would add to the background concentration level.

Since these sources are not neatly located for easy analysis of upwind contributions, the procedure normally adopted to estimate background air concentrations could not be followed. Instead, the "background" concentration was established by comparing the predicted air concentrations with the observed air concentrations. The background concentration as used in this application therefore corresponds to the observed concentration value at a monitoring site when the simulated value at this site reached a near zero value. In other words, the observed residual air concentration was assumed to arise from other sources in the modelling domain.

With this method, the assumption is made that the model performs realistically and that the residual concentration determined this way is a good reflection of the emissions not included in the simulations. In an attempt to illustrate the model accuracy, the fractional bias was calculated for each monitoring station as described in Section 5.1.6.2 of the AIRs. This methodology has been prescribed by the US EPA (U.S. EPA 1992) as an acceptable manner to illustrate the validity of atmospheric dispersion model. Given the good model performance, as measure by the fractional bias, it is assumed that the background concentration obtained using this methodology is reasonable estimates.

#### **d) Ambient impacts of secondary particulates arising from Natref emissions**

As detailed in Section 5.1.4.4, one of the reasons for selection of the CALPUFF modelling suite is the fact this this enabled inclusion of the impact of the chemical conversion of sulfur dioxide and nitrogen oxides to secondary particulates within the dispersion model results. Thus, the predicted PM<sub>10</sub> concentrations reflected in Section 5.1.8.1.3 include direct emissions of PM plus secondary particulates formed from Natref's emissions.

10 ANNEXURE A

DECLARATION OF ACCURACY OF INFORMATION – APPLICANT

Name of Enterprise: NATREF

Declaration of accuracy of information provided:

Atmospheric Impact Report in terms of section 30 of the Act.

I, Charlene Wassenaar [duly authorised], declare that the information provided in this atmospheric impact report is, to the best of my knowledge, in all respects factually true and correct. I am aware that the supply of false or misleading information to an air quality officer is a criminal offence in terms of section 51(1)(g) of the National Environmental Management: Air Quality Act (Act No. 39 of 2004).

Signed at Sasolburg on this 3<sup>rd</sup> day of December 2018

Wassenaar  
SIGNATURE

VP: SHERQ Natref  
CAPACITY OF SIGNATORY

## 11 ANNEXURE B

### DECLARATION OF INDEPENDENCE - PRACTITIONER

**Name of Practitioner:** \_Reneé von Gruenewaldt

**Name of Registration Body:** South African Council for Natural Scientific Professions

**Professional Registration No.:** 400304/07

Declaration of independence and accuracy of information provided:

#### **Atmospheric Impact Report in terms of section 30 of the Act.**

I, Reneé von Gruenewaldt, declare that I am independent of the applicant. I have the necessary expertise to conduct the assessments required for the report and will perform the work relating the application in an objective manner, even if this results in views and findings that are not favourable to the applicant. I will disclose to the applicant and the air quality officer all material information in my possession that reasonably has or may have the potential of influencing any decision to be taken with respect to the application by the air quality officer. The additional information provided in this atmospheric impact report is, to the best of my knowledge, in all respects factually true and correct. I am aware that the supply of false or misleading information to an air quality officer is a criminal offence in terms of section 51(1)(g) of this Act.

Signed at Midrand on this 6<sup>th</sup> day of March 2019



#### **SIGNATURE**

Principal Air Quality Scientist

#### **CAPACITY OF SIGNATORY**

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## APPENDIX A: COMPETENCIES FOR PERFORMING AIR DISPERSION MODELLING

All modelling tasks were performed by competent personnel. Table A-1 is a summary of competency requirements. Apart from the necessary technical skills required for the calculations, personnel competency also include the correct attitude, behaviour, motive and other personal characteristic that are essential to perform the assigned job on time and with the required diligence as deemed necessary for the successful completion of the project.

The project team included a two principal engineers, with relevant experience of 34 years and 15 years and two principal scientists with 16 years and 6 years relevant experience. One of the principal scientists managed and directed the project.

One of the principal engineers conducted verification of modelling results. This function requires a thorough knowledge of the

- meteorological parameters that influence the atmospheric dispersion processes and
- atmospheric chemical transformations that some pollutants may undergo during the dispersion process.

**Table A-1: Competencies for Performing Air Dispersion Modelling**

Competency	Task, Knowledge and Experience
Context	Communication with field workers, technicians, laboratories, engineers and scientists and project managers during the process is important to the success of the model
	Familiar with terminology, principles and interactions
	Record keeping is important to support the accountability of the model - Understanding of data collection methods and technologies
Knowledge	Meteorology: <ul style="list-style-type: none"> <li>• Obtain, review and interpret meteorological data</li> <li>• Understanding of meteorological impacts on pollutants</li> <li>• Ability to identify and describe soil, water, drainage and terrain conditions               <ul style="list-style-type: none"> <li>○ Understanding of their interaction</li> <li>○ Familiarity with surface roughness`</li> </ul> </li> <li>• Ability to identify good and bad data points/sets</li> <li>• Understanding of how to deal with incomplete/missing meteorological data</li> </ul>
	Atmospheric Dispersion models <ul style="list-style-type: none"> <li>• Select appropriate dispersion model</li> <li>• Prepare and execute dispersion model</li> <li>• Understanding of model input parameters</li> <li>• Interpret results of model</li> </ul>
	Chemical and physical interactions of atmospheric pollutants <ul style="list-style-type: none"> <li>• Familiarity with fate and transport of pollutants in air</li> <li>• Interaction of primary pollutants with other substances (natural or industrial) to form secondary pollutants</li> </ul>
	Information relevant to the model <ul style="list-style-type: none"> <li>• Identify potential pollution (emission) sources and rates</li> <li>• Gather physical information on sources such as location, stack height and diameter</li> <li>• Gather operating information on sources such as mass flow rates, stack top temperature, velocity or volumetric flow rate</li> <li>• Calculate emission rates based on collected information</li> <li>• Identify land use (urban/rural)</li> <li>• Identify land cover/terrain characteristics</li> <li>• Identify the receptor grid/site</li> </ul>
	Legislation, regulations and guidelines in regards to National Environment Management: Air Quality Act (Act No 39 of 2004), including <ul style="list-style-type: none"> <li>• Minimum Emissions Standards (Section 21 of Act)</li> <li>• National Ambient Air Quality Standards</li> <li>• Regulations Regarding Air Dispersion Modelling</li> <li>• Atmospheric Impact Report (AIR)</li> </ul>
Abilities	Ability to read and understand map information
	Ability to prepare reports and documents as necessary
	Ability to review reports to ensure accuracy, clarity and completeness

Competency	Task, Knowledge and Experience
	Communication skills
	Team skills

## APPENDIX B: COMPARISON OF STUDY APPROACH WITH THE REGULATIONS PRESCRIBING THE FORMAT OF THE ATMOSPHERIC IMPACT REPORT AND THE REGULATIONS REGARDING AIR DISPERSION MODELLING (GAZETTE NO 37804 PUBLISHED 11 JULY 2014)

The Regulations prescribing the format of the Atmospheric Impact Report (AIR) (Government Gazette No 36094; published 11 October 2013) were referenced for the air dispersion modelling approach used in this study. Table B-1 compares the AIR Regulations with the approach used in Section 5.

The promulgated Regulations regarding Air Dispersion Modelling (Gazette No. 37804, vol. 589; 11 July 2014) were consulted to ensure that the dispersion modelling process used in this assessment was in agreement with the regulations. Table B-2 compares the Air Dispersion Modelling Regulations with the approach used in Section 5. The only updates applied, following stakeholder comment, was to the receptors to include schools and clinics, as indicated on the isopleth plots in Section 5.1.8.

**Table B-1: Comparison of Regulations for the AIR with study approach**

Chapter	Name	AIR regulations requirement	Status in AIR
1	Enterprise details	<ul style="list-style-type: none"> <li>• Enterprise Details</li> <li>• Location and Extent of the Plant</li> <li>• Atmospheric Emission Licence and other Authorisations</li> </ul>	All detail included in the regulated format.
2	Nature of process	<ul style="list-style-type: none"> <li>• Listed Activities</li> <li>• Process Description</li> <li>• Unit Processes</li> </ul>	All detail included in the regulated format.
3	Technical Information	<ul style="list-style-type: none"> <li>• Raw Materials Used and Production Rates</li> <li>• Appliances and Abatement Equipment Control Technology</li> </ul>	All detail included in the regulated format.
4	Atmospheric Emissions	<ul style="list-style-type: none"> <li>• Point Source Emissions                             <ul style="list-style-type: none"> <li>• Point Source Parameters</li> <li>• Point Source Maximum Emission Rates during Normal Operating Conditions</li> <li>• Point Source Maximum Emission Rates during Start-up, Maintenance and/or Shut-down</li> </ul> </li> <li>• Fugitive Emissions</li> <li>• Emergency Incidents</li> </ul>	Point source parameters and emissions have been included (Section 4.1 and Section 4.2). Emissions released during start-up, maintenance and/or Shut-down have been discussed (Section 4.3). Management of fugitive emissions across the Natref operations has been described (Section 4.4). The history of Emergency Incidents during the period of assessment and planned management of future Emergency Incidents has been described (Section 4.5).
5	Impact of enterprise on receiving environment		
5.1	Analysis of emissions impact on human health	Must conduct dispersion modelling, must be done in accordance with Regulations; must use NAAQS	Completed as set out by the Regulations.
5.2	Analysis of emissions impact on environment	Must be undertaken at discretion of Air Quality Officer.	Literature review and analysis, where possible, included in AIR.
6	Complaints	Details on complaints received for last two years	Included
7	Current or planned air quality management interventions	Interventions currently being implemented and scheduled and approved for next 5 years.	Information on air quality interventions are included in detail in the motivation reports
8	Compliance and enforcement history	Must set out all air quality compliance and enforcement actions undertaken against the enterprise in the last 5 years. Includes directives, compliance notices, interdicts, prosecution, fines	Included

Chapter	Name	AIR regulations requirement	Status in AIR
9	Additional information		Included polar plots as an additional visualisation means of ambient air quality as monitored. Independent peer review of dispersion modelling methodology by international expert consultant.

**Table B-2: Comparison of Regulations regarding the Air Dispersion Modelling with study approach**

AIR Regulations	Compliance with Regulations	Comment
<p><b>Levels of assessment</b></p> <ul style="list-style-type: none"> <li>Level 1: where worst-case air quality impacts are assessed using simpler screening models</li> <li>Level 2: for assessment of air quality impacts as part of license application or amendment processes, where impacts are the greatest within a few kilometres downwind (less than 50km)</li> <li>Level 3: requires more sophisticated dispersion models (and corresponding input data, resources and model operator expertise) in situations: <ul style="list-style-type: none"> <li>where a detailed understanding of air quality impacts, in time and space, is required;</li> <li>where it is important to account for causality effects, calms, non-linear plume trajectories, spatial variations in turbulent mixing, multiple source types, and chemical transformations;</li> <li>when conducting permitting and/or environmental assessment process for large industrial developments that have considerable social, economic and environmental consequences;</li> <li>when evaluating air quality management approaches involving multi-source, multi-sector contributions from permitted and non-permitted sources in an airshed; or,</li> <li>when assessing contaminants resulting from non-linear processes (e.g. deposition, ground-level ozone (O<sub>3</sub>), particulate formation, visibility)</li> </ul> </li> </ul>	Level 3 assessment using CALPUFF	<p>This Lagrangian Gaussian Puff model is well suited to simulate low or calm wind speed conditions. Alternative regulatory models such as the US EPA AERMOD model treats all plumes as straight-line trajectories, which under calm wind conditions grossly over-estimates the plume travel distance.</p> <p>CALPUFF is able to perform chemical transformations. In this study the conversion of NO to NO<sub>2</sub> and the secondary formation of particulate matter were concerns.</p>
<p><b>Model Input</b></p> <p>Source characterisation</p> <p><b>Emission rates:</b> For new or modified existing sources the maximum allowed amount, volume, emission rates and concentration of pollutants that may be discharged to the atmosphere should be used</p> <p><b>Meteorological data</b></p> <p>Full meteorological conditions are recommended for regulatory applications.</p> <p>Data period</p> <p><b>Geographical Information</b></p>	<p>Yes</p> <p>Yes</p> <p>Yes</p> <p>Yes</p>	<p>Source characterisation provided in Section 5.1.7.</p> <p>Emission rates used for each scenario are provided in Section 5.1.7.</p> <p>WRF modelled meteorology (including upper air) corrected with on-site observed meteorology (surface meteorology) (Sections 5.1.4.6 and 5.1.5).</p> <p>3 years (2015 to 2017)</p>

AIR Regulations	Compliance with Regulations	Comment
Topography and land-use		Required for CALMET 3D meteorological file preparation (Section 5.1.4.6.2)
Domain and co-ordinate system	Yes	<ul style="list-style-type: none"> <li>• Dispersion modelling domain: 57 x 57 km</li> <li>• UTM co-ordinate system (WGS84) (Section 5.1.4.6.4)</li> </ul>
<p><b>General Modelling Considerations</b></p> <p>Ambient Background Concentrations, including estimating background concentrations in multi-source areas</p> <p>NAAQS analyses for new or modified sources: impact of source modification in terms of ground-level concentrations should be assessed within the context of the background concentrations and the</p> <p>Land-use classification</p> <p>Surface roughness</p> <p>Albedo</p> <p><b>Temporal and spatial resolution</b></p> <p>Receptors and spatial resolutions</p> <p>Building downwash</p> <p>Chemical transformations</p>	<p>Yes</p>	<p>Section 5.1.5.4, Section 5.1.6, and Appendix F</p> <p>Model predicted, 99<sup>th</sup> percentile ground-level concentrations compared against current observed concentrations and assessed for contribution to ambient concentrations. Used as an indication of how modifications to the plant will impact ambient concentrations. (Section 5.1.8)</p> <p>Section 5.1.4.2 and Section 5.1.4.6.2</p> <p>Computed from Land-use categories in the CALMET pre-processing step (Section 5.1.4.6.2).</p> <p>Computed from Land-use categories in the CALMET pre-processing step (Section 5.1.4.6.2).</p> <p>Sections 5.1.8 and 5.1.4.6.4</p> <p>Section 5.1.4.6.5</p> <p>Sections 5.1.4.3, Section 5.1.4.4 and Appendix D and Appendix E.</p>
<p><b>General Reporting Requirements</b></p> <p>Model accuracy and uncertainty</p> <p>Plan of study</p> <p>Air Dispersion Modelling Study Reporting Requirements</p> <p>Plotted dispersion contours</p>	<p>Yes</p> <p>Yes</p> <p>Yes</p> <p>Yes</p>	<p>Section 5.1.6, Section 5.1.9, Appendix I and Appendix I</p> <p>Section 5.1.1.1</p> <p>As per the Regulations Prescribing the Format of the Atmospheric Impact Report, Government Gazette No. 36904, Notice Number 747 of 2013 (11 October 2013) and as per the Regulations Regarding Air Dispersion Modelling (Government Gazette No. 37804 Notice R533, 11 July 2014).</p> <p>Section 5.1.8</p>

## APPENDIX C: CALMET MODEL CONTROL OPTIONS

The CALMET run type selected for this assessment has been highlighted in blue in Table C-1 below.

**Table C-1: CALMET model control options**

Run Type	Description of Run Type	Ease of Use and Representativeness	Data availability	Advantages	Disadvantages
No Observations	<ul style="list-style-type: none"> <li>•Prognostic model data, such as WRF to drive CALMET.</li> <li>•No surface or upper air observations input at all.</li> </ul>	<ul style="list-style-type: none"> <li>•Relatively simple to implement in model</li> <li>•Representative of regional meteorological conditions</li> </ul>	WRF data (Lakes Environmental) for 2015, 2016 and 2017 at 4km resolution for 200km by 200km study area (Secunda + Sasolburg)	<ul style="list-style-type: none"> <li>•Simple to implement</li> <li>•Full spatial and temporal variability</li> <li>•No overwater data required</li> <li>•Cloud cover has spatial distribution</li> <li>•Eliminates need for complicated 7 user-input site-specific variables</li> <li>•Ideal as screening run as gives very good estimate</li> </ul>	Resolution of prognostic data may potentially be too coarse to be representative of local conditions
Partial Observations	<ul style="list-style-type: none"> <li>•Prognostic model data, such as WRF to drive CALMET</li> </ul> <p>PLUS</p> <ul style="list-style-type: none"> <li>•One or more surface stations</li> </ul>	<ul style="list-style-type: none"> <li>•More difficult to implement than only prognostic (WRF) data.</li> <li>•Require 7 site-specific model parameters to be specified.</li> <li>•Difficulty in dealing with missing data.</li> <li>•Potential disagreement between prognostic and surface observations.</li> <li>•Very representative and considered 'refined modelling'</li> </ul>	<ul style="list-style-type: none"> <li>• WRF data (Lakes Environmental) for 2015, 2016 and 2017 at 4km resolution for 200km by 200km study area (Secunda + Sasolburg)</li> <li>•Sasol operated surface meteorological weather stations (3 Sasolburg<sup>3</sup> and 3 Secunda<sup>4</sup>)</li> </ul>	<ul style="list-style-type: none"> <li>•Full spatial and temporal variability</li> <li>•No overwater data required</li> <li>•Refined model run as using combined approach of numerical model and observations.</li> <li>•Ability to incorporate surface representative observation data when WRF data is too coarse to fully pick up local effects.</li> </ul>	<ul style="list-style-type: none"> <li>•Surface data, especially winds may be different to that in the WRF data file</li> <li>•User must include 7 site-specific variables</li> <li>•Data preparation and missing data</li> </ul>
Observations Only	CALMET driven solely by surface, upper air and optional overwater and precipitation stations	<ul style="list-style-type: none"> <li>•Require 7 site-specific model parameters to be specified.</li> </ul> <p>Difficulty in dealing with missing data.</p> <ul style="list-style-type: none"> <li>•Considered representative if sufficient observation stations and site-specific choice of parameters by the modeller.</li> </ul>	<ul style="list-style-type: none"> <li>•Sasol operated surface meteorological weather stations (3 Sasolburg and 3 Secunda)</li> <li>•Closest upper air monitoring station is at OR Tambo International Airport (twice-daily soundings only)</li> </ul>	Very good if upper air and surface stations are located close to the facility and if upper air data are recorded at sunrise and sunset.	<ul style="list-style-type: none"> <li>•Upper air data typically 12 hourly, poor spatial and temporal resolution</li> <li>•Model has to interpolate between 12 hour soundings</li> <li>•SOUNDINGS at incorrect time of the day.</li> </ul>

<sup>3</sup> AJ Jacobs (WS, WD, SO<sub>2</sub>, NO<sub>2</sub>, PM<sub>10</sub>, PM<sub>2.5</sub>); Leitrim (WS, WD, TEMP, AMB PRESS, RH, SO<sub>2</sub>, NO<sub>2</sub>, PM<sub>10</sub>, PM<sub>2.5</sub>) and Eco Park (WS, WD, TEMP, RH, AMB PRESS, SOL RAD, RAIN, SO<sub>2</sub>, O<sub>3</sub>, NO<sub>2</sub>, PM<sub>10</sub>, PM<sub>2.5</sub>)

<sup>4</sup> Sasol Club (WS, WD, TEMP, NO<sub>2</sub>, SO<sub>2</sub>, O<sub>3</sub>, PM<sub>10</sub>, PM<sub>2.5</sub>, CO); Bosjesspruit (WS, WD, TEMP, NO<sub>2</sub>, SO<sub>2</sub>, H<sub>2</sub>S, PM<sub>10</sub>, PM<sub>2.5</sub>) and Embalenhle (WS, WD, TEMP, NO<sub>2</sub>, SO<sub>2</sub>, PM<sub>10</sub>, PM<sub>2.5</sub>, Benzene)

Run Type	Description of Run Type	Ease of Use and Representativeness	Data availability	Advantages	Disadvantages
					•User has to deal with missing surface and upper air data

## APPENDIX D: CALPUFF MODEL CONTROL OPTIONS

The CALPUFF run type selected for this assessment has been highlighted in blue in Table D-1 below.

**Table D-1: CALPUFF model control options**

Run Type	Description of Run Type	Ease of Use and Representativeness	Data availability	Advantages	Disadvantages
Sampling Function Puff	This sampling scheme employs radically symmetric Gaussian puffs and is suitable for far field.				
Sampling Function Slug	This sampling scheme uses a non-circular puff (a "slug"), elongated in the direction of the wind during release, to eliminate the need for frequent releases of puffs. Used for near field during rapidly-varying meteorological conditions.				Takes a very long time to run.
Dispersion coefficients MDISP = 1	<ul style="list-style-type: none"> <li>Dispersion coefficients are computed from measured values of turbulence, sigma-v and sigma-w.</li> </ul>	<ul style="list-style-type: none"> <li>The user must provide an external PROFILE.DAT file containing these parameters, and select a backup method out of options 2, 3 and 4 below in case of missing data.</li> </ul>	<ul style="list-style-type: none"> <li>This measured data is not available in South Africa</li> </ul>	<ul style="list-style-type: none"> <li>Very good if data is available.</li> </ul>	<ul style="list-style-type: none"> <li>These measured parameters are not readily available in South Africa.</li> </ul>
Dispersion coefficients MDISP = 2	<ul style="list-style-type: none"> <li>Dispersion coefficients are computed from internally-calculated sigma-v, sigma-w using micrometeorological variables (<math>u^*</math>, <math>w^*</math>, <math>L</math>, etc.).</li> </ul>	<ul style="list-style-type: none"> <li>This option can simulate AERMOD-type dispersion when the user also selects the use of PDF method for dispersion in the convective boundary layer (MPDF = 1). Note that when simulating AERMOD-type dispersion, the input meteorological data must be from CALMET and cannot be ISC-type ASCII format data. The user should also be aware that under this option the</li> </ul>	<ul style="list-style-type: none"> <li>The data is obtained from WRF input information.</li> </ul>	<ul style="list-style-type: none"> <li>Based on improved theoretical work and is an improvement over Pasquill-Gifford.</li> </ul>	<ul style="list-style-type: none"> <li>The coefficients are derived from other parameters.</li> </ul>

Run Type	Description of Run Type	Ease of Use and Representativeness	Data availability	Advantages	Disadvantages
		CALPUFF model will be more sensitive to the appropriateness of the land use characterization.			
Dispersion coefficients MDISP = 3	<ul style="list-style-type: none"> <li>Pasquill-Gifford (PG) dispersion coefficients for rural areas (computed using the ISCST3 multi-segment approximation) and McElroy-Pooler (MP) coefficients in urban areas.</li> </ul>	<ul style="list-style-type: none"> <li>The current default selection is MDISP = 3, which is ISC-type dispersion. Given the demonstrated improved characterization of dispersion provided by AERMOD, and EPA's intention to replace ISC with AERMOD, use of AERMOD-like dispersion (MDISP = 2, and MPDF = 1) is also acceptable, but likely will be of most benefit for short-range complex flow applications.</li> </ul>		<ul style="list-style-type: none"> <li>Simple to use if you don't have detailed meteorological information. This option can be run using fairly basic meteorological data.</li> </ul>	<ul style="list-style-type: none"> <li>Based on discreet classification scheme (not continuous function). Based on field experiments done elsewhere, may or may not be representative of Highveld area. Previous projects done using this scheme however have provided good correlation over this area.</li> </ul>
Dispersion coefficients MDISP = 4	<ul style="list-style-type: none"> <li>Same as MDISP = 3, except PG coefficients are computed using the MESOPUFF II equations</li> </ul>				
Dispersion coefficients MDISP = 5	<ul style="list-style-type: none"> <li>CTDM sigmas are used for stable and neutral conditions. For unstable conditions, sigmas are computed as in MDISP=3 described above.</li> </ul>	<ul style="list-style-type: none"> <li>When selecting this option, the user must provide an external PROFILE.DAT file, and select a backup method out of options 2, 3 and 4 above in case of missing data.</li> </ul>			
Chemical transformation RIVAD	<ul style="list-style-type: none"> <li>Pseudo-first-order chemical mechanism for SO<sub>2</sub>, SO<sub>4</sub><sup>2-</sup>, NO, NO<sub>2</sub>, HNO<sub>3</sub>, and NO<sub>3</sub> - (RIVAD/ARM3 method)</li> </ul>	<ul style="list-style-type: none"> <li>RIVAD is a 6-species scheme wherein NO and NO<sub>2</sub> are treated separately.</li> <li>In the RIVAD scheme the conversion of SO<sub>2</sub> to sulfates is not RH-dependent.</li> <li>The conversion of NO<sub>x</sub> to nitrates is RH-dependent.</li> </ul>	<ul style="list-style-type: none"> <li>In order to use the RIVAD scheme, the user must divide the NO<sub>x</sub> emissions into NO and NO<sub>2</sub> for each source.</li> <li>Two options are specified for the ozone concentrations: (1) hourly ozone concentrations from a network of stations, or (2)</li> </ul>	<ul style="list-style-type: none"> <li>In several tests conducted to date, the results have shown no significant differences between the RIVAD and MESOPUFF II options.</li> </ul>	<ul style="list-style-type: none"> <li>User has to input the NO and NO<sub>2</sub> emissions which are not always known for all sources.</li> <li>User has to input the ozone concentrations which are not always known.</li> <li>The model is restricted to rural conditions.</li> </ul>

Run Type	Description of Run Type	Ease of Use and Representativeness	Data availability	Advantages	Disadvantages
			<p>a single user defined ozone value.</p> <ul style="list-style-type: none"> <li>The background ammonia concentrations required for the HNO<sub>3</sub>/NH<sub>4</sub>NO<sub>3</sub> equilibrium calculation can be user-specified or a default value will be used.</li> </ul>		
Chemical transformation MESOPUFF II	<ul style="list-style-type: none"> <li>Pseudo-first-order chemical mechanism for SO<sub>2</sub>, SO<sub>4</sub><sup>2-</sup>, NO<sub>x</sub>, HNO<sub>3</sub>, and NO<sub>3</sub>- (MESOPUFF II method)</li> </ul>	<ul style="list-style-type: none"> <li>MESOPUFF II is a 5-species scheme in which all emissions of nitrogen oxides are simply input as NO<sub>x</sub>.</li> <li>In the MESOPUFF II scheme, the conversion of SO<sub>2</sub> to sulfates is dependent on relative humidity (RH), with an enhanced conversion rate at high RH.</li> <li>The conversion of NO<sub>x</sub> to nitrates is RH-dependent.</li> </ul>	<ul style="list-style-type: none"> <li>The MESOPUFF II scheme assumes an immediate conversion of all NO to NO<sub>2</sub>.</li> <li>Two options are specified for the ozone concentrations: (1) hourly ozone concentrations from a network of stations, or (2) a single user defined ozone value.</li> <li>The background ammonia concentrations required for the HNO<sub>3</sub>/NH<sub>4</sub>NO<sub>3</sub> equilibrium calculation can be user-specified or a default value will be used.</li> </ul>	<ul style="list-style-type: none"> <li>In several tests conducted to date, the results have shown no significant differences between the RIVAD and MESOPUFF II options for sulfate and nitrate formation.</li> <li>The model is applicable to both urban and rural conditions.</li> </ul>	<ul style="list-style-type: none"> <li>User has to input the ozone concentrations which are not always known.</li> <li>NO to NO<sub>2</sub> conversion is not included. In model.</li> </ul>
User-specified diurnal cycles of transformation rates					
No chemical conversion					

## APPENDIX E: THE NO<sub>2</sub>/NO<sub>x</sub> CONVERSION RATIOS FOR NO<sub>2</sub> FORMATION

Scire and Borissova (2011) analysed hourly monitored NO<sub>2</sub> and NO<sub>x</sub> data for 2006 at 325 monitoring sites throughout USA (approximately 2.8 million data points for each species). These observations were grouped into a number of concentration bins and were used to compute bin maximums and bin average curves. Short-term (1-hr) NO<sub>2</sub>/NO<sub>x</sub> ratios were developed on bin-maximum data, whereas the long-term (annual average) NO<sub>2</sub>/NO<sub>x</sub> ratios were based on bin-averaged data. The method was subsequently tested using the NO<sub>2</sub>/NO<sub>x</sub> ratios applied to the observed NO<sub>x</sub> at selected stations to predict NO<sub>2</sub>, and then compared to observed NO<sub>2</sub> concentrations at that station. As illustrated in the examples, Figure E-1 and Figure E-2, using these empirical curves provide a reasonable estimate of the observed NO<sub>2</sub> can be obtained, albeit mostly more conservative. In Figure E-3, the method is compared to the assumption of 100% conversion over the short-term, which clearly illustrates the extreme conservatism, especially at elevated concentrations.

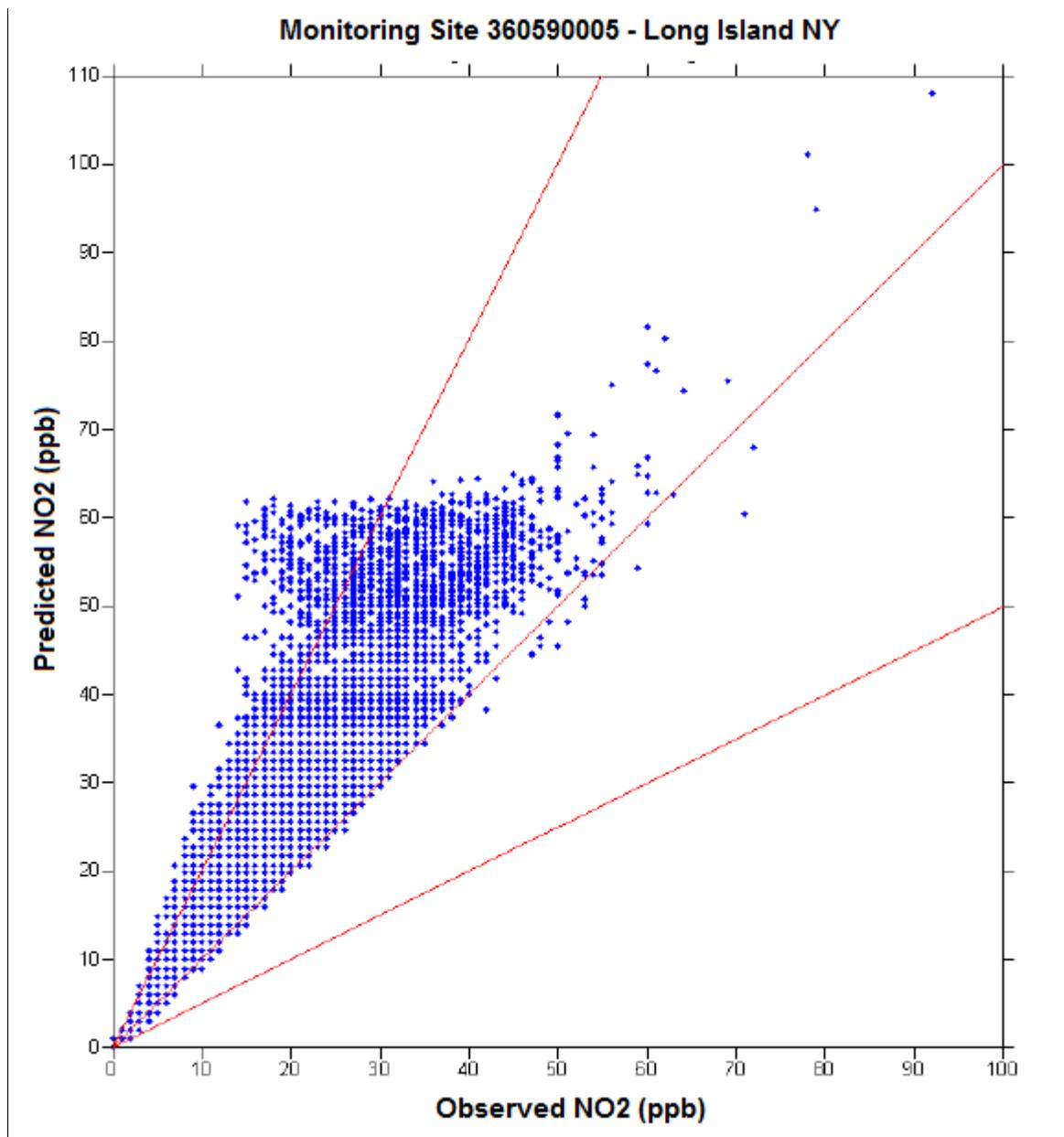


Figure E-1: Comparison of observed with predicted NO<sub>2</sub> concentrations (Long Island, NY) using the derived short-term NO<sub>2</sub>/NO<sub>x</sub> ratios (Scire and Borissova, 2011)

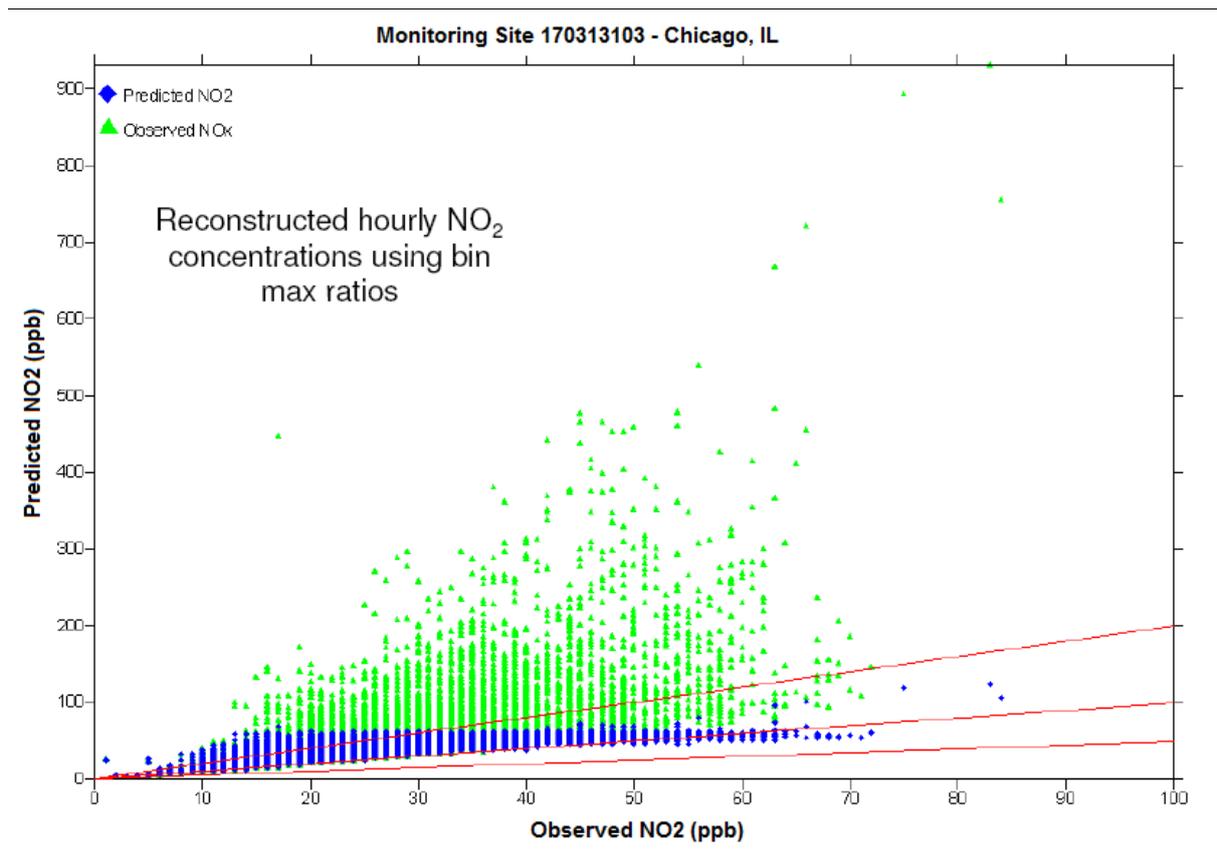


Figure E-2: Comparison of observed with predicted NO<sub>2</sub> concentrations (Chicago, IL) using the derived short-term NO<sub>2</sub>/NO<sub>x</sub> ratios (Scire and Borissova, 2011)

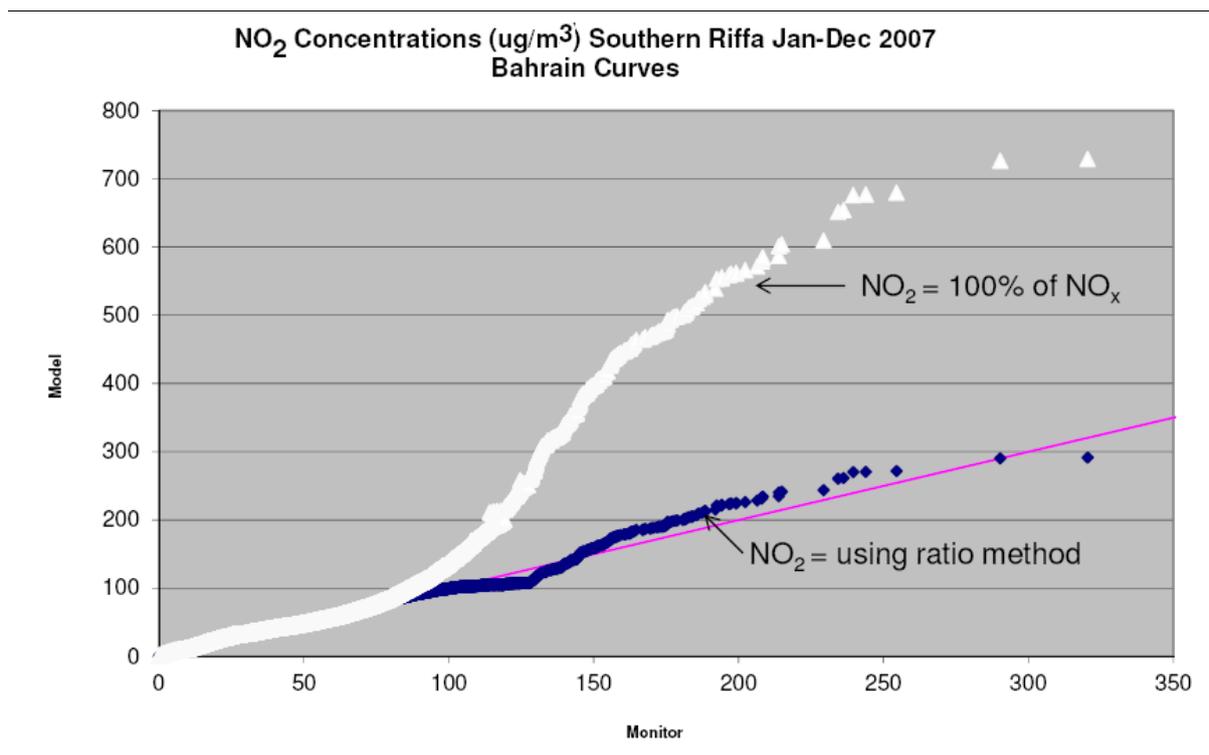


Figure E-3: Observed versus predicted NO<sub>2</sub> concentrations (Bahrain) using the derived short-term NO<sub>2</sub>/NO<sub>x</sub> ratios (Scire and Borissova, 2011)

It was decided that the NO<sub>2</sub>/NO<sub>x</sub> conversion factors described by Scire and Borissova (2011) and as given in Table E-1, will be employed in this study. Observed NO<sub>2</sub>/NO<sub>x</sub> ratios at the Sasolburg monitoring stations were also analysed and compared to the factors in the table (Figure E-1). It is shown in the table and Figure E-4, that the Scire and Borissova ratios would also be applicable in the current study since it would produce estimates similar or more conservative than if the actual NO<sub>2</sub>/NO<sub>x</sub> ratios at the site would have been used instead.

Table E-1: NO<sub>2</sub>/NO<sub>x</sub> conversion ratios for NO<sub>2</sub> formation

Bin	Concentration (µg/m <sup>3</sup> )			NO <sub>2</sub> /NO <sub>x</sub> Ratios			
				Sasolburg		Scire and Borissova 2011	
	Min	Max	Centre	AJ Jacobs 2010-2012	Ecopark 2012	Bin Average	1-Hour Max
1	0	19	9	0.658	0.521	0.7980	0.9938
2	19	38	28	0.714	0.605	0.8130	0.9922
3	38	75	56	0.657	0.501	0.7306	0.9844
4	75	113	94	0.506	0.428	0.5544	0.9094
5	113	150	132	0.380	0.305	0.4370	0.7477
6	150	188	169	0.309	0.117	0.3553	0.6085
7	188	235	212	0.265	0.311	0.3013	0.4976
8	235	282	259	0.222	0.019	0.2559	0.4173
9	282	329	306	0.208	0.114	0.2276	0.3543
10	329	376	353	0.184	0.105	0.2081	0.3056
11	376	423	400	0.216	0.164	0.1852	0.2684
12	423	470	447	0.161	0.114	0.1809	0.2404

Bin	Concentration ( $\mu\text{g}/\text{m}^3$ )			NO <sub>2</sub> /NO <sub>x</sub> Ratios			
				Sasolburg		Scire and Borissova 2011	
	Min	Max	Centre	AJ Jacobs 2010-2012	Ecopark 2012	Bin Average	1-Hour Max
13	470	517	494	0.135	0.101	0.1767	0.2194
14	517	564	541		0.153	0.1546	0.2035
15	564	611	588		0.119	0.1524	0.1912
16	611	658	635		0.071	0.1476	0.1813
17	658	705	682		0.169	0.1402	0.1726
18	705	752	729		0.157	0.1363	0.1645
19	752	846	799		0.133	0.1422	0.1527
20	846	940	893		0.164	0.1223	0.1506
21	940	1128	1034		0.164	0.1087	0.1474
22	1128	1316	1222			0.1110	0.1432
23	1316	1504	1410			0.1112	0.139
24	1504	1786	1645			0.1165	0.1337

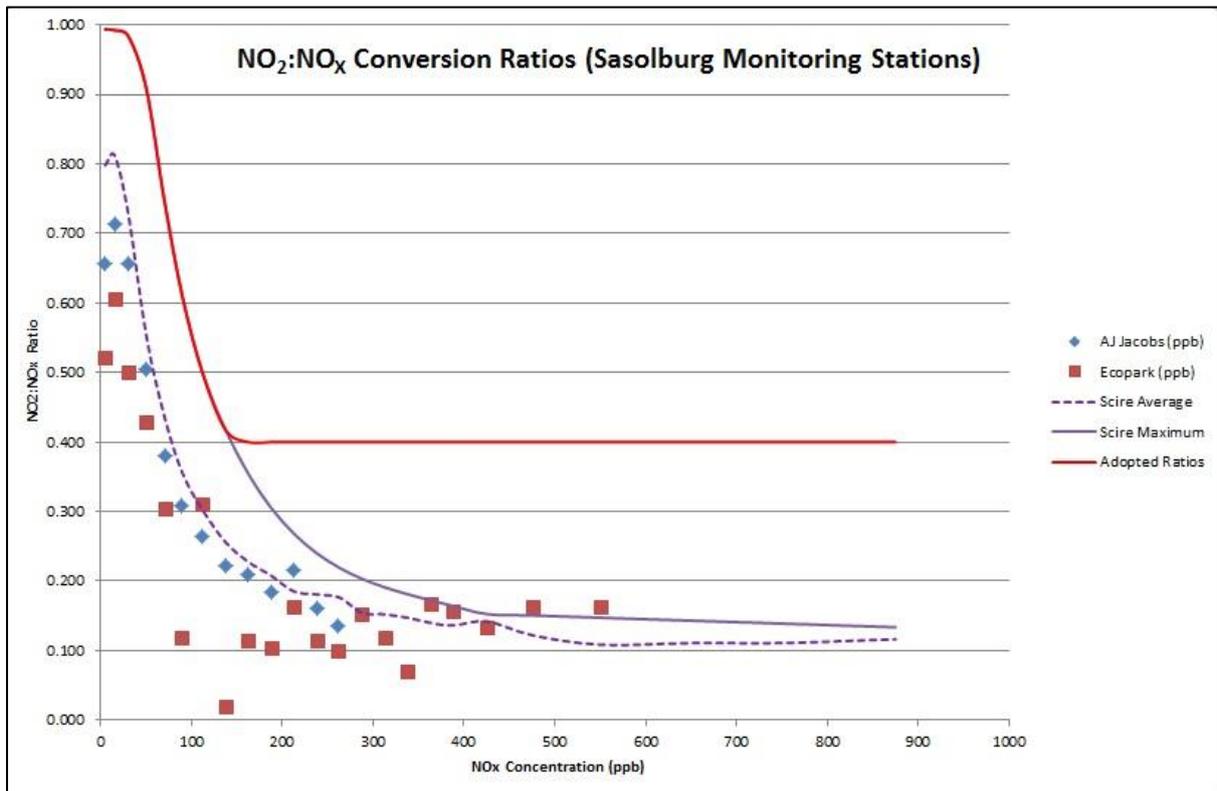


Figure E-4: NO<sub>2</sub>/NO<sub>x</sub> conversion ratios for Sasol's Sasolburg monitoring stations

## APPENDIX F: TIME SERIES PLOTS FOR THE MEASURED AMBIENT AIR QUALITY IN THE STUDY AREA

A summary of the time series plots for the measured data as provided by Sasol is given in the following section.

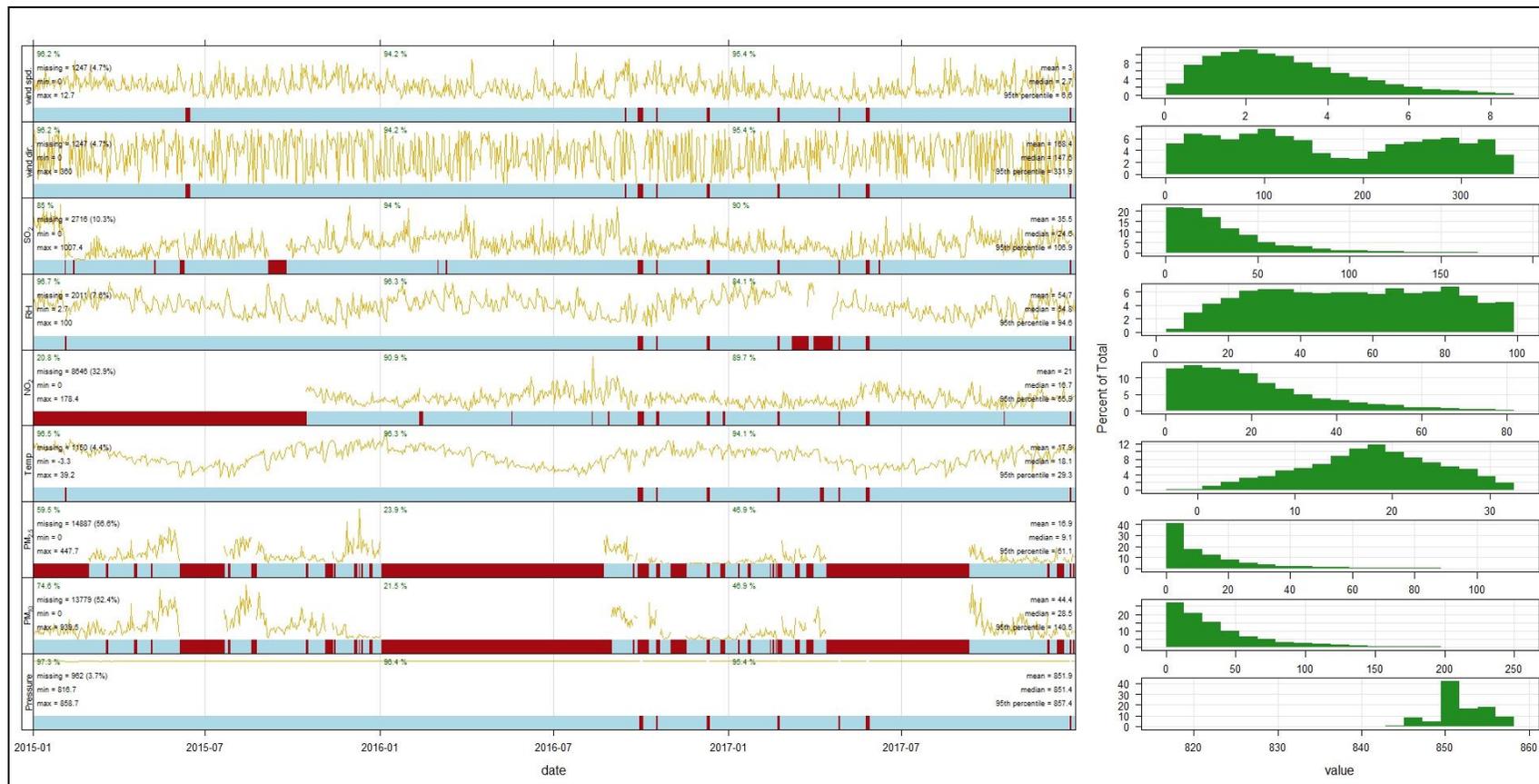


Figure F-1: Summary of meteorological and ambient air quality data received for Leitrim (2015-2017)

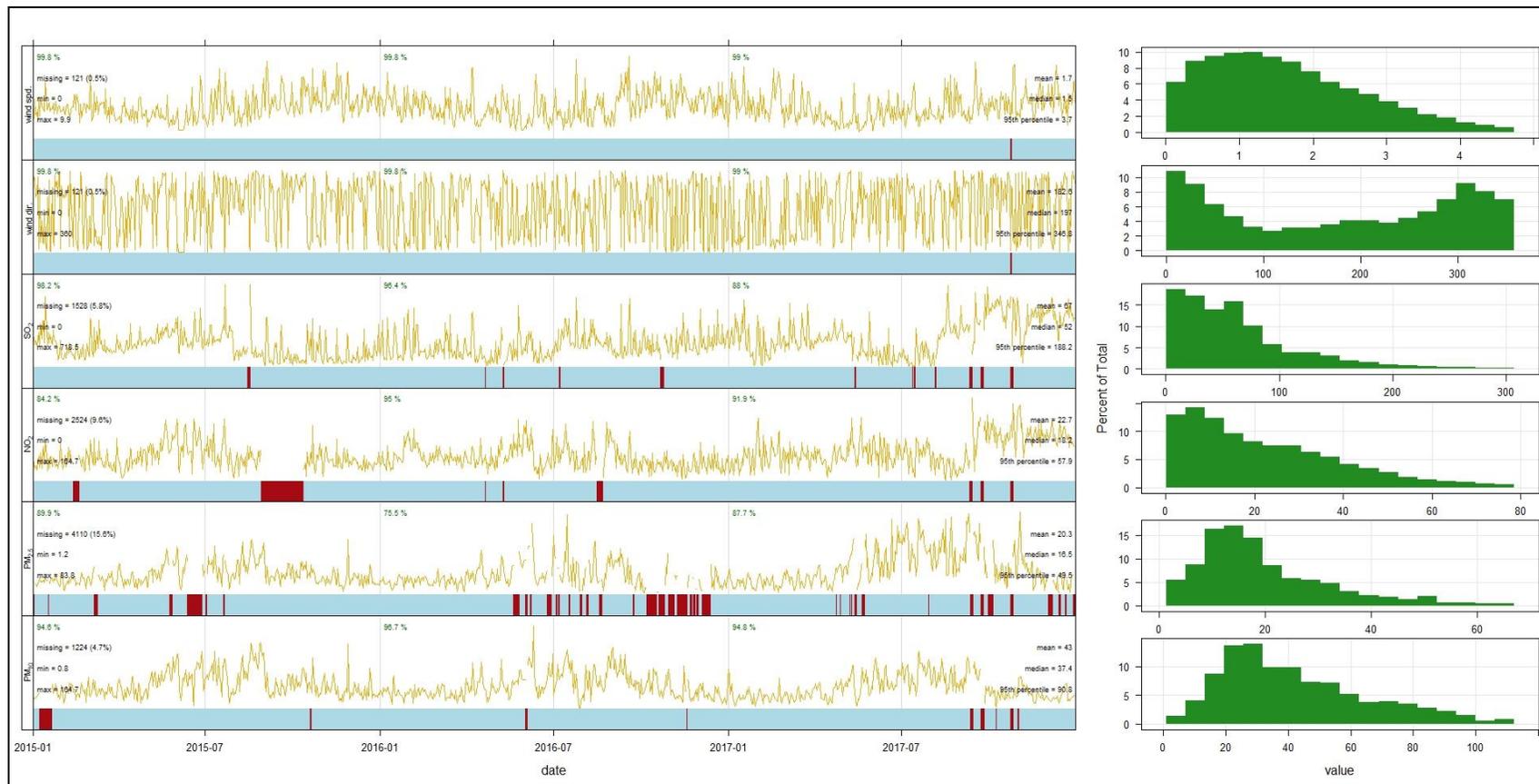


Figure F-2: Summary of meteorological and ambient air quality data received for AJ Jacobs (2015-2017)

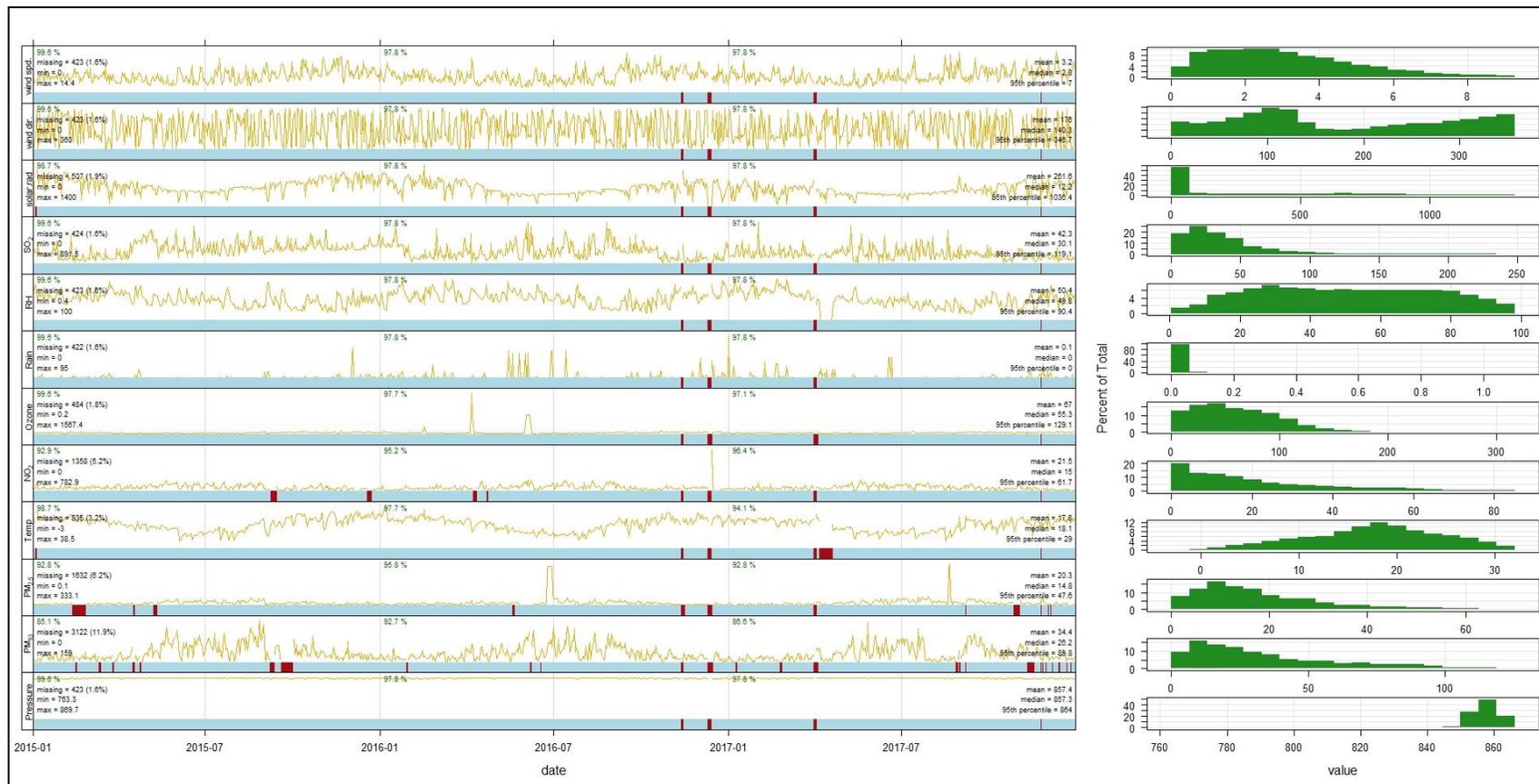


Figure F-3: Summary of meteorological and ambient air quality data received for Eco Park (2015-2017)

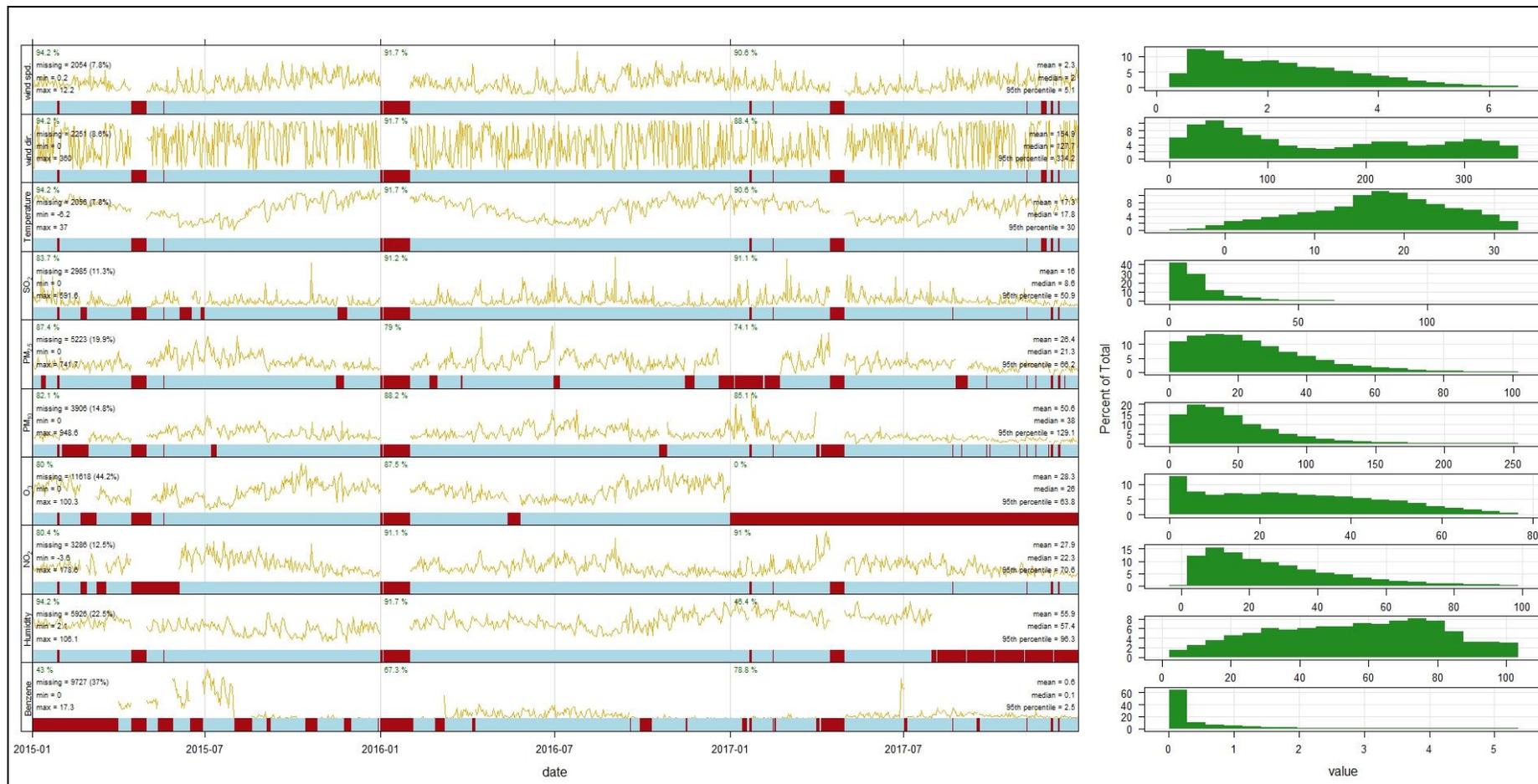


Figure F-4: Summary of meteorological and ambient air quality data received for Three Rivers (2015-2017)

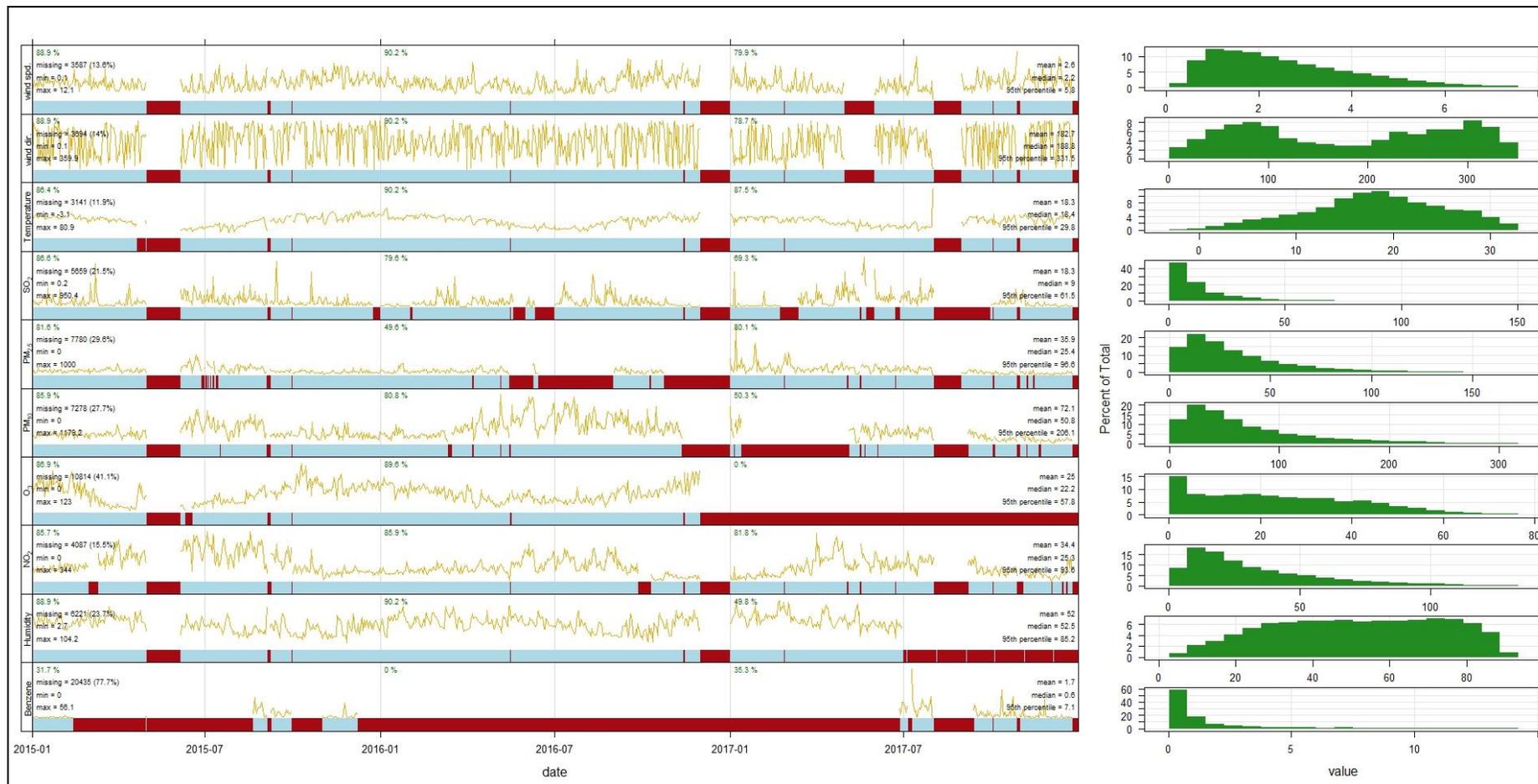


Figure F-5: Summary of meteorological and ambient air quality data received for Sharpeville (2015-2017)

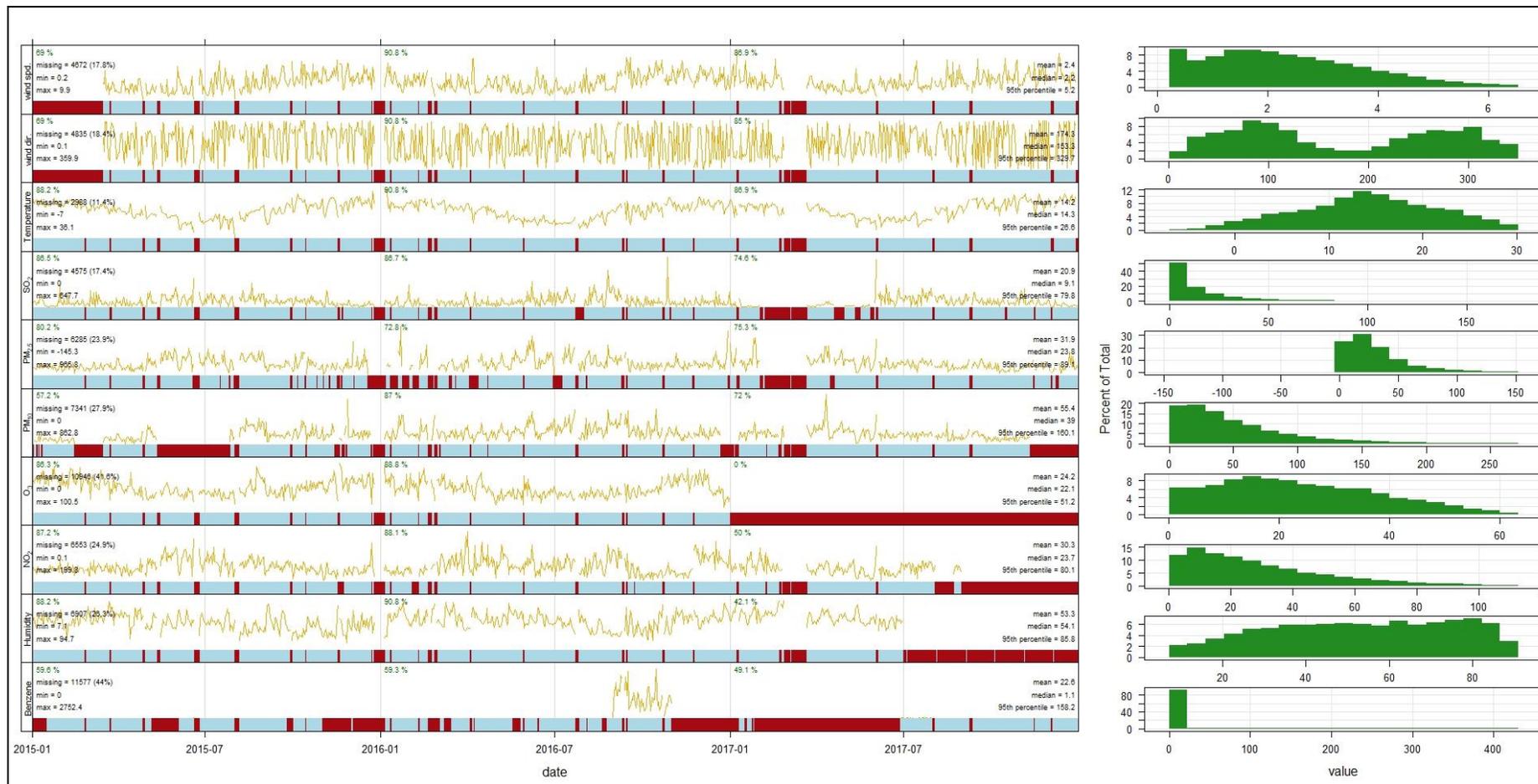


Figure F-6: Summary of meteorological and ambient air quality data received for Zamdela (2015-2017)

## APPENDIX G: PREDICTED BASELINE AND OBSERVED AIR CONCENTRATIONS

The following tables summarise the predicted baseline SO<sub>2</sub> and NO<sub>2</sub> concentrations at the Sasol and DEA monitoring site locations, respectively. The peak (maximum), 99<sup>th</sup>, 90<sup>th</sup>, 50<sup>th</sup> and annual average values are given for each of the simulated (SO and Natref combined) years, 2015, 2016 and 2017. The corresponding observed concentration values are also summarised in the tables for comparison. Estimates of background concentrations were obtained from the observed values at the ranked position when no contributions from the simulated sources were predicted.

**Table G-1: Simulated SO<sub>2</sub> concentration from routine emissions and observed SO<sub>2</sub> concentration statistics**

Description	Year	SO <sub>2</sub> Concentration (µg/m <sup>3</sup> )											
		Leitrim		AJ Jacobs		Eco Park		Three Rivers		Sharpeville		Zamdela	
		Simulated	Observed	Simulated	Observed	Simulated	Observed	Simulated	Observed	Simulated	Observed	Simulated	Observed
Maximum	2015	196.6	1007.4	435.5	603.6	176.5	881.5	37.9	591.6	65.4	950.4	337.0	414.5
	2016	254.7	515.9	454.6	676.0	157.7	842.4	31.6	474.8	59.3	512.3	344.4	647.7
	2017	187.0	425.8	409.3	718.5	311.6	891.5	66.6	539.3	75.8	462.8	290.8	356.1
	<i>Average</i>	212.8	649.7	433.2	666.0	215.3	871.8	45.4	535.2	66.8	641.8	324.1	472.8
99 <sup>th</sup> Percentile	2015	65.4	185.0	156.0	284.1	33.4	239.4	10.7	110.1	12.9	135.8	101.1	172.7
	2016	68.6	204.6	157.2	307.3	53.3	261.6	10.2	163.3	15.3	127.1	98.2	185.3
	2017	66.8	172.6	197.7	320.6	45.7	230.4	11.7	141.6	14.0	180.7	96.1	165.6
	<i>Average</i>	66.9	187.4	170.3	304.0	44.1	243.8	10.9	138.3	14.1	147.9	98.4	174.6
90 <sup>th</sup> Percentile	2015	22.9	82.3	4.3	111.2	0.7	89.9	0.5	30.3	0.4	38.3	31.8	52.4
	2016	22.1	78.5	7.1	120.8	1.2	82.5	0.5	30.5	0.6	34.0	29.9	52.6
	2017	22.4	70.3	12.6	173.4	1.2	65.5	0.5	36.2	0.7	49.0	30.0	44.3
	<i>Average</i>	22.4	77.0	8.0	135.2	1.0	79.3	0.5	32.3	0.6	40.4	30.6	49.8
50 <sup>th</sup> Percentile	2015	0.0	20.0	0.0	46.4	0.0	42.8	0.0	8.0	0.0	10.9	0.1	9.2
	2016	0.0	28.4	0.0	40.7	0.0	28.2	0.0	7.6	0.0	7.0	0.1	9.8
	2017	0.0	24.6	0.0	78.0	0.0	21.2	0.0	10.1	0.0	8.8	0.0	8.2
	<i>Average</i>	0.0	24.3	0.0	55.0	0.0	30.7	0.0	8.6	0.0	8.9	0.1	9.1
Annual Average	2015	5.7	33.3	5.7	56.3	1.1	51.5	0.4	14.5	0.5	19.1	8.1	21.4
	2016	5.7	39.3	6.9	57.1	1.8	41.8	0.4	15.5	0.6	15.2	8.1	22.1
	2017	5.5	33.5	9.4	89.7	1.8	33.4	0.5	17.9	0.6	20.8	7.8	18.7
	<i>Average</i>	5.7	35.4	7.3	67.7	1.6	42.2	0.5	16.0	0.6	18.4	8.0	20.7
Background (observed value when simulation indicated little)	2015		26.7		64.3		72.7		22.4		30.3		10.4
	2016		36.6		54.3		59.1		21.3		22.8		10.9
	2017		30.0		101.3		44.3		26.2		34.4		9.9

Description	Year	SO <sub>2</sub> Concentration (µg/m <sup>3</sup> )											
		Leitrim		AJ Jacobs		Eco Park		Three Rivers		Sharpeville		Zamdela	
		Simulated	Observed	Simulated	Observed	Simulated	Observed	Simulated	Observed	Simulated	Observed	Simulated	Observed
contribution (0.1 µg/m <sup>3</sup> )	Average		31.1		73.3		58.7		23.3		29.2		10.4

**Table G-2: Simulated NO<sub>2</sub> concentration from routine emissions and observed NO<sub>2</sub> concentration statistics**

Description	Year	NO <sub>2</sub> Concentration (µg/m <sup>3</sup> )											
		Leitrim		AJ Jacobs		Eco Park		Three Rivers		Sharpeville		Zamdela	
		Simulated	Observed	Simulated	Observed	Simulated	Observed	Simulated	Observed	Simulated	Observed	Simulated	Observed
Maximum	2015	97.8	178.4	269.8	127.4	97.5	782.9	36.3	178.6	54.8	344.0	193.6	168.1
	2016	138.9	140.7	248.5	125.4	94.9	373.1	43.5	148.4	54.3	176.8	272.3	199.8
	2017	144.2	117.4	249.2	164.7	174.6	439.8	57.3	178.2	54.9	104.0	144.4	141.7
	Average	127.0	145.5	255.8	139.2	122.3	531.9	45.7	168.4	54.6	208.3	203.4	169.9
99 <sup>th</sup> Percentile	2015	57.8	64.9	94.2	79.6	36.4	85.1	12.6	104.6	17.7	156.7	63.8	100.4
	2016	58.4	87.2	104.8	73.3	48.0	86.0	12.2	92.1	19.1	104.7	61.6	123.2
	2017	57.5	77.9	135.3	81.4	46.8	84.2	14.1	95.1	18.4	55.9	61.1	91.3
	Average	57.9	76.7	111.4	78.1	43.7	85.1	12.9	97.3	18.4	105.8	62.2	105.0
90 <sup>th</sup> Percentile	2015	22.8	39.0	10.7	46.3	1.2	52.9	0.6	64.5	0.6	96.3	38.4	62.4
	2016	22.1	47.8	15.8	42.8	1.8	51.1	0.6	53.1	1.0	62.7	39.1	73.4
	2017	22.9	42.9	22.6	52.1	1.8	49.2	0.7	54.3	0.9	34.1	36.5	55.8
	Average	22.6	43.2	16.3	47.1	1.6	51.1	0.6	57.3	0.8	64.4	38.0	63.9
50 <sup>th</sup> Percentile	2015	0.0	17.3	0.0	15.3	0.0	15.9	0.0	24.8	0.0	31.3	0.1	24.6
	2016	0.0	17.6	0.0	16.1	0.0	15.0	0.0	21.9	0.0	22.6	0.1	24.2

Description	Year	NO <sub>2</sub> Concentration (µg/m <sup>3</sup> )											
		Leitrim		AJ Jacobs		Eco Park		Three Rivers		Sharpeville		Zamdela	
		Simulated	Observed	Simulated	Observed	Simulated	Observed	Simulated	Observed	Simulated	Observed	Simulated	Observed
	2017	0.0	15.4	0.0	25.1	0.0	14.4	0.0	20.8	0.0	11.6	0.1	21.3
	<i>Average</i>	<i>0.0</i>	<i>16.8</i>	<i>0.0</i>	<i>18.8</i>	<i>0.0</i>	<i>15.1</i>	<i>0.0</i>	<i>22.5</i>	<i>0.0</i>	<i>21.8</i>	<i>0.1</i>	<i>23.4</i>
Annual Average	2015	6.0	21.2	5.2	21.0	1.2	22.3	0.5	31.5	0.7	43.9	8.0	30.1
	2016	6.0	22.8	6.6	20.3	1.7	21.5	0.5	26.4	0.8	29.7	8.3	32.6
	2017	5.9	19.2	8.2	26.6	1.8	20.5	0.6	26.3	0.8	15.7	7.6	26.4
	<i>Average</i>	<i>6.0</i>	<i>21.1</i>	<i>6.7</i>	<i>22.7</i>	<i>1.6</i>	<i>21.5</i>	<i>0.6</i>	<i>28.1</i>	<i>0.8</i>	<i>29.8</i>	<i>8.0</i>	<i>29.7</i>
Background (observed value when simulation indicated little contribution (0.1 µg/m <sup>3</sup> ))	2015		19.3		23.3		39.2		53.8		77.1		24.6
	2016		20.6		20.5		33.4		43.6		48.9		24.2
	2017		18.9		30.1		32.8		44.6		27.0		22.2
	<i>Average</i>		<i>19.6</i>		<i>24.6</i>		<i>35.1</i>		<i>47.3</i>		<i>51.0</i>		<i>23.6</i>

## APPENDIX H: MANAGEMENT OF UNCERTAINTIES

### Dispersion Model Uncertainties

In the US EPA Guideline on Air Quality Models (U.S. EPA, 2017), the need to address the uncertainties associated with dispersion modelling is acknowledged as an important issue that should be considered. The US Guideline divides the uncertainty associated with dispersion model predictions into two main types (U.S. EPA, 2017), as follows:

- Reducible uncertainty, which results from (1) Uncertainties in the input values of the known conditions (i.e., emission characteristics and meteorological data); (2) errors in the measured concentrations which are used to compute the concentration residuals; and (3) inadequate model physics and formulation. The “reducible” uncertainties can be minimized through better (more accurate and more representative) measurements and better model physics.
- Inherent uncertainty is associated with the stochastic (turbulent) nature of the atmosphere and its representation (approximation) by numerical models. Models predict concentrations that represent an ensemble average of numerous repetitions for the same nominal event. An individual observed value can deviate significantly from the ensemble value. This uncertainty may be responsible for a  $\pm 50\%$  deviation from the measured value.

Atmospheric dispersion models are often criticised for being inadequate since “...it is only a model approximating reality”, and therefore include inherent uncertainty. Both reducible and inherent uncertainties mean that dispersion modelling results may over- or under-estimate measured ground-level concentrations at any specific time or place. However, the US EPA Guideline on Air Quality Models (U.S. EPA, 2017) also states that:

*“Models are more reliable for estimating longer time-averaged concentrations than for estimating short-term concentrations at specific locations; and the models are reasonably reliable in estimating the magnitude of highest concentrations occurring sometime, somewhere within an area. For example, errors in highest estimated concentrations of  $\pm 10$  to 40 percent are found to be typical, certainly well within the often-quoted factor-of-two accuracy that has long been recognized for these models.”*

To minimise the overall uncertainty, but specifically the “reducible uncertainty”, the following simple principles were followed in the investigation:

- Understanding the objectives of the investigation;
- Demonstrating that the model inputs are as correct as possible;
- Understanding and stating the model performance limitations;
- Demonstrating that the modelling process has been conducted appropriately and in line with both local DEA requirements and international practice;
- Including any validating information from monitoring that might be available; and,
- To be conservative in cases where there is greater uncertainty (e.g. conversion of NO to NO<sub>2</sub>).

Although the existence of model uncertainty is well-accepted, it does not exclude the use of dispersion modelling results in making important air quality impact decisions. The uncertainties should simply be acknowledged and understood that, given their inherent uncertainty, current dispersion models are a “best-case” approximation of what are otherwise very complex physical processes in the atmosphere. An accepted dispersion model (i.e., CALPUFF) was selected for the analysis to minimize some of these uncertainties. The US EPA states that when dispersion models such as CALPUFF are used to assess ground-level concentration and when a sufficiently large number of meteorological conditions are considered, the modelling results should ideally fall well within the often quoted “factor of two” accuracy for these modelled (U.S. EPA, 2017).

## Validation of Predictions

Model verification and validation (V&V) are the primary processes for quantifying and building credibility in numerical models. There are distinct differences between the two processes, as described below:

- Verification is the process of determining that a model implementation accurately represents the developer's conceptual description of the model and its solution.
- Validation is the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.

Whilst V&V cannot prove that a model is correct and accurate for all possible scenarios, it can provide evidence that the model is sufficiently accurate for its intended use.

A rigorous V&V programme was not completed as part of the study; however, regular sanity checks on model results and comparisons with observations were done, as discussed in Section 5.1.6. An attempt was also made to quantify the level of agreement between observed data and model prediction, as well as the predictive accuracy of the model once the necessary adjustments have been made (such as including the estimated background concentrations). In this regard, the CALPUFF model's performance was evaluated by comparing the modelling results for the years 2015, 2016 and 2017 to the monitoring data collected over the same time period. In particular, the predicted SO<sub>2</sub> and NO<sub>2</sub> concentrations arising from both the SO and Natref plant were included in the comparison.

The performance evaluation was completed using the fractional bias method, since this statistical technique is one of the evaluation methods recommended by the U.S. EPA for determining dispersion model performance (U.S. EPA 1992). The fractional bias was computed for SO<sub>2</sub> and NO<sub>2</sub> as predicted and observed at monitoring stations within the study area. The fractional biases of the means were shown to be well within a factor of two, which the U.S. EPA consider to be a reasonable performance target for a dispersion model before it is used for refined regulatory analysis (U.S. EPA 1992).

## Scenario Simulations

Since the focus of the study has been to illustrate the relative changes with the introduction of different emission conditions (i.e. emission rates, exit gas temperatures and velocities), whilst maintaining the same stack heights and diameters, it is expected that the model errors would mostly be carried between the different modelling scenarios. Therefore, expressing the changes as incremental and relative to the baseline scenario, it is expected that these errors would be mostly cancel each other out.

## Ambient Monitoring Uncertainty

Sasol operates a total of four ambient air quality monitoring stations in and around Sasolburg, namely at Sasol 1 Fence Line, AJ Jacobs, Leitrim and Eco Park. No data was provided for the Sasol 1 Fence Line monitoring station. The DEA operate three monitoring stations in the study area, namely Zamdela, Three Rivers and Sharpeville. Data from the Sasol and DEA monitoring stations for 2015, 2016 and 2017 were included in this investigation.

All of the abovementioned Sasol monitoring stations are ISO/IEC17025 accredited, to ensure data integrity and data quality as well as to ensure that the data obtained from the monitoring stations are representative of the ambient air when measured. Data availability and credibility is maximised through:

- Regular (at least on a weekly basis) visits of the monitoring stations to ensure the stations are functioning properly.
- Dynamic calibrations are conducted on at a quarterly basis, however where possible more frequent calibrations have been done.
- Certified calibration gas is used and obtained from reputable vendors
- Inter-laboratory comparisons are done between Sasol's Sasolburg and Secunda monitoring stations as well as between Sasolburg, Secunda and a third-party calibration laboratory.
- Participation in the National Metrological Laboratory's national inter-laboratory comparisons to ensure that the system is in line with the rest of the accredited laboratories in South Africa.

Although the ISO/IEC 17025 System requires a quarterly data availability of 80%, Sasol's internal data availability, tracked on a monthly Scorecard, is a monthly data availability of 90%.

Based on the uncertainty calculations completed as per the ISO/IEC17025 requirements, Sasol's uncertainty in measurements on its ambient air quality monitoring stations is between 3% and 5% with a level of confidence of 95%. This has been confirmed through inter-laboratory comparisons and is confirmed on a regular basis.

### Upper Air Meteorological Data

Although meteorological data from the monitoring stations described in the previous section are available for input into the CALPUFF dispersion model, there is a lack of upper air meteorology. Furthermore, it is anticipated that the wind observations at AJ Jacobs may be compromised due to nearby trees and building structures (see Section 5.1.5.1). The lack of appropriate meteorological information is often the single most important limiting factor in modelling accuracy. It is also the most subjective in deciding just how many data are needed, from which location and how accurate they must be.

The CALMET wind field model requires, as a minimum, meteorological data from at least one surface and an upper air station. This information is then used to "seed" the three-dimensional wind field with an initial solution of a relatively simple mass conservation model. CALMET does not include momentum, energy, or moisture conservation equations, and is therefore classified as a diagnostic model.

It is expected, that a wind field developed using all the parameters that could influence the flow, thermal and turbulence mechanisms should improve the accuracy of the dispersion predictions. For simulated data, the Weather Research and Forecasting mesoscale model (known as WRF) was used. The WRF Model is a next-generation mesoscale numerical weather prediction system designed for both atmospheric research and operational forecasting needs. It features two dynamical cores, a data assimilation system, and a software architecture facilitating parallel computation and system extensibility. The model serves a wide range of meteorological applications across scales from tens of meters to thousands of kilometres. WRF can generate atmospheric simulations using real data (observations, analyses) or idealized conditions. WRF offers operational forecasting a flexible and computationally-efficient platform, while providing recent advances in physics, numeric, and data assimilation contributed by developers across the very broad research community.

WRF data for the study domain was purchased from Lakes Environmental that has proven record of generating WRF data ready for use in the CALMET modelling suite. The dataset included the years 2015, 2016 and 2017 at 4 km resolution for a 200 km by 200 km study area. The model setup used for WRF was provided by Lakes Environmental and is included in Appendix K.

The WRF model together with the meteorological observations provide a 'first-guess field', which is then modified by the CALMET diagnostic model to take account of terrain and land-use features that are at a smaller spatial scale than the terrain

used by the prognostic model. The main purpose of this approach is to increase the horizontal resolution of the meteorological fields.

### **Emission Inventory Uncertainty**

In addition to meteorological input data, the uncertainty associated with the emissions inventory needs to be accommodated in the results. All emissions used in the simulations of the baseline condition were based on iso-kinetic measurement campaigns.

Natref makes use of reputable sampling companies for its third party measurement campaign. All third party (and *ad hoc*) sampling requests (or requirements) for Natref has to comply with AQA Section 21, Schedule 2 of the Listed Activities and Minimum Emission Standard. Furthermore, Natref has, as far as possible, standardised on US EPA sampling methodologies. Analyses of the samples are also done by an ISO/IEC17025 accredited laboratory to further control the quality of the results.

Where *ad hoc* sampling is done, Natref's philosophy is aligned with the requirements of the AQA Section 21, namely that all point sources must be sampled at least once a year.

#### Third-Party Emission Monitoring

The uncertainty associated with third-party emission's measurements is considered to be up to 10% with a level of confidence of 95%. This uncertainty is based on the isokineticity of the isokinetic sampling, as well as the uncertainty associated with the sample taking and chemical analysis of gaseous components.

According to the Natref quality control system, all third-party contractors for isokinetic sampling need to comply with the following control criteria:

- Their entire sampling staffs undergo the training associated with the UK-based Monitoring Certification Scheme (MCERTS): Manual Stack emissions monitoring program (MCERTS 2011);
- An electronic automated sampler is used for all isokinetic sampling;
- The pitot tubes used for sampling are calibrated at least on a quarterly basis;
- The pneumatic pressure sensors on the sampler are also calibrated on at least a quarterly basis; and
- The dry gas meters are checked on a regular basis and replaced every 6 months.

#### Ad-Hoc Emissions Sampling

SANAS is compiling an accreditation system for *ad hoc* sampling and as soon as this system is in place, the uncertainty of the measurements will be confirmed; however it is not expected to be higher than 10%.

The Minimum Emission Standards requires that sampling be conducted at normal operating conditions; therefore the emissions information included in the dispersion model is aligned with normal operating conditions on site. The sampling schedule is communicated to the plant managers with the aim of having process conditions as representative as possible to normal operations. Sampling upset conditions often poses a challenge from both a logistical and safety point of view, since safety requirements require as few people as possible on the plant during severe upset conditions and therefore sampling cannot be done during such conditions.

#### PM<sub>2.5</sub> and PM<sub>10</sub> Air Emissions

All particulate matter was assumed to be PM<sub>2.5</sub> since it was not possible to establish the PM<sub>2.5</sub>/PM<sub>10</sub> split.

Non-Natref Air Emissions

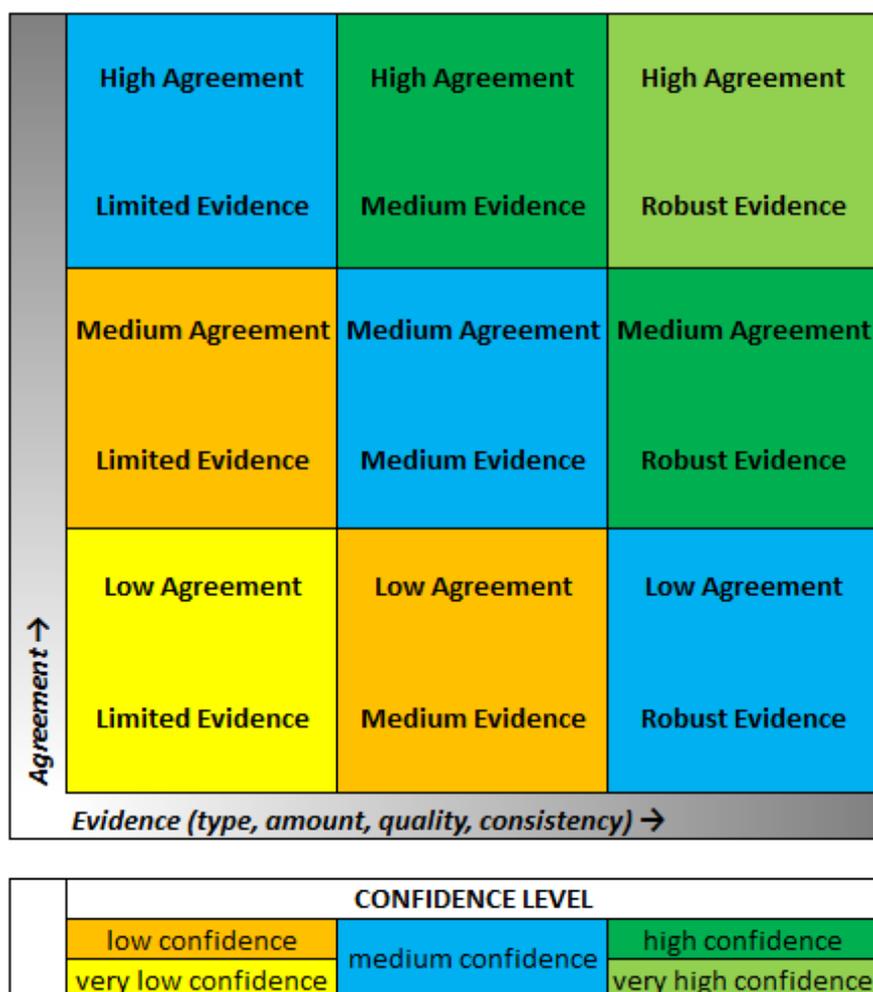
No attempt was made to estimate the emissions from non-industrial activities within regional communities. Instead, the community contribution (and other sources) of a particular compound was discussed in Section 5.1.5.4. and Section 5.1.6.

## APPENDIX I: GUIDANCE NOTE ON TREATMENT OF UNCERTAINTIES

The Intergovernmental Panel on Climate Change (IPCC) produced a Guidance Note for lead authors of the IPCC Fifth Assessment Report on consistent treatment of uncertainties. These notes define a common approach and calibrated language that can be used broadly for developing expert judgments and for evaluating and communicating the degree of certainty in findings of the assessment process. Communicating the degree of certainty in key findings relies on expressing the:

- Confidence in the validity of a finding, based on the type, amount, quality, and consistency of evidence (e.g., mechanistic understanding, theory, data, models, expert judgment) and the degree of agreement. Confidence is expressed qualitatively.
- Quantified measures of uncertainty in a finding expressed probabilistically (based on statistical analysis of observations or model results, or expert judgment).

The Guidance Note proposes the use of the following dimensions to evaluate the validity of a finding: the type, amount, quality, and consistency of evidence (summary terms: “limited,” “medium,” or “robust”), and the degree of agreement (summary terms: “low,” “medium,” or “high”), as summarised in the figure below.



**Figure I-1: A depiction of evidence and agreement statements and their relationship to confidence. Confidence increases towards the top-right corner as suggested by the increasing strength of shading. Generally, evidence is most robust when there are multiple, consistent independent lines of high-quality evidence.**

Generally, evidence is most robust when there are multiple, consistent independent lines of high-quality evidence. The guide further provides advice for a traceable account describing the evaluation of evidence and agreement, as follows:

- For findings with high agreement and robust evidence, present a level of confidence or a quantified measure of uncertainty.
- For findings with high agreement or robust evidence, but not both, assign confidence or quantify uncertainty when possible. Otherwise, assign the appropriate combination of summary terms for your evaluation of evidence and agreement (e.g., robust evidence, medium agreement).
- For findings with low agreement and limited evidence, assign summary terms for your evaluation of evidence and agreement.
- In any of these cases, the degree of certainty in findings that are conditional on other findings should be evaluated and reported separately.

A level of confidence is expressed using five qualifiers: “very low,” “low,” “medium,” “high,” and “very high.” It synthesizes the author teams’ judgments about the validity of findings as determined through evaluation of evidence and agreement. Figure I-1 depicts summary statements for evidence and agreement and their relationship to confidence. There is flexibility in this relationship; for a given evidence and agreement statement, different confidence levels could be assigned, but increasing levels of evidence and degrees of agreement are correlated with increasing confidence. Confidence cannot necessarily be assigned for all combinations of evidence and agreement in Figure I-1. Presentation of findings with “low” and “very low” confidence should be reserved for areas of major concern, and the reasons for their presentation should be carefully explained. Confidence should not be interpreted probabilistically, and it is distinct from “statistical confidence.” Additionally, a finding that includes a probabilistic measure of uncertainty does not require explicit mention of the level of confidence associated with that finding if the level of confidence is “high” or “very high.”

Likelihood, as defined in Table I-1, provides calibrated language for describing quantified uncertainty. It can be used to express a probabilistic estimate of the occurrence of a single event or of an outcome (e.g., a climate parameter, observed trend, or projected change lying in a given range). Likelihood may be based on statistical or modelling analyses, elicitation of expert views, or other quantitative analyses.

**Table I-1: Likelihood scale**

Term	Likelihood of the Outcome
Virtually certain	99-100% probability
Very likely	90-100% probability
Likely	66-100% probability
About as likely as not	33 to 66% probability
Unlikely	0-33% probability
Very unlikely	0-10% probability
Exceptionally unlikely	0-1% probability

The categories defined in this table can be considered to have “fuzzy” boundaries. A statement that an outcome is “likely” means that the probability of this outcome can range from  $\geq 66\%$  (fuzzy boundaries implied) to 100% probability. This implies that all alternative outcomes are “unlikely” (0-33% probability). When there is sufficient information, it is preferable to specify the full probability distribution or a probability range (e.g., 90-95%) without using the terms in Table I-1. “About as likely as not” should not be used to express a lack of knowledge.

## APPENDIX J: SENSITIVE RECEPTORS INCLUDED IN THE DISPERSION MODEL SIMULATIONS

Table J-1: Discrete sensitive receptors included in the dispersion model simulations

Receptor code name	Receptor details	Distance from centre of operations (km)
Leitrim	Sasol Leitrim monitoring station	5.1
AJ Jacobs	Sasol AJ Jacobs monitoring station	3.5
EcoPark	Sasol EcoPark monitoring station	3.8
Three Rivers	VTAPA Three Rivers monitoring station	21.8
Sharpeville	VTAPA Sharpeville monitoring station	13.0
Zamdela	VTAPA Zamdela monitoring station	4.2
34	HTS Secondary School	2.3
43	Sasolburg Provincial Hospital	3.0
52	Sasolburg Clinic	3.2
24	Lumiere Primary School	3.3
14	AJ Jacobs Primary School	3.3
19	Fonteine Primary School	3.4
25	Malakabeng Primary School	3.6
15	Bofula-Tshepe Primary School	4.0
29	Tsatsi Primary School	4.0
32	Cedar Secondary School	4.0
51	Zamdela Hospital Zumayear	4.1
42	Vaalpark Hospital	4.1
38	Sasolburg High School	4.1
49	Clinic A Zamdela	4.2
33	Fakkal Secondary School	4.3
37	Nkopoleng Secondary School	4.3
36	Kahobotjha-sakubusha Secondary School	4.3
35	Iketsetseng Secondary School	4.3
48	Clinic B Zamdela	4.3
39	Vaalpark Articon Secondary School	4.4
20	Isaac Mhlambi Primary School	4.4
26	Noord Primary School	4.5
44	Zamdela Community Clinic	4.9
30	Vaalpark Primary School	5.0
28	Theha Setjhaba Primary	5.2
18	Credo Primary School	5.3
31	Afrikaans Hoërskool	5.6
22	Leewspruit Primary	5.6
23	Lehutso Primary School	5.7
50	Harry Gwala Clinic   Creche	5.7
21	Kopanelang Thuto Primary School	8.3
41	Vaal Christian Secondary	10.0
40	Pele-ya-pele Secondary School	10.5
27	Taaibos Primary School	11.3
17	Vukuzake Primary School	12.3
16	Bokantsho Primary School	20.0

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**LAKES ENVIRONMENTAL WRF MODELING**

**DRAFT**

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**1 Introduction**

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This document provides a brief description of WRF modeling at *Lakes Environmental* and the type of outputs generated. Our WRF modeling focuses on generating high resolution data with enough information to create meteorological input files for the CALPUFF and AERMOD modeling systems.

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**2 WRF Description**

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The Weather Research and Forecasting model (WRF) is a prognostic meteorology model developed in a collaborative partnership between the U.S. National Center for Atmospheric Research (NCAR), the National Centers for Environmental Prediction (NCEP), and others. The WRF model is a limited-area, non-hydrostatic, terrain-following sigma-coordinate model designed to simulate or predict mesoscale and regional-scale atmospheric circulation.



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### 3 WRF Processing Specifications

#### 3.1 Input of Meteorological Data

WRF does not directly use conventional meteorological data from airport reports. Instead, the model uses objective analysis of global weather reports. Objective analysis is a process of analyzing the observed data and outputting them into a regular grid. The meteorological field is “balanced” to account for the energy and momentum equations of the atmosphere. These objective analyses are products of global models, which are maintained by national weather centers or federal agencies such as UKMO (United Kingdom Meteorological Office) or US NCEP.

Lakes Environmental used the NCEP Global Forecast System (GFS) 0.5-degree resolution data (approximately 50-km resolution) for input into WRF. GFS 0.5-deg data is given every 6 hours at 00, 06, 12, and 18Z.

Sea Surface Temperature (SST) data comes from the GFS 0.5 degree data but updated daily as each WRF simulation is done for 24 hours.

#### 3.2 Nested Grids Domains

WRF uses a nested grid approach allowing an area of interest to be modeled without the penalty of excessive run times created by having a fine grid over the entire modeling domain. Depending on the application, Lakes Environmental employs 12-km or 4-km grid spacing at the highest resolution (inner grid).

Tables 1 presents the grid dimensions and number of grid points that that are commonly used.

**Table 1. WRF Nested Domain Grids**

Domain	Resolution (km)	Number of Grid Points in X and Y
Domain 1	36	31 x 31
Domain 2	12	31 x 31
Domain 3 (if necessary)	4	31 x 31



### 3.3 WRF Physics Options

The WRF model provides many modeling options which can greatly affect the final output. In Table 2 below, we have listed the physics options most commonly used for the WRF processing.

**Table 2. Physics Options Used for WRF Modeling**

WRF Physics Options		
#	Type	Options Used
1	Microphysics	WSM 3-class scheme mp_physics = 3
2	Long-wave Radiation	RRTM Logwave scheme ra_lw_physics = 1
3	Short-wave Radiation	Dudhia Shortwave ra_sw_physics = 1
4	Surface Layer	Monin-Obukhov (MM5 MRF PBL) sf_sfclay_physics = 1
5	Land Surface	Unified Noah Land Surface model sf_surface_physics = 2
6	Planetary Boundary Layer	Yonsei University scheme (YSU) bl_pbl_physics = 1
7	Cumulus parameterization	Betts-Miller-Janjic scheme cu_physics = 2

See link below to the UCAR web site for descriptions and references of WRF physics options:

[http://www2.mmm.ucar.edu/wrf/users/wrfv3.5/phys\\_references.html](http://www2.mmm.ucar.edu/wrf/users/wrfv3.5/phys_references.html)

### 3.4 Additional WRF Modeling Information

The information below describes other modeling parameters taken into account for *Lakes Environmental* WRF processing:

- WRF-ARW and WPS models Version 3.6
- Map projection in Lambert Conformal Conic (LCC)
- 35 ETA vertical pressure levels
- USGS 24 land use category data

In addition to the above options, a spin up time of 6 hours for each daily run was used. This means that every 24-hour run was composed of 30 hours where the 6 preceding hours are used for proper daily initialization. The initialization process discards these 6 initial hours which are not saved in the output as part of the meteorological modeling run.

### 3.5 WRF Output for AERMET

The US EPA Mesoscale Model Interface Program (MMIF) is a tool that retrieves data from NCAR's WRF-ARW model output in netCDF format and generates surface and upper air data files that can be used by the US EPA AERMET model (meteorological pre-processor for the US EPA AERMOD air dispersion model).

Data for use in AERMET/AERMOD are extracted from the innermost domain for the center of the grid cell closest to the user-defined latitude/longitude coordinate. Outer domains are used only to provide information to the innermost domain.

The latest version of the MMIF program is used. Table 3 contains a description of the files that were generated by the MMIF program where METxxxxx is the order number, yyyy is the starting year, and zzzz is the ending year.

**Table 3. Files Generated by MMIF**

#	File Name	Description
1	METxxxxx_AERMET_ yyyy-zzzz.IN1	AERMET Stage 1 Input File
2	METxxxxx_AERMET_ yyyy-zzzz.IN2	AERMET Stage 2 Input File
3	METxxxxx_AERMET_ yyyy-zzzz.IN3	AERMET Stage 3 Input File
4	METxxxxx_AERMET_ yyyy-zzzz.DAT	Onsite Surface Met File
5	METxxxxx_AERMET_ yyyy-zzzz.FSL	FSL Upper Air Met File



### 3.6 WRF Output for CALMET

CALWRF is a tool that retrieves data from NCAR's WRF-ARW model output in netCDF format and creates a 3D.DAT file suitable for input into the CALMET model. The CALWRF output forms a grid covering the requested modeling domain with the requested resolution of either 4 km or 12 km. CALMET is a 3-D diagnostic meteorological pre-processor for CALPUFF model. CALPUFF is an advanced non-steady-state air quality dispersion model. CALWRF, CALMET, and CALPUFF are from Exponent. See below additional information on the CALWRF executable currently in use at Lakes Environmental:

- CALWRF.EXE, Version 2.0.1, Level 130418
- Generates 3D.DAT file in Version 2.1 format

The output from CALWRF is an ASCII file, known as the 3D.DAT format, which contains output variables for each hour, for each pressure level, and for each grid cell. Table 4 below describes the output variables.

**Table 4. Variables Available in 3D.DAT File**

#	Parameter	Units
1	Pressure	(mb)
2	Elevation	(m above mean sea level)
3	Temperature	(K)
4	Wind direction	(deg)
5	Wind speed	(m/s)
6	Vertical wind velocity	(m/s)
7	Relative humidity	(%)
8	Vapor mixing ratio	(g/kg)
9	Cloud mixing ratio	(g/kg)
10	Rain mixing ratio	(g/kg)

In addition, Table 5 describes the surface variables reported for each hour and each grid cell under the 3D.DAT file.

**Table 5. Surface Variables Available in 3D.DAT File**



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#	Parameter	Units
1	Sea level pressure	(hPa)
2	Total rainfall accumulated for the past hour	(cm)
3	Snow cover indicator	-
4	Short wave radiation at the surface	(W / m <sup>2</sup> )
5	Long wave radiation at the top	(W / m <sup>2</sup> )
6	Air temperature at 2 m	(K)
7	Specific humidity at 2 m	(g/kg)
8	Wind direction of 10 m wind	(deg)
9	Wind speed of 10 m wind	(m/s)
10	Sea surface temperature	(K)

### 3.7 WRF Output for CALPUFF

The Mesoscale Model Interface Program (MMIF) converts prognostic meteorological model output fields to formats required for direct input into dispersion models. The utility was developed by ENVIRON International Corporation for the USEPA and is distributed via the USEPA's website. The utility reads data from NCAR's WRF-ARW model output in netCDF format and creates data in a user-specified format.

MMIF can be used to generate data for direct input to the CALPUFF model bypassing the CALMET model entirely. Output can be processed for use in either CALPUFF version 5.8.x or CALPUFF version 6 / 7. MMIF generates three sets of files:

- **Projection File:** This file contains information on the domain, projection, and met grid to be used in the CALPUFF project.
- **Terrain Grid File:** This is a gridded file containing terrain elevations (from mean sea level) to be used in the extraction of base elevations for sources and receptors in the CALPUFF project.
- **CALPUFF-Ready Meteorological Data Files:** The meteorological data to be input to CALPUFF.

#### 4 Additional Information

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If you require any further information, please contact us at [support@weblakes.com](mailto:support@weblakes.com). When contacting us, please provide the met data order number.

For more information about the WRF meteorological model, please visit the site below:

<http://www.wrf-model.org/index.php>



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