



AIRSHED
PLANNING PROFESSIONALS

Atmospheric Impact Report: Natref

Project done on behalf of **National Petroleum Refineries of South Africa (Pty) Ltd.**

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Revision Record

Revision Number	Date	Reason for Revision
Rev 0	October 2018	Draft for client review
Rev 1	November 2018	Update of short-term impacts for alternative scenario and incorporation of comments from client
Rev 2	November 2018	Update of impact results
Rev 3	November 2018	Incorporation of client comments
Rev 4	February 2019	Re-wording of the scenario's
Rev 5	March 2019	Incorporation of client comments

Preface

The Natref Facility (Natref) is required to comply with the Minimum Emissions Standards, which came into effect in terms of Section 21 of the National Environment Management: Air Quality Act (Act No 39 of 2004) on 1 April 2010 and subsequently replaced by GN893, of 22 November 2013. The Minimum Emission Standards were subsequently amended, and the amendments were promulgated on 22 November 2013 (Government Gazette No. 37054), replacing the 2010 regulations. These standards require the refinery operations to comply with standards for “new plant” by 1 April 2020. Guided by the technical investigations, Natref intends to apply for the postponements of the Compliance Timeframes as provided for in Regulation 11 of the Minimum Emission Standards in cases where compliance with the relevant standard can ultimately be achieved but not within the prescribed timeframe. In support of the submissions and to fulfil the requirements for these applications stipulated in the Air Quality Act and the Minimum Emissions Standards, an Atmospheric Impact Report (AIR) is required to substantiate the motivations for the postponement application.

At the Natref Refinery in Sasolburg, imported crude oil is converted into “white products” such as petrol and diesel. The main air pollutants from the Natref operations include sulfur dioxide (SO₂), nitric oxide (NO) and nitrogen dioxide (NO₂) collectively known as NO_x, particulate matter (PM) and volatile organic compounds (VOC).

Airshed Planning Professionals (Pty) Ltd (hereafter referred to as Airshed) was appointed by Natref to provide independent and competent services for the compilation of an Atmospheric Impact Report as set out in the Regulations Prescribing the Format of the Atmospheric Impact Report (Government Gazette No. 36904, 11 October 2013). The tasks to be undertaken consist of:

- 1) Review of emissions inventory and identification of any gaps in the emissions inventory. It is preferable that gaps be estimated using an agreed emission estimation technique.
- 2) Prepare meteorological input files for use in one or more dispersion model to cover the Natref site. Sasol will provide surface meteorological data and ambient air quality data from the Sasol ambient air quality monitoring stations. Surface meteorological data for three years, as required by the Dispersion Modelling Guidelines for Level 3 Assessments (Government Gazette No 37804 published 11 July 2014), is available for ambient air quality monitoring stations.
- 3) Preparation of one or more dispersion model set up with Natref’s emissions inventory capable of running various scenarios for each of the point sources as specified by Natref. The intent is to model delta impacts of the various emission scenarios against an acceptable measured airshed baseline.
- 4) Airshed will validate the dispersion model based on a fractional bias approach.
- 5) It is anticipated that three scenarios be modelled:
 - a. Scenario 1 – 100% SRU availability
 - b. Scenario 2 – 99% SRU availability, compliance to the legislative requirement as stipulated within the Listed Activities and Minimum Emissions Standards (for new plant standards).
 - c. Scenario 3 – 95% SRU availability as per current Natref AEL requirement.
- 6) Comparison of dispersion modelling results with the National Ambient Air Quality Standards (NAAQS).
- 7) A report detailing the methodology used and model setup must be compiled for purposes of a peer review, which Natref will contract independently.
- 8) Interactions with the Environmental Assessment Practitioner (EAP) to provide all necessary inputs into the EAP’s compilation of documentation in support of Natref’s application. Airshed will attend all Public Participation meetings scheduled by the EAP to address any queries pertaining to the dispersion model.

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Abbreviations

AGO	Atmospheric Gas Oil
AIR	Atmospheric Impact Report
AQA	Air quality act
AQMS	Air quality monitoring stations
APCS	Air pollution control systems
ARM	Ambient Ratio Method
ASG	Atmospheric Studies Group
BPIP	Building Profile Input Program
C₆H₆	Benzene
CDU	Crude Distillation Unit
CO	Carbon monoxide
CO₂	Carbon dioxide
DEA	Department of Environmental Affairs
DHC	Distillate Hydrocracker
FCC	Fluidized Catalytic Cracker
ft	Feet
g	Gram
gal	Gallon
g/s	Gram per second
HNO₃	Nitric acid
H₂S	Hydrogen Sulfide
HVGO	Heavy Vacuum Gas Oil
IPCC	Intergovernmental Panel on Climate Change
LMo	Monin-Obukhov length
LSR	Light straight run (light Naphtha)
LPG	Liquefied Petroleum Gas
m	Meter
m²	Square Meter
m³	Cubic Meter
MES	Minimum Emission Standards
m/s	Meters per second
MVGO	Medium Vacuum Gas Oil
NAAQS	National Ambient Air Quality Standards (as a combination of the NAAQ Limit and the allowable frequency of exceedance)
NEMA	National Environmental Management Act
NEMAQA	National Environmental Management Air Quality Act
NH₃	Ammonia
NO	Nitrogen oxide
NO₂	Nitrogen dioxide
NO_x	Oxides of nitrogen
O₃	Ozone
OH	Hydroxyles
OLM	Ozone Limiting Method
PBL	Planetary boundary layer

Pb	Lead
PM	Particulate matter
PM₁₀	Particulate matter with diameter of less than 10 µm
PM_{2.5}	Particulate matter with diameter of less than 2.5 µm
ppb	Parts per billion
RCD	Reduced Crude Desulfurisation
SO₂	Sulfur dioxide ⁽¹⁾
SO₄	Sulfates ⁽¹⁾
SWS	Sour Water Stripper
US EPA	United States Environmental Protection Agency
USGS	United States Geological Survey
VOC	Volatile organic compound
WRF	The Weather Research and Forecasting Mesoscale Model
yr	Year
Z₀	Roughness length
µ	micro
°C	Degrees Celsius

Note:

- (1) The spelling of "sulfur" has been standardised to the American spelling throughout the report. "The International Union of Pure and Applied Chemistry, the international professional organisation of chemists that operates under the umbrella of UNESCO, published, in 1990, a list of standard names for all chemical elements. It was decided that element 16 should be spelled "sulfur". This compromise was to ensure that in future searchable data bases would not be complicated by spelling variants. (IUPAC. Compendium of Chemical Terminology, 2nd ed. (the "Gold Book"). Compiled by A. D. McNaught and A. Wilkinson. Blackwell Scientific Publications, Oxford (1997). XML on-line corrected version: <http://goldbook.iupac.org> (2006) created by M. Nic, J. Jirat, B. Kosata; updates compiled by A. Jenkins. ISBN 0-9678550-9-8.doi: 10.1351/goldbook")

Glossary

Advection	Transport of pollutants by the wind
Airshed	An area, bounded by topographical features, within which airborne contaminants can be retained for an extended period
Algorithm	A mathematical process or set of rules used for calculation or problem-solving, which is usually undertaken by a computer
Assessment of environmental effects	A piece of expert advice submitted to regulators to support a claim that adverse effects will or will not occur as a result of an action, and usually developed in accordance with section 88 of the Resource Management Act 1991
Atmospheric chemistry	The chemical changes that gases and particulates undergo after they are discharged from a source
Atmospheric dispersion model	A mathematical representation of the physics governing the dispersion of pollutants in the atmosphere
Atmospheric stability	A measure of the propensity for vertical motion in the atmosphere
Building wakes	Strong turbulence and downward mixing caused by a negative pressure zone on the lee side of a building
Calm / stagnation	A period when wind speeds of less than 0.5 m/s persist
Cartesian grid	A co-ordinate system whose axes are straight lines intersecting at right angles
Causality	The relationship between cause and effect
Complex terrain	Terrain that contains features that cause deviations in direction and turbulence from larger-scale wind flows
Configuring a model	Setting the parameters within a model to perform the desired task
Convection	Vertical movement of air generated by surface heating
Convective boundary layer	The layer of the atmosphere containing convective air movements
Data assimilation	The use of observations to improve model results – commonly carried out in meteorological modelling
Default setting	The standard (sometimes recommended) operating value of a model parameter
Diagnostic wind model (DWM)	A model that extrapolates a limited amount of current wind data to a 3-D grid for the current time. It is the 'now' aspect, and makes the model 'diagnostic'.
Diffusion	Clean air mixing with contaminated air through the process of molecular motion. Diffusion is a very slow process compared to turbulent mixing.
Dispersion	The lowering of the concentration of pollutants by the combined processes of advection and diffusion
Dispersion coefficients	Variables that describe the lateral and vertical spread of a plume or a puff
Dry deposition	Removal of pollutants by deposition on the surface. Many different processes (including gravity) cause this effect.

Atmospheric Impact Report: Natref

1 ENTERPRISE DETAILS

1.1 Enterprise Details

The details of Natref's Operations are summarised in Table 1-1. The contact details of the responsible person, the Emission Control Officer, are provided in Table 1-2.

Table 1-1: Enterprise details

Enterprise Name	National Petroleum Refiners of South Africa (Pty) Ltd.
Trading as	NATREF
Type of Enterprise	Company
Company Registration Number	1967/012994/07
Registered Address	Northern Industries, Jan Haak Road, Sasolburg
Telephone Number (General)	016 940 9111
Fax Number (General)	016 940 2503
Industry Type/Nature of Trade	Petrochemical refinery
Land Use Zoning as per Town Planning Scheme	Petroleum Refinery
Land Use Rights if Outside Town Planning Scheme	Industrial

Table 1-2: Contact details of responsible person

Responsible Person	Charlene Wassenaar (Vice President, SHERQ)
Telephone Number	016 940 2446
Cell Number	083 405 0741
Fax Number	016 940 2503
Email Address	charlene.wassenaar@natref.com
After Hours Contact Details	083 405 0741

1.2 Location and Extent of the Plant

Table 1-3: Location and extent of the plant

Physical Address of the Plant	Northern Industries, Jan Haak Road, Sasolburg
Description of Site (Where no Street Address)	N/A
Coordinates of Approximate Centre of Operations	The geographical co-ordinates have been excluded for security reasons but will be made available to the DEA under confidentiality arrangements.
Extent	2.037 km ²
Elevation Above Sea Level	1498 m
Province	Free State
Metropolitan/District Municipality	Fezile Dabi District Municipality
Local Municipality	Metsimaholo
Designated Priority Area	Vaal Triangle Airshed Priority Area (VTAPA)

1.3 Atmospheric Emission Licence and other Authorisations

The following authorisations, permits and licences related to air quality management are applicable:

- Atmospheric Emission License:
 - FDDM-MET-2013-17-P2
- Other:
 - None

2 NATURE OF THE PROCESS

2.1 Listed Activities

A summary of listed activities currently undertaken at Natref is provided in Table 2-1.

Table 2-1: Listed activities

Category of Listed Activity	Sub-category of the Listed Activity	Description of the Listed Activity
2	2.1	Combustion installations
	2.2	Catalytic cracking units
	2.3	Sulfur recovery units
	2.4	Storage and handling of petroleum products

2.2 Process Description

General

National Petroleum Refiners of South Africa (Pty) Ltd (Natref), South Africa's only inland crude oil refinery, is jointly owned by Sasol South Africa (Pty) Ltd and Total South Africa (Pty) Ltd and is located in Sasolburg, Free State.. The refinery was founded in 1968 and commissioned in 1971. Natref employs more than 600 permanent employees in Sasolburg and 80 employees at its Durban product storage facility. The refinery is situated in the Metsimaholo Local Municipality which is part of the Fezile Dabi District Municipality. Because the refinery is inland, approximately ± 600 km from the crude oil vessel offloading facilities in Durban, imported crude oil has to be pumped from Durban to the Natref facility via a pipeline.

Natref serves a market that has a limited requirement for heavy fuel oil products. With its inland location and due to the abundance of coal, the refinery's market for heavy fuel oil is limited. The refinery therefore has a process configuration that allows significant conversion of the bottom-of-the-barrel crude to saleable products, e.g. Liquid Petroleum Gas, gasoline, jet fuel, diesel, fuel oil and bitumen. The refinery uses the bottoms upgrading refining process using medium gravity crude oil and giving the refinery the capability of producing 20 percent more white product than conventional coastal refineries that have market outlets for heavy fuel oil. Conversion of vacuum residue to white products (diesel, petrol, jet fuel and LPG) was a necessity from the start. Thus, in addition to a conventional Fluidized Catalytic Cracking (FCC) unit, the refinery is equipped with a Distillate Hydrocracker (DHC) and black oil Reduced Crude Desulfurisation (RCD) Units. The refinery also produces various grades of Bitumen.

Crude Distillation Unit (CDU)

Raw Crude Oil (incorporating all fractions from LPG, Light and Heavy Naphtha, Jet fuel, Diesel, Gas Oils, Vacuum Gas Oils and Vacuum Residue) is fed into the unit. The oil feed is heated in heat exchangers which recover heat from the product streams as well as in furnaces and at various stages within the plant, different products are fractionated from the feed stream. LPG and Light Naphtha are the first to be separated in the Crude Preflash Column and fed to the Debutaniser. Within the Atmospheric Crude Distillation Column itself, Heavy Naphtha, Jet fuel, Light Diesel, Heavy Diesel and Atmospheric Gas Oil (AGO) is removed. The remainder, Atmospheric Residue, is fed through to the Vacuum Preflash Column and then to the Vacuum column, which produce various cuts of gas oils and vacuum residue.

Fluidised Catalytic Cracking (FCC)

The Natref FCC is a resid-type cracker, whereby the predominant part of the FCC feed is residual material, i.e. 70 % RCD products and 30% gasoils including the heavy product from the DHC.

The residual material is converted to various products in the reactor. Predominant reactions are cracking reactions whereby paraffins are converted to shorter paraffins and olefins. The products from the FCC are unsaturated LPG, LFCC to Petrol Blending, Light Cycle Oil to the Diesel Hydrotreater and Slurry for Fuel oil blending.

Naphtha Unifiner and Platformer

A catalytic reforming process used in the Platformer to convert low quality heavy naphtha in the presence of hydrogen, requires the input of heat in furnaces to convert the feed into a high octane petrol component. Octane improvement, the main function of the reforming process is brought about by the chemical re-arrangement of the low octane molecules into hydrocarbon components of a high octane value. Hydrogen which is produced in the Platformer as a by-product is supplied to the hydrotreating and hydrocracking units in the refinery after purification in a membrane section.

Diesel Unifiner

Diesel Hydrotreating is a catalytic refining process employing a catalyst, together with a hydrogen rich gas to:

- decompose sulfur, nitrogen and oxygen compounds
- to remove metallic compounds found in the hydrocarbon fractions and
- to provide hydrogen saturation of olefinic compounds found in the feedstock.

Diesel Unifiner is mainly employed to refine high sulfur diesel feedstock to low sulfur diesel product which requires high temperature catalytic conversion where the high feed temperature to the reactor is supplied by a furnace.

Reduced Crude Desulfurisation (RCD)

The Reduced Crude Desulfurisation (RCD) process is a catalytic hydrogenation process, which upgrades the heavy petroleum fractions (Atmospheric Residue and Vacuum Residue) by removing contaminants (sulfur, metals, etc.) requiring high temperature and pressure. The high temperatures are achieved by heating in a furnace. The product is fed to the FCC for further processing to white products.

Distillate Hydrocracker (DHC)

The DHC is used to crack Gas oils from the Crude Distillation Unit in the presence of Hydrogen to produce jet fuel and diesel as well as a light naphtha (LSR - routed to petrol blending) and heavy naphtha (routed to the Platformer unit). The heavy product from the unit is routed to the FCC. The high temperatures required for the cracking reactions are achieved by means of heating the feed in furnaces.

HF Alkylation

The aim of the Alkylation unit is to produce a high octane petrol blending component from unsaturated and saturated LPG in the presence of Hydrofluoric Acid as catalyst.

Butamer

The Butamer unit is designed to convert normal butane feed into an isomerase product, rich in isobutane. This isobutane is required as feed to the HF Alkylation unit.

Hydrogen Reformer

The objective of the unit is to produce hydrogen for consumption by consumers (DHC/RCD/DU/Butamer). The feed to the unit is mainly saturated gas (from the Amine unit) although propane (vaporized) can also supplement the feed. The steam reformer converts the hydrocarbon components (such as methane, ethane and propane) into hydrogen and CO/CO₂. The CO is converted to CO₂ which is then routed to the CO₂ plant for purification and sold as a by-product. The temperature required for the reactions is achieved by means of a furnace.

Amine Treating

The off gases from the refinery units are routed to this unit for removal of H₂S using MEA. The H₂S rich stripped gas is routed to the Sulfur unit where liquid Sulfur is produced. The H₂S free gas is used in the refinery as fuel in the various furnaces as well as feed to the Hydrogen unit (saturated off gas).

Sour Water Stripper (SWS)

The Hydrotreating and Hydrocracking units require water injection in the process equipment to prevent fouling. This water is recovered and sent to the Sour Water Stripper (SWS) to remove H₂S and NH₃ which is present in this water. The recovered H₂S and NH₃ is sent to the Sulfur unit for conversion.

Sulfur Recovery Unit

The purpose of the Sulfur Recovery Unit is to convert H₂S rich gas received from the Amine Units and the Sour Water Stripper off-gas to elemental sulfur. The Claus type process produces maximum conversion to elemental sulfur in the reactors of the unit. The liquid sulfur which is produced is dispatched to external customers.

Utilities

The refinery processes require steam as a form of energy for pumps and heating. This steam is produced in waste heat boilers in the refinery units and in 3 main boilers in the Utilities area. A Demineralisation unit supplies demineralised water for this steam production. In addition condensate is recovered from the units and recycled to the boilers. Fuel oil is supplied to the refinery units as fuel in some furnaces and boilers. Fuel gas from the Amine unit is distributed in the refinery as fuel in furnaces. Four cooling towers supply cooling water to the refinery units.

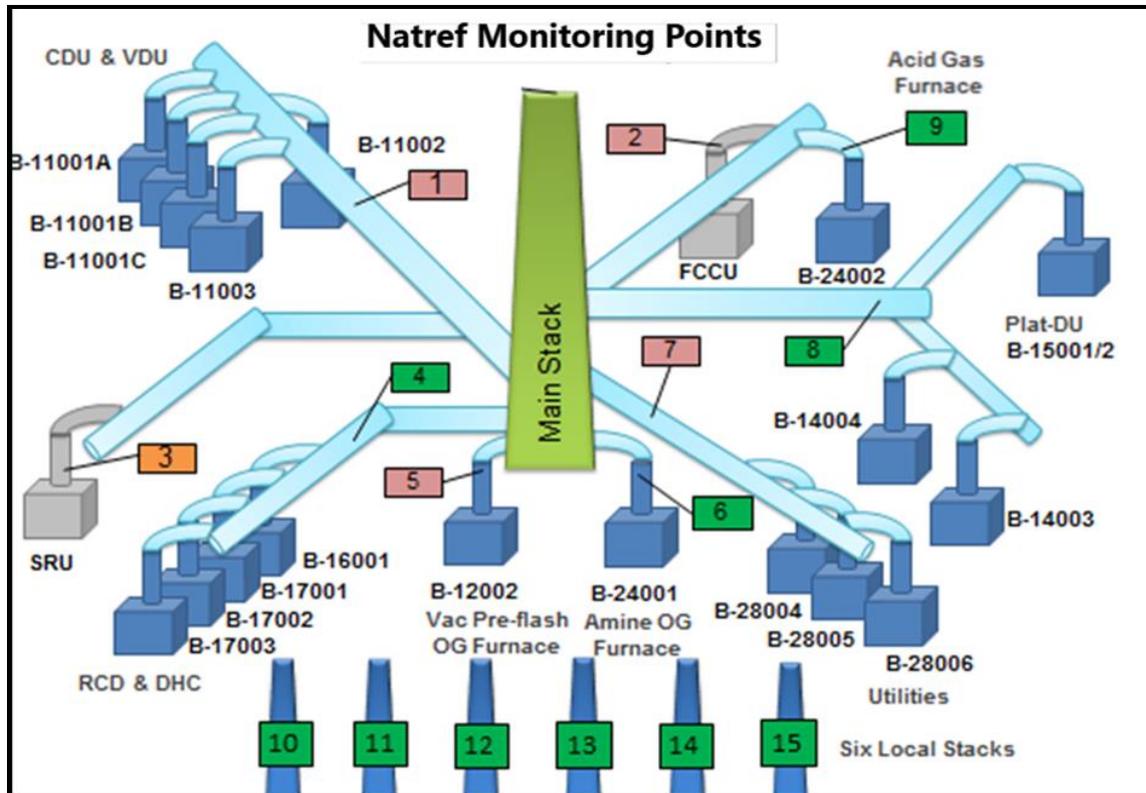
Storage Facilities

The storage facilities consist of raw material (crude oil) storage, intermediate storage and final storage tanks.

Raw material, Intermediate and final products are stored in fixed roof or floating roof tanks depending on the size of the tank, vapour pressure of the product and the service of the tank. Intermediate product is used for further processing in the various refinery units or for blending into final product from where it may be dispatched via road, rail or pipeline.

Floating roof tanks with a diameter of greater than 20 m are equipped with primary and secondary seals to minimise fugitive emissions.

The Diagram below illustrates Natref's monitoring points as per AEL requirements.



2.3 Unit Processes

Unit process considered listed activities under the National Environmental Management Air Quality Act (NEMAQA) are summarised in Table 2-2.

Table 2-2: List of unit processes considered listed activities under NEMAQA

Name of the Unit Process	Unit Process Function	Batch or Continuous Process	Listed Activity Sub-category
Crude Distillation Unit	Atmospheric distillation of crude oil	Continuous	2
Vacuum Distillation Unit	Vacuum distillation is distillation at conditions where the pressure above the liquid mixture to be distilled is reduced to less than its vapour pressure (usually less than atmospheric) causing evaporation of the least volatile liquid(s) (those with the highest boiling points) at lower temperature and hence more energy efficient distillation.	Continuous	2
Fluidised Catalytic Cracker Unit	The Fluidised Catalytic Cracking processes allow for the production of "light" products such as liquid petroleum gas and gasoline from heavier crude oil distillation fractions such as gas oil and residues. Fluid Catalytic Cracking produces a high yield of gasoline and liquid petroleum gas.	Continuous	2

Name of the Unit Process	Unit Process Function	Batch or Continuous Process	Listed Activity Sub-category
Mercox	Mercox treatment is mercaptan oxidation. It is a proprietary catalytic chemical process developed by UOP (Universal Oil Products) and used to remove mercaptans from LPG, Propane, Butane, Kerosene and petrol components by converting the mercaptans to liquid hydrocarbon disulphides.	Continuous	2
Distillate Hydrocracker	The Distillate Hydrocracker Unit catalytically cracks vacuum distillate (lube oil type components) into petrol, jet fuel and diesel under a hydrogen partial pressure of 160 bar and a temperature of 450°C.	Continuous	2
Diesel Unifiner	The purpose of this unit is to remove sulfur from diesel to reduce the sulfur dioxide (SO ₂) emissions that result from using those fuels in automotive vehicles, aircraft and rail road locomotives and other forms of fuel combustion.	Continuous	2
Naphtha Unifiner / Platformer	The Naphtha Unifiner removes sulfur and nitrogen compounds and saturate olefins in the light naphtha. The Unifiner uses the hydrogen from platformate to remove the undesirable compounds and supplies the feed to the Platformer. The platforming unit converts the low octane naphtha from Unifiner to high octane reformate by conversion of straight chain compounds into cyclic compounds.	Continuous	2
Reduced Crude Desulfurisation	The Reduced Crude Desulfurisation unit operates at elevated temperature (~400°C) and pressure (~200Bar). The unit catalytically hydro-desulfurises, demetalises and cracks vacuum residue (road tar and heavy fuel oil) into feedstock that can be treated in the fluidised catalytic cracking unit where LPG, petrol, kerosene and diesel are produced.	Continuous	2
PPU4	The PPU4 Unit separates propane (sold as a final product) from propylene. The propylene is sold as a feedstock to neighbouring industry Safripol.	Continuous	2
Bitumen Blower	In order to produce bitumen that will soften at a higher temperature than an equivalent penetration Bitumen, severe air blowing is required. The product is therefore also known as 'air-blown' or 'oxidised' bitumen. Typically the blower feedstock has a lower initial boiling point than other bitumen grades.	Batch	2
Sour Water Stripper	The Sour Water Stripper is used to force both Hydrogen Sulphide and Ammonia out of the water phase into a gas phase. Sulfur is recovered from the gas phase "Acid Gas" in the Sulfur Recovery Unit.	Continuous	2
Amine Scrubbing and Sulfur Recovery Unit	Hydrogen sulphide present in gas streams is separated by means of selective chemical absorption in the Amine unit and sent to the Claus Sulfur Recovery Unit (SRU) for conversion into elemental sulfur. The resultant "sweet gas" is used as Refinery Fuel Gas. Waste Water Stripper Off gas is also routed to the SRU. The acid gas, rich in H ₂ S, is passed through a combustion chamber at 1380°C to combust ammonia impurities and to convert H ₂ S to liquid sulfur.	Continuous	2
Alkylation Unit	Alkylation is a process that combines olefins with iso-butane using a catalyst, HF acid in this case, to produce alkylate. Alkylate is highly flammable and is blended into petrol to boost its octane. The unit operates in tandem with the Butamer Unit that produces iso-butane as feed for the Alkylation Unit.	Continuous	2
Crude, Intermediate, Final Product Tanks, Spheres and Bullets	Storage of raw materials, intermediate and final products used and produced in the refinery.	Continuous	2
Road and Rail Loading Facilities	Facilities for loading road tankers and rail tankers with LPG, Petrol, Diesel, Jet Fuel, Fuel Oil, Slurry and Bitumen.	Batch	2

Name of the Unit Process	Unit Process Function	Batch or Continuous Process	Listed Activity Sub-category
Stacks	Natref has one main stack at 145m from where refinery off-gasses are vented off into the atmosphere. Natref has also seven local stacks when including the 55m FCCU stack which is used under start-up, shut-down and abnormal operating conditions.	<ul style="list-style-type: none"> • Main Stack and six local stacks have continuous emissions; and • FCCU local stack is batch emission process 	2
Flares	Flares are used as safety devices to manage abnormal operating conditions, start-up and to shut down the refinery units safely.	Batch	2
Vapour Recovery Unit	The purpose of the VRU is to control and reduce the emissions of hydrocarbons to the atmosphere caused by loading of petroleum products into road and rail tankers.	Continuous	2

3 TECHNICAL INFORMATION

Raw material consumption rates are tabulated in Table 3-1. Pollution abatement technologies employed at Natref listed activities are provided in Table 3-2.

3.1 Raw Materials Used and Production Rates

Table 3-1: Raw materials used in the production

Raw Material Type	Process	Maximum Permitted Consumption Rate	Design Consumption Rate	Actual Consumption Rate	Rate Unit
Crude	Refining	6 307 200 m ³ /year	720 m ³ /h	650 m ³ /h	As indicated

3.2 Appliances and Abatement Equipment Control Technology

Table 3-2: Appliances and abatement equipment control technology

Appliance Name	Abatement Appliance Type	Appliance function / purpose
LE-CSGC-10W Low NO _x Burners	Callidus Scepter	NO _x reduction
Sulfur Recovery Plant	Lurgi - Fluor Revamp	Sulfur reduction
CO ₂ Plant	Air Products/ AFROX	CO ₂ reduction
CO Boiler	Babcock	CO reduction
Vapour Recovery Unit	Cool Sorption Unit	VOC reduction

4 ATMOSPHERIC EMISSIONS

The establishment of a comprehensive emission inventory formed the basis for the assessment of the air quality impacts from Natref on the receiving environment.

Point source parameters for Natref stacks are provided in Table 4-1. A locality map indicating the position of Natref in relation to surrounding residential and industrial areas is provided in Figure 4-1.



Figure 4-1: Locality map of Natref in relation to surrounding residential and industrial areas

4.1 Point Source Parameters

Table 4-1: Point source parameters for stacks

Point Source Number	Point Source Name	Point Source Coordinates		Height of Release above Ground (m)	Height above Nearby Building (m)	Diameter at Stack Tip or Vent Exit (m)	Actual Gas Exit Temperature (°C)	Actual Gas Volumetric Flow Rate (m ³ /hr.)	Actual Gas Exit Velocity (m/s)	%O ₂	Type of Emission (Continuous /Batch)
		Latitude	Longitude								
N1	Main Stack	-26.8060667	27.857458	145.00	not applicable	5.500	255	700 000	10	11.48	Continuous
N2	B14001	-26.8070778	27.858400	26.51	not applicable	1.372	400	22 600	5.03	8.43	Continuous
N3	B14002	-26.8069528	27.858480	24.56	not applicable	1.016	280	9 600	3.29	16.00	Continuous
N4	B14005	-26.8067722	27.858233	62.00	not applicable	1.866	230	36 900	4.21	4.74	Continuous
N5	B14006	-26.8066444	27.858672	27.42	not applicable	1.676	280	18 300	2.48	10.11	Continuous
N6	B17004	-26.8064944	27.857019	20.02	not applicable	0.914	310	7 800	3.6	6.74	Continuous
N7	B25001	-26.8062639	27.856189	19.15	not applicable	1.518	320	198 000	30.8	8.84	Continuous

4.2 Point Source Maximum Emission Rates during Normal Operating Conditions

Table 4-2: Point source emission rates during normal operating conditions for stacks

Point Source Number	Point Source Name	Pollutant Name	Average Emission Rate		Duration of Emission
			¹ Emission Concentration (mg/Nm ³)	Averaging Period	
N1	Main Stack	Particulates	No longer a point of compliance due to definition.	N/A	Continuous
		SO ₂	No longer a point of compliance due to definition.		
		NO _x as NO ₂	No longer a point of compliance due to definition.		
N2	B14001	Particulates	120	Daily	Continuous
		SO ₂	1700		
		NO _x as NO ₂	1700		
N3	B14002	Particulates	120	Daily	Continuous
		SO ₂	1700		
		NO _x as NO ₂	1700		
N4	B14005	Particulates	120	Daily	Continuous
		SO ₂	1700		
		NO _x as NO ₂	1700		
N5	B14006	Particulates	120	Daily	Continuous
		SO ₂	1700		
		NO _x as NO ₂	1700		
N6	B17004	Particulates	120	Daily	Continuous
		SO ₂	1700		
		NO _x as NO ₂	1700		

Point Source Number	Point Source Name	Pollutant Name	Average Emission Rate		Duration of Emission
			¹ Emission Concentration (mg/Nm ³)	Averaging Period	
N7	B25001	Particulates	120	Daily	Continuous
		SO ₂	1700		
		NO _x as NO ₂	1700		

Note:

1 - The above concentrations are AEL limits and not actual emission rates

Table 4-3 provides the average emission rates per process unit that feeds into the main stack.

Table 4-3: Unit process emission rates during normal operating conditions

Process Unit Source Number	Process Unit Source Name	Pollutant Name	Average Emission Rate		Duration of Emission
			¹ Emission Concentration (mg/Nm ³)	Averaging Period	
N8	B11001A, B11001B, B11001C and B11002	Particulates	120	Daily	Continuous
		SO ₂	1700		
		NO _x as NO ₂	1700		
N9	B28004, B28006 and B28005	Particulates	350	Daily	Continuous
		SO ₂	1700		
		NO _x as NO ₂	1700		
N10	B12002	Particulates	120	Daily	Continuous
		SO ₂	5800		
		NO _x as NO ₂	1700		
N11	B14003, B14004, B15001 and B15002	Particulates	120	Daily	Continuous
		SO ₂	1700		

Process Unit Source Number	Process Unit Source Name	Pollutant Name	Average Emission Rate		Duration of Emission
			¹ Emission Concentration (mg/Nm ³)	Averaging Period	
		NO _x as NO ₂	1700		
N12	B16001, B17001, B17002 and B17003	Particulates	120	Daily	Continuous
		SO ₂	1700		
		NO _x as NO ₂	1700		
N13	B24001	Particulates	120	Daily	Intermittent
		SO ₂	1700		
		NO _x as NO ₂	1700		
N14	B24002	Particulates	120	Daily	Intermittent
		SO ₂	1700		
		NO _x as NO ₂	1700		

* For point sources where periodic compliance measurements are made, these measurements are conducted in accordance with the methods prescribed in Schedule A of the MES.

Note:

1 - The above concentrations are AEL limits and not actual emission rates

4.3 Point Source Maximum Emission Rates during Start-up, Maintenance and/or Shut-down

Natref conducts periodic measurements which make it difficult to establish maximum emissions during start up, shut down, maintenance or upset conditions, since periodic measurements cannot pinpoint exactly when the maximum will occur. The main reason maximum values cannot be predicted with periodic sampling, in Natref's case, is that the sampling methods prescribe fixed time periods during which a sample must be taken. In addition, timing of specific conditions leading to an absolute maximum emission rate is not predictable, meaning that the sampling period and the conditions resulting in the upsets are unlikely to occur concurrently; hence, it cannot be guaranteed that a maximum emission rate will be reached at a specific condition.

4.4 Fugitive Emissions

Natref manages fugitive emissions through a Leak Detection and Repair (LDAR) program. These emissions emanate from various pressurized process equipment. A third party contractor is contracted to conduct leak detection, with the help of a "sniffer" device and an infrared camera, to identify and quantify the leaks associated with various process emissions. The report results are then included in the maintenance plan and the leaking process devices are repaired according to the maintenance schedule. This process has been operational for a period exceeding five years.

A second external third party service provider conducts Natref's VOC monitoring of emissions from area sources like API basins, ponds, storage tanks, loading and unloading of products. This is done by exposing Radiello™ cartridges to ambient air at strategic locations and around the fence-line perimeter. Cartridges are then collected and sent to an independent external laboratory for analysis after which a report is issued to Natref.

Table 4-4: Area source emission rates during normal operating conditions for tanks calculated using the US EPA TANKS model

Tank ID	Tank source	Pollutant Name	Maximum Release Rate (grams per second)	Average Annual Release Rate (tonnes per annum)	Emission Hours	Type of Emission (Continuous / Intermittent)	Wind Dependent (Yes / No)
1	F29059	Total VOC	6.42E-01	20.2	24 hours	Continuous	Yes
		Benzene	1.85E-02	0.6	24 hours	Continuous	Yes
2	F29106	Total VOC	2.16E-01	6.8	24 hours	Continuous	Yes
		Benzene	5.86E-03	0.2	24 hours	Continuous	Yes
3	F29112	Total VOC	5.15E-01	16.2	24 hours	Continuous	Yes
		Benzene	1.40E-02	0.4	24 hours	Continuous	Yes
4	F29117	Total VOC	5.12E-01	16.1	24 hours	Continuous	Yes
		Benzene	1.48E-02	0.5	24 hours	Continuous	Yes
5	F29118	Total VOC	3.79E-01	12.0	24 hours	Continuous	Yes
		Benzene	9.95E-03	0.3	24 hours	Continuous	Yes
6	F29119	Total VOC	5.11E-01	16.1	24 hours	Continuous	Yes
		Benzene	1.37E-02	0.4	24 hours	Continuous	Yes
7	F29006	Total VOC	1.75E-01	5.5	24 hours	Continuous	Yes
		Benzene	1.14E-02	0.4	24 hours	Continuous	Yes
8	F29007	Total VOC	1.75E-01	5.5	24 hours	Continuous	Yes
		Benzene	1.14E-02	0.4	24 hours	Continuous	Yes
9	F29008	Total VOC	1.75E-01	5.5	24 hours	Continuous	Yes
		Benzene	1.14E-02	0.4	24 hours	Continuous	Yes

Tank ID	Tank source	Pollutant Name	Maximum Release Rate (grams per second)	Average Annual Release Rate (tonnes per annum)	Emission Hours	Type of Emission (Continuous / Intermittent)	Wind Dependent (Yes / No)
10	F29009	Total VOC	5.64E+00	177.8	24 hours	Intermittent	Yes
		Benzene	6.20E-02	2.0	24 hours	Intermittent	Yes
11	F29010	Total VOC	8.18E+00	258.0	24 hours	Intermittent	Yes
		Benzene	9.00E-02	2.8	24 hours	Intermittent	Yes
12	F29011	Total VOC	5.64E+00	177.8	24 hours	Intermittent	Yes
		Benzene	6.20E-02	2.0	24 hours	Intermittent	Yes
13	F29012	Total VOC	2.92E-01	9.2	24 hours	Continuous	Yes
		Benzene	1.75E-03	0.1	24 hours	Continuous	Yes
14	F29013	Total VOC	2.92E-01	9.2	24 hours	Continuous	Yes
		Benzene	1.75E-03	0.1	24 hours	Continuous	Yes
15	F29014	Total VOC	2.23E-01	7.0	24 hours	Continuous	Yes
		Benzene	1.34E-03	0.0	24 hours	Continuous	Yes
16	F29047	Total VOC	3.80E-01	12.0	24 hours	Continuous	Yes
		Benzene	9.81E-03	0.3	24 hours	Continuous	Yes
17	F29029	Total VOC	4.96E-02	1.6	24 hours	Continuous	Yes
		Benzene	6.45E-05	0.0	24 hours	Continuous	Yes
18	F29030	Total VOC	3.05E-01	9.6	24 hours	Continuous	Yes
		Benzene	1.83E-03	0.1	24 hours	Continuous	Yes
19	F29101	Total VOC	8.20E-02	2.6	24 hours	Continuous	Yes
		Benzene	1.07E-04	0.0	24 hours	Continuous	Yes
20	F29102	Total VOC	6.75E-02	2.1	24 hours	Continuous	Yes
		Benzene	8.77E-05	0.0	24 hours	Continuous	Yes
21	F29107	Total VOC	4.85E-02	1.5	24 hours	Continuous	Yes
		Benzene	6.31E-05	0.0	24 hours	Continuous	Yes
22	F29108	Total VOC	5.06E-02	1.6	24 hours	Continuous	Yes
		Benzene	6.57E-05	0.0	24 hours	Continuous	Yes
23	F29109	Total VOC	4.89E-02	1.5	24 hours	Continuous	Yes
		Benzene	6.35E-05	0.0	24 hours	Continuous	Yes
24	F29113	Total VOC	6.88E-02	2.2	24 hours	Continuous	Yes
		Benzene	8.95E-05	0.0	24 hours	Continuous	Yes
25	F29114	Total VOC	7.41E-02	2.3	24 hours	Continuous	Yes
		Benzene	9.64E-05	0.0	24 hours	Continuous	Yes

Table 4-5: Tank area source emission estimation information

Area Source	Basis for Emission Rates
All tanks	US EPA AP-42 TANKS Software, based on AP-42 Section 7.1, Organic Liquid Storage Tanks

4.5 Emergency Incidents

Emergency incidents on the site are handled through standard operating procedures governing the actions that need to take place, as well as defining the responsibilities of the parties involved in managing the incident. Part of any environmental incident/emergency response, the environmental respondent will evaluate the incident and then classify it according to an

internal ranking as well as against relevant legislative requirements which will then trigger the necessary reporting requirements. The Natref NEMA Section 30 reportable incidents, related to air emissions in the past five years, are included in the table below.

Table 4-6: Emergency Incidents

Date of Incident	Incident	Nature and cause of the incident	Actions undertaken immediately to minimize impact	Actions undertaken to prevent recurrence
22 May 2017	Explosion and fire at Hydrogen compressor	Unexpected release of Hydrogen from Hydrogen Booster compressor, which resulted in an explosion and fire.	<ul style="list-style-type: none"> • Inspection of two similar compressors • Full investigation of incident 	<ul style="list-style-type: none"> • Implement a gas detection system with alarms and trips
19 March 2013	SRU unplanned shutdown	The SRU tripped on high pressure resulting in the unit shutdown.	<ul style="list-style-type: none"> • Natref cut back feed throughput to minimum on all SO₂ producing units. • Ambient air quality was monitored. 	<ul style="list-style-type: none"> • Improve the integrity of the Sulphur plant.

5 IMPACT OF ENTERPRISE ON THE RECEIVING ENVIRONMENT

5.1 Analysis of Emissions' Impact on Human Health

The report includes the results for three emission scenarios per pollutant, in order to establish the delta impacts against air quality limit values. The scenarios are as follows:

- *Scenario 1*: modelling conducted based on 100% SRU availability
- *Scenario 2*: modelling conducted based on 99% SRU availability (theoretically complying with New Plant Standards)
- *Scenario 3*: assuming 95% SRU availability.

5.1.1 Study Methodology

5.1.1.1 Study Plan

The study methodology may conveniently be divided into a “preparatory phase” and an “execution phase”. The basic methodology followed in this assessment is provided in Figure 5-1.

The preparatory phase included the following basic steps prior to performing the actual dispersion modelling and analyses:

1. Understand Scope of Work
2. Assign Appropriate Specialists
3. Review of legal requirements (e.g. dispersion modelling guideline)
4. Prepare a Plan of Study for Peer Review
5. Decide on Dispersion Model

The Regulations Regarding Air Dispersion Modelling (Gazette No 37804 published 11 July 2014) was referenced for the dispersion model selection (Appendix B).

Three Levels of Assessment are defined in the Regulations Regarding Air Dispersion Modelling:

- Level 1: where worst-case air quality impacts are assessed using simpler screening models
- 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)
- Level 3: require more sophisticated dispersion models (and corresponding input data, resources and model operator expertise) in situation:
 - where a detailed understanding of air quality impacts, in time and space, is required;
 - where it is important to account for causality effects, calms, non-linear plume trajectories, spatial variations in turbulent mixing, multiple source types & chemical transformations;
 - when conducting permitting and/or environmental assessment process for large industrial developments that have considerable social, economic and environmental consequences;
 - when evaluating air quality management approaches involving multi-source, multi-sector contributions from permitted and non-permitted sources in an airshed; or,
 - when assessing contaminants resulting from non-linear processes (e.g. deposition, ground-level O₃, particulate formation, visibility)

The models recommended for Level 3 assessments are CALPUFF or SCIPUFF. In this study, CALPUFF was selected for the following reasons (as referenced in Figure 5-1 - Model Aspects to Consider and Dispersion Models):

- This Lagrangian Gaussian Puff model is also 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 over-estimates the plume travel distance (Busini *et al.*, 2012; Gulia *et al.* 2015; Lakes Environmental, 2017).
- CALPUFF is able to perform chemical transformations. In this study the conversion of NO to NO₂ and the secondary formation of particulate matter was a concern.

The execution phase (i.e. dispersion modelling and analyses) firstly involves gathering specific information in relation to the emission source(s) and site(s) to be assessed. This includes:

- Source information: Emission rate, exit temperature, volume flow, exit velocity, etc.;
- Site information: Site building layout, terrain information, land use data;
- Meteorological data: Wind speed, wind direction, temperature, cloud cover, mixing height;
- Receptor information: Locations using discrete receptors and/or gridded receptors.

The model uses this specific input data to run various algorithms to estimate the dispersion of pollutants between the source and receptor. The model output is in the form of a predicted time-averaged concentration at the receptor. These predicted concentrations are compared with the relevant ambient air quality standard or guideline. Post-processing can be carried out to produce percentile concentrations or contour plots that can be prepared for reporting purposes.

The following steps were followed for the execution phase of the assessment:

- Decide on meteorological data input (Figure 5-1 - CALMET). A summary of the model control options for CALMET is provided in Appendix C. Refer to Section 5.1.4.6.
- Prepare all meteorological model input files (Figure 5-1 - CALMET)
 - Surface meteorological files
 - WRF meteorological files
 - Topography
 - Land Use
- Select control options in meteorological model (Figure 5-1 - CALMET)
 - Dispersion coefficients
 - Vertical levels
 - Receptor grid
- *Feedback to Project Team and revise where necessary*
- Review emissions inventory and ambient measurements
- *Feedback to Project Team and revise where necessary*
- Decide on dispersion model controls and module options (Figure 5-1 - CALPUFF). A summary of the model control options for CALPUFF is provided in Appendix D. Refer to Section 5.1.4.6
- Decide on dispersion module options (Figure 5-1 - CALPUFF).
 - Sulfate and nitrate formation module (MESOPUFF or RiVAD)
 - NO₂ formation (MESOPUFF or RiVAD)
 - Model resolution
- *Feedback to Project Team and revise where necessary*
- Decide on modelling domain and receptor locations (Figure 5-1 – CALPUFF and Simulations)
- *Feedback to Project Team and revise where necessary*
- Prepare all dispersion model input files (Figure 5-1 - CALPUFF)
 - Control options
 - Measured ambient O₃ and NH₃ for chemical transformation module

- Meteorology
 - Source data
 - Receptor grid and discrete receptors
- Review all modelling input data files and fix where necessary
- Simulate source groups per pollutant and calculate air concentration levels for regular and discrete grid locations for the following scenarios (Figure 5-1 – Simulations):
 - Scenario 1: 100% SRU availability
 - Scenario 2: 99% SRU availability (reflecting theoretical compliance with “New Plant” standards)
 - Scenario 3: 95% SRU availability
- Compare against National Ambient Air Quality Standards (NAAQS)
- Preparation of draft AIR
- Preparation of final AIR.

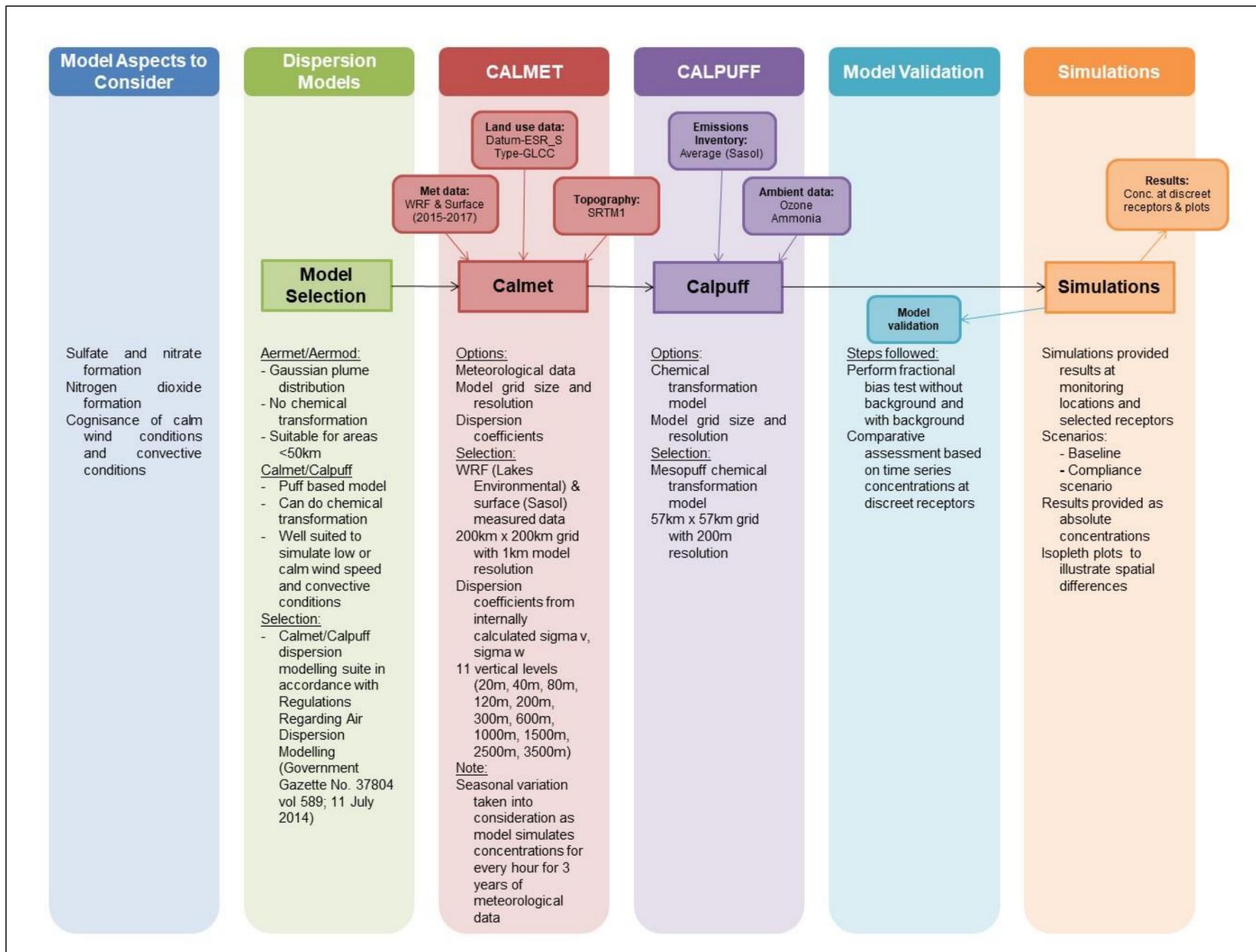


Figure 5-1: The basic study methodology followed for the assessment

5.1.1.2 Emission Scenarios

In order to assess the impact of the postponements for which Natref is applying, three emissions scenarios were modelled, with the results throughout the AIR presented as illustrated in Figure 5-2.

1. **Scenario 1**, reflective of 100% SRU availability. Source emissions were provided as averages of measurements taken from periodic emission monitoring during normal operating conditions. This scenario is represented by the first column in the presentation of all AIR graphs (shown in blue in Figure 5-2). Source emissions were derived from 3rd parties and accredited (ISO/IEC17025) laboratories. Emissions measurements follow the requirements prescribed in Schedule A of GN 893.
2. **Scenario 2** reflects emission conditions when the SRU operates at 99% availability (theoretical compliance with the 2020 new plant standards). This scenario is then represented by the second column in the presentation of all AIR graphs (shown in green in Figure 5-2).
3. **Scenario 3** assumes the SRU operates at 95% availability. This scenario is represented by the third column in the presentation of all AIR graphs (shown in purple in Figure 5-2).

In Figure 5-2, the arrow in the green bar reflects the predicted delta (change) in ambient impacts with the SRU operating at 100% availability to operating at 99% availability. For Scenario 3, the arrow on the purple bar represents the theoretical delta increase in ambient impacts when the SRU is operating with 95% availability, compared with the theoretical scenario of the SRU operating with 100% availability. The orange dot in Figure 5-2 represents physically measured ambient air quality, reflective of the total impact of all sources in the vicinity, as the 99th percentile recorded value over the averaging period. On a given day, there is a 99% chance that the actual measured ambient air quality would be lower than this value, but this value is reflected for the purpose of aligning with modelling requirements. The orange line represents the applicable NAAQS.

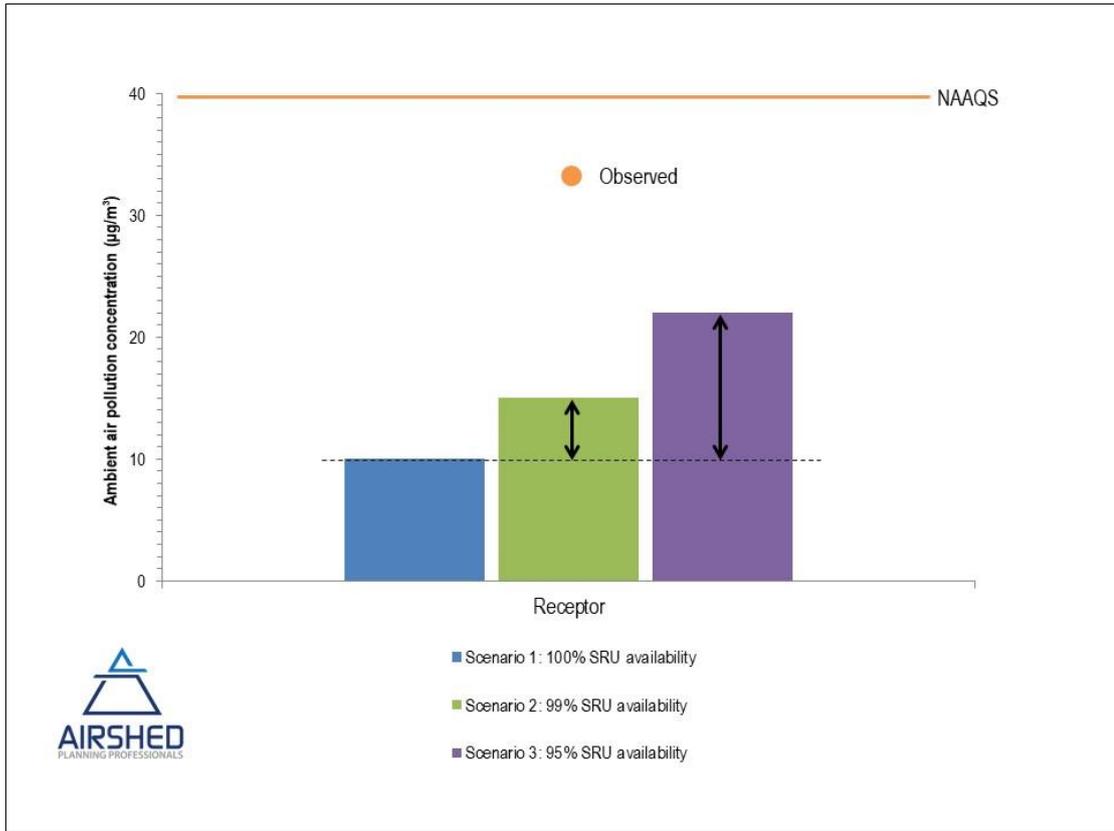


Figure 5-2: Schematic displaying how the dispersion modelling scenarios are presented, for each monitoring station receptor in the modelling domain

5.1.1.3 CALPUFF/CALMET Modelling Suite

As discussed in the previous section, the CALPUFF model was selected for use in the current investigation to predict maximum short-term (1 and 24-hour) and annual average ground-level concentrations at various receptor locations within the computational domain. CALPUFF is a multi-layer, multi-species non-steady-state puff dispersion model that can simulate the effects of time- and space-varying meteorological conditions on pollutant transport, transformation, and removal (Scire *et al.*, 2000a). It can accommodate arbitrarily varying point source, area source, volume source, and line source emissions. The CALPUFF code includes algorithms for near-source effects such as building downwash, transitional plume rise, partial plume penetration, sub grid scale terrain interactions as well as longer range effects such as pollutant removal due to wet scavenging and dry deposition, chemical transformation, vertical wind shear, overwater transport and coastal interaction effects.

The model is intended for use on scales from tens of metres to hundreds of kilometres from a source (US EPA 1998). The CALPUFF model allows the user to select from a number of calculation options, including a choice of dispersion coefficient and chemical transformation formulations. The different dispersion coefficient approaches accommodated in the CALPUFF model include:

- stability-based empirical relationships such as the Pasquill-Gifford or McElroy-Pooler dispersion coefficients;
- turbulence-based dispersion coefficients (based on measured standard deviations of the vertical and crosswind horizontal components of the wind); and
- similarity theory to estimate the turbulent quantities using the micrometeorological variables calculated by CALMET

The most desirable approach is to use turbulence-based dispersion coefficients using measured turbulent velocity variances or intensity components, if such data are readily available and they are of good quality. However, since reliable turbulent measurements are generally not available, the next best recommendation is to use the similarity approach.

CALPUFF includes parameterized chemistry modules for the formation of secondary sulfate and nitrate from the oxidation of the emitted primary pollutants, SO₂ and NO_x. The conversion processes are assumed to be linearly dependent (first-order) on the relevant primary species concentrations. Two options are included, namely the MESOPUFF II and RIVAD/ARM3 chemistry options. In both options, a fairly simple stoichiometric thermodynamic model is used to estimate the partitioning of total inorganic nitrate between gas-phase nitric acid and particle-phase ammonium nitrate. Ammonia and O₃ concentrations are required as background values to the model.

CALPUFF uses dry deposition velocities to calculate the dry deposition of gaseous and particulate pollutants to the surface. These dry deposition velocities can either be user-specified or calculated internally in CALPUFF. A resistance-based model is used for the latter option. For gaseous pollutants, the resistances that are considered are the atmospheric resistance, the deposition layer resistance, and the canopy resistance. For particles, a gravitational settling term is included, and the canopy resistance is assumed to be negligible. CALPUFF uses the scavenging coefficient approach to parameterize wet deposition of gases and particles. The scavenging coefficient depends on pollutant characteristics (e.g., solubility and reactivity), as well as the precipitation rate and type of precipitation. The model provides default values for the scavenging coefficient for various species and two types of precipitation (liquid and frozen). These values may be overridden by the user.

CALPUFF also has the capability to model the effects of vertical wind shear by explicitly allowing different puffs to be independently advected by their local average wind speed and direction, as well as by optionally allowing well-mixed puffs to split into two or more puffs when across-puff shear becomes important. Another refinement is an option to use a probability density function (pdf) model to simulate vertical dispersion during convective conditions.

The CALPUFF modelling system consists of a number of software components, as summarised in Table 5-1, however only CALMET and CALPUFF contain the simulation engines to calculate the three-dimensional atmospheric boundary layer conditions and the dispersion and removal mechanisms of pollutants released into this boundary layer. The other components are mainly used to assist with the preparation of input and output data. Table 5-1 also includes the development versions of each of the codes used in this investigation.

Table 5-1: Summary description of CALPUFF/CALMET model suite with versions used in the investigation

Module	Version	Description
CALMET	V6.5.0	Three-dimensional, diagnostic meteorological model
CALPUFF	V7.2.1	Non-steady-state Gaussian puff dispersion model with chemical removal, wet and dry deposition, complex terrain algorithms, building downwash, plume fumigation and other effects.
CALPOST	V7.1.0	A post-processing program for the output fields of meteorological data, concentrations and deposition fluxes.
CALSUM	V7.0.0	Sums and scales concentrations or wet/dry fluxes from two or more source groups from different CALPUFF runs
PRTMET	V4.495	Lists selected meteorological data from CALMET and creates plot files
POSTUTIL	V7.0.0	Processes CALPUFF concentration and wet/dry flux files. Creates new species as weighted combinations of modelled species; merges species from different runs into a single output file; sums and scales results from different runs; repartitions nitric acid/nitrate based on total available sulfate and ammonia.

Module	Version	Description
TERREL	V7.0.0	Combines and grids terrain data
CTGPROC	V7.0.0	Processes and grids land use data
MAKEGEO	V3.2	Merges land use and terrain data to produce the geophysical data file for CALMET

A summary of the main CALMET and CALPUFF control options are given in Appendices D and E, respectively.

5.1.2 Legal Requirements

5.1.2.1 Atmospheric Impact Report

In the event where an application for postponement is being made, Section 21 of NEM: Air Quality Act (AQA), Regulations 11 and 12 state:

1. An application for postponement may be made to the National Air Quality Officer
2. The application contemplated in Regulation 11 must include, amongst others, an Atmospheric Impact Report.

The format of the Atmospheric Impact Report is stipulated in the Regulations Prescribing the Format of the AIR, Government Gazette No. 36904, Notice Number 747 of 2013 (11 October 2013) (Appendix B; Table B-1).

Sasol and Natref appointed Airshed to compile this AIR to meet the requirements of Regulation 12 (Postponement of compliance time frames) of the Listed Activities and Associated MES (Government Gazette No. 37054, 22 November 2013) (Appendix B; Table B-1).

5.1.2.2 National Ambient Air Quality Standards

Modelled concentrations will be assessed against NAAQS (Table 5-2), where they are prescribed by South African legislation. Where no NAAQS exists for a relevant non-criteria pollutant, health screening effect levels based on international guidelines are used. These are discussed with the results of dispersion modelling in Section 5.1.8.

Table 5-2: National Ambient Air Quality Standards

Pollutant	Averaging Period	Concentration ($\mu\text{g}/\text{m}^3$)	Frequency of Exceedance	Compliance Date
Benzene (C_6H_6)	1 year	5	0	1 January 2015
Carbon Monoxide (CO)	1 hour	30000	88	Immediate
	8 hour ^(a)	10000	11	Immediate
Lead (Pb)	1 year	0.5	0	Immediate
Nitrogen Dioxide (NO_2)	1 hour	200	88	Immediate
	1 year	40	0	Immediate
Ozone (O_3)	8 hour ^(b)	120	11	Immediate
Inhalable particulate matter less than	24 hour	40	4	Immediate until 31 December 2029
	24 hour	25	4	1 January 2030

Pollutant	Averaging Period	Concentration ($\mu\text{g}/\text{m}^3$)	Frequency of Exceedance	Compliance Date
2.5 μm in diameter (PM _{2.5})	1 year	20	0	Immediate until 31 December 2029
	1 year	15	0	1 January 2030
Inhalable particulate matter less than 10 μm in diameter (PM ₁₀)	24 hour	75	4	Immediate
	1 year	40	0	Immediate
Sulfur Dioxide (SO ₂)	10 minutes	500	526	Immediate
	1 hour	350	88	Immediate
	24 hour	125	4	Immediate
	1 year	50	0	Immediate

Notes:

- (a) Calculated on 1 hour averages.
- (b) Running average.

5.1.2.3 National Dust Control Regulations

South Africa's Draft National Dust Control Regulations were published on 27 May 2011 with the dust fallout standards passed and subsequently published on 1 November 2013 (Government Gazette No. 36974). These are called the National Dust Control Regulations (NDCR). The purpose of the regulations is to prescribe general measures for the control of dust in all areas including residential and light commercial areas. Acceptable dustfall rates according to the regulations are summarised in Table 5-3.

Table 5-3: Acceptable dustfall rates

Restriction areas	Dustfall rate (D) in $\text{mg}/\text{m}^2\text{-day}$ over a 30 day average	Permitted frequency of exceedance
Residential areas	$D < 600$	Two within a year, not sequential months.
Non-residential areas	$600 < D < 1\ 200$	Two within a year, not sequential months.

The regulations also specify that the method to be used for measuring dustfall and the guideline for locating sampling points shall be ASTM D1739 (1970), or equivalent method approved by any internationally recognized body. It is important to note that dustfall is assessed for nuisance impact and not inhalation health impact.

A revised Draft National Dust Control Regulations were published on 25 March 2018 (Government Gazette No. 41650) which references the same acceptable dustfall rates but refers to the latest version of the ASTM D1739 method to be used for sampling.

5.1.3 Regulations Regarding Air Dispersion Modelling

Air dispersion modelling provides a cost-effective means for assessing the impact of air emission sources, the major focus of which is to determine compliance with the relevant ambient air quality standards. Regulations regarding Air Dispersion Modelling were promulgated in Government Gazette No. 37804 vol. 589; 11 July 2014, and recommend a suite of dispersion

models to be applied for regulatory practices as well as guidance on modelling input requirements, protocols and procedures to be followed. The Regulations Regarding Air Dispersion Modelling are applicable:

- (a) in the development of an air quality management plan, as contemplated in Chapter 3 of the AQA;
- (b) in the development of a priority area air quality management plan, as contemplated in Section 19 of the AQA;
- (c) in the development of an atmospheric impact report, as contemplated in Section 30 of the AQA; and,
- (d) in the development of a specialist air quality impact assessment study, as contemplated in Chapter 5 of the AQA.

The Regulations have been applied to the development of this report. The first step in the dispersion modelling exercise requires a clear objective of the modelling exercise and thereby gives clear direction to the choice of the dispersion model most suited for the purpose. Chapter 2 of the Regulations present the typical levels of assessments, technical summaries of the prescribed models (SCREEN3, AERSCREEN, AERMOD, SCIPUFF, and CALPUFF) and good practice steps to be taken for modelling applications.

Dispersion modelling provides a versatile means of assessing various emission options for the management of emissions from existing or proposed installations. Chapter 3 of the Regulations prescribe the source data input to be used in the models.

Dispersion modelling can typically be used in the:

- Apportionment of individual sources for installations with multiple sources. In this way, the individual contribution of each source to the maximum ambient predicted concentration can be determined. This may be extended to the study of cumulative impact assessments where modelling can be used to model numerous installations and to investigate the impact of individual installations and sources on the maximum ambient pollutant concentrations.
- Analysis of ground level concentration changes as a result of different release conditions (e.g. by changing stack heights, diameters and operating conditions such as exit gas velocity and temperatures).
- Assessment of variable emissions as a result of process variations, start-up, shut-down or abnormal operations.
- Specification and planning of ambient air monitoring programmes which, in addition to the location of sensitive receptors, are often based on the prediction of air quality hotspots.

The above options can be used to determine the most cost-effective strategy for compliance with the NAAQS. Dispersion models are particularly useful under circumstances where the maximum ambient concentration approaches the ambient air quality limit value and provide a means for establishing the preferred combination of mitigation measures that may be required including:

- Stack height increases;
- Reduction in pollutant emissions through the use of air pollution control systems (APCS) or process variations;
- Switching from continuous to non-continuous process operations or from full to partial load.

Chapter 4 of the Regulations prescribe meteorological data input from onsite observations to simulated meteorological data. The chapter also gives information on how missing data and calm conditions are to be treated in modelling applications. Meteorology is fundamental for the dispersion of pollutants because it is the primary factor determining the diluting effect of the atmosphere. Therefore, it is important that meteorology is carefully considered when modelling.

New generation dispersion models, including models such as AERMOD and CALPUFF¹, simulate the dispersion process using planetary boundary layer (PBL) scaling theory. PBL depth and the dispersion of pollutants within this layer are influenced by specific surface characteristics such as surface roughness, albedo and the availability of surface moisture:

- Roughness length (z_0) is a measure of the aerodynamic roughness of a surface and is related to the height, shape and density of the surface as well as the wind speed.
- Albedo is a measure of the reflectivity of the Earth's surface. This parameter provides a measure of the amount of incident solar radiation that is absorbed by the Earth/atmosphere system. It is an important parameter since absorbed solar radiation is one of the driving forces for local, regional, and global atmospheric dynamics.
- The Bowen ratio provides measures of the availability of surface moisture injected into the atmosphere and is defined as the ratio of the vertical flux of sensible heat to latent heat, where sensible heat is the transfer of heat from the surface to the atmosphere via convection and latent heat is the transfer of heat required to evaporate liquid water from the surface to the atmosphere.

Topography is also an important geophysical parameter. The presence of terrain can lead to significantly higher ambient concentrations than would occur in the absence of the terrain feature. In particular, where there is a significant relative difference in elevation between the source and off-site receptors large ground level concentrations can result. Thus the accurate determination of terrain elevations in air dispersion models is very important.

The modelling domain would normally be decided on the expected zone of influence; the latter extent being defined by the predicted ground level concentrations from initial model runs. The modelling domain must include all areas where the ground level concentration is significant when compared to the air quality limit value (or other guideline). Air dispersion models require a receptor grid at which ground-level concentrations can be calculated. The receptor grid size should include the entire modelling domain to ensure that the maximum ground-level concentration is captured and the grid resolution (distance between grid points) sufficiently small to ensure that areas of maximum impact adequately covered. No receptors however should be located within the property line as health and safety legislation (rather than ambient air quality standards) is applicable within the site.

Chapter 5 provides general guidance on geophysical data, model domain and coordinates system required in dispersion modelling, whereas Chapter 6 elaborates more on these parameters as well as the inclusion of background air concentration data. The chapter also provides guidance on the treatment of NO_2 formation from NO_x emissions, chemical transformation of sulfur dioxide into sulfates and deposition processes.

Chapter 7 of the Regulations outline how the plan of study and modelling assessment reports are to be presented to authorities. A comparison of how this study met the requirements of the Regulations is provided in Appendix B.

5.1.4 Atmospheric Dispersion Processes

CALPUFF initiates the simulation of point source plumes with a calculation of buoyant plume rise as discussed below in Section 5.1.4.1. Transport winds are extracted from the meteorological data file at the location of the stack and at the effective plume height (stack height plus plume rise). For near-field effects, the height of the plume in transition to the final plume height is taken into account. The puff release rate is calculated internally, based on the transport speed and the distance to the closest receptor.

¹ The CALMET modelling system require further geophysical parameters including surface heat flux, anthropogenic heat flux and leaf area index (LAI).

As the puff is transported downwind, it grows due to dispersion and wind shear, and the trajectory is determined by advection winds at the puff location and height at each time step. The pollutant mass within each puff is initially a function of the emission rate from the original source. The pollutant mass is also subject to chemical transformation, washout by rain and dry deposition, when these options are selected, as is the case in this application. Chemical transformation and removal are calculated based on a one-hour time step.

Both wet and dry deposition fluxes are calculated by CALPUFF, based on a full resistance model for dry deposition and the use of precipitation rate-dependent scavenging coefficients for wet deposition. Pollutant mass is removed from the puff due to deposition at each time step. For the present modelling analyses, most options were set at "default" values, including the MESOPUFF II transformation scheme² and the treatment of terrain.

5.1.4.1 *Plume Buoyancy*

Gases leaving a stack mix with ambient air and undergo three phases namely the initial phase, the transition phase and the diffusion phase (Figure 5-3). The initial phase is greatly determined by the physical properties of the emitted gases. These gases may have momentum as they enter the atmosphere and are often heated and therefore warmer than the ambient air. Warmer gases are less dense than the ambient air and are therefore buoyant. A combination of the gases' momentum and buoyancy causes the gases to rise (vertical jet section, in Figure 5-3). In the Bent-Over Jet Section, entrainment of the cross flow is rapid because, by this time, appreciable growth of vortices has taken place. The self-generated turbulence causes mixing and determines the growth of plume in the thermal section. This is referred to as plume rise and allows air pollutants emitted in this gas stream to be lifted higher in the atmosphere. Since the plume is higher in the atmosphere and at a further distance from the ground, the plume will disperse more before it reaches ground level. With greater volumetric flow and increased exit gas temperatures, the plume centreline would be higher than if either the volumetric flow or the exit gas temperature is reduced. The subsequent ground level concentrations would therefore be lower.

² A sensitivity study was carried out with the RIVAD II transformation scheme to examine the performance of the different approaches to calculating the SO₂ to SO₄ and NO_x to NO₃ transformation rates. The concentrations from the RIVAD II and the MESOPUFF II transformation schemes showed no real bias with the secondary particulate formation varying by -41% to 31% for the two schemes.

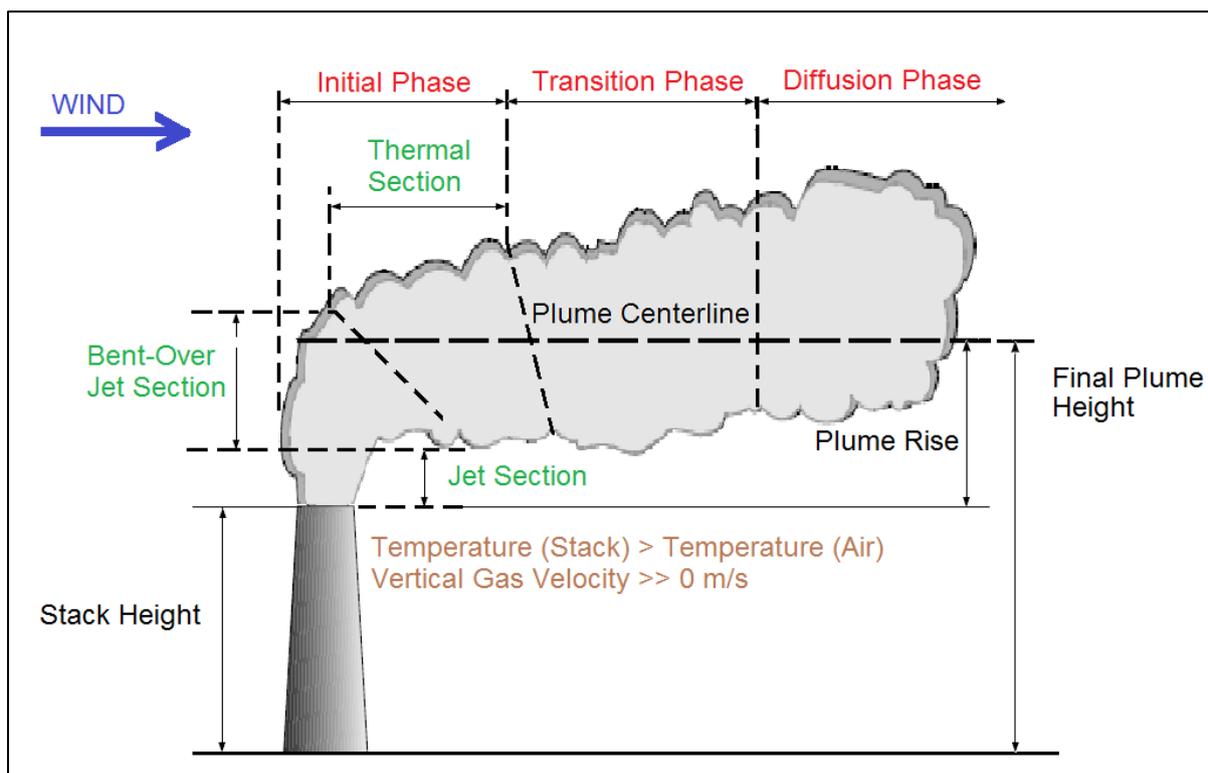


Figure 5-3: Plume buoyancy

This is particularly important in understanding some of the dispersion model results in Section 5.1.8.

5.1.4.2 Urban & Rural Conditions

Land use information is important to air dispersion modelling, firstly to ensure that the appropriate dispersion coefficients and wind profiles (specified as surface roughness) are used, and secondly, that the most appropriate chemical transformation models are employed. Urban conditions result in different dispersion conditions than in rural areas, as well as changing the vertical wind profiles. Urban conditions are also generally associated with increased levels of VOCs, thereby influencing chemical equilibria between the photochemical reactions of NO_x , CO and O_3 .

It can be appreciated that the definition of urban and rural conditions for the dispersion coefficients and wind profiles, on the one hand, and chemical reactions on the other, may not be the same. Nonetheless, it was decided to use the US Environmental Protection Agency's (US EPA's) guideline on air dispersion models (US EPA 2005), to classify the surrounding land-use as rural or urban based on the Auer method, which is strictly recommended for selecting dispersion coefficients.

The classification scheme is based on the activities within a 3 km radius of the emitting stack. Areas typically defined as rural include residences with grass lawns and trees, large estates, metropolitan parks and golf courses, agricultural areas, undeveloped land and water surfaces. An area is defined as urban if it has less than 35% vegetation coverage or the area falls into one of the use types in Table 5-4.

Table 5-4: Definition of vegetation cover for different developments (US EPA 2005)

Urban Land-Use		
Type	Development Type	Vegetation Cover
I1	Heavy industrial	Less than 5%
I2	Light/moderate industrial	Less than 10%

Urban Land-Use		
Type	Development Type	Vegetation Cover
C1	Commercial	Less than 15%
R2	Dense/multi-family	Less than 30%
R3	Multi-family, two storeys	Less than 35%

According to this classification scheme, the study area is classified as urban.

5.1.4.3 Nitrogen Dioxide Formation

Of the several species of nitrogen oxides, only NO₂ is specified in the NAAQS. Since most sources emit uncertain ratios of these species and these ratios change further in the atmosphere due to chemical reactions, a method for determining the amount of NO₂ in the plume must be selected.

Estimation of this conversion normally follows a tiered approach, as discussed in the Regulations Regarding Air Dispersion Modelling (Government Gazette No. 37804, published 11 July 2014), which presents a scheme for annual averages:

Tier 1: Total Conversion Method

Use any of the appropriate models recommended to estimate the maximum annual average NO₂ concentrations by assuming a total conversion of NO to NO₂. If the maximum NO_x concentrations are less than the NAAQS for NO₂, then no further refinement of the conversion factor is required. If the maximum NO_x concentrations are greater than the NAAQS for NO₂, or if a more "realistic" estimate of NO₂ is desired, proceed to the second tier level.

Tier 2: Ambient Ratio Method (ARM) - Multiply NO_x by a national ratio of NO₂/NO_x = 0.80

Assume a wide area quasi-equilibrium state and multiply the Tier 1 empirical estimate NO_x by a ratio of NO₂/NO_x = 0.80. The ratio is recommended for South Africa as the conservative ratio based on a review of ambient air quality monitoring data from the country. If representative ambient NO and NO₂ monitoring data is available (for at least one year of monitoring), and the data is considered to represent a quasi-equilibrium condition where further significant changes of the NO/NO₂ ratio is not expected, then the NO/NO₂ ratio based on the monitoring data can be applied to derive NO₂ as an alternative to the national ratio of 0.80.

In the Total Conversion Method, the emission rate of all NO_x species is used in the dispersion model to predict ground-level concentrations of total NO_x. These levels of NO_x are assumed to exist as 100% NO₂ and are directly compared to the NAAQS for NO₂. If the NAAQS are met, the Tier 2 methods are not necessary.

Although not provided in the Regulations (Section 5.1.3), the conversion of NO to NO₂ may also be based on the amount of ozone available within the volume of the plume. The NO₂/NO_x conversion ratio is therefore coupled with the dispersion of the plume. This is known as the Ozone Limiting Method (OLM). Use of onsite ozone data is always preferred for the OLM method.

Ideally, the NO₂ formation should be dealt with in the dispersion model. CALPUFF has one such a module, known as the RIVAD / ARM3 chemical formulations. The RIVAD / ARM3 chemical formulations option in the CALPUFF model can be used to calculate NO₂ concentrations directly in rural (non-urban) areas (Morris et al., 1988). The RIVAD / ARM3 option incorporates the effect of chemical and photochemical reactions on the formation of nitrates and other deposition chemicals. However, since the study area could be classified as urban (Section 5.1.4.2), the RIVAD / ARM3 chemical formulations should not be used.

Whilst the MESOPUFF II chemical transformation scheme, which is also included in the CALPUFF model accommodates NO_x reactions, these are only considering the formation of nitrates and not the NO /NO₂ reactions.

Given all of the above limitations, it was decided to employ the Ambient Ratio Method (ARM), i.e. the second version of the DEA Tier 2 option. The ARM ambient ratio method is based upon the premise that the NO₂/NO_x ratio in a plume changes as it is transported but attains an equilibrium value some distance away from the source (Scire and Borissova, 2011). In their study, Scire and Borissova analysed hourly monitored NO₂ and NO_x data for 2006 at 325 monitoring sites throughout USA, which amounted to approximately 2.8 million data points for each species. These observations were grouped into a number of concentration ranges (bins), and the binned data were used to compute bin maximums and bin average curves. Short-term (1-hr) NO₂/NO_x ratios were subsequently developed based on bin-maximum data. Similarly, long-term (annual average) NO₂/NO_x ratios were based on bin-averaged data. The method was tested using the NO₂/NO_x ratios applied to the observed NO_x at selected stations to predict NO₂, and then compared to observed NO₂ concentrations at that station. The comparison of NO₂ derived from observed NO_x using these empirical curves was shown to be a conservative estimate of observed NO₂, whilst at the same time arriving at a more realistic approximation than if simply assuming a 100% conversion rate. More details of the adopted conversion factors are given in Appendix E.

5.1.4.4 *Particulate Formation*

CALPUFF includes two chemical transformation schemes for the calculation of sulfate and nitrate formation from SO₂ and NO_x emissions. These are the MESOPUFF II and the RIVAD / ARM3 chemical formulations. Whilst the former scheme is not specifically restricted to urban or rural conditions; the latter was developed for use in rural conditions. Since the study area could be classified as urban (Section 5.1.5), the RIVAD / ARM3 chemical formulations should not be used. The chemical transformation scheme chosen for this analysis was therefore the MESOPUFF II scheme. As described in the CALPUFF User Guide it is a "pseudo first-order chemical reaction mechanism" and involves five pollutant species namely SO₂, sulfates (SO₄), NO_x, nitric acid (HNO₃) and particulate nitrate. CALPUFF calculates the rate of transformation of SO₂ to SO₄, and the rate of transformation of NO_x to NO₃, based on environmental conditions including the ozone concentration, atmospheric stability, solar radiation, relative humidity, and the plume NO_x concentration. The daytime reaction formulation depends on solar radiation and the transformation increases non-linearly with the solar radiation (see the SO₂ to SO₄ transformation rate equation (equation 2-253 in the CALPUFF User Guide). At night, the transformation rate defaults to a constant value of 0.2% per hour. Calculations based on these formulas show that the transformation rate can reach about 3 per cent per hour at noon on a cloudless day with 100 ppb of ozone.

With the MESOPUFF-II mechanism, NO_x transformation rates depend on the concentration levels of NO_x and O₃ (equations 2-254 and 2-255 in the CALPUFF User Guide) and both organic nitrates (RNO₃) and HNO₃ are formed. According to the scheme, the formation of RNO₃ is irreversible and is not subject to wet or dry deposition. The formation of HNO₃, however, is reversible and is a function of temperature and relative humidity. The formation of particulate nitrate is further determined through the reaction of HNO₃ and NH₃. Background NH₃ concentrations are therefore required as input to calculate the equilibrium between HNO₃ and particulate nitrate. At night, the NO_x transformation rate defaults to a constant value of 2.0% per hour. Hourly average ozone and ammonia concentrations were included as input in the CALPUFF model to facilitate these sulfate and nitrate formation calculations.

The limitation of the CALPUFF model is that each puff is treated in isolation, i.e. any interaction between puffs from the same or different points of emission is not accounted for in these transformation schemes. CALPUFF first assumes that ammonia reacts preferentially with sulfate, and that there is always sufficient ammonia to react with the entire sulfate present within a single puff. The CALPUFF model performs a calculation to determine how much NH₃ remains after the particulate sulfate has been formed and the balance would then be available for reaction with NO₃ within the puff. The formation of particulate nitrate

is subsequently limited by the amount of available NH_3 . Although this may be regarded a limitation, in this application the particulate formation is considered as a group and not necessarily per species.

5.1.4.5 Ozone Formation

Similar to sulphate, nitrate and nitrogen dioxide, O_3 can also be formed through chemical reactions between pollutants released into the atmosphere. As a secondary pollutant, O_3 is formed in the lower part of the atmosphere, from complex photochemical reactions following emissions of precursor gases such as NO_x and VOCs (Seinfeld and Pandis, 1998). O_3 is produced during the oxidation of CO and hydrocarbons by hydroxyls (OH) in the presence of NO_x and sunlight (Seinfeld and Pandis, 1998). The rate of ozone production can therefore be limited by CO, VOCs or NO_x . In densely populated regions with high emissions of NO_x and hydrocarbons, rapid O_3 production can take place and result in a surface air pollution problem. In these urban areas O_3 formation is often VOC-limited. O_3 is generally NO_x -limited in rural areas and downwind suburban areas.

O_3 concentration levels have the potential to become particularly high in areas where considerable O_3 precursor emissions combine with stagnant wind conditions during the summer, when high insolation and temperatures occur (Seinfeld and Pandis, 1998). The effects of sunlight on O_3 formation depend on its intensity and its spectral distribution.

The main sectors that emit ozone precursors are road transport, power and heat generation plants, household (heating), industry, and petrol storage and distribution. In many urban areas, O_3 nonattainment is not caused by emissions from the local area alone. Due to atmospheric transport, contributions of precursors from the surrounding region can also be important. The transport of O_3 is determined by meteorological and chemical processes which typically extend over spatial scales of several hundred kilometres. Thus, in an attempt to study O_3 concentrations in a local area, it is necessary to include regional emissions and transport. This requires a significantly larger study domain with the inclusion of a significantly more comprehensive emissions inventory of NO_x and VOCs sources (e.g. vehicle emissions in Gauteng). Such a collaborative study was not within the scope of this report.

5.1.4.6 Model Input

5.1.4.6.1 Meteorological Input Data

The option of Partial Observations was selected for the CALMET wind field model which used both simulated and observed meteorological data (refer to Appendix C for all CALMET control options). 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 period 2015 to 2017 on a 4 km horizontal resolution for a 200 km by 200 km was used. An evaluation of the WRF data is provided in Table 5-6 with the benchmark for the WRF data provided in Table 5-5. This evaluation was undertaken for a point extracted at OR Tambo (see Figure 5-8). OR Tambo was selected for the evaluation as it is expected that the data quality at this weather station is of high standard. From the evaluation, the daily average WRF results for the period 2015 to 2017 were within the benchmarks for model evaluation, with the exception of wind direction (WRF providing value of 36

degrees for the gross error where benchmark is at ≤ 30 degrees) and temperature (WRF providing value of 2.22 K for the gross error where the benchmark is at ≤ 2 K and -1.27 K for the mean bias where benchmark is at $\leq \pm 0.5$ K).

Table 5-5: Benchmarks for WRF Model Evaluation

	Wind Speed	Wind Direction	Temperature	Humidity
IOA	≥ 0.6		≥ 0.8	≥ 0.6
RMSE	≤ 2 m/s			
Mean Bias	$\leq \pm 0.5$ m/s	$\leq \pm 10$ deg	$\leq \pm 0.5$ K	$\leq \pm 1$ g/kg
Gross Error		≤ 30 deg	≤ 2 K	≤ 2 g/kg

Table 5-6: Daily evaluation results for the WRF simulations for the 2015-2017 extracted at OR Tambo^(a)

	Wind Speed	Wind Direction	Temperature	Humidity
IOA	0.60		0.84	0.6
RMSE	1.55			
Mean Bias	0.05	0.39	-1.27	-0.54
Gross Error		36.26	2.22	1.11

(a) Values that do not meet the benchmark is provided in bold

A comparison of wind roses from measured meteorological data at OR Tambo (Figure 5-4) to WRF data (extracted at OR Tambo) (Figure 5-5) is provided below. The measured wind direction at OR Tambo has a higher frequency of winds from the north and lower frequency of winds from the north-northeast to east than the WRF data. The gross error for wind direction could influence the CALPUFF simulated pollutant concentrations by up to 36 degrees. This is limited by the inclusion of measured wind speed and direction at surface stations near Natref.

A comparison of monthly temperature profiles from measured meteorological data at OR Tambo to WRF data (extracted at OR Tambo) is provided in Figure 5-6. The measured temperature data is higher than the WRF data. This could result in the CALPUFF model underpredicting concentrations as the plume is not exposed to as much buoyancy in the atmosphere.

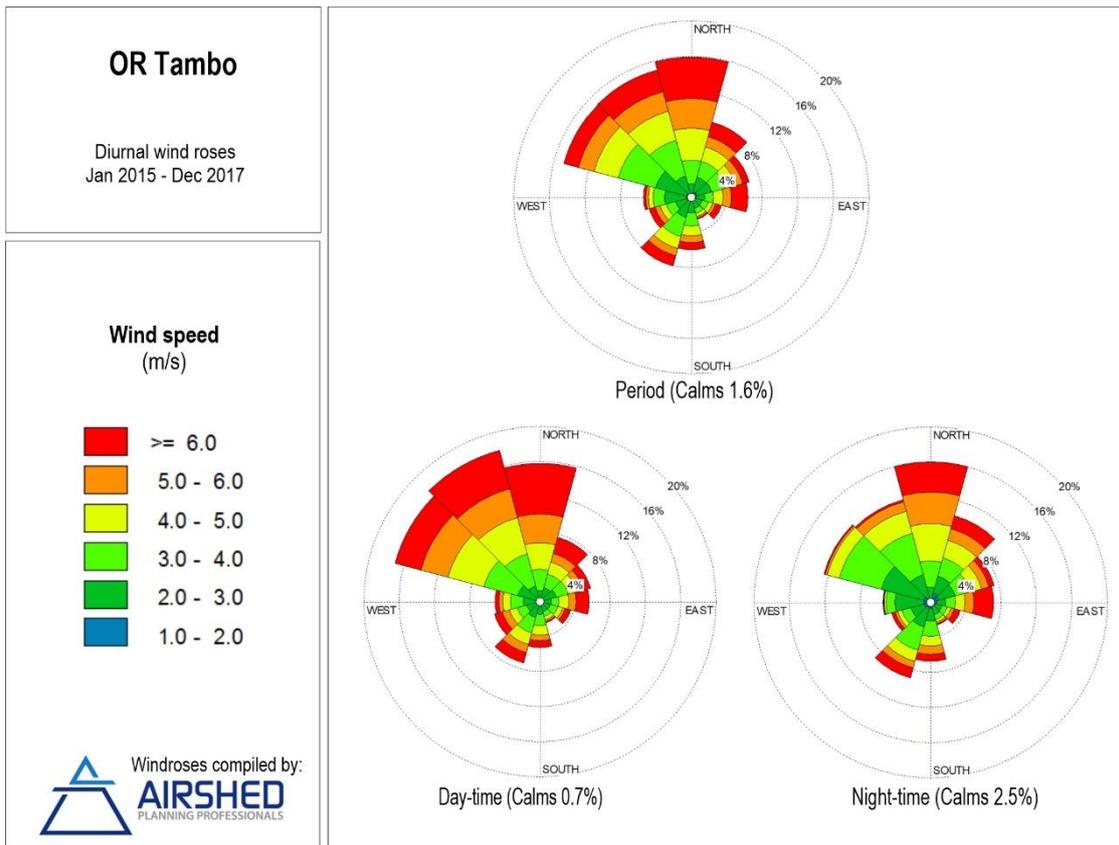


Figure 5-4: Period, day- and night-time wind rose for OR Tambo for the period 2015 - 2017

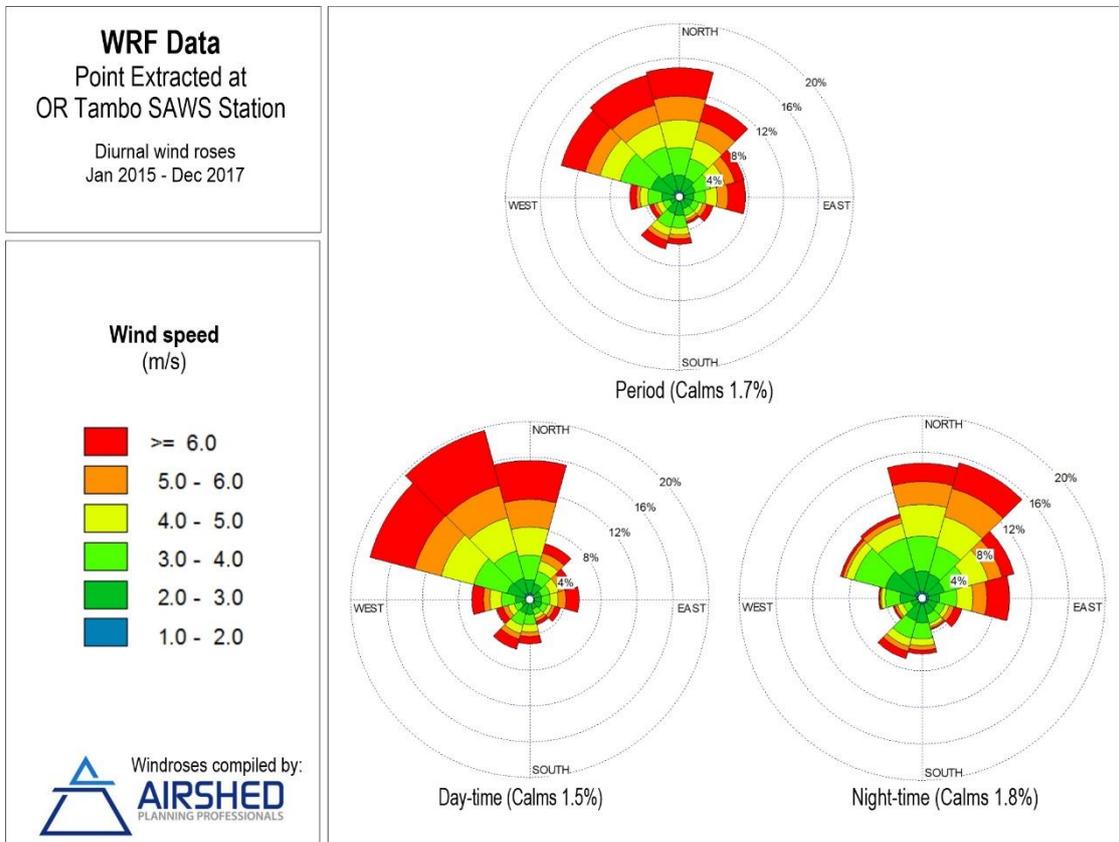


Figure 5-5: Period, day- and night-time wind rose for WRF data as extracted at OR Tambo for the period 2015 - 2017

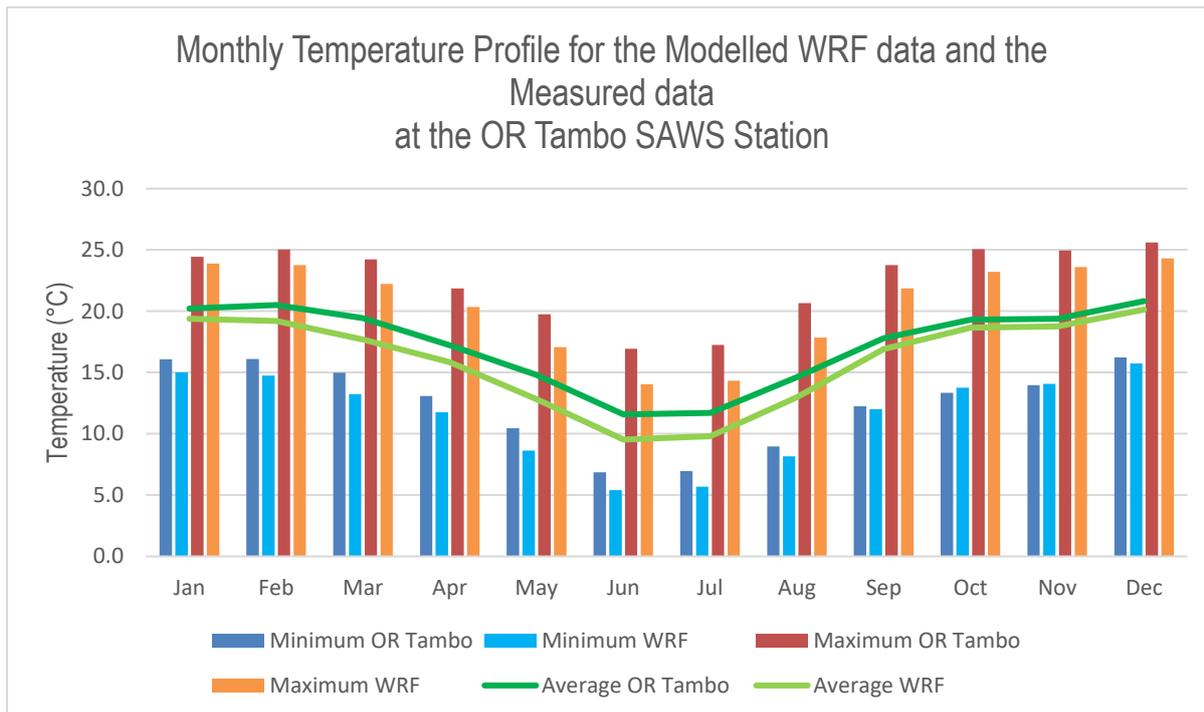


Figure 5-6: Monthly temperature profile for WRF data as extracted at OR Tambo and measured data from OR Tambo SAWS station data for the period 2015 – 2017

WRF data was supplemented with surface field observations from three monitoring stations operated by Sasol in the Sasolburg area and three monitoring stations operated by Sasol in the Secunda area. Meteorological parameters provided for the Sasol monitoring stations in the Sasolburg area are provided in Table 5-7.

Table 5-7: Meteorological parameters provided for the Sasol monitoring stations in the Sasolburg area

Monitoring Station	Latitude	Longitude	Closest Residential Area	Meteorology						
				WD	WS	Temp	RH	Press	SR	Rain
Eco Park	-26.778	27.837	Vaalpark	✓	✓	✓	✓	✓	✓	✓
AJ Jacobs	-26.822778	27.826111	Sasolburg	✓	✓					
Leitrim	-26.850278	27.874167	Sasolburg	✓	✓	✓	✓	✓		

WD: Wind direction
 WS: Wind speed
 Temp: Temperature
 RH: Relative humidity
 Press: Surface pressure
 SR: Solar radiation

An evaluation of the WRF data at the Eco Park monitoring station location is provided in Table 5-8. From the evaluation, the daily average WRF results for the period 2015 to 2017 were within the benchmarks for model evaluation, with the exception of wind direction (WRF providing value of -18 degrees mean bias where the benchmark is $\leq \pm 10$ degrees and 46 degrees for the gross error where benchmark is at ≤ 30 degrees) and temperature (WRF providing value of 2.27 K for the gross error where the benchmark is at ≤ 2 K and -0.81 K for the mean bias where benchmark is at $\leq \pm 0.5$ K). The gross error and mean bias for wind direction is limited by the inclusion of measures wind direction near Natref.

Table 5-8: Daily evaluation results for the WRF simulations for the 2015-2017 extracted at Eco Park^(a)

	Wind Speed	Wind Direction	Temperature	Humidity
IOA	0.64		0.88	0.56
RMSE	1.72			
Mean Bias	0.41	-18.48	-0.81	0.47
Gross Error		46.76	2.27	1.20

(a) Values that do not meet the benchmark is provided in bold

Figure 5-7 and Figure 5-8 provides examples of the CALMET layer 1 (up to 20 m above surface) wind vector plots from the CALMET data for 15 May 2015 at 05:00 and 2 February 2015 at 05:00 respectively. The spatial variations in the wind field over parts of the domain are due to terrain effects which are to be expected during this part of the diurnal cycle.

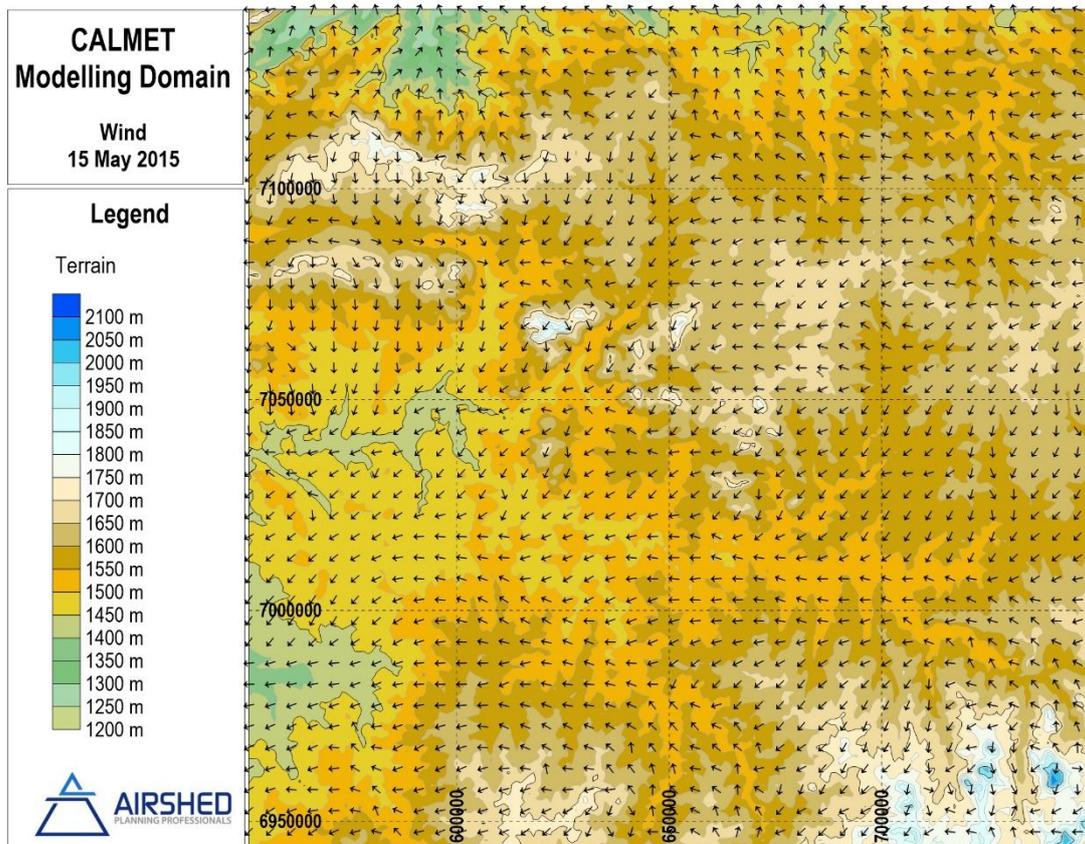


Figure 5-7: CALMET Layer 1 wind vector plot for 15 May 2015 at 05:00

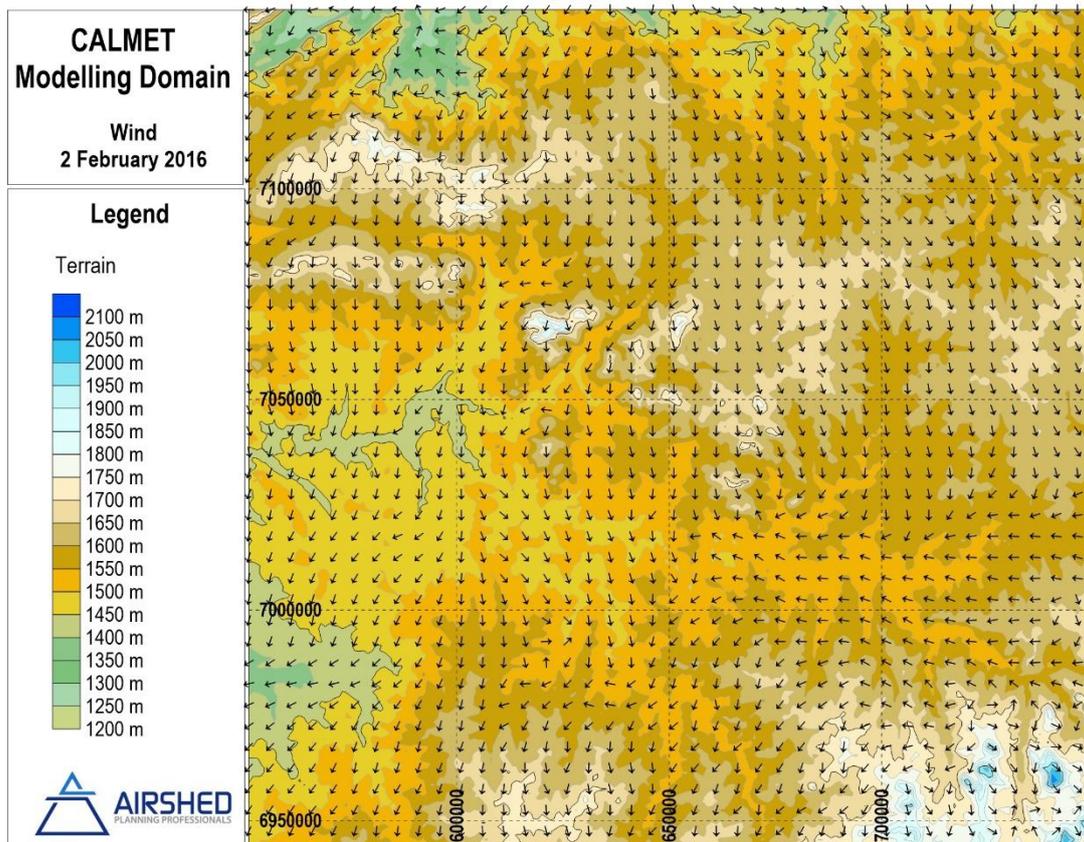


Figure 5-8: CALMET Layer 1 wind vector plot for 2 February 2016 at 05:00

5.1.4.6.2 Land Use and Topographical Data

Readily available terrain and land cover data for use in CALMET was obtained via the Lakes Environmental CALPUFF View interface. Use was made of Shuttle Radar Topography Mission (SRTM) (30 m, 1 arc-sec) terrain data and Global Land Cover Characterization (GLCC) land use data for Africa.

Figure 5-9 provides the terrain contours and land use categories over the entire CALMET domain and the location of the CALPUFF computational domain.

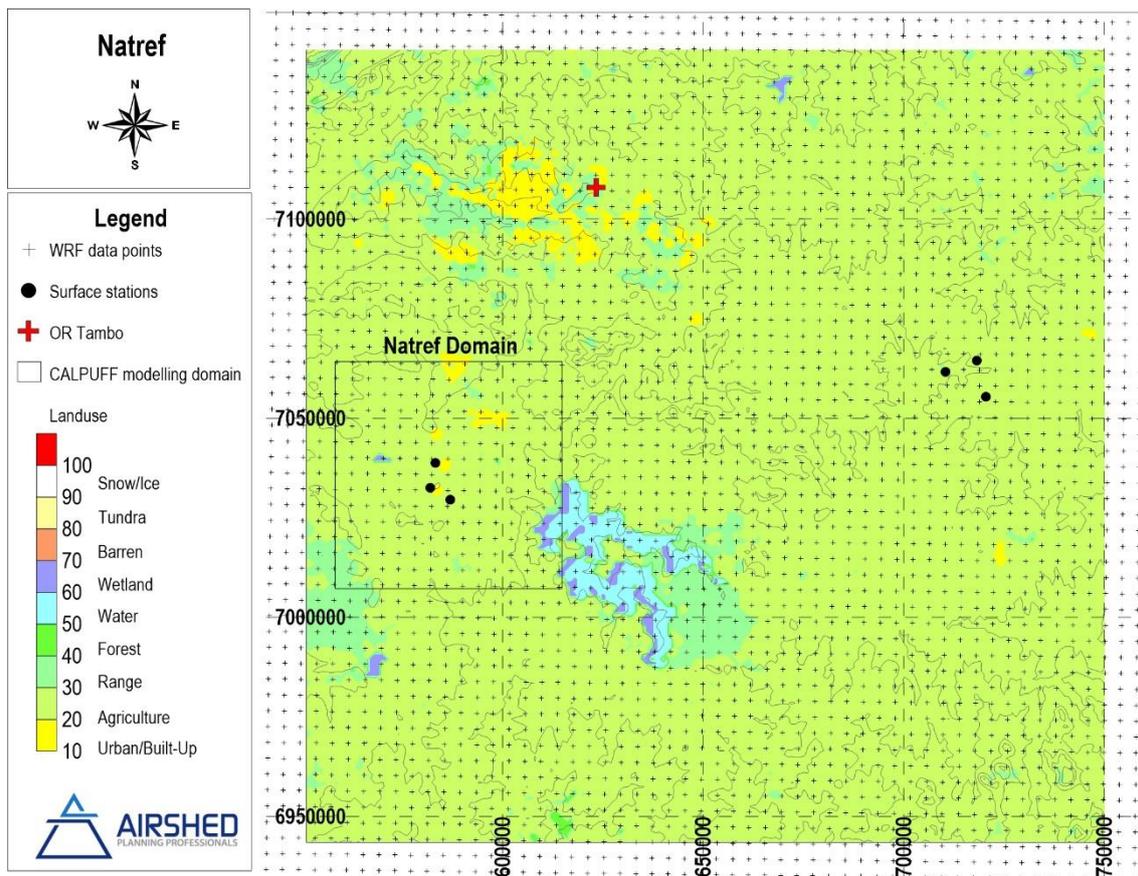


Figure 5-9: Land use categories, terrain contours, meteorological WRF grid points and surface station locations displayed on 200 x 200 km CALMET domain (1 km resolution)

5.1.4.6.3 Dispersion Coefficients

The option of dispersion coefficients from internally calculated sigma v, sigma w using micrometeorological variables (u^* , w^* , L , etc.) was selected (refer to Appendix D for all CALPUFF control options).

5.1.4.6.4 Grid Resolution and Model Domain

The CALMET modelling domain included an area of 200 km by 200 km with a grid resolution of 1 km. The vertical profile included 11 vertical levels up to a height of 3 500 m. The CALPUFF model domain selected for the sources at Natref included an area of 57 km by 57 km with a grid resolution of 200 m. This area was selected based on the area of impact around Sasolburg simulated during an assessment undertaken for the Vaal Triangle Airshed Priority Area.

5.1.4.6.5 Building Downwash

The impact of building downwash on ground-level pollutant concentrations was evaluated using "ScreenView" - a Tier 1 screening model which includes the same building downwash scheme as CALPUFF. For the most conservative simulation of downwind concentrations "ScreenView" was used with a full meteorological set. The screening exercise assessed the individual impact of three sources selected based on location; stack height; proximity to nearby buildings (excluding complex pipework structures); and, proximity to receptors. The baseline emission parameters (temperature, release height, exit

velocities, etc.) were used in combination with three theoretical building heights (10, 15, and 20 m). A single emission rate (1 m/s) was used to simulate the ground-level concentrations at automated distances between 1 m and 5 000 m from the sources, at 100 m intervals.

The screening assessment indicated that building downwash did not affect downwind concentration as a result of the emissions from tall stacks (75 m). Sources with lower release heights (15 m and 20 m) were found to increase ground-level concentrations downwind of the source where the scale of increase was dependent on the height of the near-by building. The distance after which simulated ground-level concentrations matched levels for comparative simulations where building downwash was not included was a minimum of 1 800 m.

Building downwash was not accounted for in the dispersion modelling of stack emission sources, based on the findings from the screening evaluation, and on the basis that the nearest receptor is approximately 2 300m away from the Natref facility, and the minimum stack height is 20 m.

5.1.5 *Atmospheric Dispersion Potential*

Meteorological mechanisms govern the dispersion, transformation, and eventual removal of pollutants from the atmosphere. The analysis of hourly average meteorological data is necessary to facilitate a comprehensive understanding of the dispersion potential of the site. The horizontal dispersion of pollution is largely a function of the wind field. The wind speed determines both the distance of downward transport and the rate of dilution of pollutants. A summary of the measured meteorological data is given in Appendix F.

Sasol currently operates four meteorological stations in the Sasolburg area (viz. Sasol 1 Fence Line, Eco Park, AJ Jacobs and Leitrim). For this assessment, data from the Sasol operated meteorological stations at Eco Park, AJ Jacobs and Leitrim was provided for the period 2015 to 2017. Parameters useful in describing the dispersion and dilution potential of the site (i.e. wind speed, wind direction, temperature and atmospheric stability) are subsequently discussed.

5.1.5.1 *Surface Wind Field*

Wind roses comprise 16 spokes, which represent the directions from which winds blew during a specific period. The colours used in the wind roses below, reflect the different categories of wind speeds; the red area, for example, representing winds >6m/s. The dotted circles provide information regarding the frequency of occurrence of wind speed and direction categories. The frequency with which calms occurred, i.e. periods during which the wind speed was below 1 m/s are also indicated.

The period wind field and diurnal variability (2015 to 2017) for the three Sasol operated meteorological stations in the Sasolburg area is provided in Figure 5-10 to Figure 5-12.

The predominant flow field at Eco Park is from the east-southeast (~12% frequency of occurrence). During day-time conditions winds from the north-western sector increases while winds from the east-southeast are more frequent during night-time conditions (Figure 5-10).

The predominant wind direction at AJ Jacobs is from the north-northeast (~11% frequency of occurrence) (Figure 5-11). Very little wind is measured from the south-eastern sector. During day-time conditions winds from the western sector increase while

winds from the north-northeast are more frequent during night-time conditions. A higher frequency of low-speed winds (1-2 m/s) and calm conditions (less than 1 m/s) was measured at this monitoring station.

The predominant wind direction at Leitrim is from the north-northeast and east (~10% frequency of occurrence). During day-time conditions winds from the western sector increase while winds from the east, south-southeast and north-northeast are more frequent during night-time conditions (Figure 5-12).

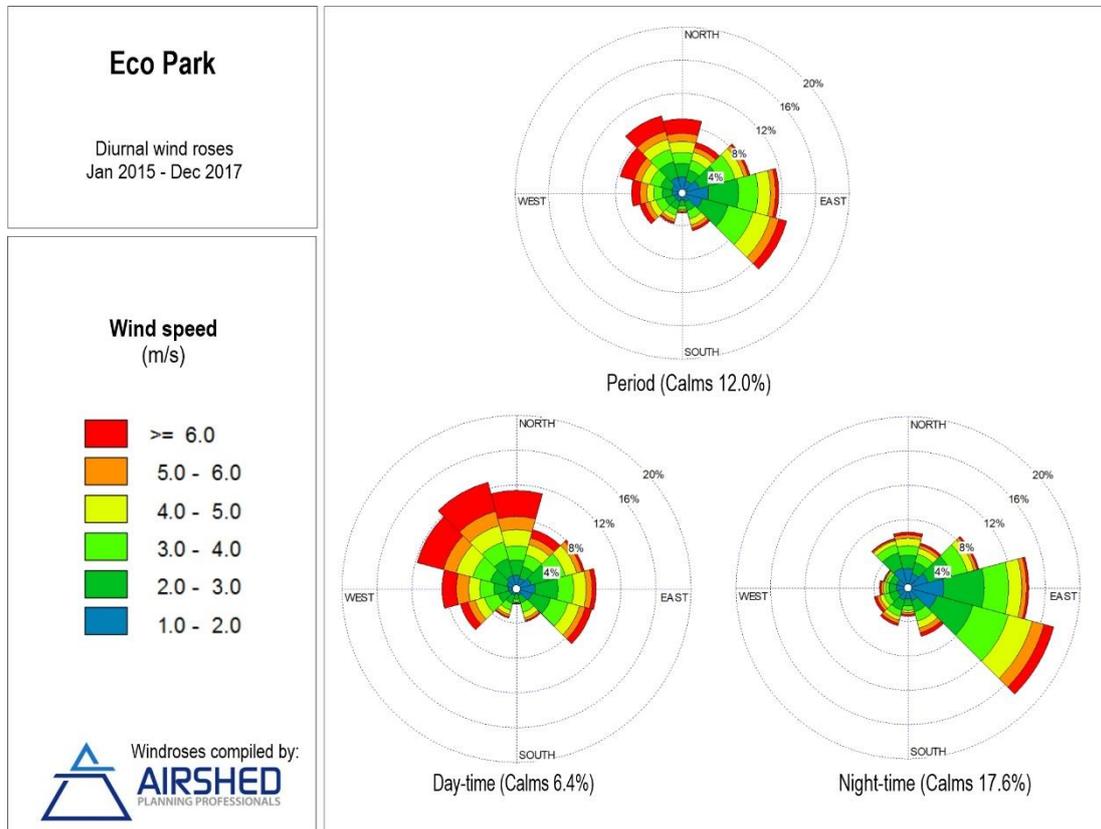


Figure 5-10: Period, day- and night-time wind rose for Eco Park for the period 2015 - 2017

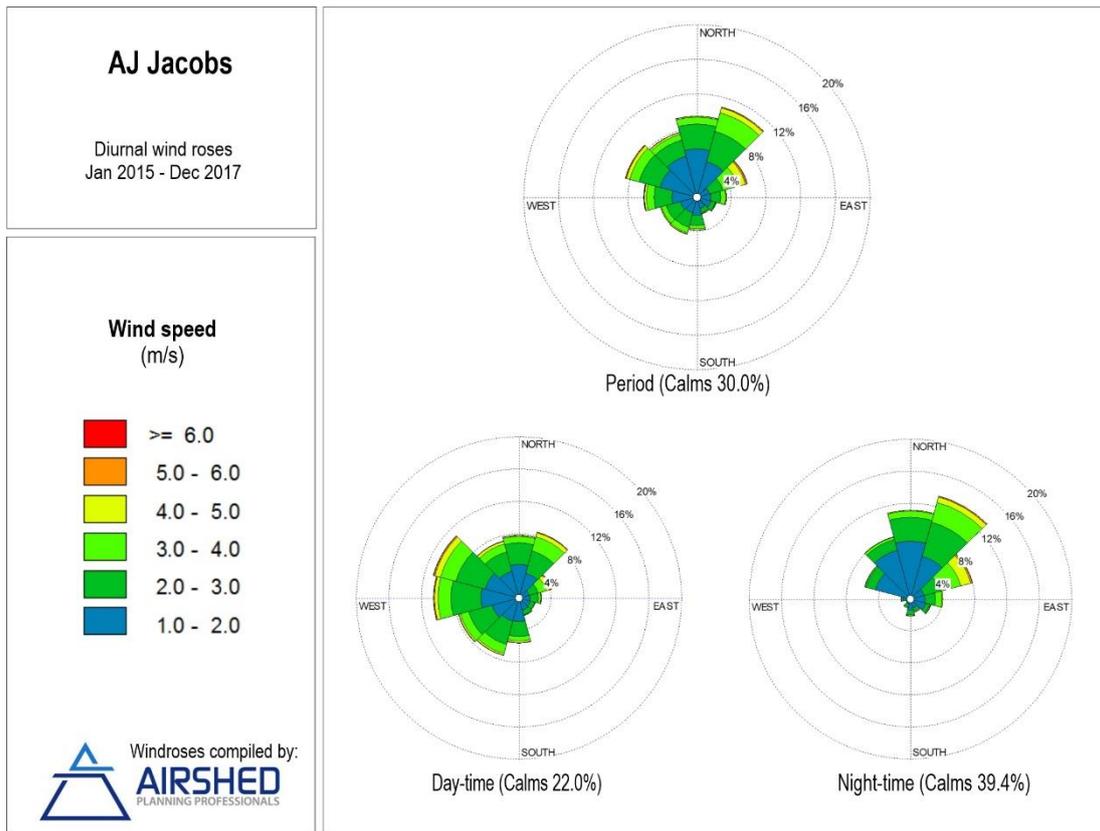


Figure 5-11: Period, day- and night-time wind rose for AJ Jacobs for the period 2015 - 2017

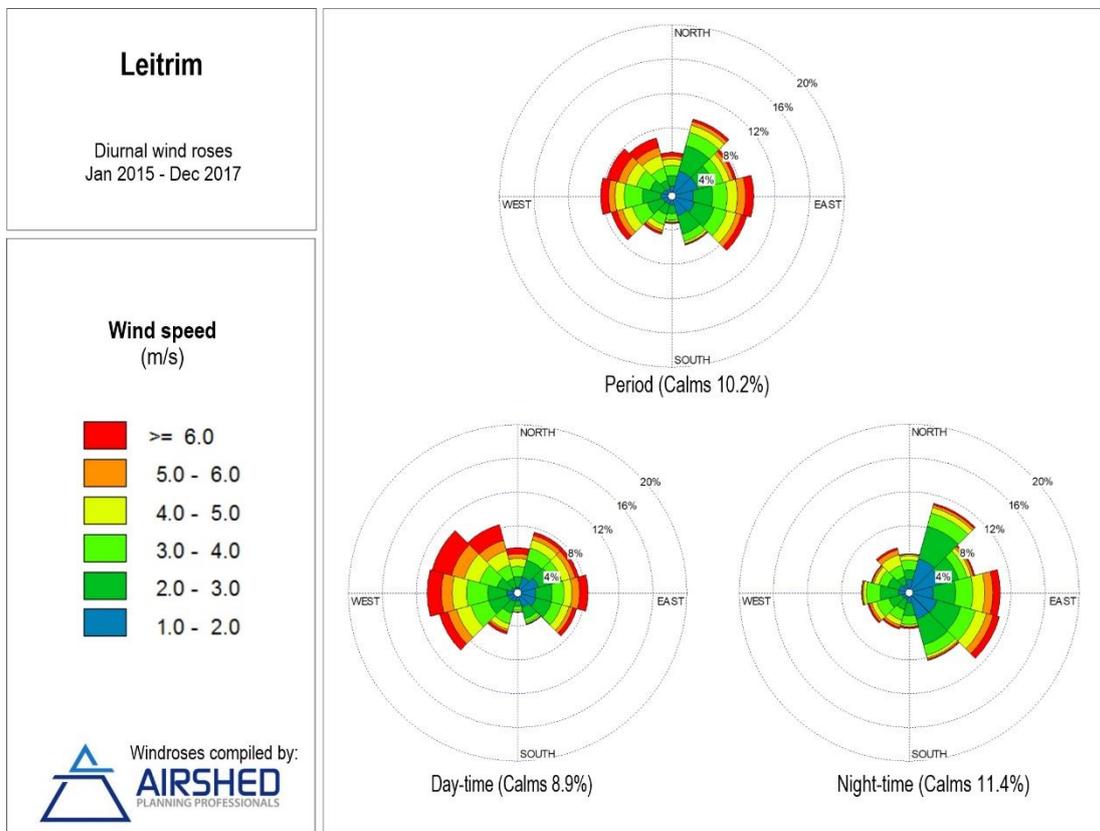


Figure 5-12: Period, day- and night-time wind rose for Leitrim for the period 2015 - 2017

5.1.5.2 Temperature

Air temperature is important, both for determining the effect of plume buoyancy (the larger the temperature difference between the emission plume and the ambient air, the higher the plume can rise), and determining the development of the mixing and inversion layers.

The average monthly temperature trends are presented in Figure 5-13 and Figure 5-14 for Eco Park and Leitrim respectively. Monthly mean and hourly maximum and minimum temperatures are given in Table 5-9.

Table 5-9: Monthly temperature summary (2015 - 2017)

Hourly Minimum, Hourly Maximum and Monthly Average Temperatures (°C) (2015 - 2017)												
	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Eco Park												
Minimum	17.2	16.7	14.7	11.6	6.8	4.0	3.9	5.7	11.4	13.2	14.3	17.1
Maximum	27.1	27.6	26.3	24.2	21.8	19.1	19.3	22.8	25.8	27.3	27.1	28.1
Average	22.1	21.9	20.3	17.5	14.0	11.0	11.2	14.2	18.4	20.3	20.8	22.4
Leitrim												
Minimum	17.3	16.7	14.6	11.6	7.1	4.6	4.0	5.6	10.8	13.4	14.1	17.0
Maximum	27.4	28.4	26.6	24.4	22.2	19.2	19.7	23.2	25.8	27.7	27.3	28.4
Average	22.2	22.3	20.3	17.8	14.2	11.4	11.4	14.3	18.1	20.6	20.7	22.5

Average temperatures ranged between 11 °C and 22.5 °C. The highest temperatures occurred in December and the lowest in July. During the day, temperatures increase to reach maximum at around 15:00 in the afternoon. Ambient air temperature decreases to reach a minimum at around 07:00 i.e. just before sunrise.

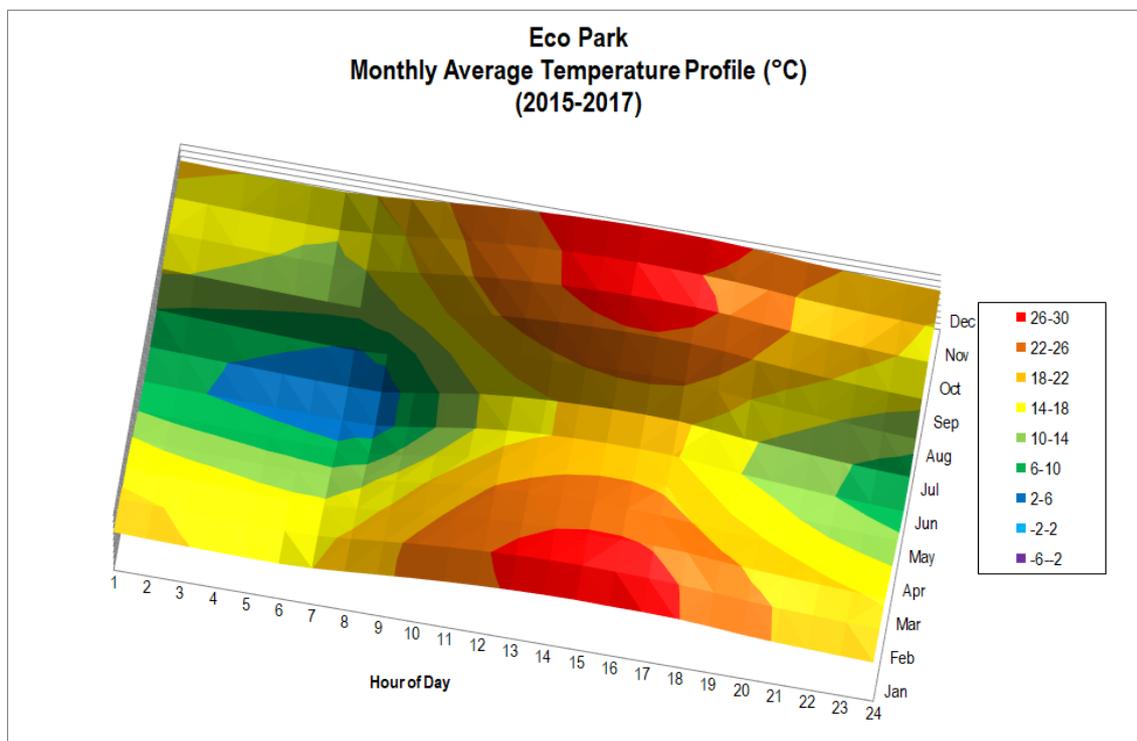


Figure 5-13: Monthly average temperature profile for Eco Park (2015 – 2017)

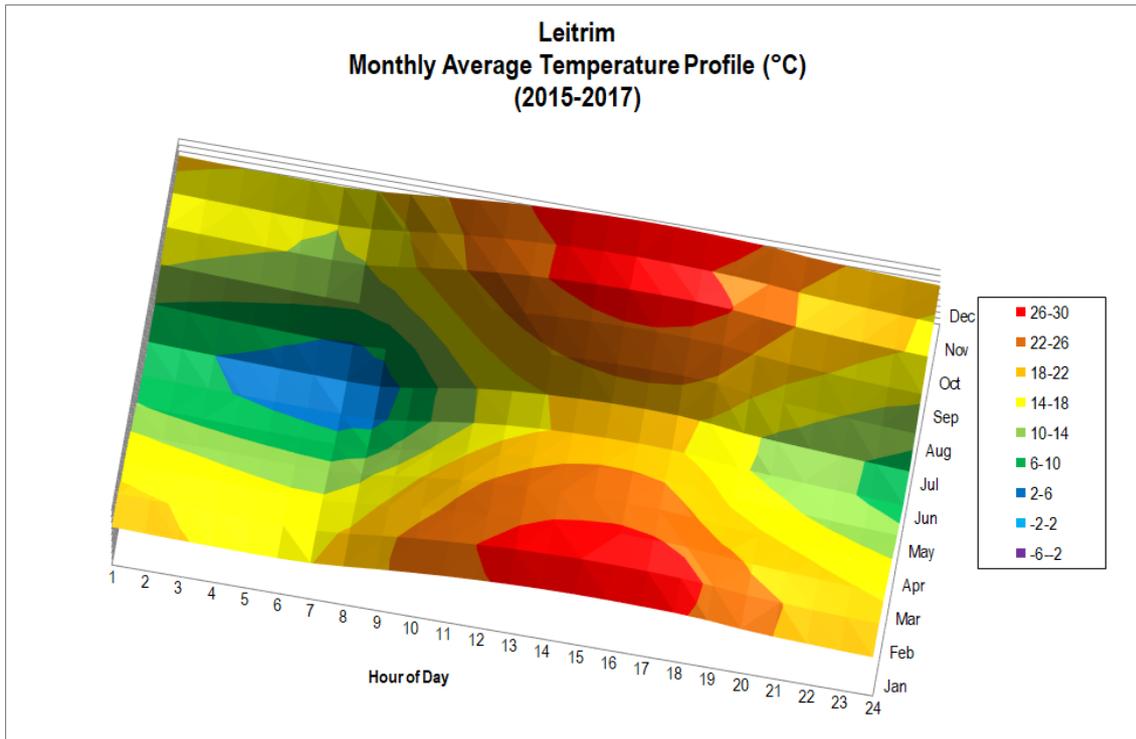


Figure 5-14: Monthly average temperature profile for Leitrim (2015 – 2017)

5.1.5.3 Atmospheric Stability

The atmospheric boundary layer properties are described by two parameters; the boundary layer depth and the Monin-Obukhov length.

The Monin-Obukhov length (L_{Mo}) provides a measure of the importance of buoyancy generated by the heating of the ground and mechanical mixing generated by the frictional effect of the earth's surface. Physically, it can be thought of as representing the depth of the boundary layer within which mechanical mixing is the dominant form of turbulence generation (CERC, 2004). The atmospheric boundary layer constitutes the first few hundred metres of the atmosphere. During daytime, the atmospheric boundary layer is characterised by thermal turbulence due to the heating of the earth's surface. Night-times are characterised by weak vertical mixing and the predominance of a stable layer. These conditions are normally associated with low wind speeds and lower dilution potential.

Diurnal variation in atmospheric stability, as calculated from on-site data (Tiwary and Colls, 2010), and described by the inverse Monin-Obukhov length and the boundary layer depth is provided in Figure 5-15. The highest concentrations for ground level, or near-ground level releases from non-wind dependent sources would occur during weak wind speeds and stable (night-time) atmospheric conditions.

For elevated releases, unstable conditions can result in very high concentrations of poorly diluted emissions close to the stack. This is called looping (Figure 5-15 (c)) and occurs mostly during daytime hours. Neutral conditions disperse the plume fairly equally in both the vertical and horizontal planes and the plume shape is referred to as coning (Figure 5-15 (b)). Stable conditions prevent the plume from mixing vertically, although it can still spread horizontally and is called fanning (Figure 5-14 (a)) (Tiwary & Colls, 2010).

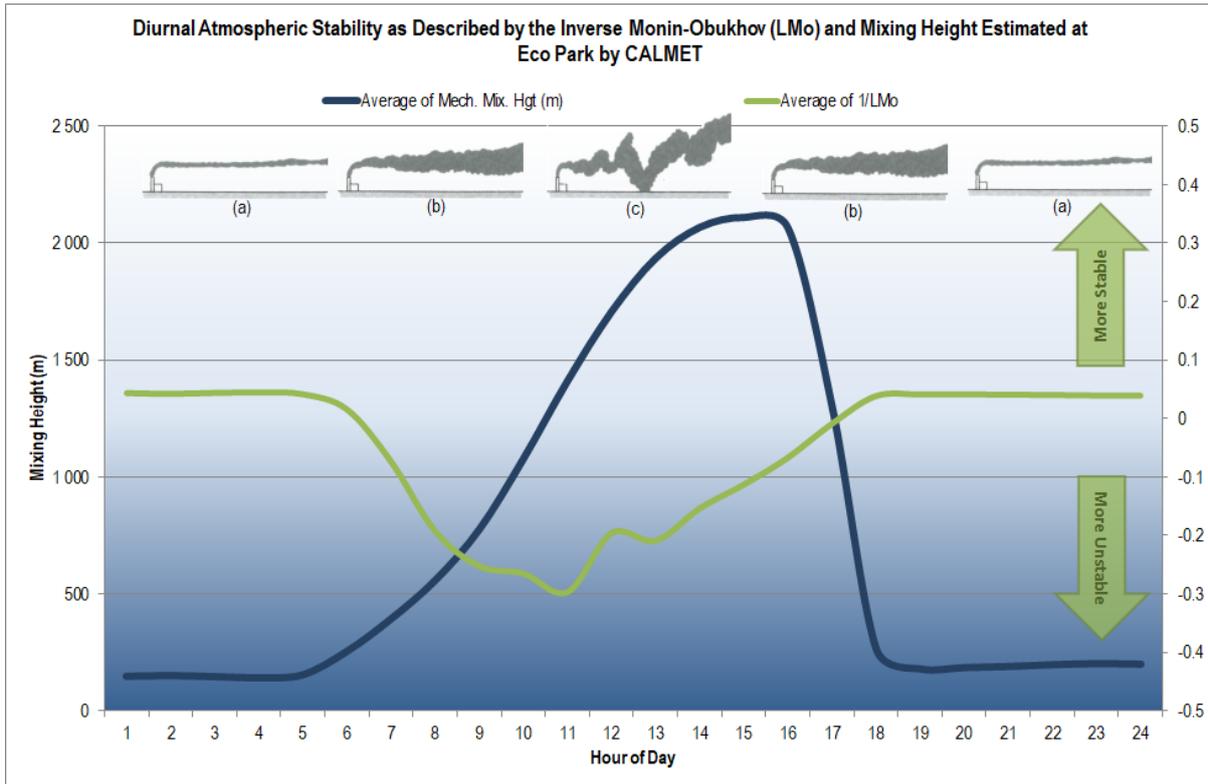


Figure 5-15: Diurnal atmospheric stability (extracted from CALMET at the Eco Park monitoring point)

5.1.5.4 Air Quality Monitoring data

A summary of ambient data measured at Leitrim, AJ Jacobs and Eco Park for the period 2015 – 2017 is provided in Table 5-11, Table 5-12 and Table 5-13 respectively. A summary of ambient air quality data recorded at the DEA stations - Three Rivers, Sharpeville, and Zamdela - is provided in Table 5-14, Table 5-15, and Table 5-16. Time series of the measured ambient air quality data is provided in Appendix F.

Table 5-10: Summary of the ambient NH₃ measurements at Fence Line for the period 2010-2012 (units: µg/m³)

Period	Hourly				Annual Average
	Max	99 th Percentile	90 th Percentile	50 th Percentile	
NH ₃					
2010	231.34	65.19	6.59	0.59	4.74
2011	270.11	82.68	15.98	1.10	6.60
2012	236.77	88.22	23.29	5.18	10.11
Average	246.07	78.69	15.28	2.29	7.15
NOTE:					
* Ammonia is no longer monitored at the Sasol monitoring stations and therefore data for the most recent available period was used.					

Table 5-11: Summary of the ambient measurements at Leitrim for the period 2015-2017 (units: µg/m³)

Period	Availability	Hourly				Annual Average	No of recorded hourly exceedances
		Max	99 th Percentile	90 th Percentile	50 th Percentile		
NO ₂							
2015	21%	178.4	64.9	39.0	17.3	21.2	1
2016	91%	140.7	87.2	47.8	17.6	22.8	-
2017	90%	117.4	77.9	42.9	15.4	19.2	-
Average			76.7	43.2	16.8	21.1	

Period	Availability	Hourly				Annual Average	No of recorded hourly exceedances
		Max	99 th Percentile	90 th Percentile	50 th Percentile		
SO₂							
2015	85%	1007.4	185.0	82.3	20.0	33.3	4
2016	94%	515.9	205.8	78.5	28.4	39.4	15
2017	90%	425.8	172.6	70.3	24.6	33.5	2
Average			187.8	77.0	24.3	35.4	
Period	Availability	Daily				Annual Average	No of recorded daily exceedances
		Max	99 th Percentile	90 th Percentile	50 th Percentile		
SO₂							
2015	85%	46.1	40.5	26.9	11.2	33.3	-
2016	94%	45.7	38.2	23.7	14.4	39.4	-
2017	90%	37.1	30.6	22.2	11.8	33.5	-
Average			36.4	24.2	12.4	35.4	
PM₁₀							
2015	81%	192.1	153.4	106.0	37.7	49.2	57
2016	24%	129.9	121.6	100.9	12.7	38.5	21
2017	52%	193.5	142.4	80.4	29.4	38.0	22
Average			139.1	95.8	26.6	41.9	
PM_{2.5}							
2015	65%	117.0	75.2	50.0	19.3	24.2	5
2016	26%	59.8	58.5	37.2	2.9	12.6	8
2017	52%	49.7	39.1	22.3	8.1	10.5	2
Average			57.6	36.5	10.1	15.8	

Table 5-12: Summary of the ambient measurements at AJ Jacobs for the period 2015-2017 (units: µg/m³)

Period	Availability	Hourly				Annual Average	No of recorded hourly exceedances
		Max	99 th Percentile	90 th Percentile	50 th Percentile		
NO₂							
2015	86%	127.4	79.6	46.3	15.3	21.0	-
2016	95%	125.4	73.5	42.9	16.1	20.3	-
2017	92%	164.7	81.4	52.1	25.1	26.6	-
Average			78.1	47.1	18.8	22.7	
SO₂							
2015	98%	603.6	284.1	111.1	46.3	56.3	34
2016	96%	676.0	307.7	121.1	41.0	57.2	54
2017	88%	718.5	320.6	173.4	78.0	89.7	56
Average			304.1	135.2	55.1	67.7	
Period	Availability	Daily				Annual Average	No of recorded daily exceedances
		Max	99 th Percentile	90 th Percentile	50 th Percentile		
SO₂							
2015	98%	224.6	152.9	104.5	53.5	56.3	14
2016	96%	188.0	162.1	103.0	49.1	57.2	23
2017	88%	220.6	194.5	160.0	80.5	89.7	91
Average			169.9	122.5	61.0	67.7	
PM₁₀							
2015	96%	124.6	119.9	81.1	39.5	46.4	48
2016	99%	154.9	105.1	76.1	37.7	43.1	39
2017	98%	107.3	94.6	74.0	33.4	38.9	32
Average			106.5	77.1	36.9	42.8	
PM_{2.5}							
2015	93%	51.0	48.2	30.9	16.1	18.3	-
2016	82%	73.7	54.2	33.4	15.2	17.9	14
2017	93%	75.8	69.9	49.7	19.9	24.8	66
Average			57.5	38.0	17.1	20.4	

Table 5-13: Summary of the ambient measurements at Eco Park for the period 2015-2017 (units: µg/m³)

Period	Availability	Hourly				Annual Average	No of recorded hourly exceedances
		Max	99 th Percentile	90 th Percentile	50 th Percentile		
NO₂							
2015	84%	782.9	85.1	52.9	15.9	22.3	2
2016	98%	373.1	85.9	51.1	15.0	21.5	6
2017	98%	439.8	84.2	49.2	14.4	20.5	3
Average			85.1	51.1	15.1	21.5	
SO₂							
2015	96%	881.5	239.4	89.9	42.8	51.5	31
2016	98%	842.4	261.8	82.6	28.3	41.9	41
2017	98%	891.5	230.4	65.5	21.2	33.4	35
Average			243.8	79.3	30.8	42.2	
Period	Availability	Daily				Annual Average	No of recorded daily exceedances
		Max	99 th Percentile	90 th Percentile	50 th Percentile		
SO₂							
2015	96%	131.0	117.6	86.1	48.8	51.5	1
2016	98%	144.3	128.1	81.5	36.3	41.9	5
2017	98%	145.6	100.9	60.4	30.0	33.4	2
Average			115.5	76.0	38.3	42.2	
PM₁₀							
2015	93%	150.4	126.1	83.0	27.5	37.2	45
2016	98%	131.1	117.9	69.5	27.2	33.1	29

Period	Availability	Hourly				Annual Average	No of recorded hourly exceedances
		Max	99 th Percentile	90 th Percentile	50 th Percentile		
2017	96%	145.5	98.3	68.5	23.3	31.4	29
Average			112.6	71.9	26.5	34.0	
PM_{2.5}							
2015	95%	61.7	52.6	35.2	14.7	18.2	-
2016	98%	312.9	308.8	32.9	13.3	20.6	23
2017	97%	331.9	69.8	46.1	16.3	22.0	50
Average			143.7	38.1	14.7	20.3	
O₃							
2015	98%	124.1	109.7	85.5	58.7	58.3	
2016	99%	1567.4	728.0	91.3	58.0	79.5	
2017	99%	112.3	108.0	85.3	60.0	61.2	
Average			315.2	87.4	58.9	67.0	

Table 5-14: Summary of the ambient measurements at Three Rivers for the period 2015-2017 (units: µg/m³)

Period	Availability	Hourly				Annual Average	No of recorded hourly exceedances
		Max	99 th Percentile	90 th Percentile	50 th Percentile		
NO₂							
2015	80%	178.6	104.6	64.5	24.8	31.5	-
2016	91%	148.4	92.1	53.0	21.8	26.4	-
2017	91%	178.2	95.1	54.3	20.8	26.3	-
Average			97.3	57.3	22.5	28.1	
SO₂							
2015	53%	592.0	110.1	30.3	8.0	14.5	5
2016	91%	474.8	163.1	30.4	7.6	15.5	7
2017	91%	539.3	141.5	36.2	10.1	17.9	9
Average			138.3	32.3	8.6	16.0	
Benzene							
2015	37%	17.3	6.7	3.7	0.4	1.2	
2016	83%	11.6	3.0	1.2	0.1	0.4	
2017	79%	13.2	2.8	0.8	0.1	0.3	
Average			4.2	1.9	0.2	0.7	
CO							
2015	83%	5710	1808	715	260	352	-
2016	91%	5250	1482	896	496	587	-
2017	44%	3769	1632	979	549	658	-
Average			1641	863	435	532	
Period	Availability	Daily				Annual Average	No of recorded daily exceedances
		Max	99 th Percentile	90 th Percentile	50 th Percentile		
SO₂							
2015	53%	105.2	55.4	26.9	10.8	14.5	-
2016	91%	117.7	67.3	32.7	11.0	15.5	-
2017	91%	114.2	72.4	33.0	14.3	17.9	-
Average			65.0	30.9	12.0	16.0	
PM₁₀							
2015	82%	144.2	119.3	84.3	46.2	51.4	54
2016	90%	174.2	130.1	101.8	53.7	61.1	87
2017	90%	248.4	177.6	63.5	32.0	38.6	24
Average			142.3	83.3	43.9	50.4	
PM_{2.5}							
2015	87%	76.6	69.7	45.7	25.6	27.7	5
2016	82%	96.5	61.8	45.8	26.0	28.7	58
2017	78%	83.0	60.1	34.7	21.0	22.1	18
Average			63.8	42.0	24.2	26.2	

O ₃							
2015	80%	127.8	105.2	85.0	55.9	55.6	
2016	89%	122.8	104.0	83.9	55.5	56.4	
2017	45%	107.5	76.3	64.4	43.7	44.0	
Average			95.2	77.8	51.7	52.0	

Table 5-15: Summary of the ambient measurements at Sharpeville for the period 2015-2017 (units: µg/m³)

Period	Availability	Hourly				Annual Average	No of recorded hourly exceedances
		Max	99 th Percentile	90 th Percentile	50 th Percentile		
NO₂							
2015	86%	344.0	156.7	96.3	31.3	43.9	15
2016	86%	176.8	104.7	62.7	22.6	29.7	-
2017	82%	195.5	105.2	64.1	21.8	29.6	-
Average			122.2	74.4	25.2	34.4	
SO₂							
2015	87%	950.4	135.8	38.2	10.9	19.1	16
2016	80%	512.3	127.1	34.0	7.0	15.2	3
2017	69%	462.8	180.7	49.0	8.8	20.8	6
Average			147.9	40.4	8.9	18.4	
Benzene							
2015	32%	25.9	12.2	3.1	0.5	1.3	
2016	0%						
2017	35%	56.1	16.8	5.4	0.8	2.1	
Average			14.5	4.3	0.6	1.7	
CO							
2015	87%	6420	3492	1516	512	712	-
2016	88%	7684	3724	1903	739	968	-
2017	44%	5736	3317	1647	701	893	-
Average			3511	1688	651	858	
Period	Availability	Daily				Annual Average	No of recorded daily exceedances
		Max	99 th Percentile	90 th Percentile	50 th Percentile		
SO₂							
2015	87%	135.0	94.0	36.5	13.4	19.1	2
2016	80%	97.6	74.5	33.5	9.7	15.2	-
2017	69%	147.1	106.6	46.5	12.4	20.8	1
Average			91.7	38.8	11.8	18.4	
PM₁₀							
2015	89%	178.0	153.6	110.3	53.8	62.8	83
2016	86%	251.0	234.8	166.9	84.6	95.9	185
2017	56%	188.5	130.5	84.1	41.8	46.7	36
Average			173.0	120.4	60.1	68.5	
PM_{2.5}							
2015	88%	138.4	97.9	60.6	31.8	36.5	27
2016	53%	81.7	77.2	47.1	29.7	31.6	43
2017	90%	322.4	151.1	68.3	34.6	39.4	131
Average			108.7	58.7	32.0	35.8	
O₃							
2015	88%	127.8	107.3	83.5	52.1	51.3	
2016	91%	107.9	103.8	72.9	45.9	48.3	
2017	50%	99.3	96.5	81.5	49.6	52.5	
Average			102.5	79.3	49.2	50.7	

Table 5-16: Summary of the ambient measurements at Zamdela for the period 2015-2017 (units: $\mu\text{g}/\text{m}^3$)

Period	Availability	Hourly				Annual Average	No of recorded hourly exceedances
		Max	99 th Percentile	90 th Percentile	50 th Percentile		
NO₂							
2015	87%	168.1	100.4	62.4	24.6	30.1	-
2016	88%	199.8	123.7	73.7	24.3	32.7	-
2017	50%	141.7	91.3	55.8	21.3	26.4	-
Average			105.2	64.0	23.4	29.7	
SO₂							
2015	87%	414.5	172.7	52.4	9.2	21.4	5
2016	87%	647.7	187.1	52.9	9.9	22.2	5
2017	75%	356.1	165.5	44.3	8.2	18.7	2
Average			175.1	49.8	9.1	20.7	
Benzene							
2015	63%	16.3	11.6	4.2	1.0	1.8	
2016	67%	2752.4	638.8	220.8	0.9	59.5	
2017	49%	31.5	25.9	7.7	1.3	3.1	
Average			225.4	77.6	1.1	21.4	
CO							
2015	73%	7187	3889	1267	491	652	-
2016	84%	12691	4860	1491	645	858	-
2017	38%	7690	3965	1432	703	845	-
Average			4238	1397	613	785	
Period	Availability	Daily				Annual Average	No of recorded daily exceedances
		Max	99 th Percentile	90 th Percentile	50 th Percentile		
SO₂							
2015	87%	105.1	68.2	43.6	17.9	21.4	-
2016	87%	180.7	81.1	44.9	17.2	22.2	2
2017	75%	171.8	68.9	41.9	13.0	18.7	1
Average			75.3	44.5	17.8	22.3	
PM₁₀							
2015	57%	221.9	125.2	88.7	40.3	46.0	35
2016	92%	175.3	165.2	106.5	57.2	64.7	106
2017	76%	245.2	133.1	74.7	46.5	49.4	26
Average			141.1	90.0	48.0	53.3	
PM_{2.5}							
2015	80%	93.6	73.2	54.2	26.0	30.0	11
2016	82%	138.4	95.8	58.7	30.9	35.0	92
2017	83%	105.9	89.8	45.9	26.9	29.7	64
Average			86.3	52.9	27.9	31.6	
O₃							
2015	94%	95.7	88.0	71.3	49.1	50.4	
2016	95%	91.8	83.3	67.4	43.9	45.9	
2017	41%	77.4	71.8	53.0	35.0	35.7	
Average			81.0	63.9	42.7	44.0	

The following graphs summarise the observed concentrations of SO₂, NO₂ and PM₁₀ at the six monitoring sites (Leitrim, AJ Jacobs, Eco Park, Three Rivers, Sharpeville, and Zamdela) monitoring stations for the years 2015, 2016 and 2017. The NAAQS have been included in the graphs for:

- SO₂ hourly (88 hourly exceedances of 350 $\mu\text{g}/\text{m}^3$) and daily average (4 daily exceedances of 125 $\mu\text{g}/\text{m}^3$)
- NO₂ hourly average (88 hourly exceedances of 200 $\mu\text{g}/\text{m}^3$); and,
- PM₁₀ daily average (4 daily exceedances of 75 $\mu\text{g}/\text{m}^3$; 2015 standards).

The hourly 99th percentiles for SO₂ were below the limit value of 350 µg/m³ at all stations for all three years (Figure 5-16 to Figure 5-21). The daily 99th percentiles for SO₂ were exceeded at AJ Jacobs for 2015, 2016 and 2017 (Figure 5-23) and at Eco Park in 2016 (Figure 5-24) but were below the limit value (125 µg/m³) at Leitrim, Three Rivers, Sharpeville and Zamdela stations for all three years (Figure 5-22 and Figure 5-25 to Figure 5-27).

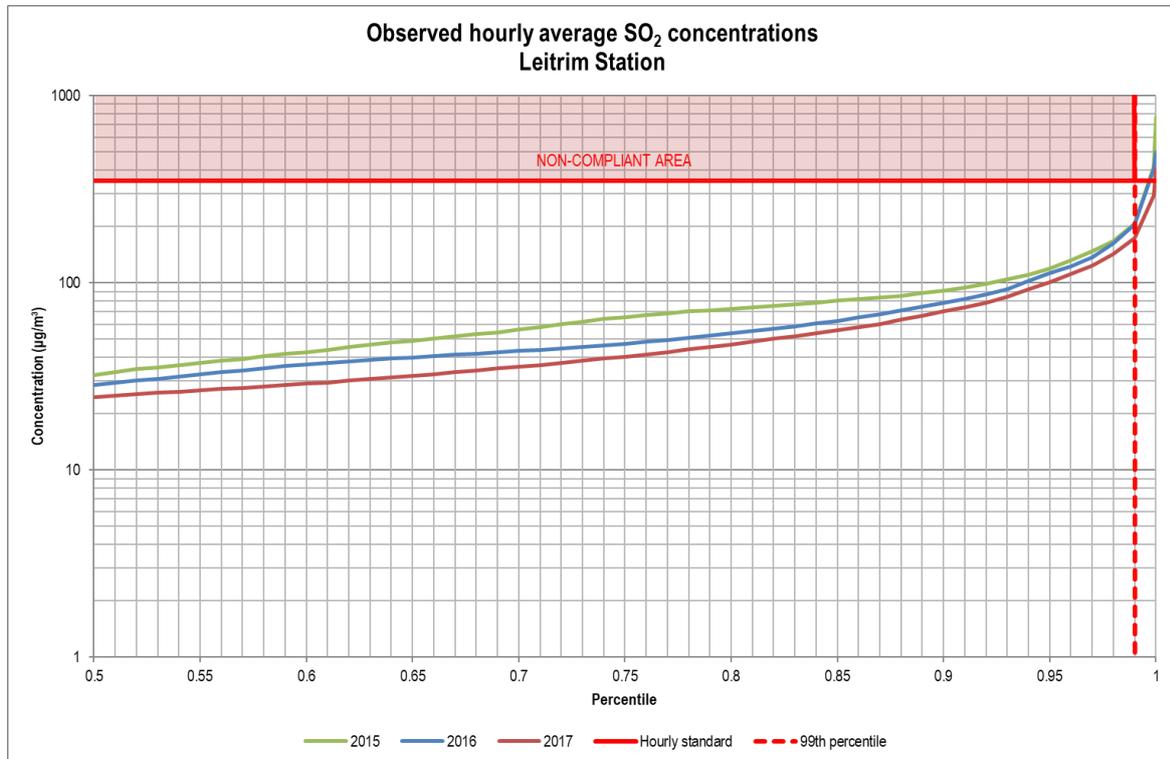


Figure 5-16: Observed hourly average SO₂ concentrations at Leitrim

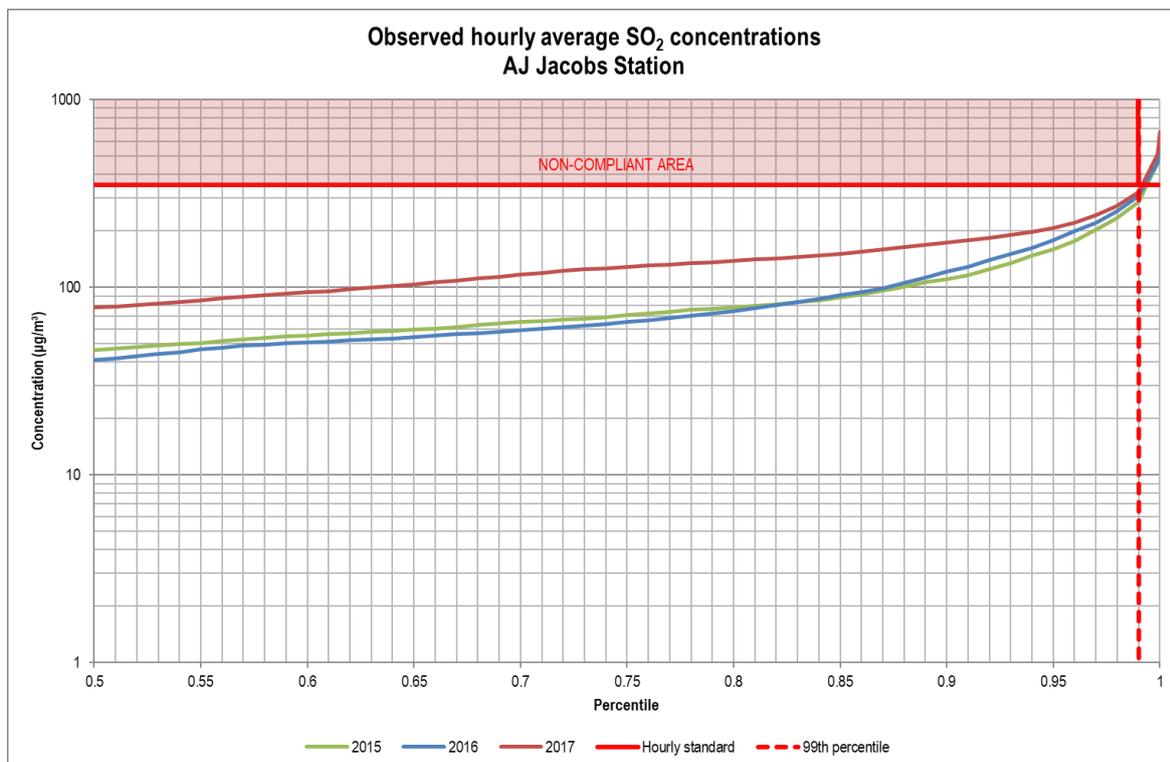


Figure 5-17: Observed hourly average SO₂ concentrations at AJ Jacobs

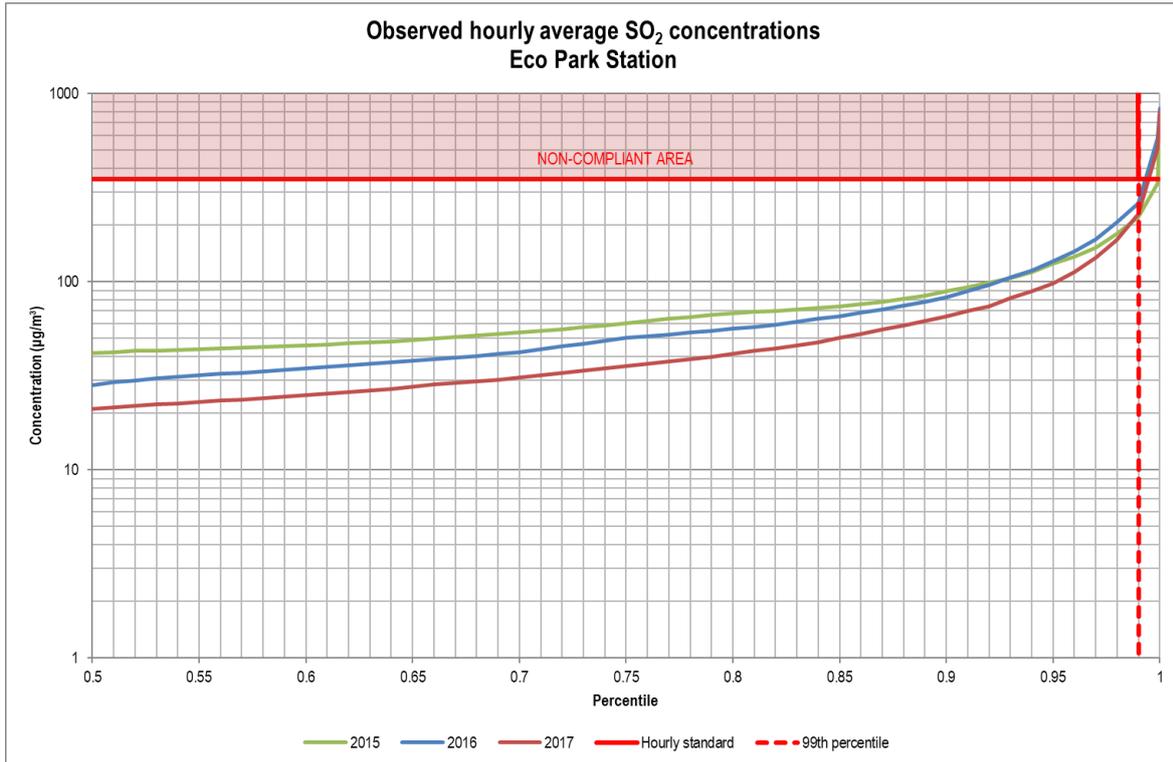


Figure 5-18: Observed hourly average SO₂ concentrations at Eco Park

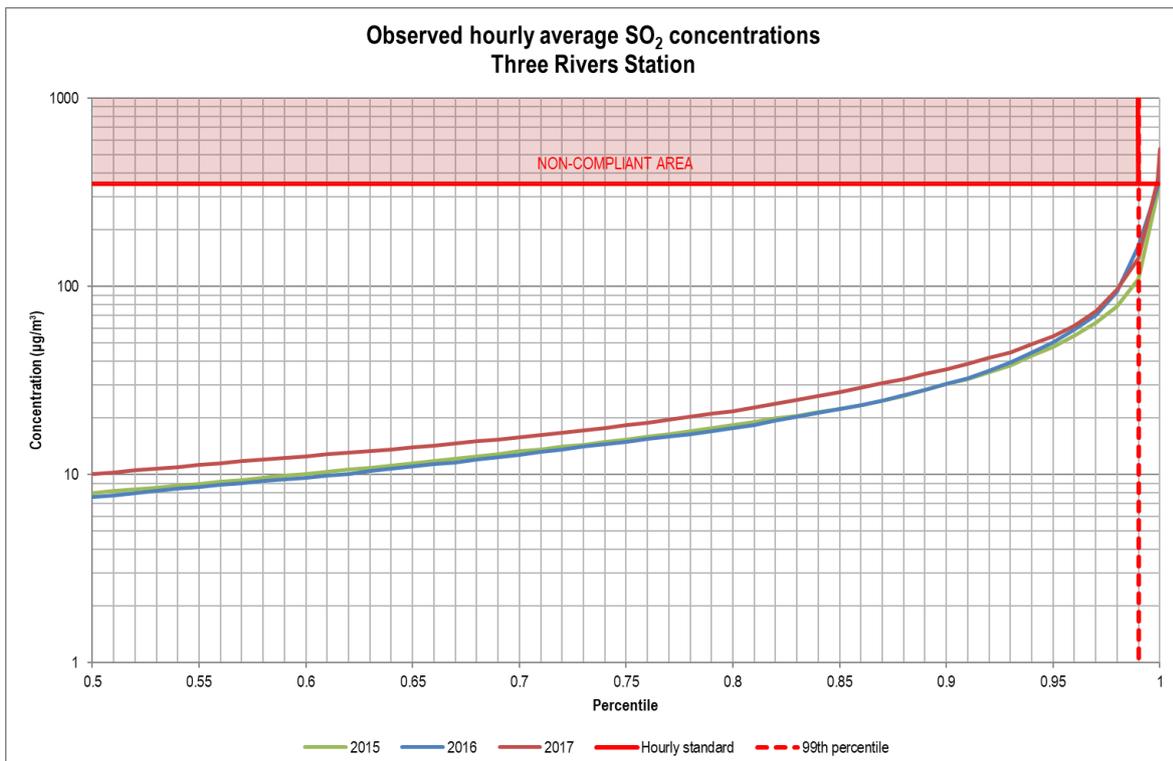


Figure 5-19: Observed hourly average SO₂ concentrations at Three Rivers

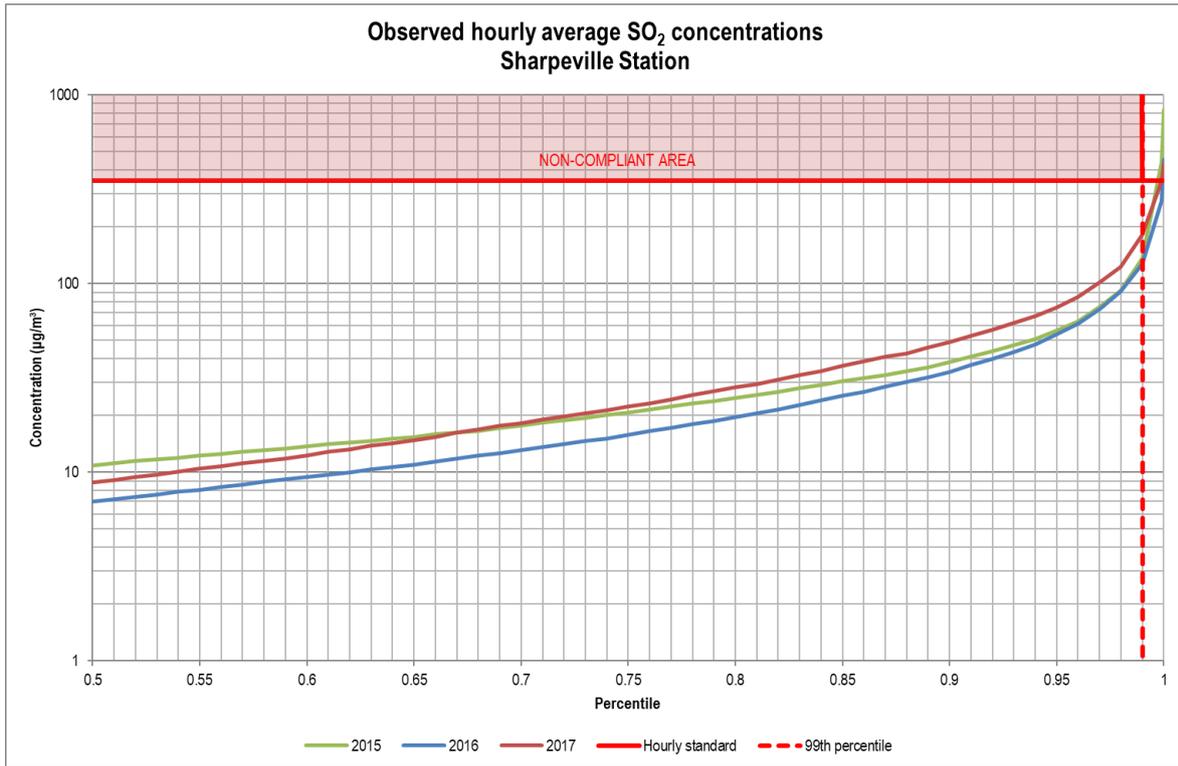


Figure 5-20: Observed hourly average SO₂ concentrations at Sharpeville

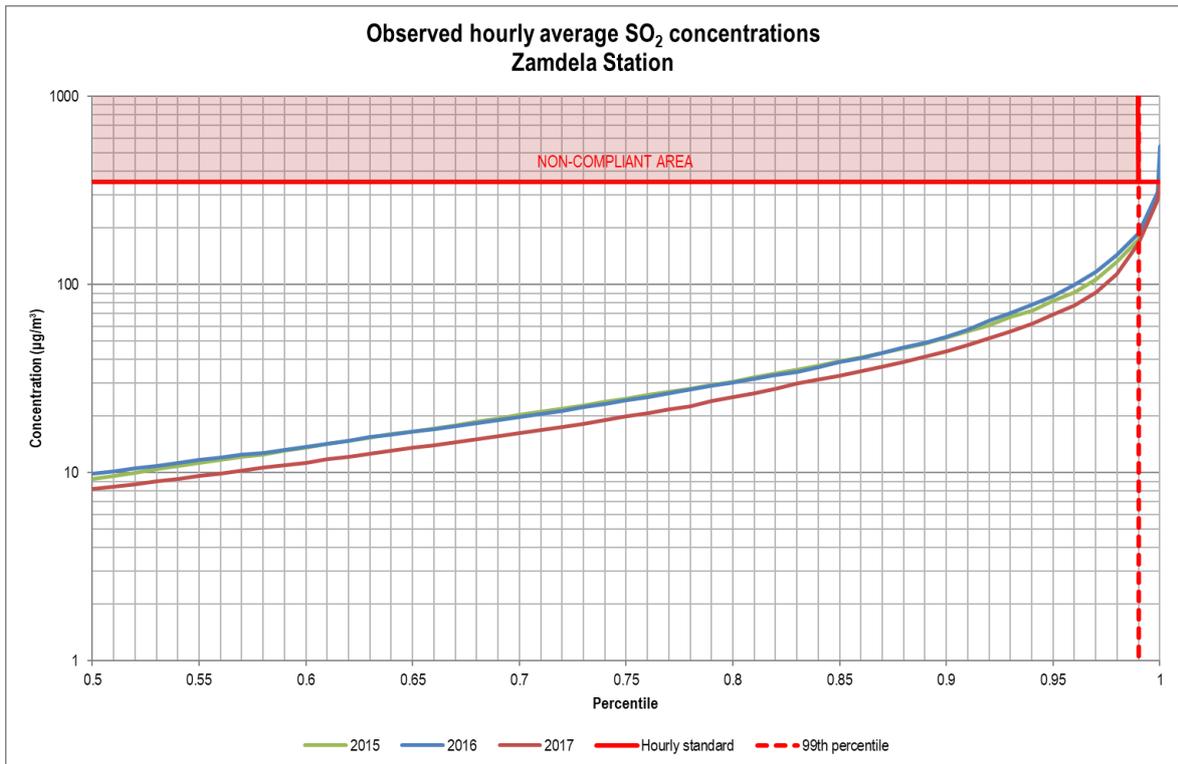


Figure 5-21: Observed hourly average SO₂ concentrations at Zamdela

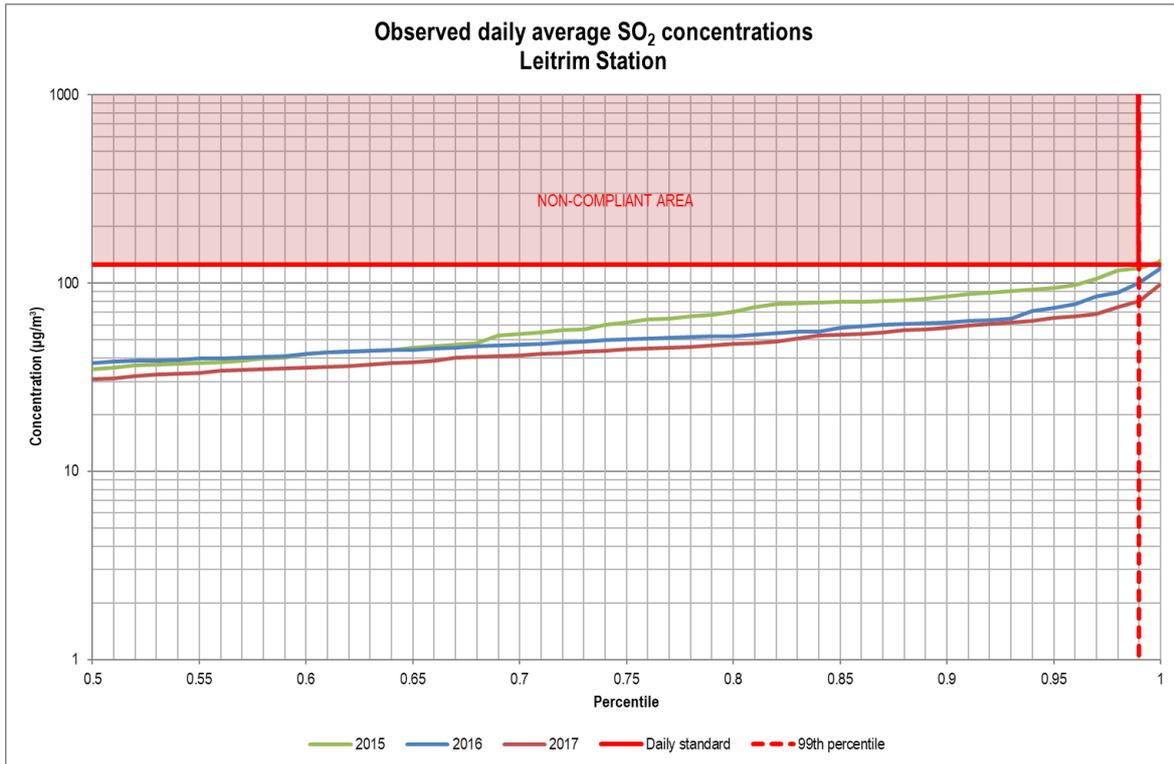


Figure 5-22: Observed daily average SO₂ concentrations at Leitrim

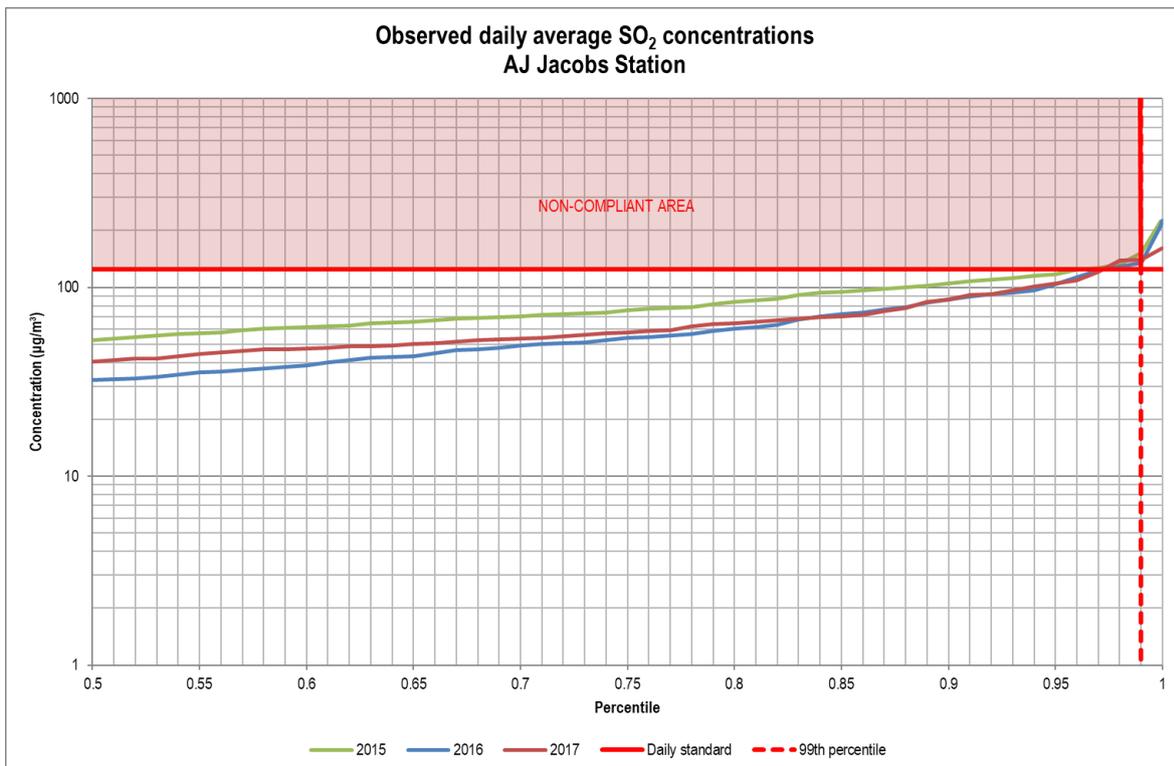


Figure 5-23: Observed daily average SO₂ concentrations at AJ Jacobs

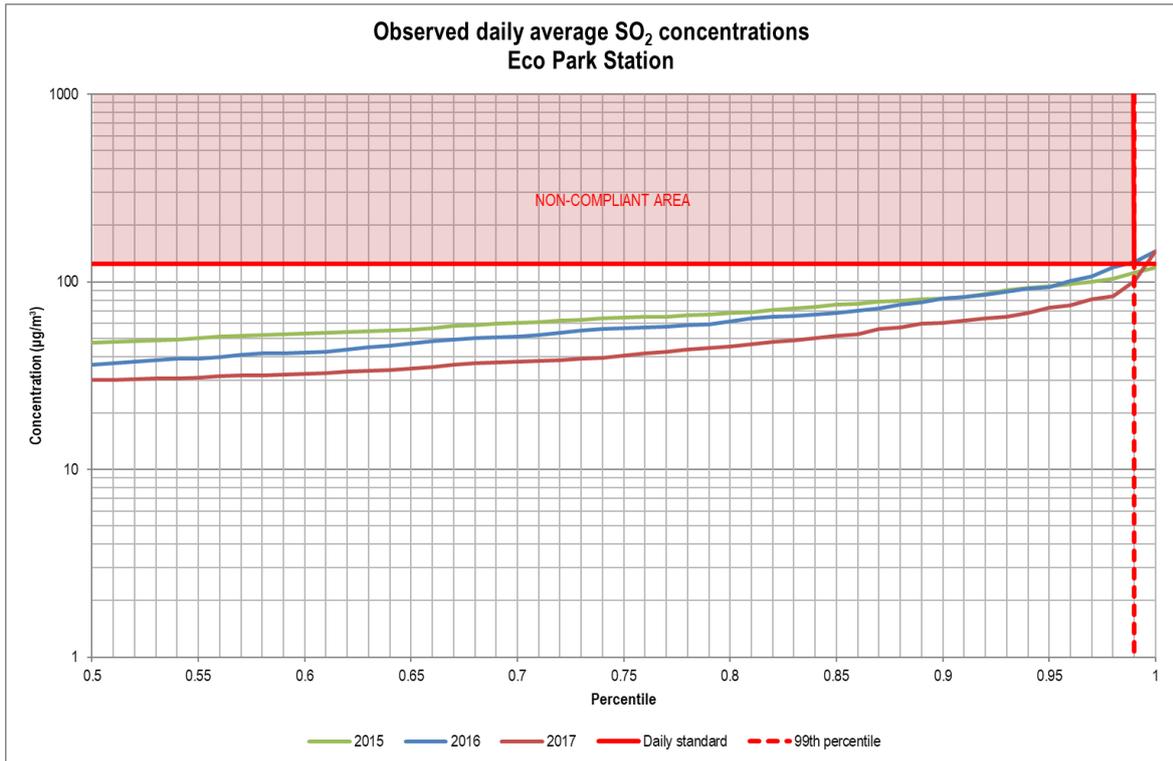


Figure 5-24: Observed daily average SO₂ concentrations at Eco Park

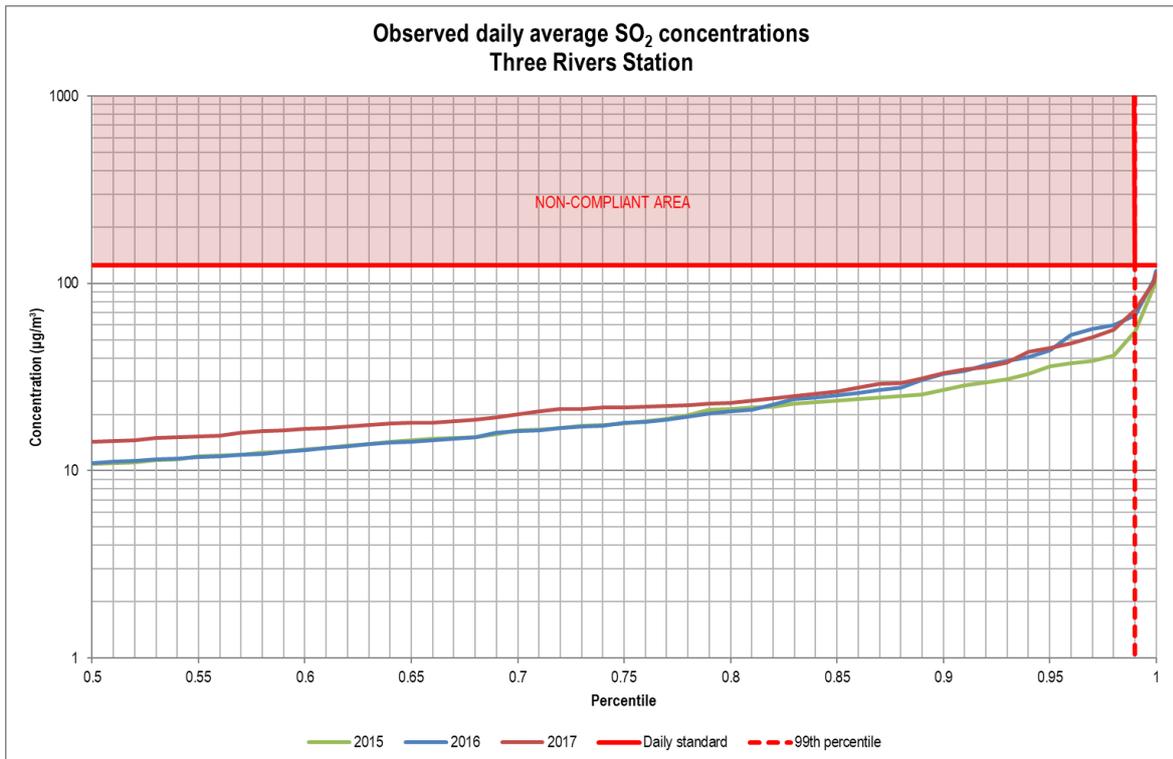


Figure 5-25: Observed daily average SO₂ concentrations at Three Rivers

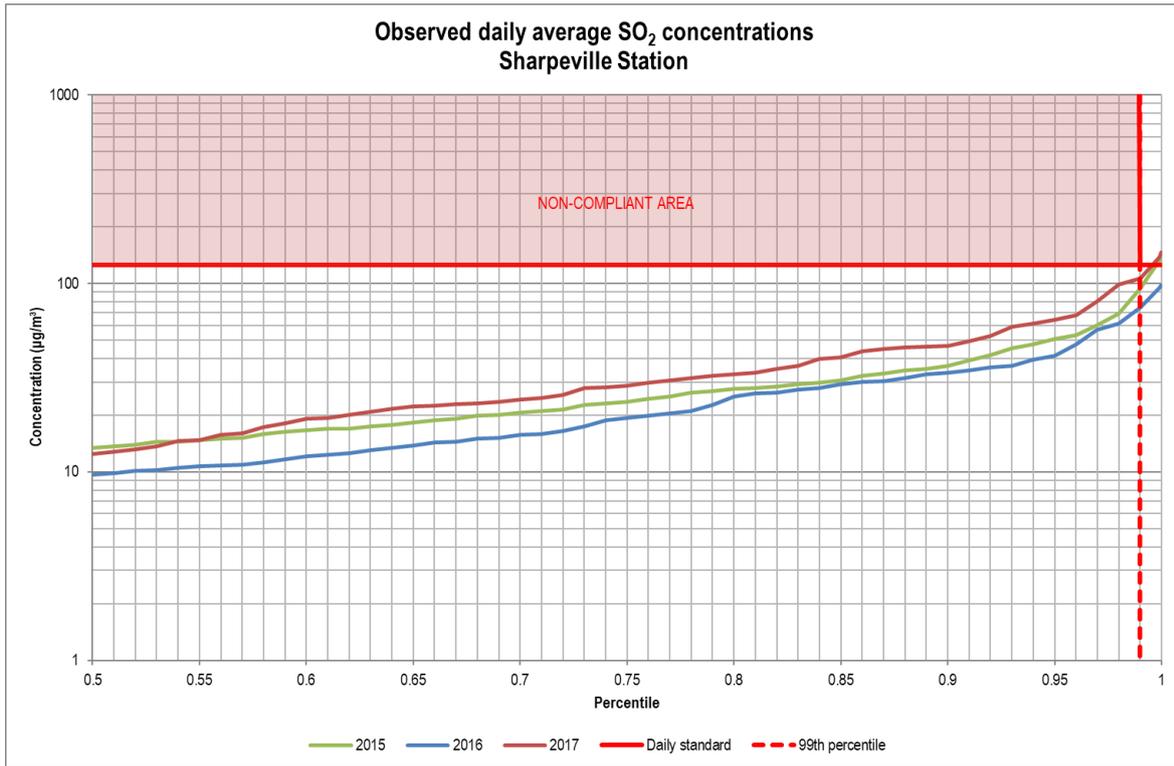


Figure 5-26: Observed daily average SO₂ concentrations at Sharpeville

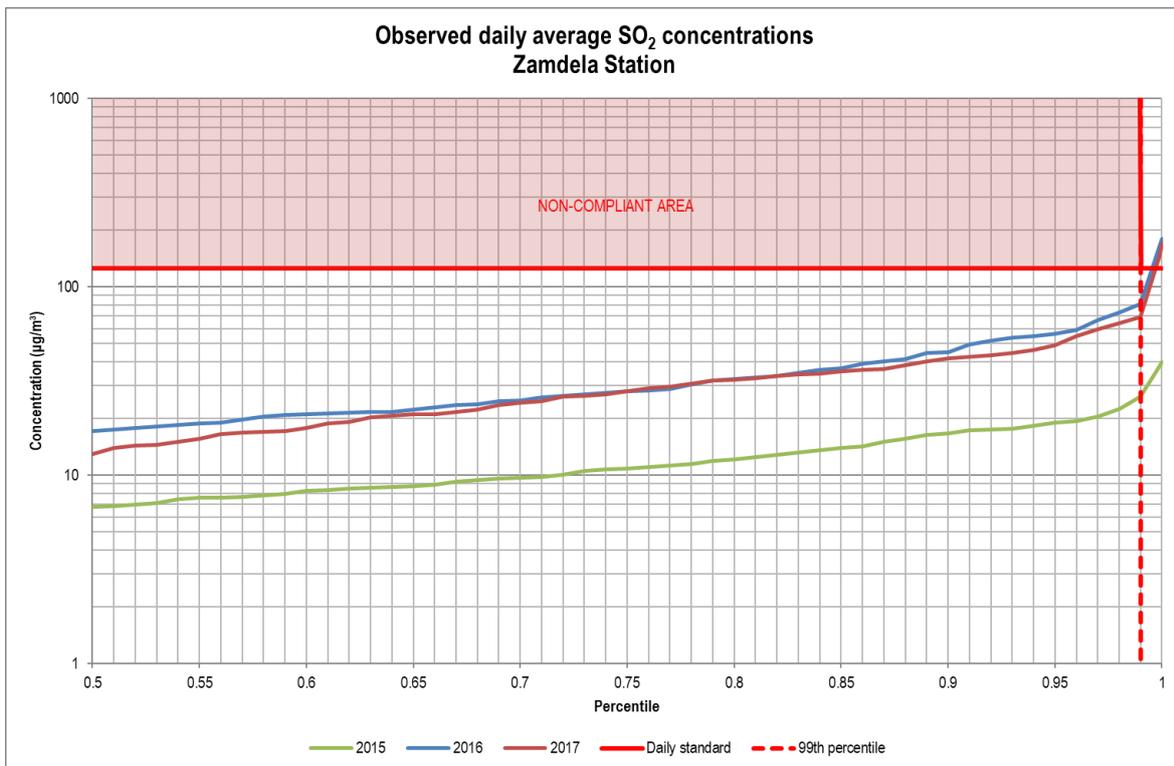


Figure 5-27: Observed daily average SO₂ concentrations at Zamdela

The hourly 99th percentiles for NO₂ were below the limit value (200 µg/m³) at all stations and for all three years (Figure 5-28 to Figure 5-33).

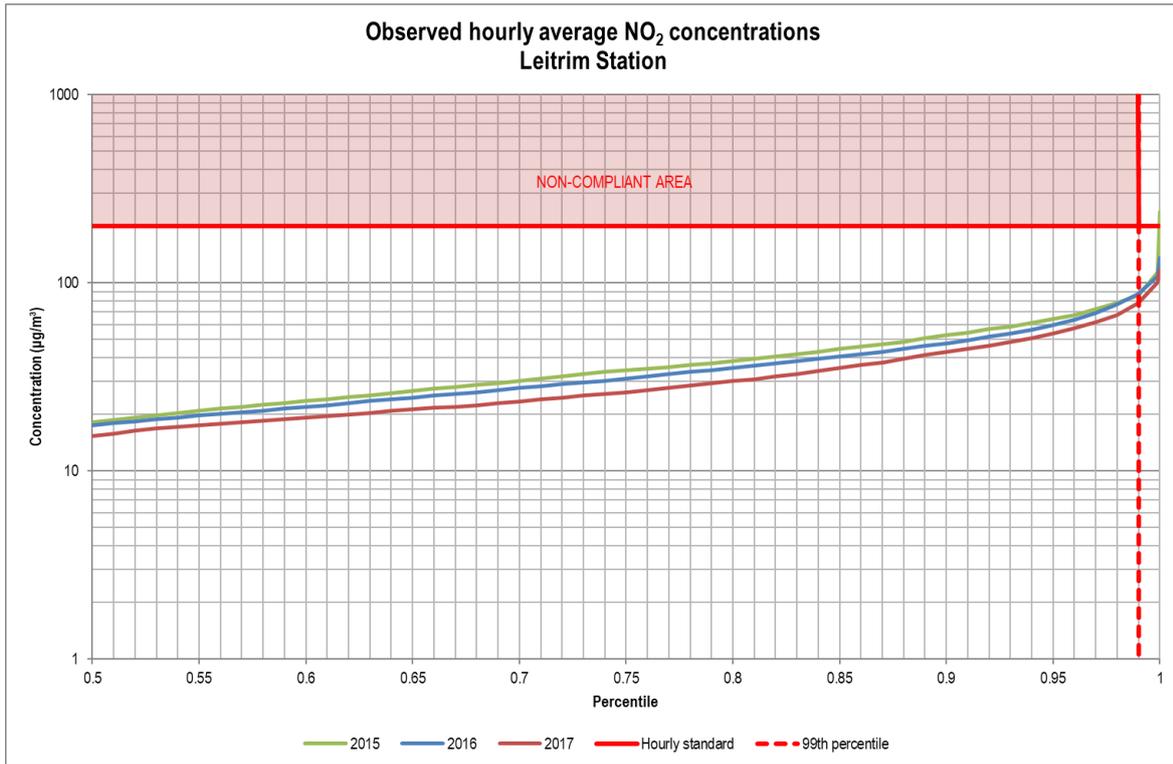


Figure 5-28: Observed hourly average NO₂ concentrations at Leitrim

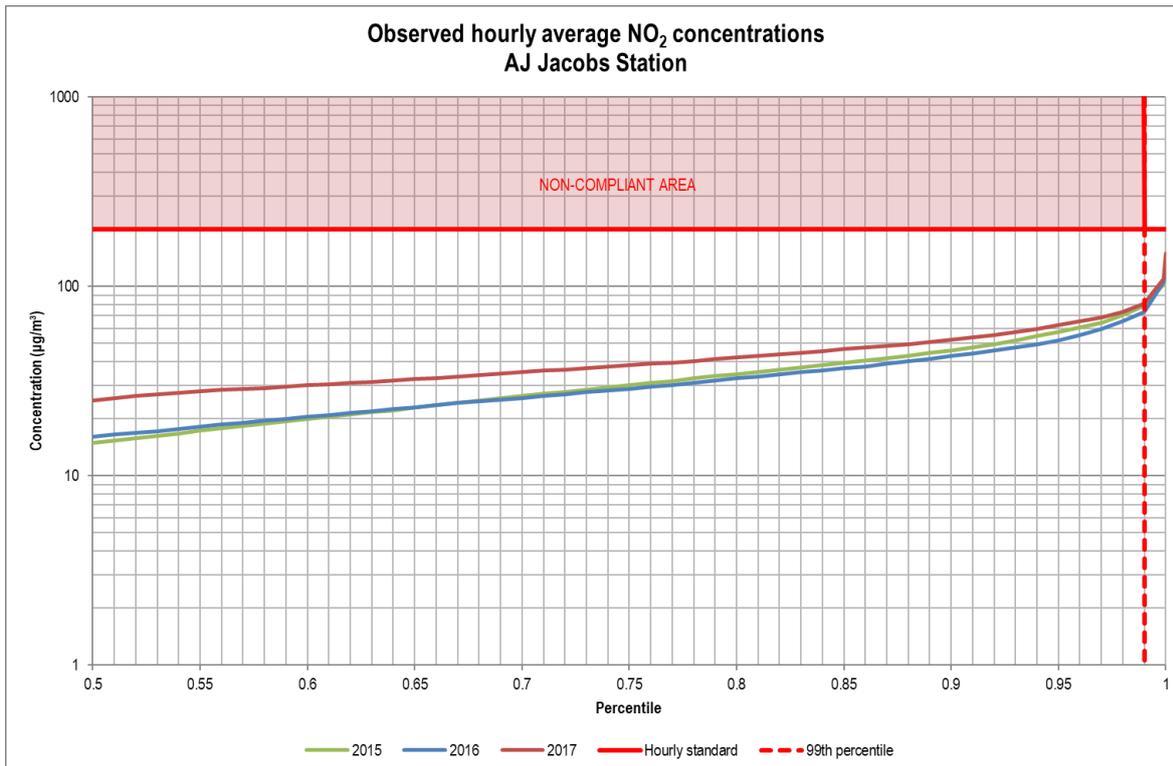


Figure 5-29: Observed hourly average NO₂ concentrations at AJ Jacobs

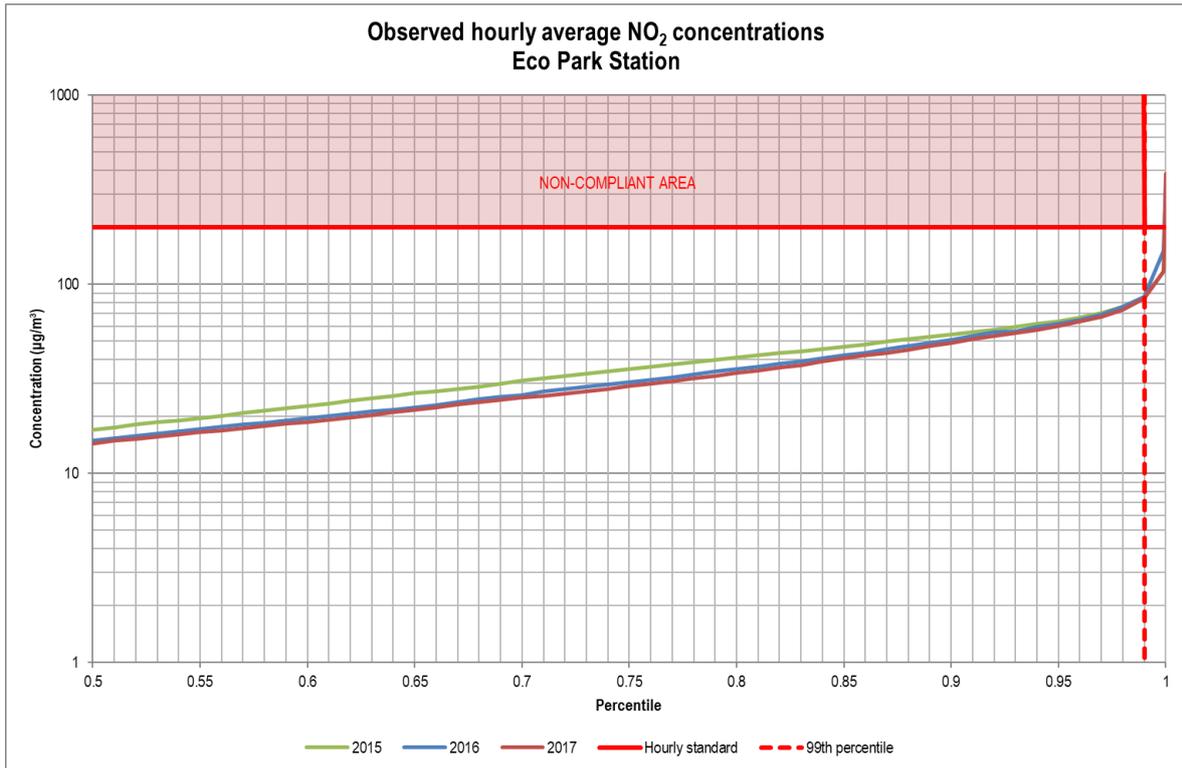


Figure 5-30: Observed hourly average NO₂ concentrations at Eco Park

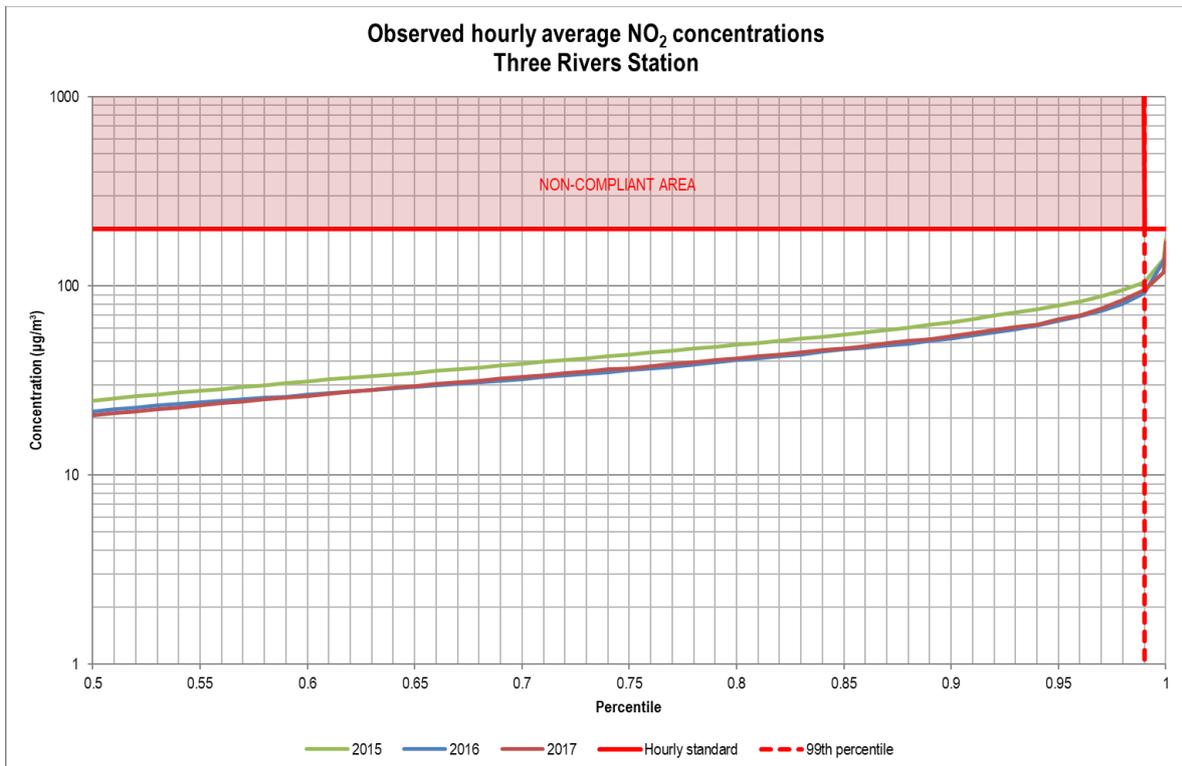


Figure 5-31: Observed hourly average NO₂ concentrations at Three Rivers

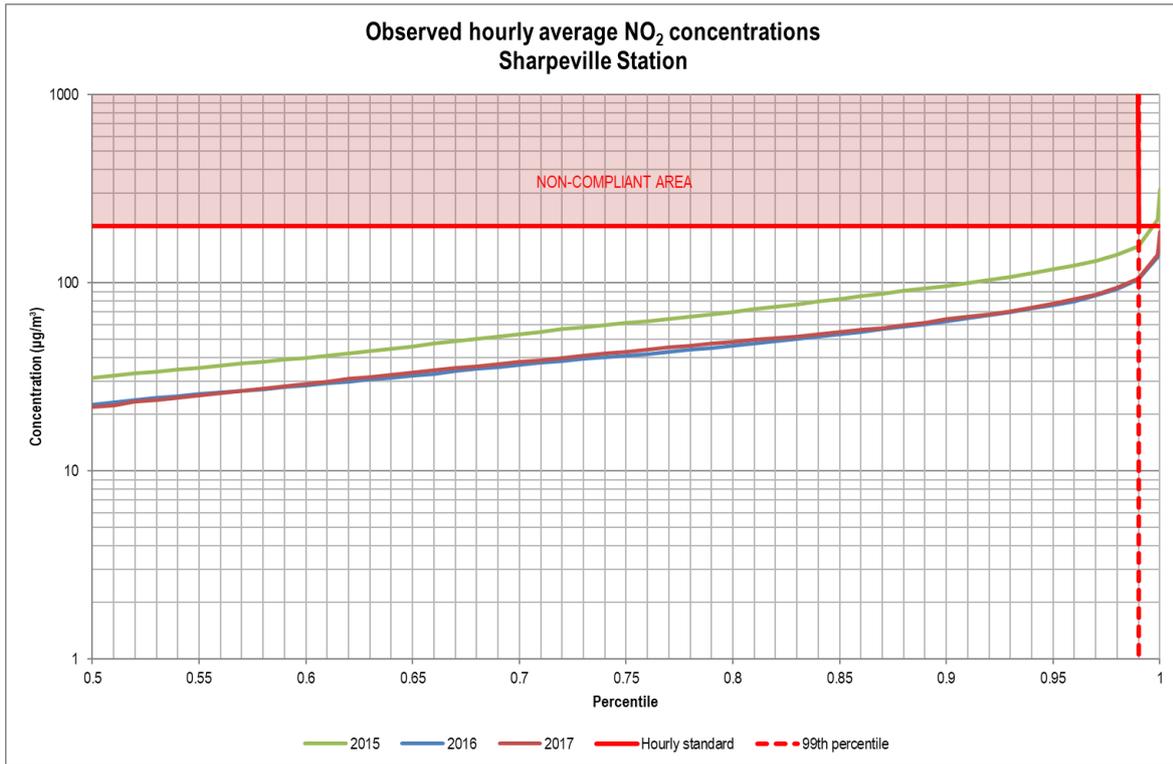


Figure 5-32: Observed hourly average NO₂ concentrations at Sharpeville

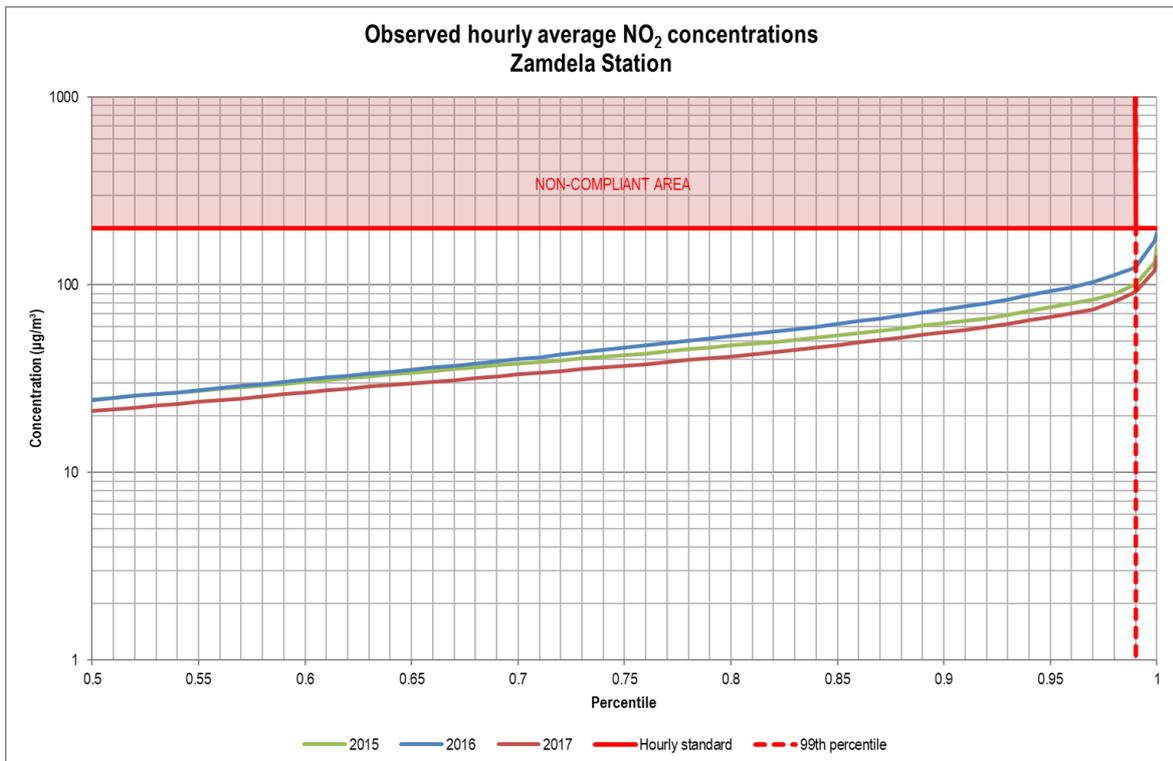


Figure 5-33: Observed hourly average NO₂ concentrations at Zamdela

The daily 99th percentiles for PM₁₀ exceeded the limit value (75 µg/m³; 2015 standard) at all stations and for all three years (Figure 5-34 to Figure 5-39). Non-compliance varied between 3% and 50% of the three years assessed.

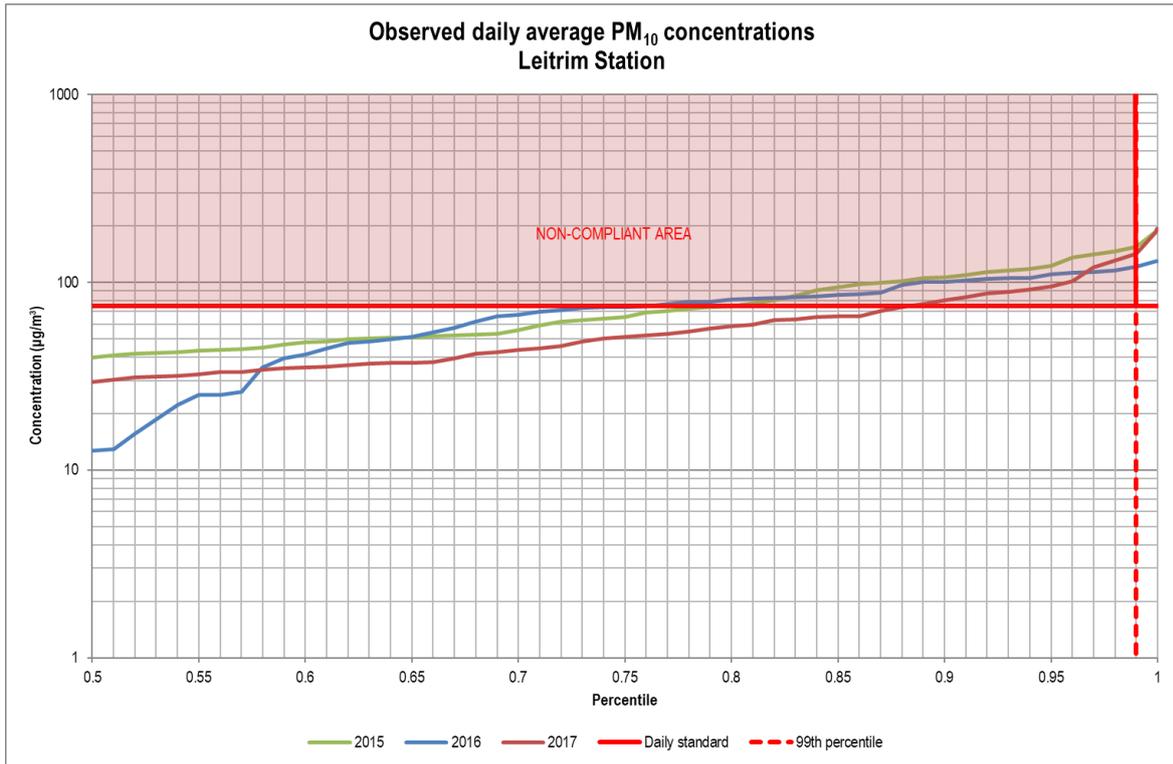


Figure 5-34: Observed daily average PM₁₀ concentrations at Leitrim

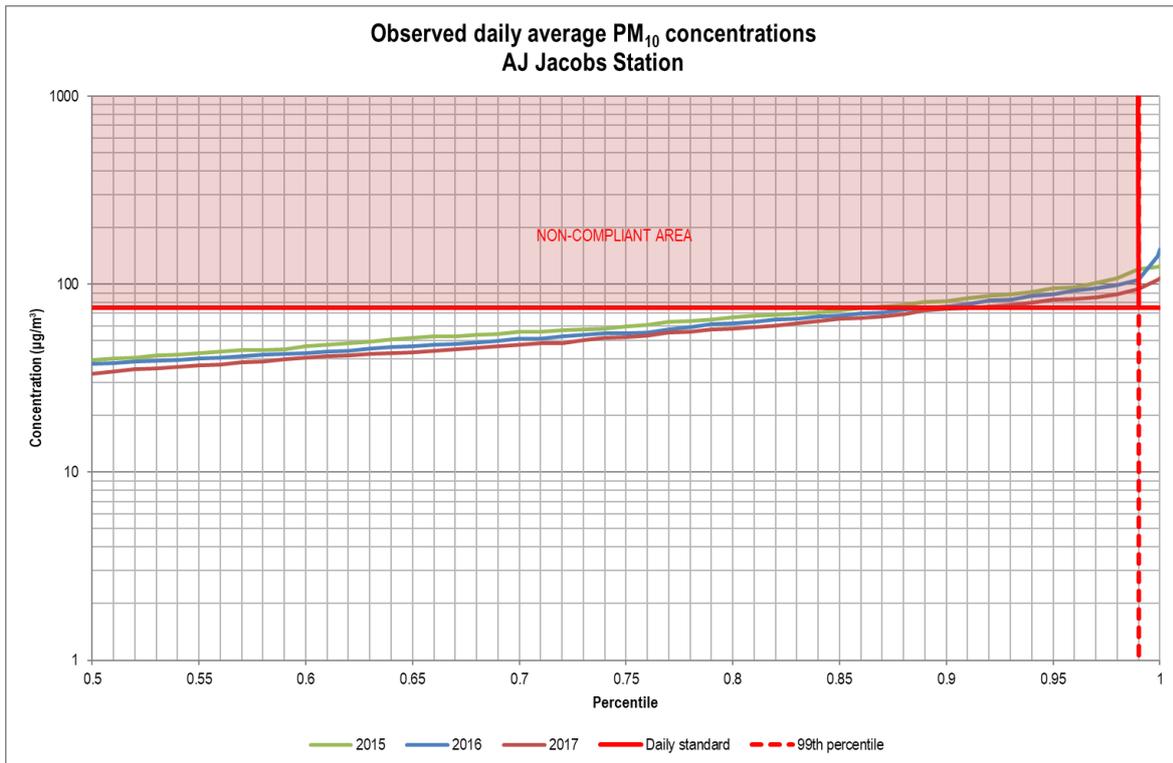


Figure 5-35: Observed daily average PM₁₀ concentrations at AJ Jacobs

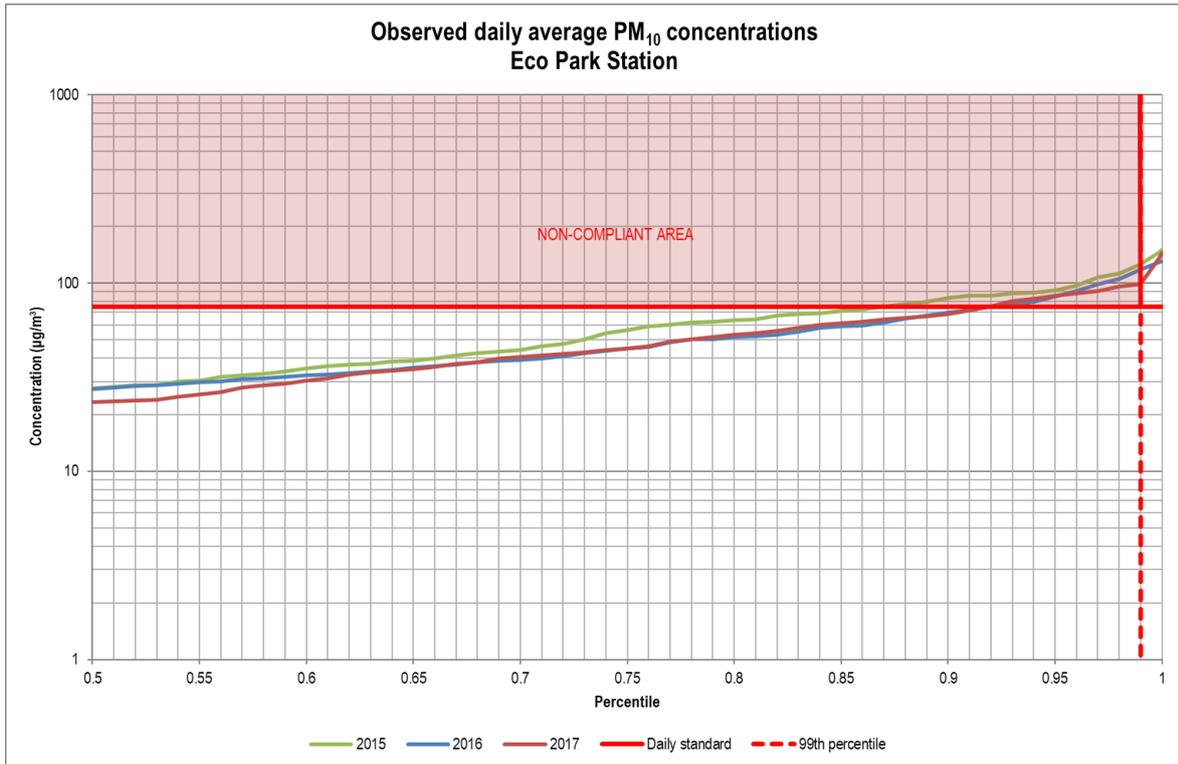


Figure 5-36: Observed daily average PM₁₀ concentrations at Eco Park

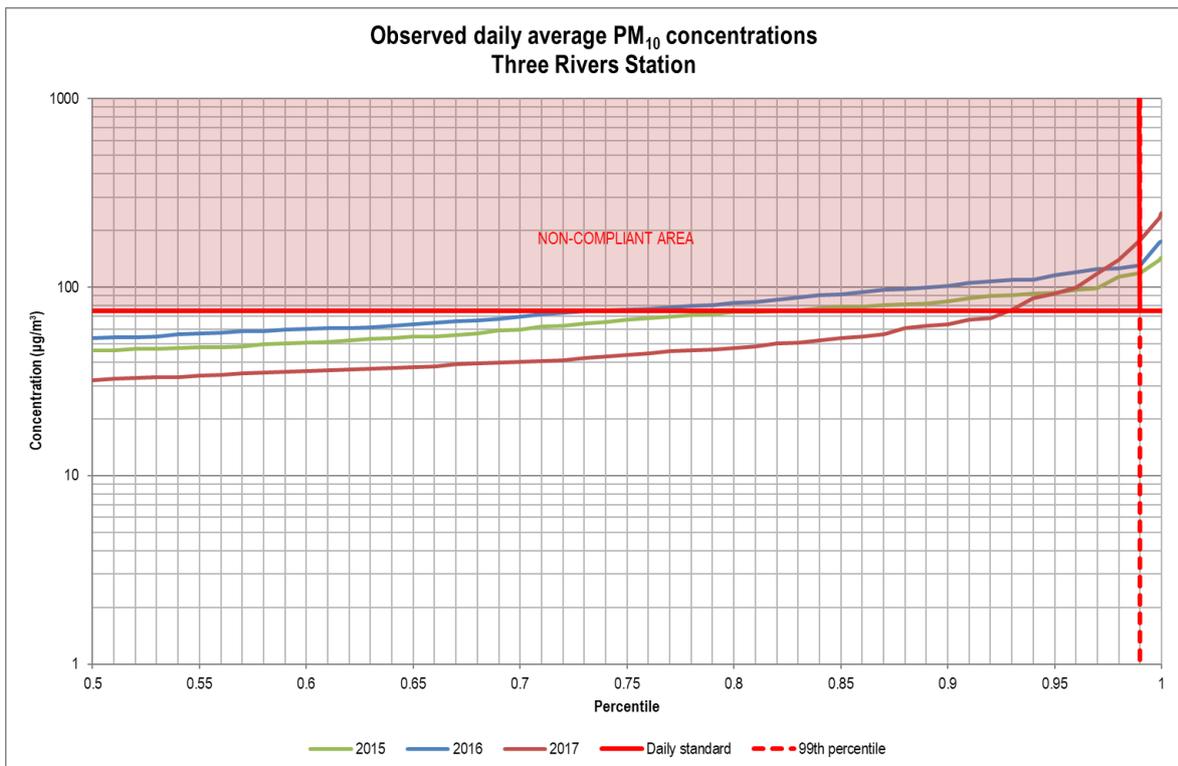


Figure 5-37: Observed daily average PM₁₀ concentrations at Three Rivers

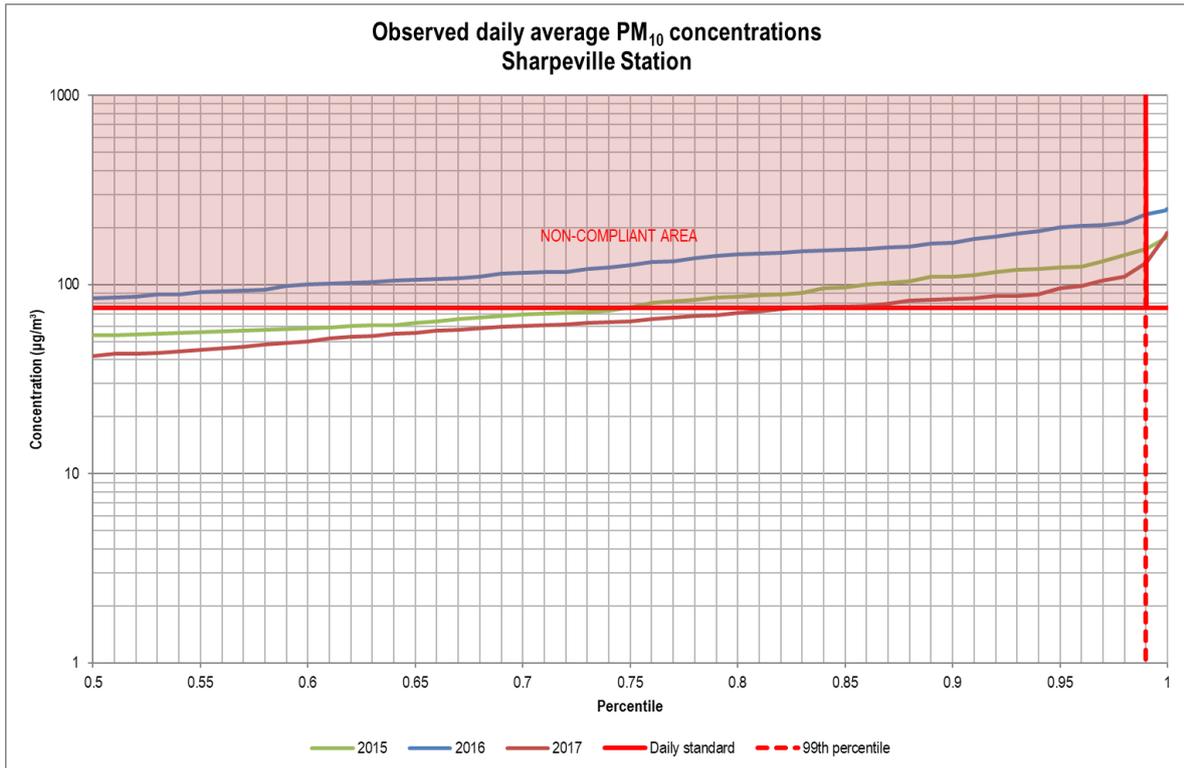


Figure 5-38: Observed daily average PM₁₀ concentrations at Sharpeville

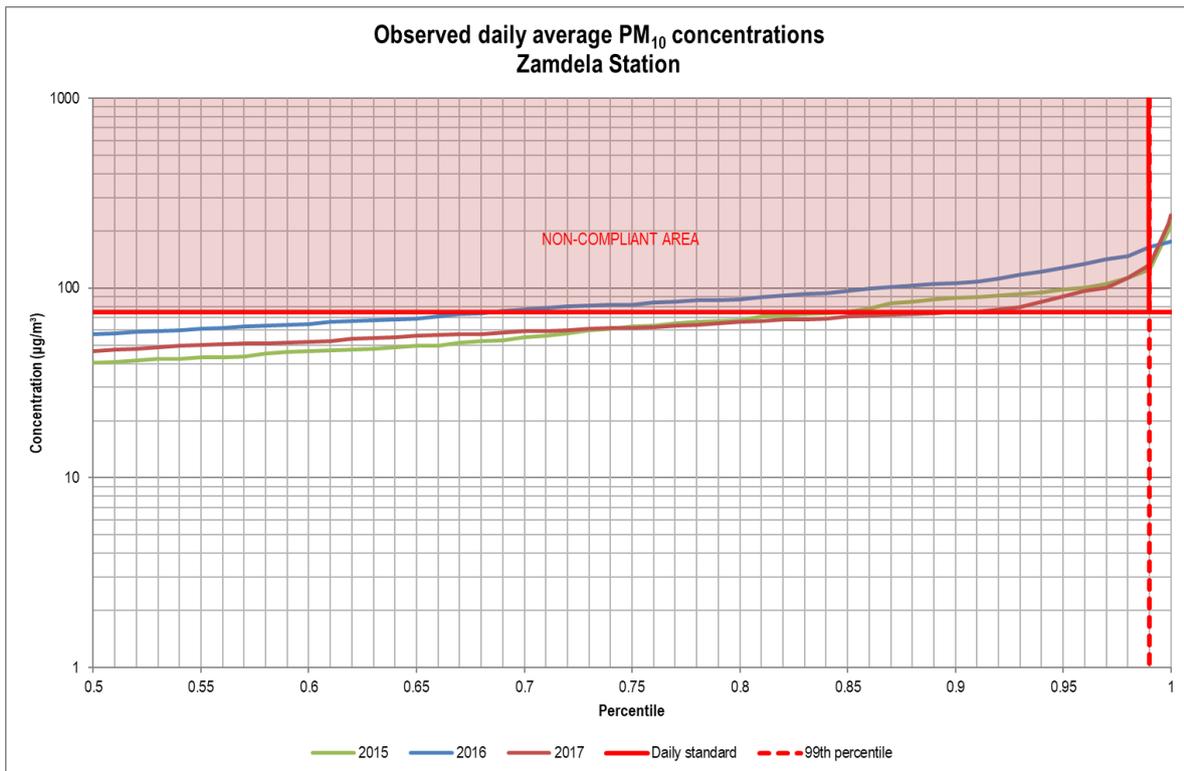


Figure 5-39: Observed daily average PM₁₀ concentrations at Zamdela

Time variation plots (mean with 95% confidence interval) of ambient SO₂, NO₂, and particulate matter (PM₁₀ and PM_{2.5}) concentrations measured the six monitoring stations show the variation of these pollutants over a daily, weekly and annual cycles (Figure 5-40 to Figure 5-51). The daily SO₂ show a typically industrial signature with increased SO₂ concentrations as

just before midday due to the break-up of an elevated inversion layer, in addition to the development of daytime convective conditions causing the plume to be brought down to ground level relatively close to the point of release from tall stacks. Increased NO₂ concentrations during peak traffic times (07:00 to 08:00 and 16:00 to 18:00) illustrate the contribution of vehicle emissions to the ambient NO₂ concentrations. The winter (June, July and August) elevation of SO₂ and NO₂ shows the contribution of residential fuel burning to the ambient SO₂ and NO₂ concentrations.

Monthly variation of particulate matter shows elevated concentrations during winter months due to the larger contribution from domestic fuel burning, dust from uncovered soil and the lack of the settling influence of rainfall (Figure 5-46 and Figure 5-51).

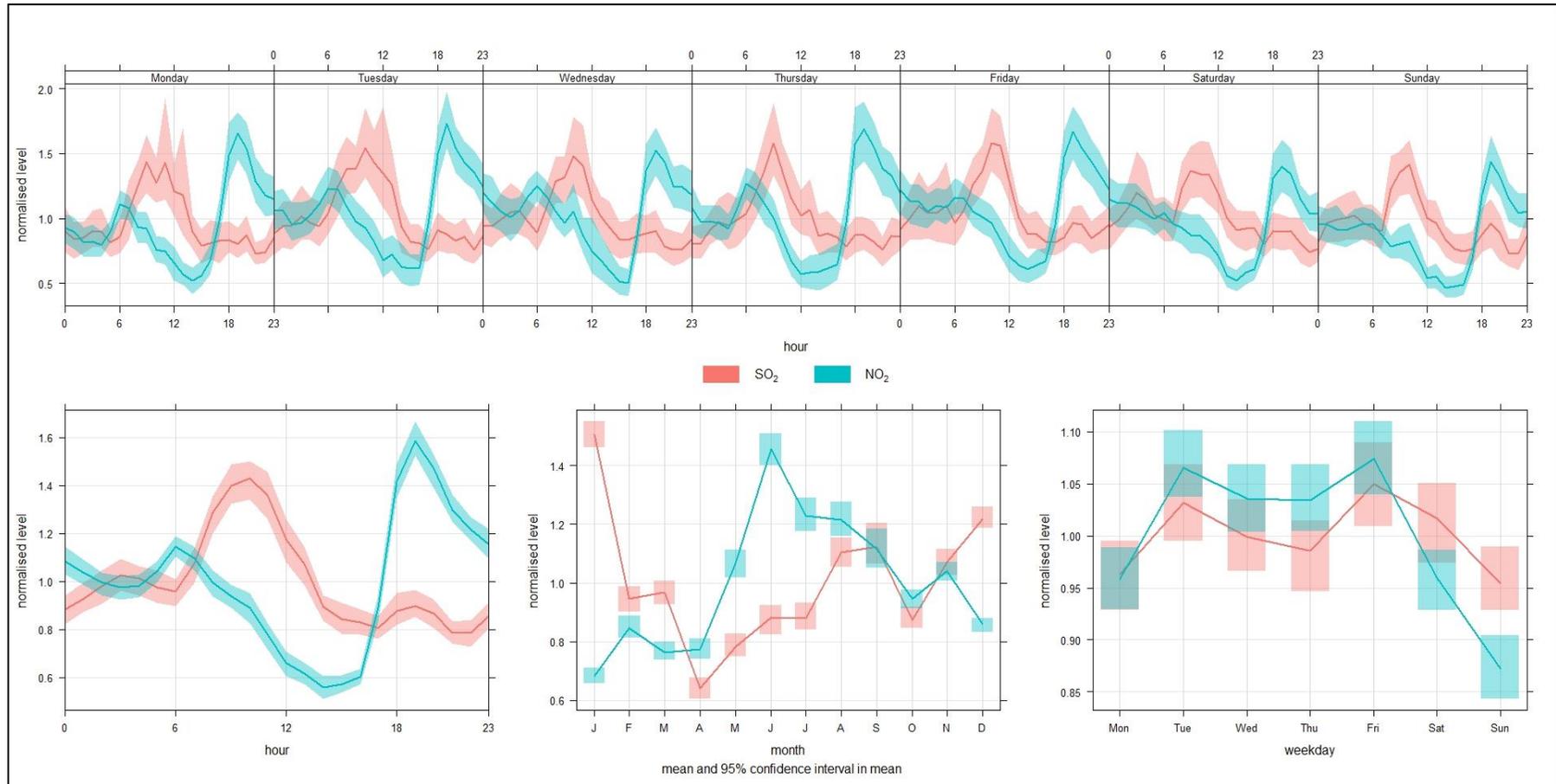


Figure 5-40: Time variation plot of observed SO₂ and NO₂ concentrations at Leitrim (shaded area indicates 95th percentile confidence interval)

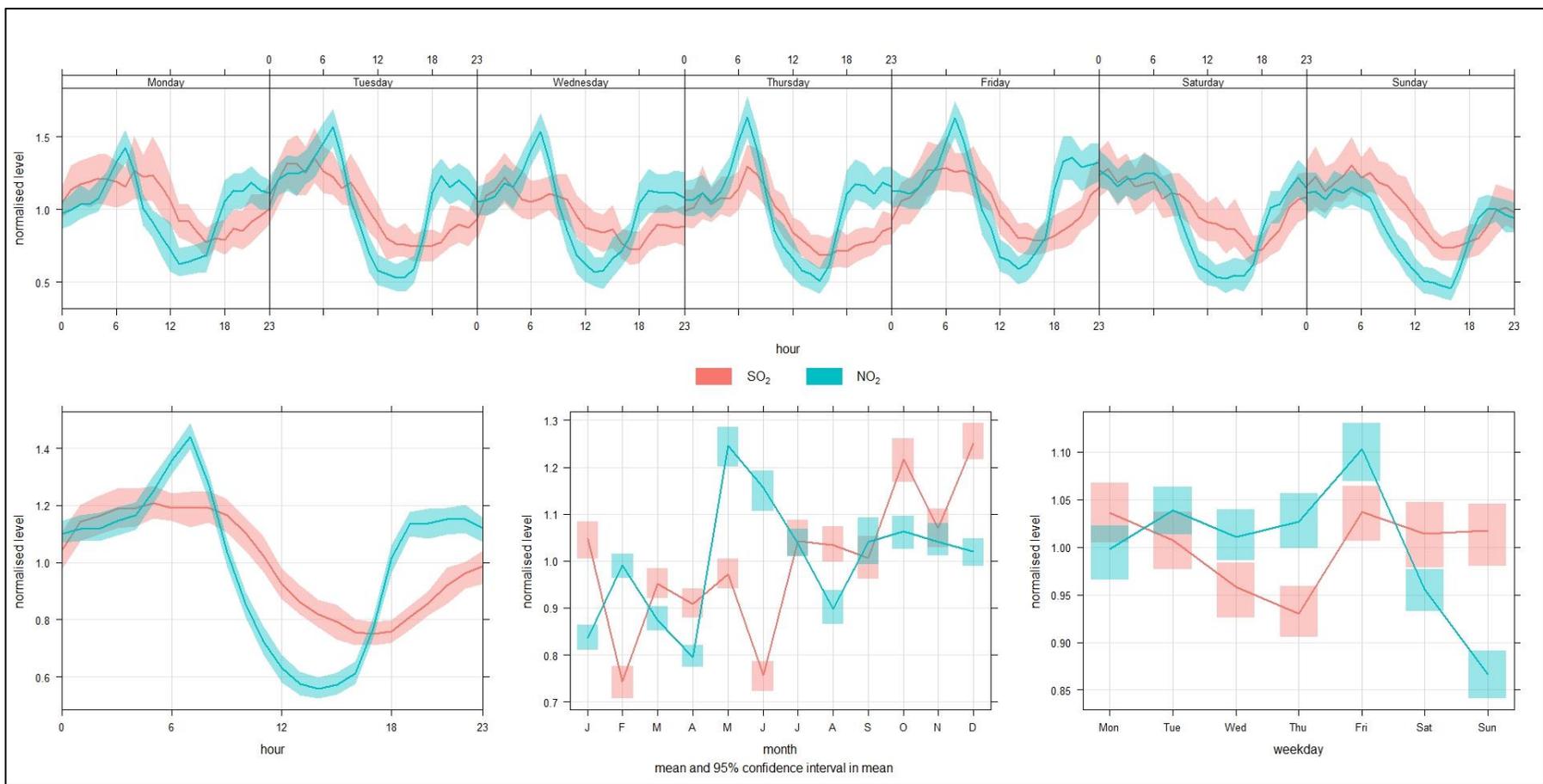


Figure 5-41: Time variation plot of observed SO₂ and NO₂ concentrations at AJ Jacobs (shaded area indicates 95th percentile confidence interval)

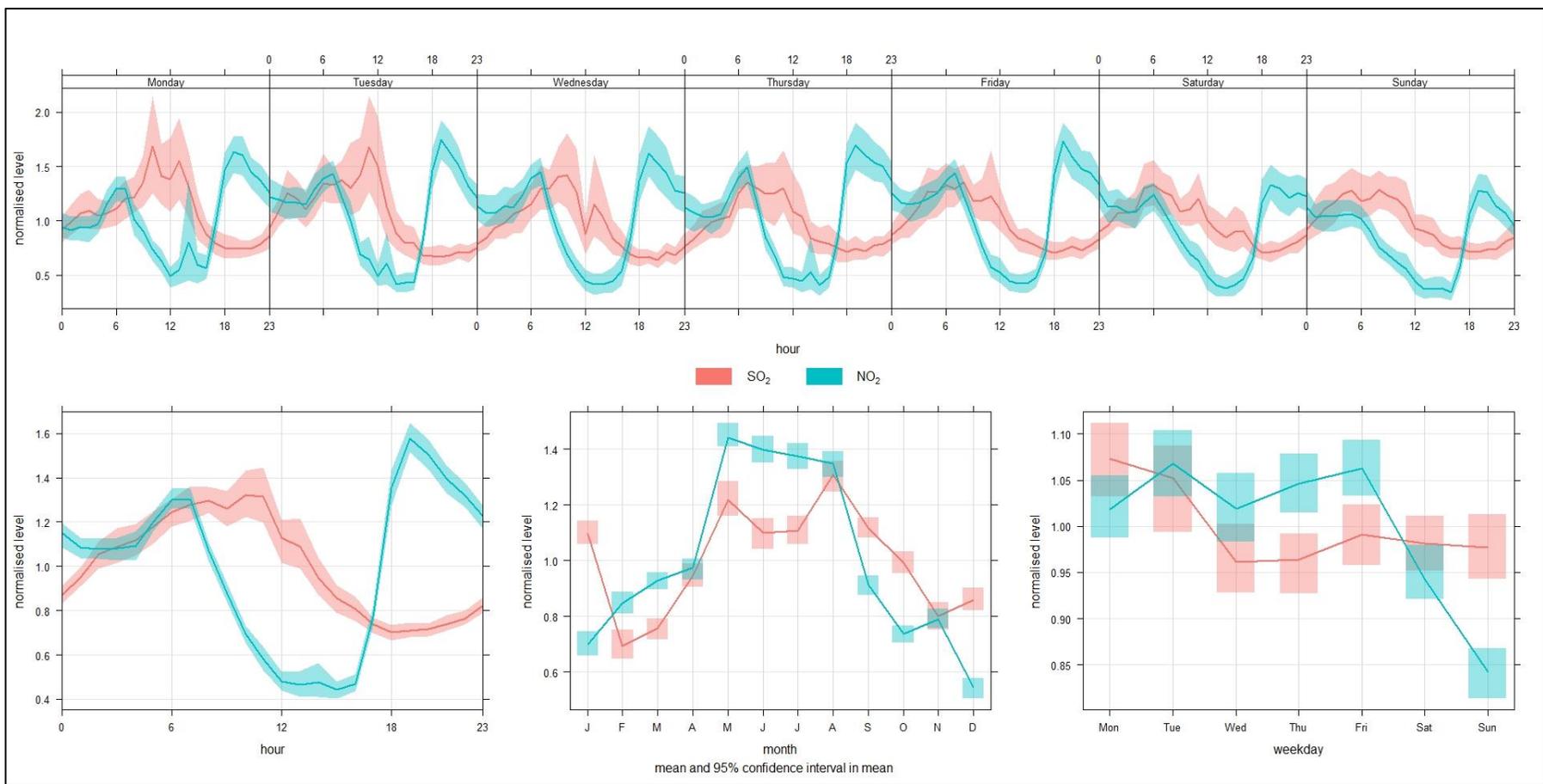


Figure 5-42: Time variation plot of observed SO₂ and NO₂ concentrations at Eco Park (shaded area indicates 95th percentile confidence interval)

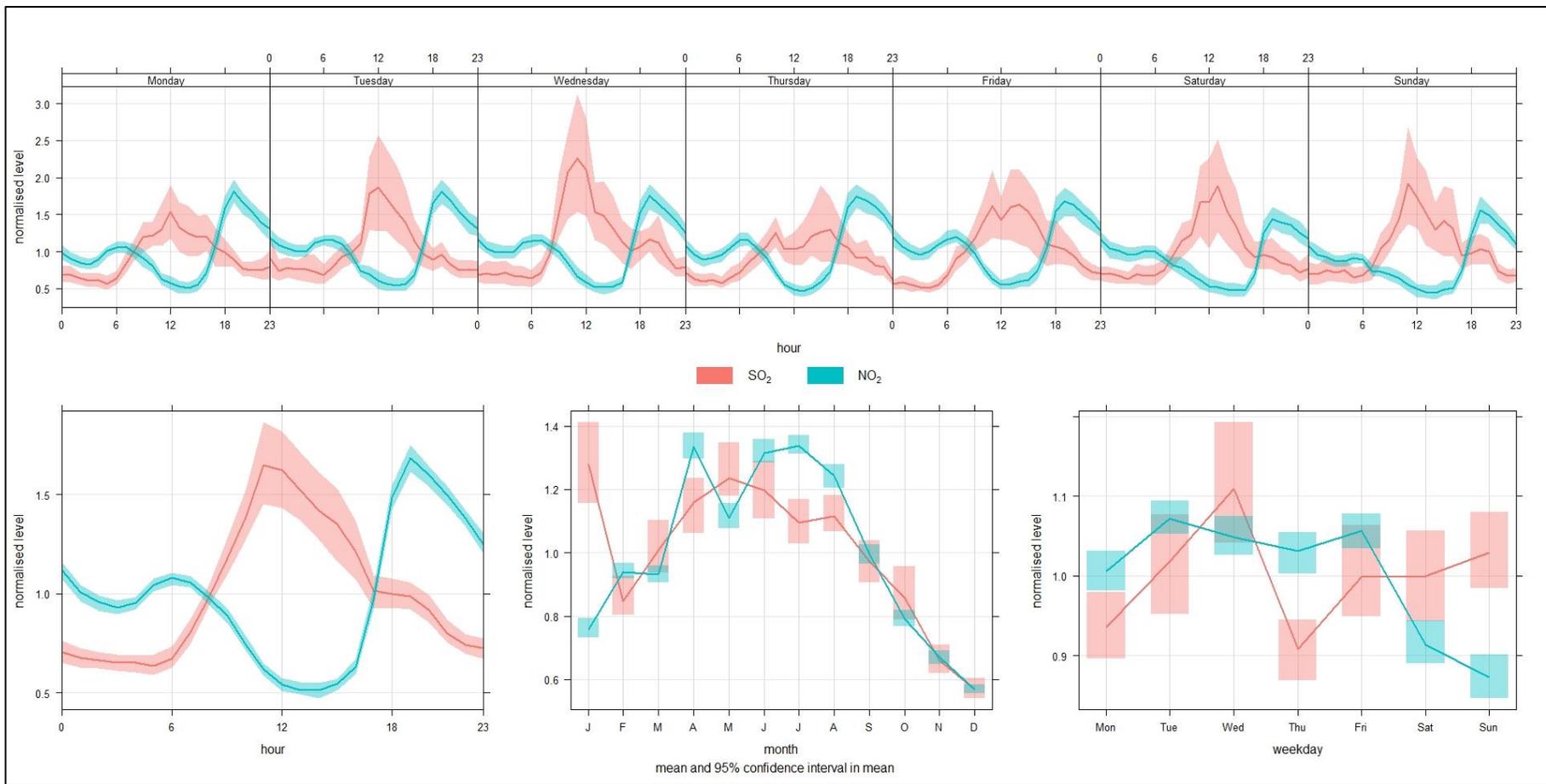


Figure 5-43: Time variation plot of observed SO₂ and NO₂ concentrations at Three Rivers (shaded area indicates 95th percentile confidence interval)

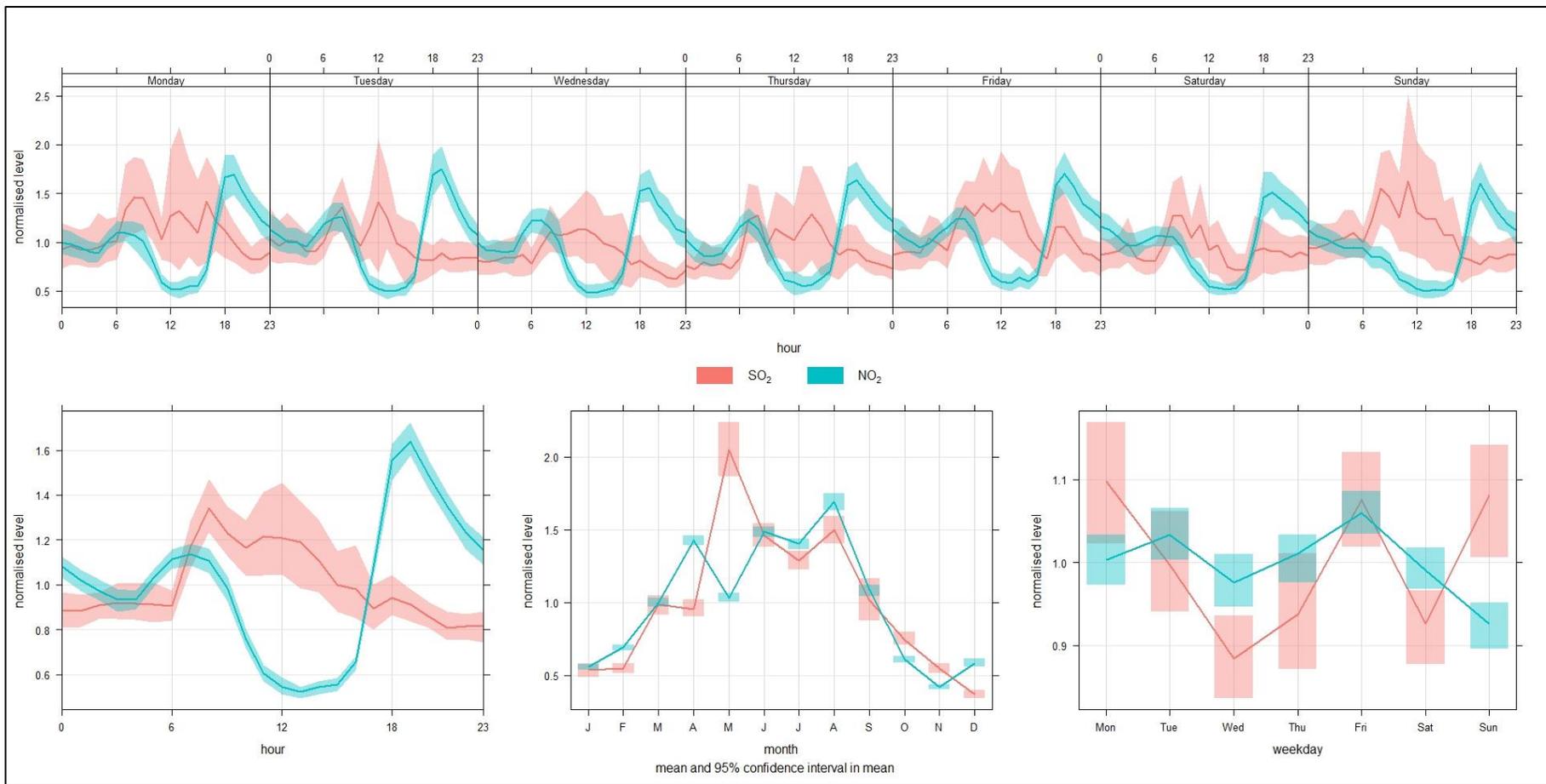


Figure 5-44: Time variation plot of observed SO₂ and NO₂ concentrations at Sharpeville (shaded area indicates 95th percentile confidence interval)

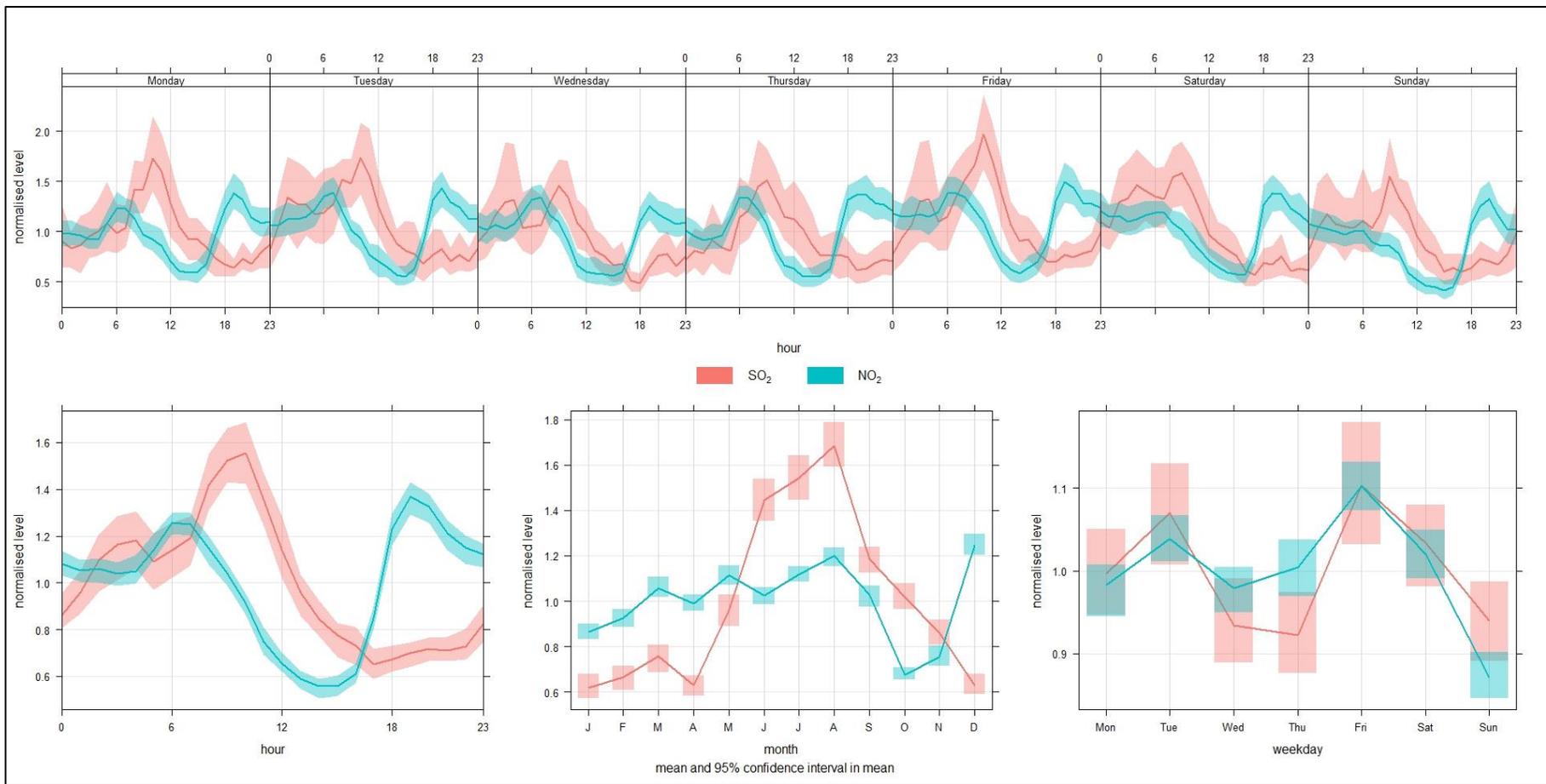


Figure 5-45: Time variation plot of observed SO₂ and NO₂ concentrations at Zamdela (shaded area indicates 95th percentile confidence interval)

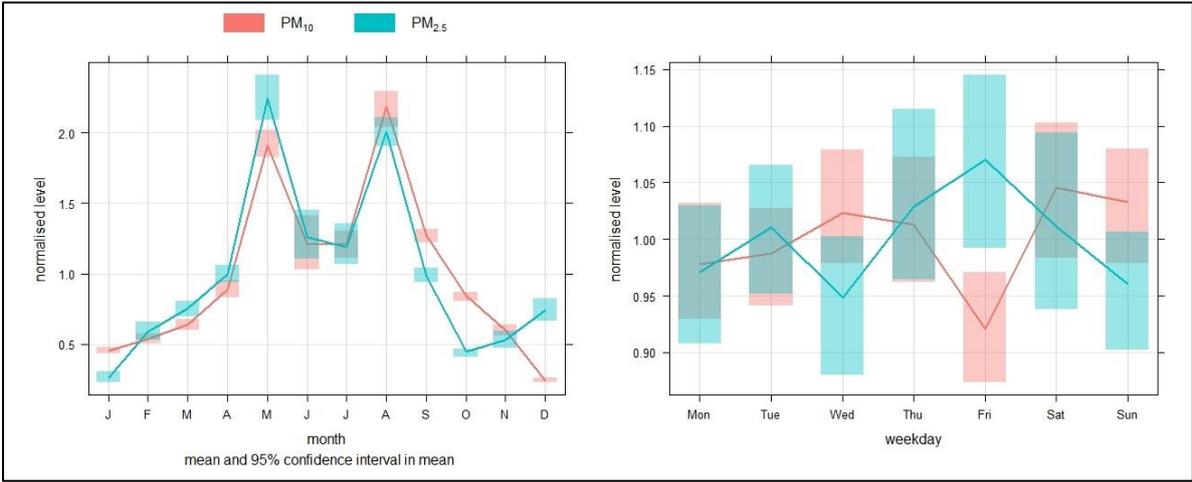


Figure 5-46: Time variation plot of normalised observed PM₁₀ and PM_{2.5} concentrations at Leitrim

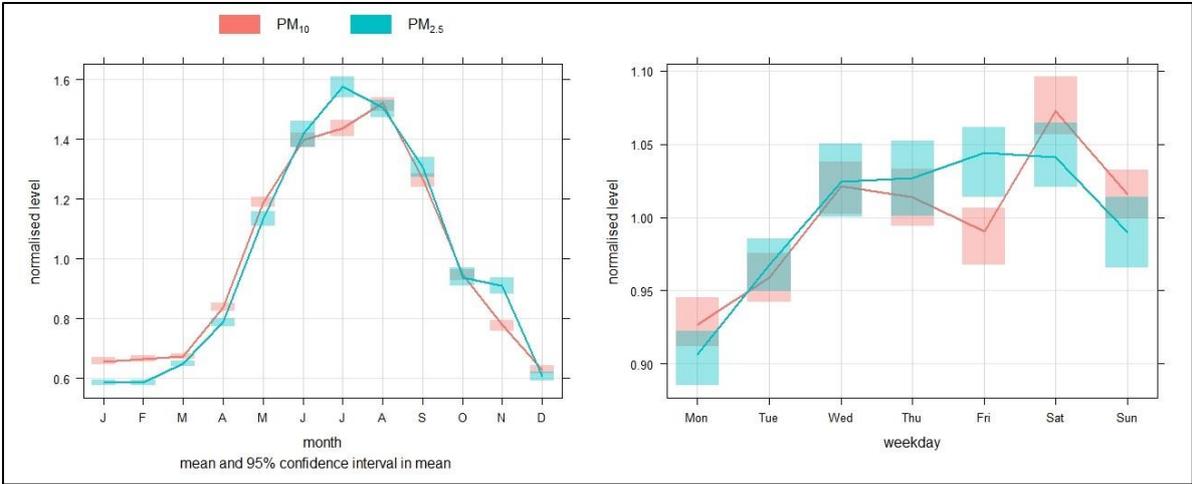


Figure 5-47: Time variation plot of normalised observed PM₁₀ and PM_{2.5} concentrations at AJ Jacobs

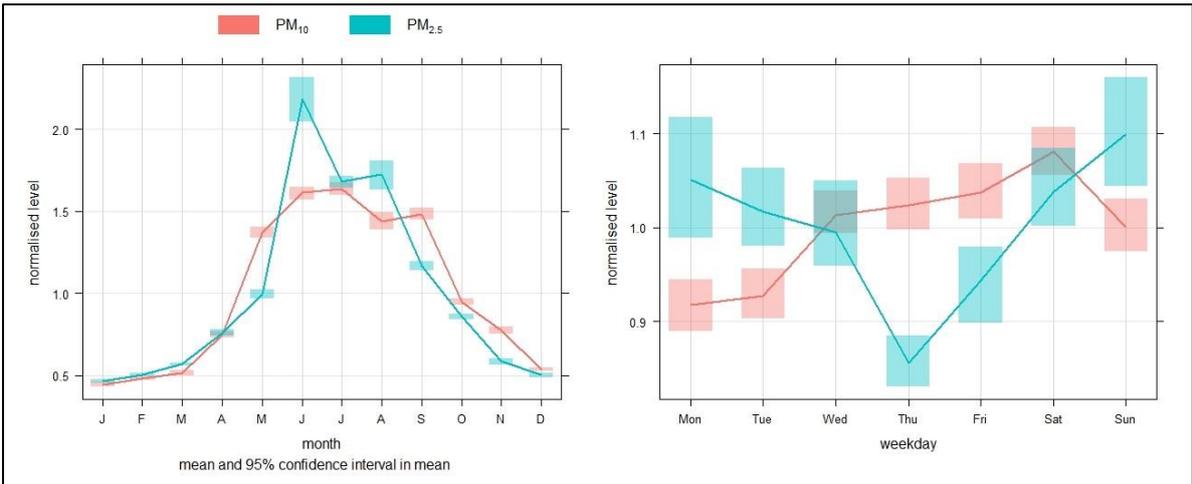


Figure 5-48: Time variation plot of normalised observed PM₁₀ and PM_{2.5} concentrations at Eco Park

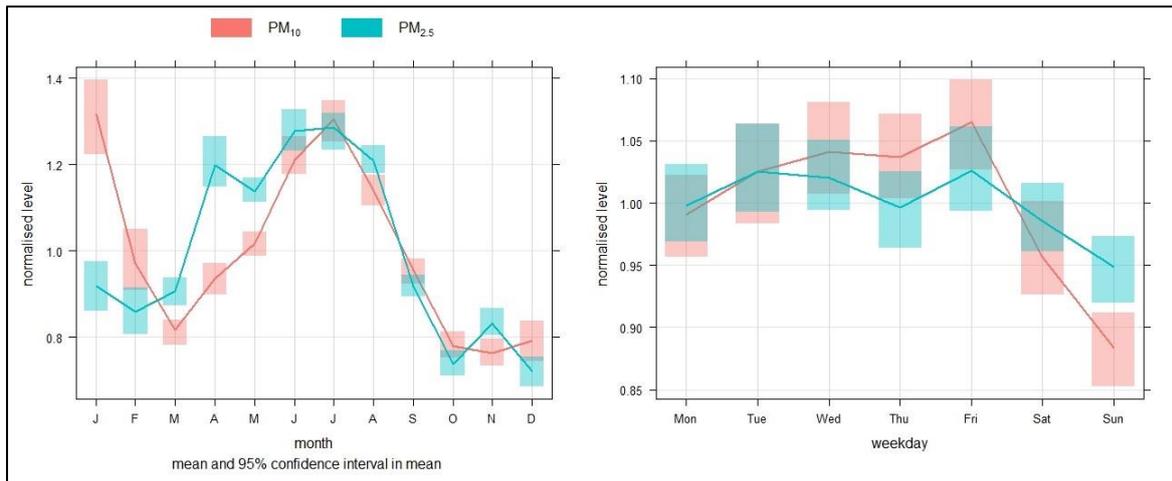


Figure 5-49: Time variation plot of normalised observed PM₁₀ and PM_{2.5} concentrations at Three Rivers

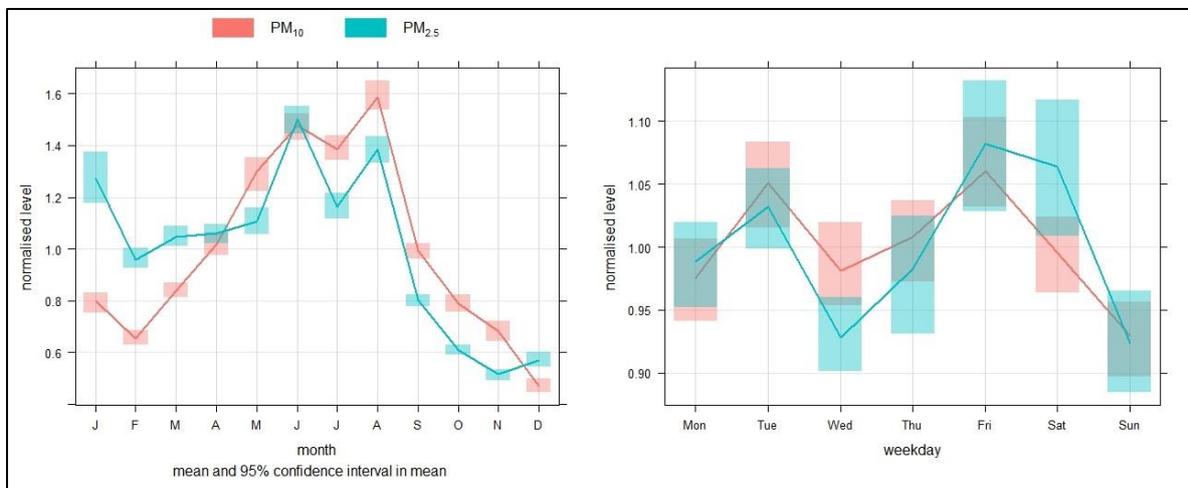


Figure 5-50: Time variation plot of normalised observed PM₁₀ and PM_{2.5} concentrations at Sharpeville

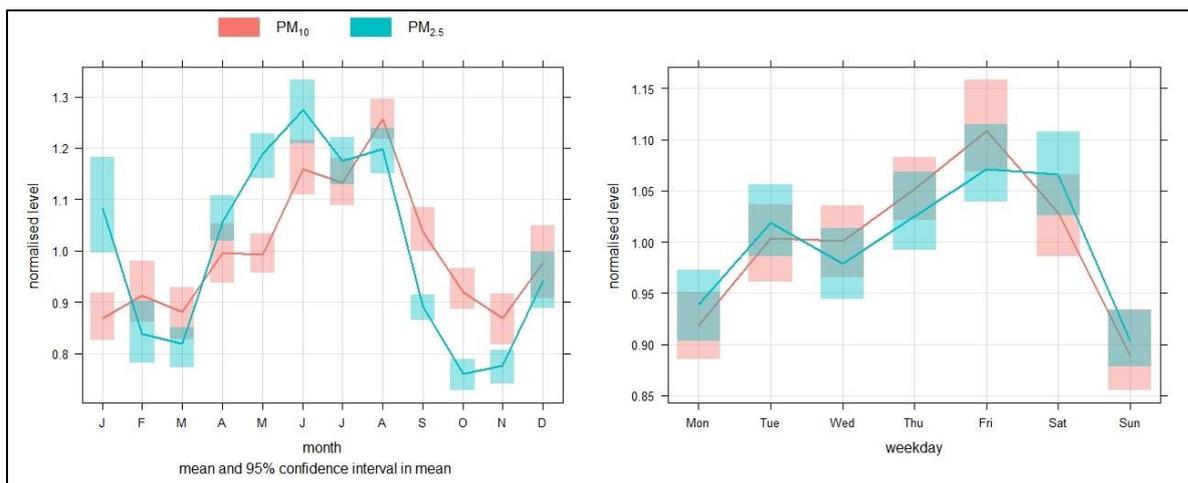


Figure 5-51: Time variation plot of normalised observed PM₁₀ and PM_{2.5} concentrations at Zamdela

5.1.6 Model Performance

5.1.6.1 Understanding of Observed Concentrations

An analysis of the observed SO₂, NO₂ and PM₁₀ concentrations at six monitoring stations was completed, in which the concentration values were categorised into wind speed and direction bins for different concentrations. This information is most easily visualised as polar plots, where the centre of the polar plot refers to the location of the monitoring station, as shown in Figure 5-52 for Leitrim and Figure 5-54 for Eco Park for SO₂ observations (other stations Figure 5-55 to Figure 5-57). The corresponding NO₂ analyses are summarised in Figure 5-58 to Figure 5-63. Polar plots for PM analyses are presented in Figure 5-64 and Figure 5-69.

These polar plots (Carslaw and Ropkins, 2012; Carslaw, 2013) provide an indication of the directional contribution as well as the dependence of concentrations on wind speed. Whereas the directional display is fairly obvious, i.e. when higher concentrations are shown to occur in a certain sector, e.g. east and south for SO₂ at Eco Park (Figure 5-54), it is understood that most of the high concentrations occur when winds blow from that sector (i.e. east or south). When the high concentration pattern is more symmetrical around the centre of the plot, it is an indication that the contributions are near-equally distributed, as is displayed for SO₂ in Figure 5-55.

Furthermore, since the observed concentrations have also been categorised according to wind speed categories, it provides an indication of the plume height. As explained in Section 5.1.4.1 (plume buoyancy), stronger winds reduce the amount of plume rise, and may effectively increase ground level concentrations. However, since an increased wind speed also enhances plume dispersion, a concentration maximum would be reached for a wind speed where the plume rise and dilution effects cancel each other. These conditions would be different for day- and night-time atmospheric stabilities. It is expected that high ground level concentrations from elevated stacks would be more prevalent during stronger wind speeds during stable conditions than daytime, convective conditions, when the plume buoyancy is often not as effective in lifting the plume centreline. Low-level emissions behave differently, and higher concentrations would normally be observed during weak-wind conditions.

The SO₂ concentrations observed at Leitrim (Figure 5-52) show elevated concentrations occurring with north-easterly winds above 5 m/s. Other SO₂ contributions originate to the north-west of the Leitrim station. The dominant contribution of median SO₂ concentrations above 100 µg/m³ originate to the north-east of the AJ Jacobs at wind speeds between 2 m/s and 8 m/s (Figure 5-53). Natref operations are located north-west of the AJ Jacobs monitoring station and contribute to the SO₂ concentrations from this direction. The SO₂ concentrations observed at Eco Park (Figure 5-54) indicate that most of the high concentrations occur with easterly winds between 6 m/s and 10 m/s. Albeit not as high as the concentrations from the easterly sector, the observations also show elevated concentrations from an southerly direction. The Three Rivers station recorded relatively low median hourly SO₂ concentrations from all directions (Figure 5-55). Median SO₂ concentrations above 50 µg/m³ originate from the east and north-west at wind speeds above 2 m/s at the Sharpeville station (Figure 5-56). The Zamdela station recorded elevated SO₂ concentrations (above 100 µg/m³) at wind speeds above 6 m/s from the north-east (Figure 5-57). Other SO₂ contributions originate to the north-west and north of the Zamdela station.

The NO₂ concentrations observed at Leitrim (Figure 5-58) indicate that most of the elevated concentrations occur from the north-westerly winds of between 2 m/s and 6 m/s, northerly winds at winds less than 2 m/s or above 10 m/s. Since vehicular exhaust emissions are significant NO₂ contributors, the observations from the northern sector most likely indicates this source. Median NO₂ concentrations originate to the north-east of the AJ Jacobs at all wind speeds (Figure 5-59). The NO₂ concentrations observed at Eco Park (Figure 5-60) showed higher concentrations occurring during relatively weak winds of about 2 m/s and at higher wind speeds around 10 m/s, primarily from the south-south-west of the station. Median NO₂

concentrations observed at the Three Rivers station showed a local source at low wind speeds contributing NO₂ concentrations of approximately 50 µg/m³ (Figure 5-61). Higher NO₂ concentrations were recorded during high wind speeds (above 8 m/s) from the east of the Three Rivers station. A similar pattern of a local NO₂ source at low wind speeds is evident at the Sharpeville station (Figure 5-62), while NO₂ concentrations above 50 µg/m³ originate to the west-north-west of the Sharpeville station at wind speeds 8 m/s. Median NO₂ concentrations measured at the Zamdela station show contributions of NO₂ above 50 µg/m³ from the north-west and north east at all wind speeds (Figure 5-63).

Elevated particulate concentrations at Leitrim show contributions from the north and north-west at higher (between 8 and 10 m/s) wind speeds (Figure 5-64). At low wind speeds (2 m/s or less) the almost symmetrical plot shows a local contribution, most likely a result of community activities. Elevated particulate matter concentrations at AJ Jacobs are shown to originate from the northerly sector at wind speeds above 3 m/s (Figure 5-65). Other sources of particulate matter contribute to concentrations of approximately 50 µg/m³ from localised sources at wind speeds below 1 m/s. Particulate concentrations observed at the Eco Park station are lower than at the other stations, where the sources of elevated concentrations (greater than 40 µg/m³) are located to the north-west of the station (Figure 5-66). Other particulate sources are also located to the north-east and south-west of the Eco Park station contributing at lower wind speeds (5 to 10 m/s). A local source also contributes at low wind speeds. The Three Rivers station recorded elevated particulate concentrations from almost all directions at wind speeds greater than 3 m/s (Figure 5-67). A local source contributes at wind speeds lower than 2 m/s. Similarly, the Sharpeville station recorded elevated particulate concentrations from nearly all wind directions at speeds greater than 4 m/s, with the southerly direction showing the lower particulate concentrations (Figure 5-68). A local source (possibly community activities) is a large contributor at low wind speeds (less than 2 m/s). Particulate concentrations recorded at the Zamdela show high concentrations from the north-west and north-east, at high wind speeds (above 4 m/s), and a local source at low wind speeds (Figure 5-69). Sources in the south-westerly sector contribute the lowest concentrations, especially at higher wind speeds.

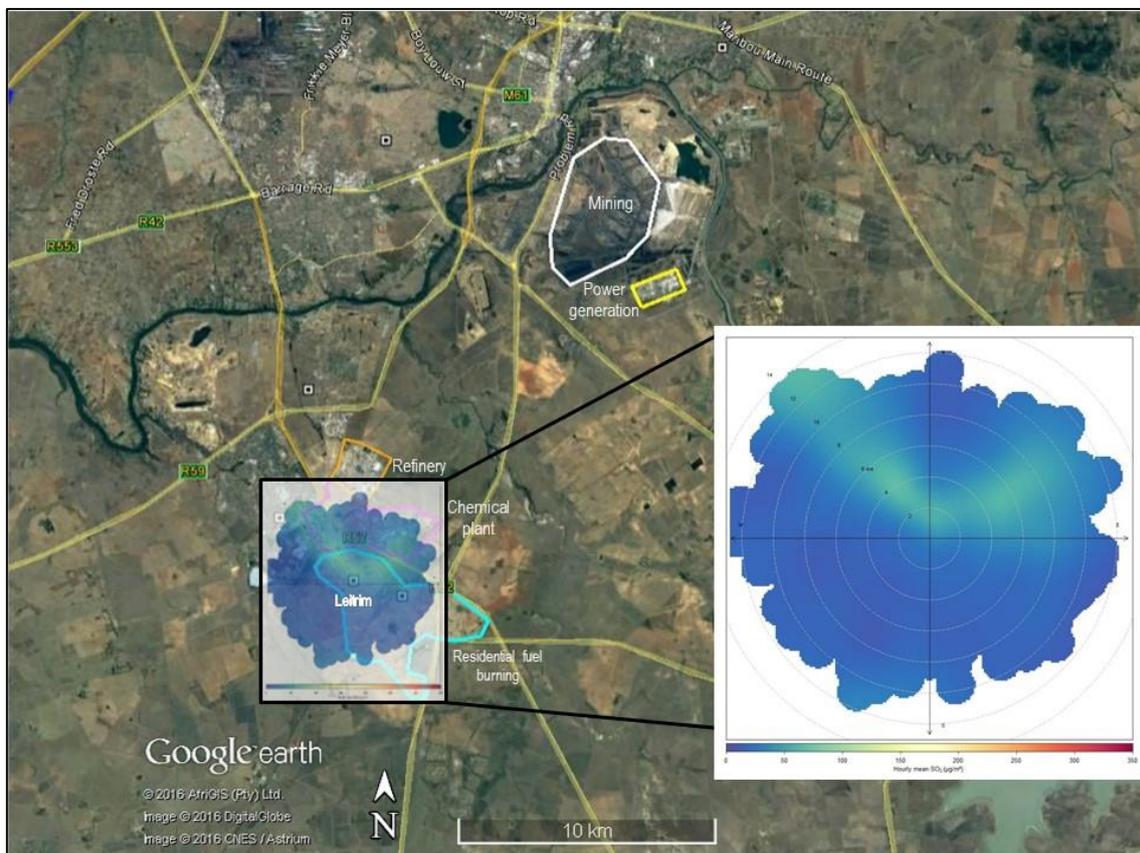


Figure 5-52: Polar plot of hourly median SO₂ concentration observations at Leitrim for 2015 to 2017

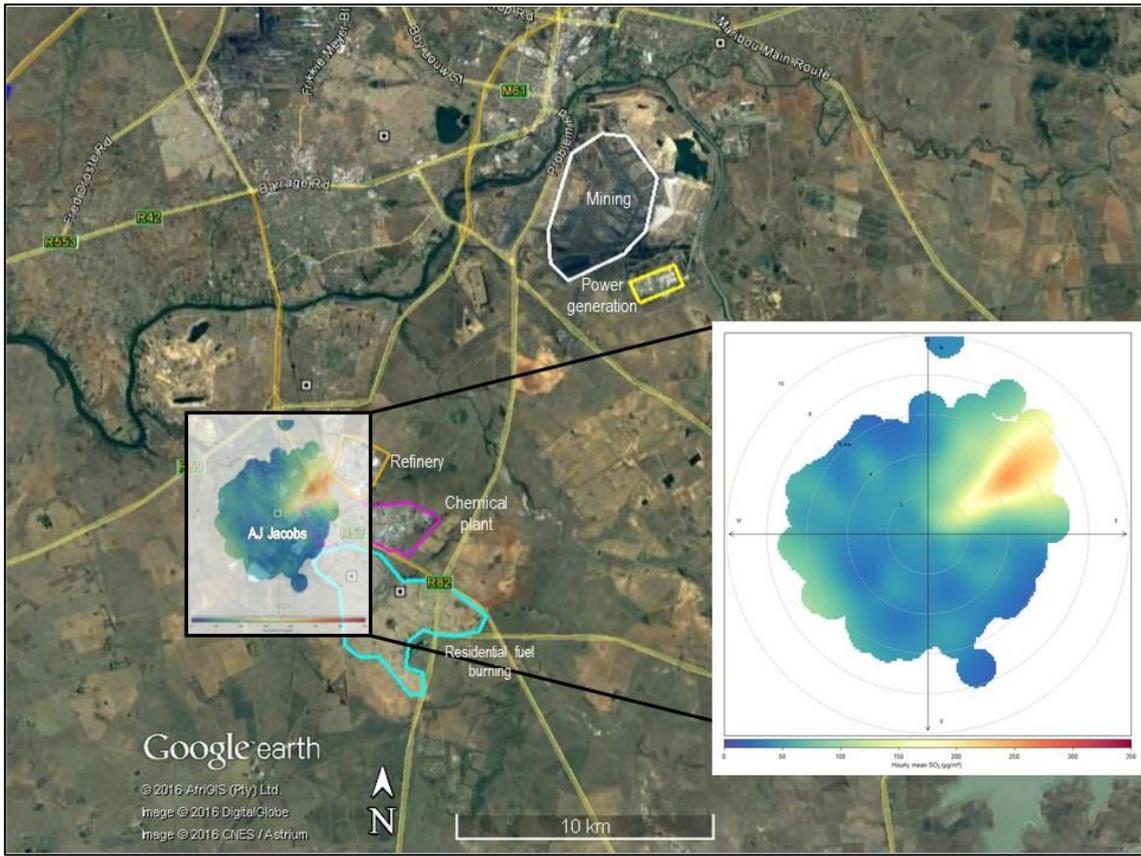


Figure 5-53: Polar plot of hourly median SO₂ concentration observations at AJ Jacobs for 2015 to 2017

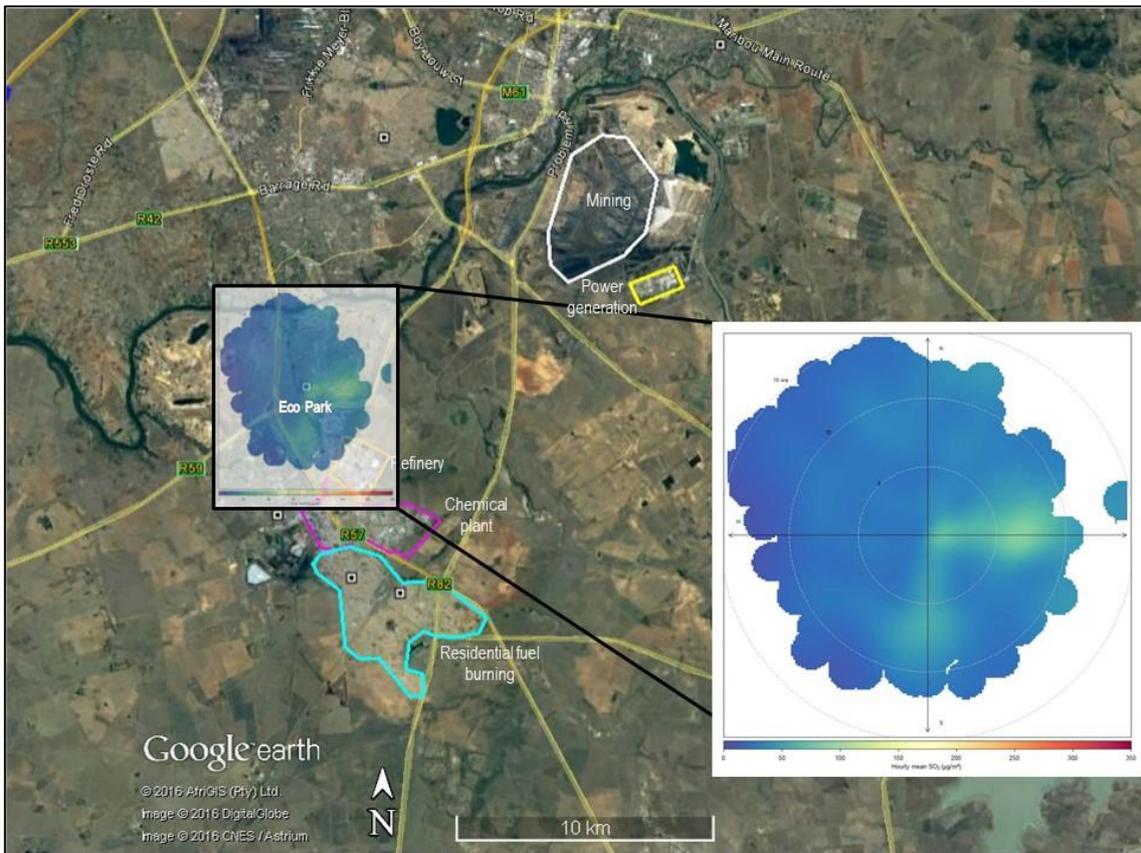


Figure 5-54: Polar plot of hourly median SO₂ concentration observations at Eco Park for 2015 to 2017

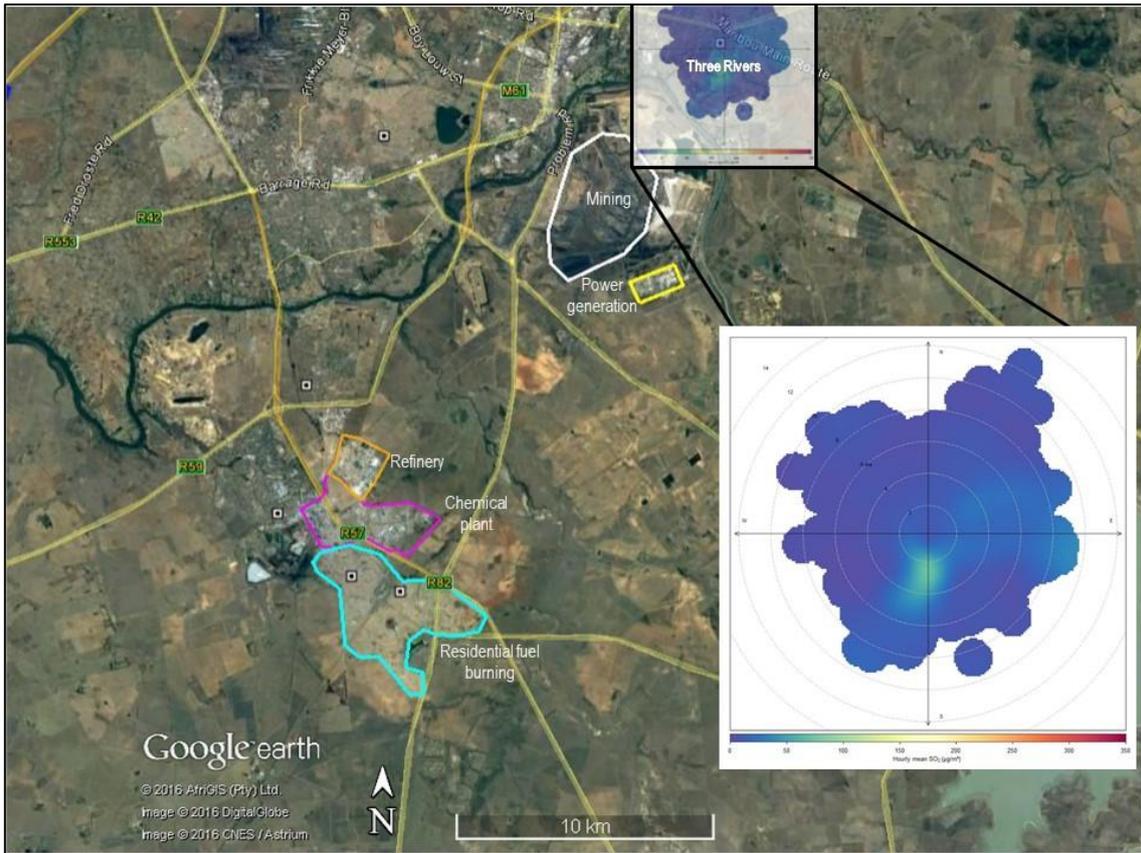


Figure 5-55: Polar plot of hourly median SO₂ concentration observations at Three Rivers for 2015 to 2017

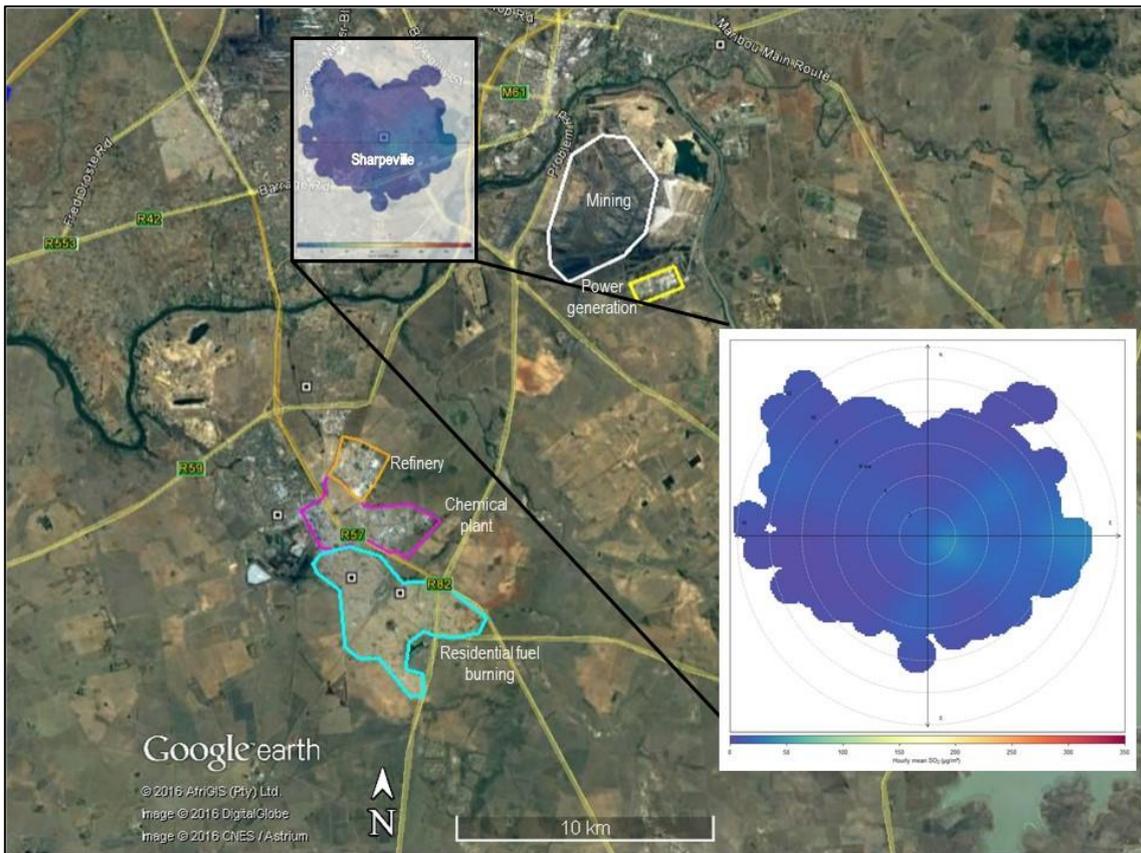


Figure 5-56: Polar plot of hourly median SO₂ concentration observations at Sharpeville for 2015 to 2017

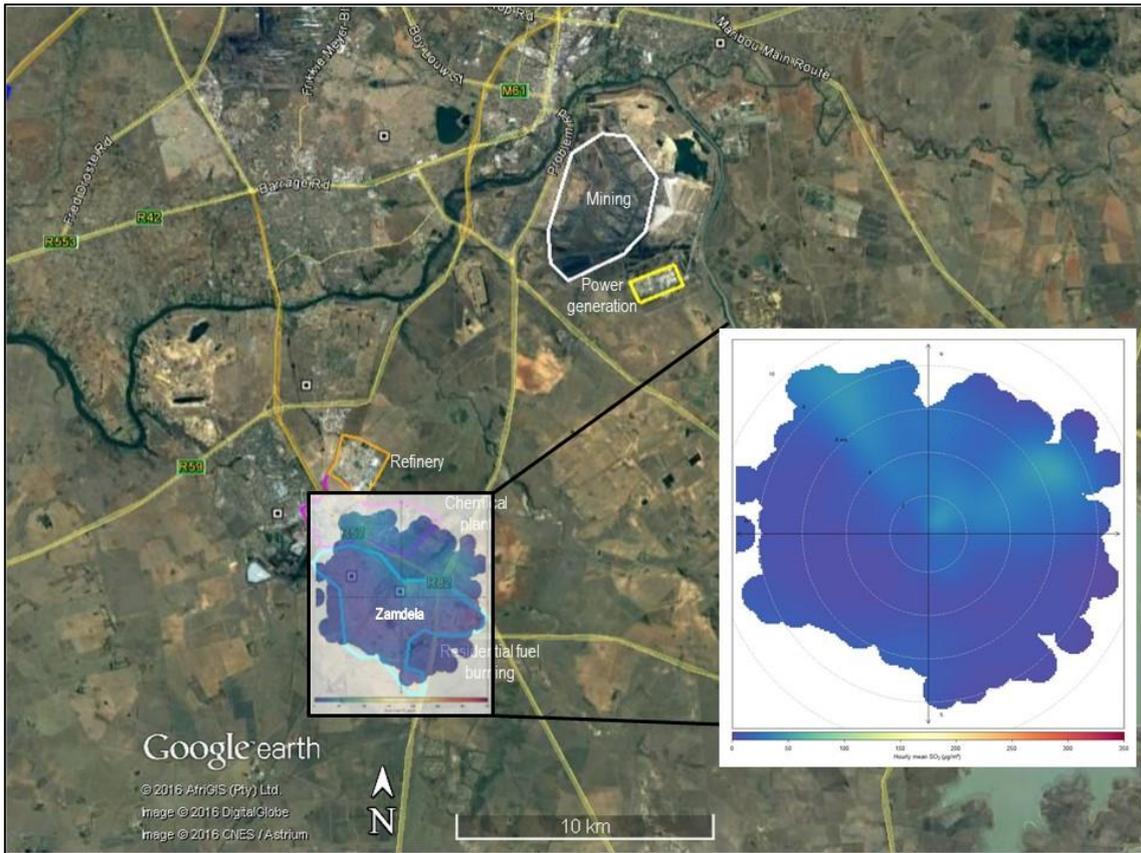


Figure 5-77: Polar plot of hourly median SO₂ concentration observations at Zamdela for 2015 to 2017

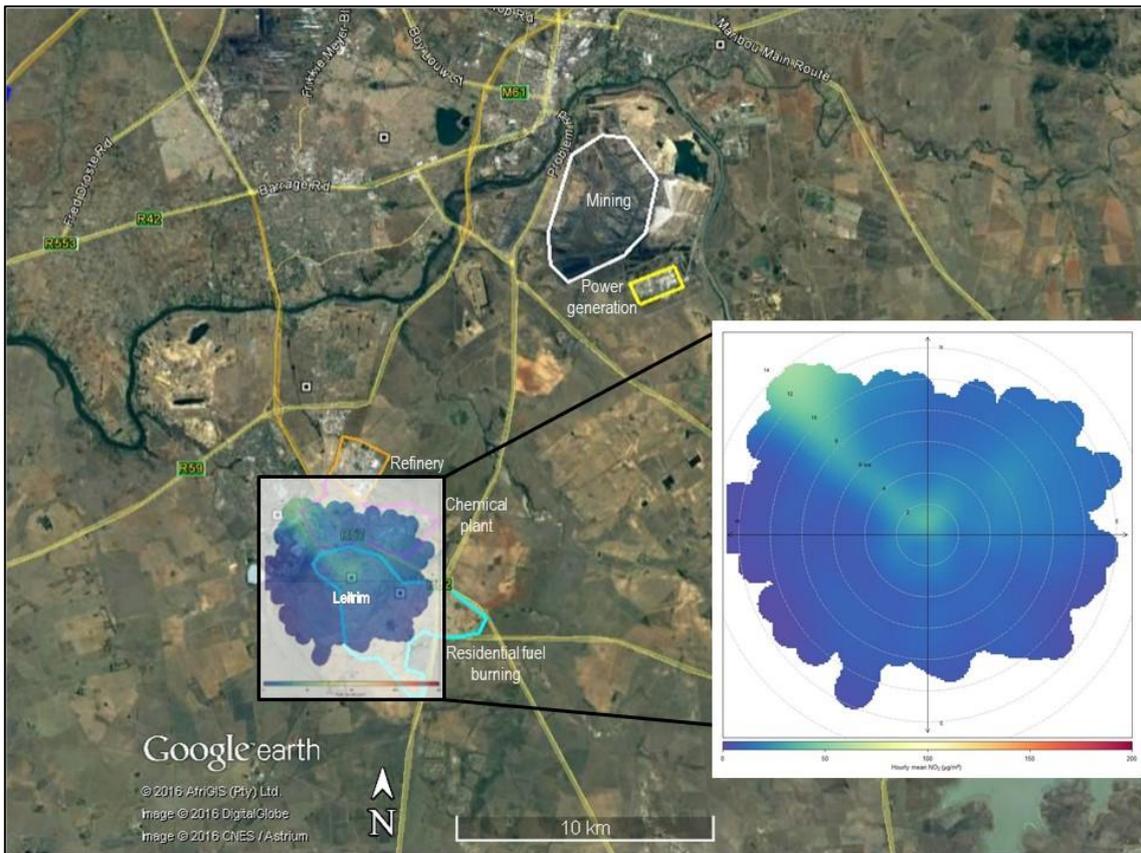


Figure 5-78: Polar plot of hourly median NO₂ concentration observations at Leitrim for 2015 to 2017

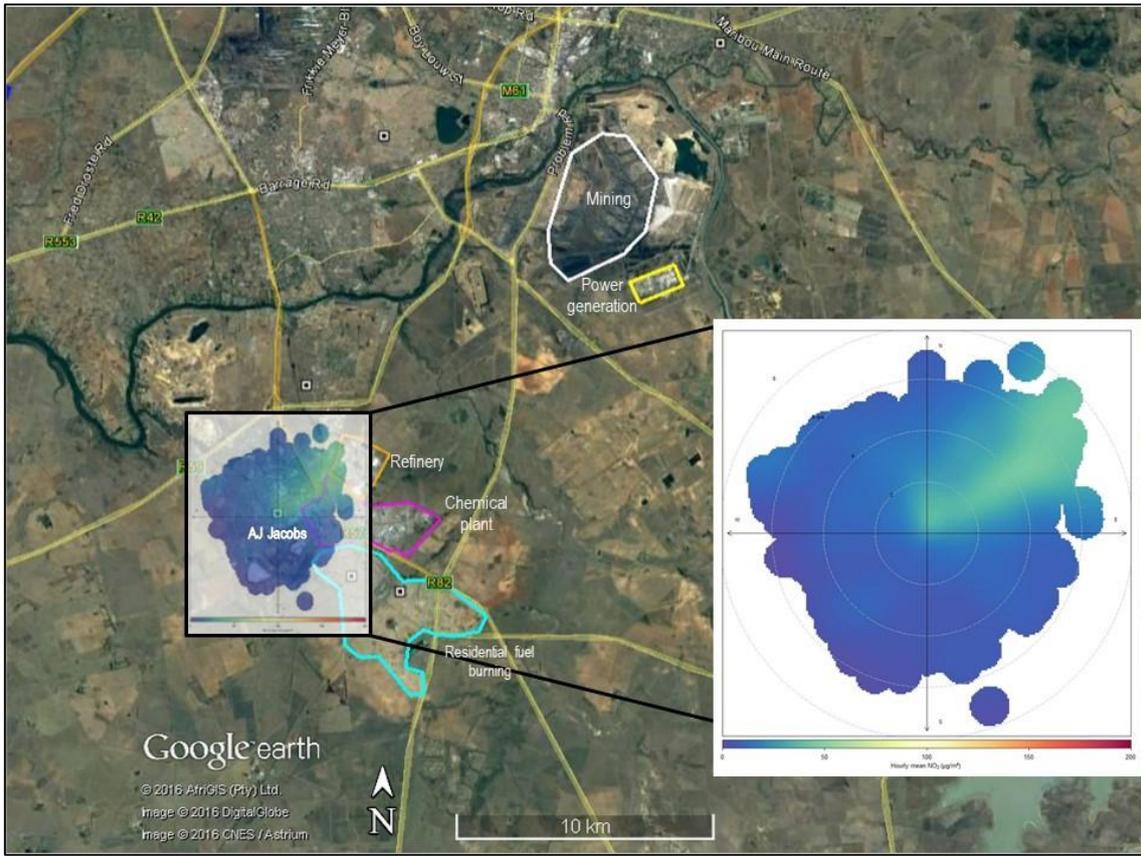


Figure 5-59: Polar plot of hourly median NO₂ concentration observations at AJ Jacobs for 2015 to 2017

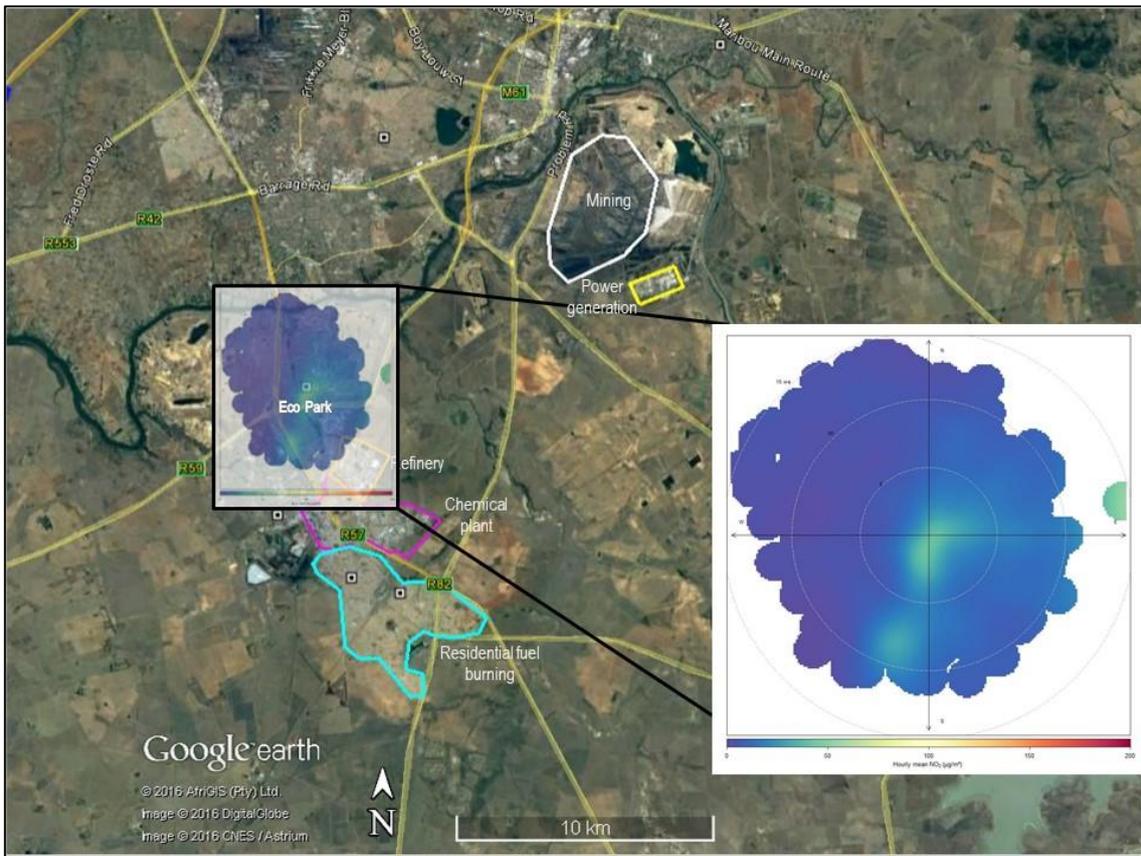


Figure 5-60: Polar plot of hourly median NO₂ concentration observations at Eco Park for 2015 to 2017

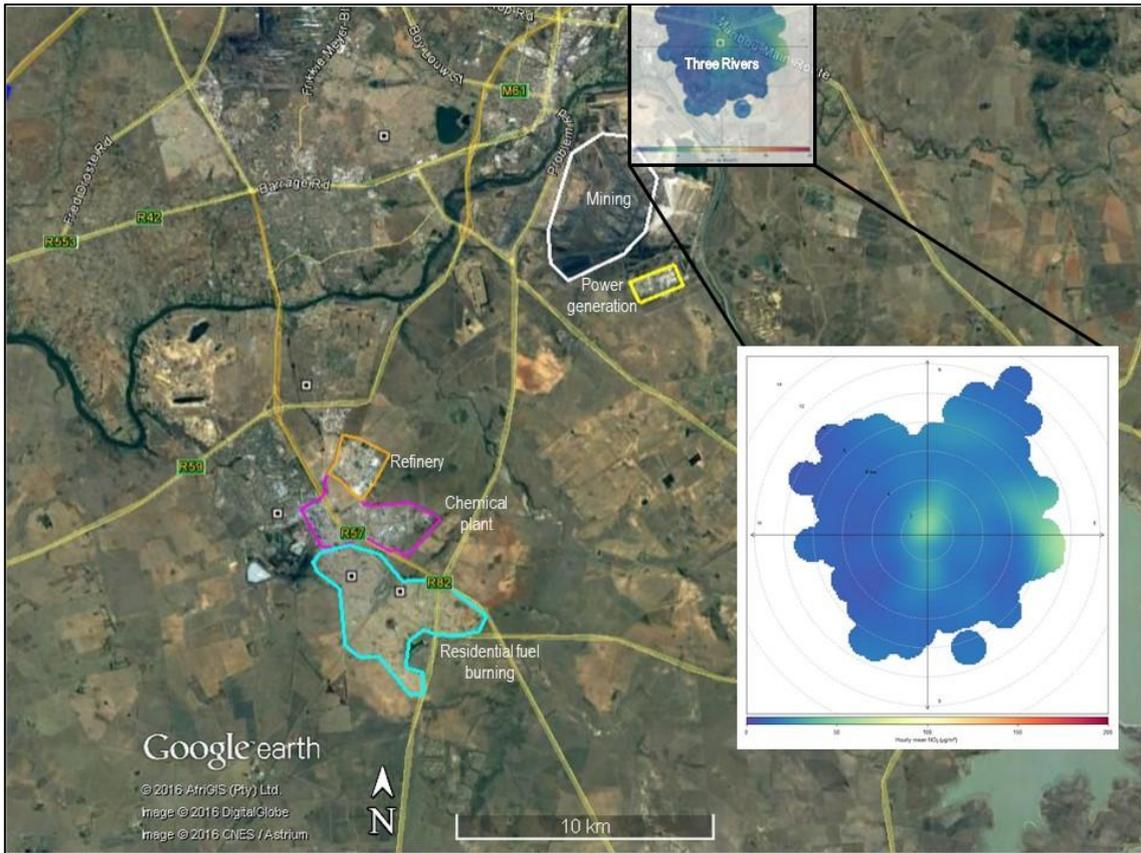


Figure 5-61: Polar plot of hourly median NO₂ concentration observations at Three Rivers for 2015 to 2017

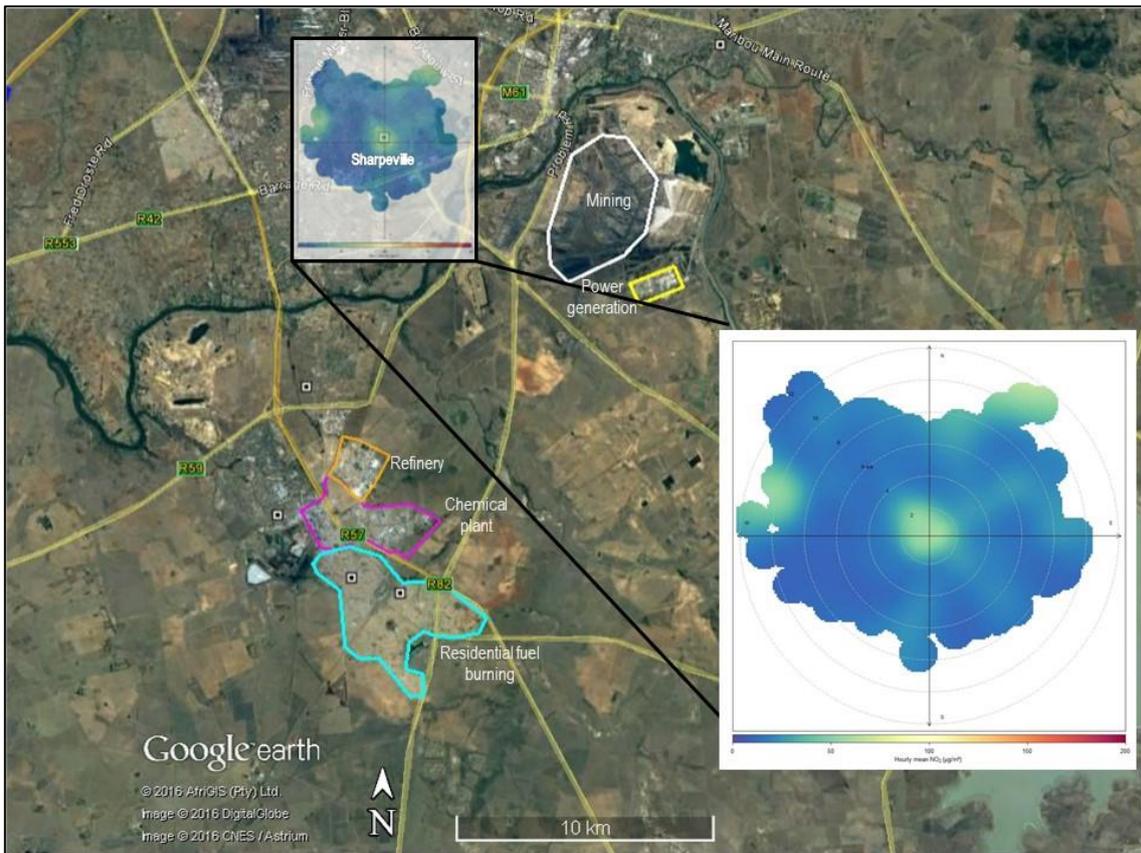


Figure 5-62: Polar plot of hourly median NO₂ concentration observations at Sharpeville for 2015 to 2017

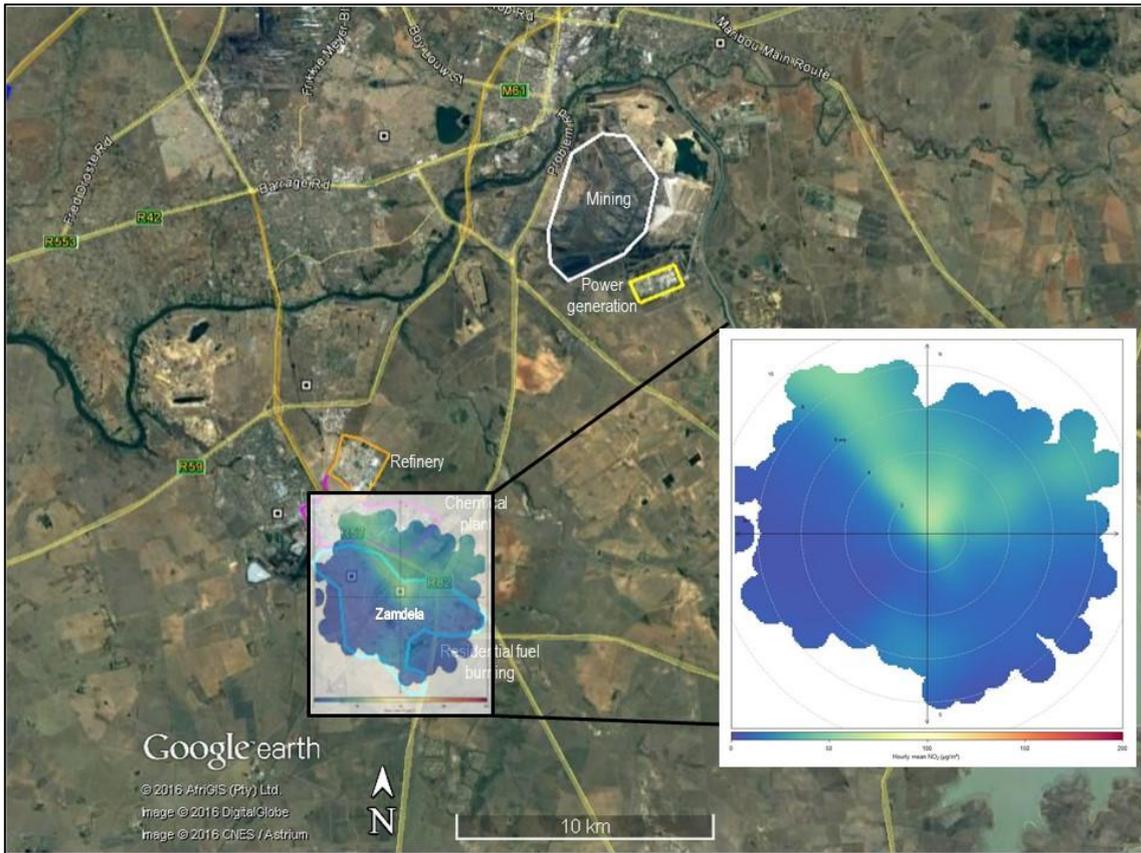


Figure 5-63: Polar plot of hourly median NO₂ concentration observations at Zamdela for 2015 to 2017

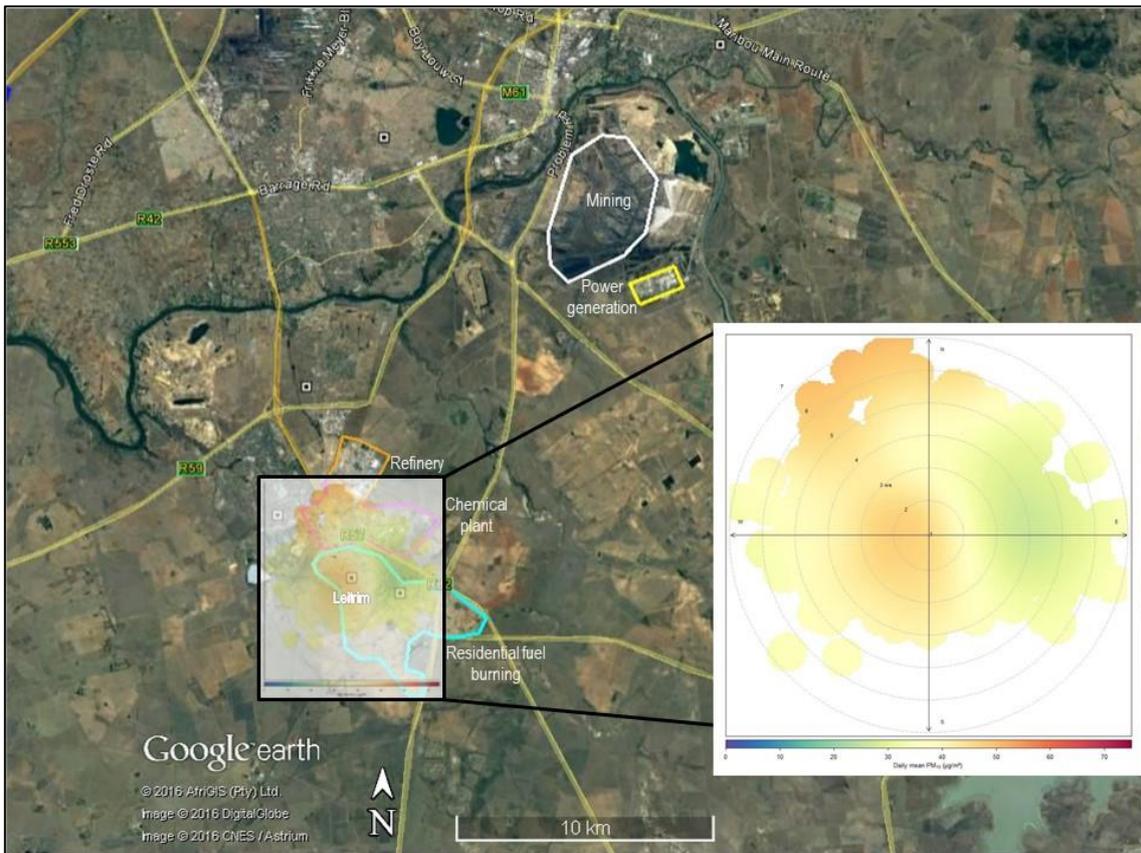


Figure 5-64: Polar plot of hourly median PM₁₀ concentration observations at Leitrim for 2015 to 2017

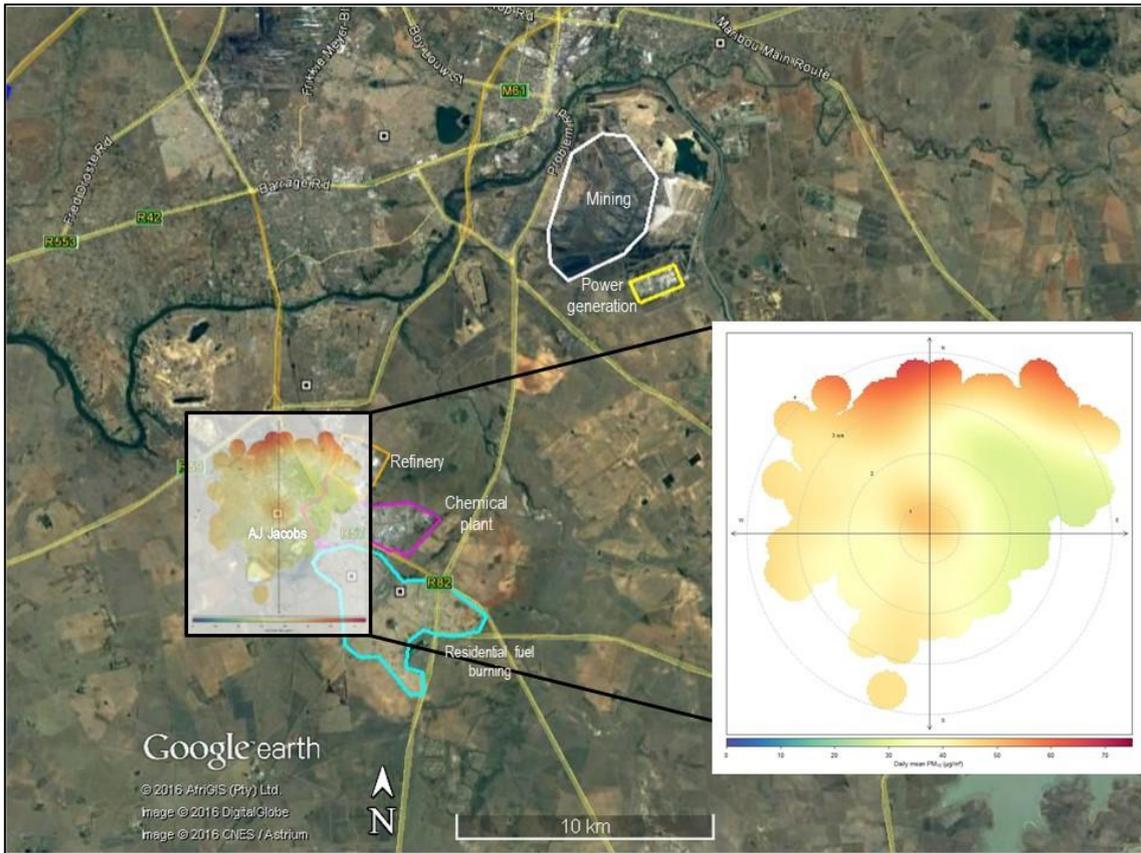


Figure 5-65: Polar plot of hourly median PM₁₀ concentration observations at AJ Jacobs for 2015 to 2017

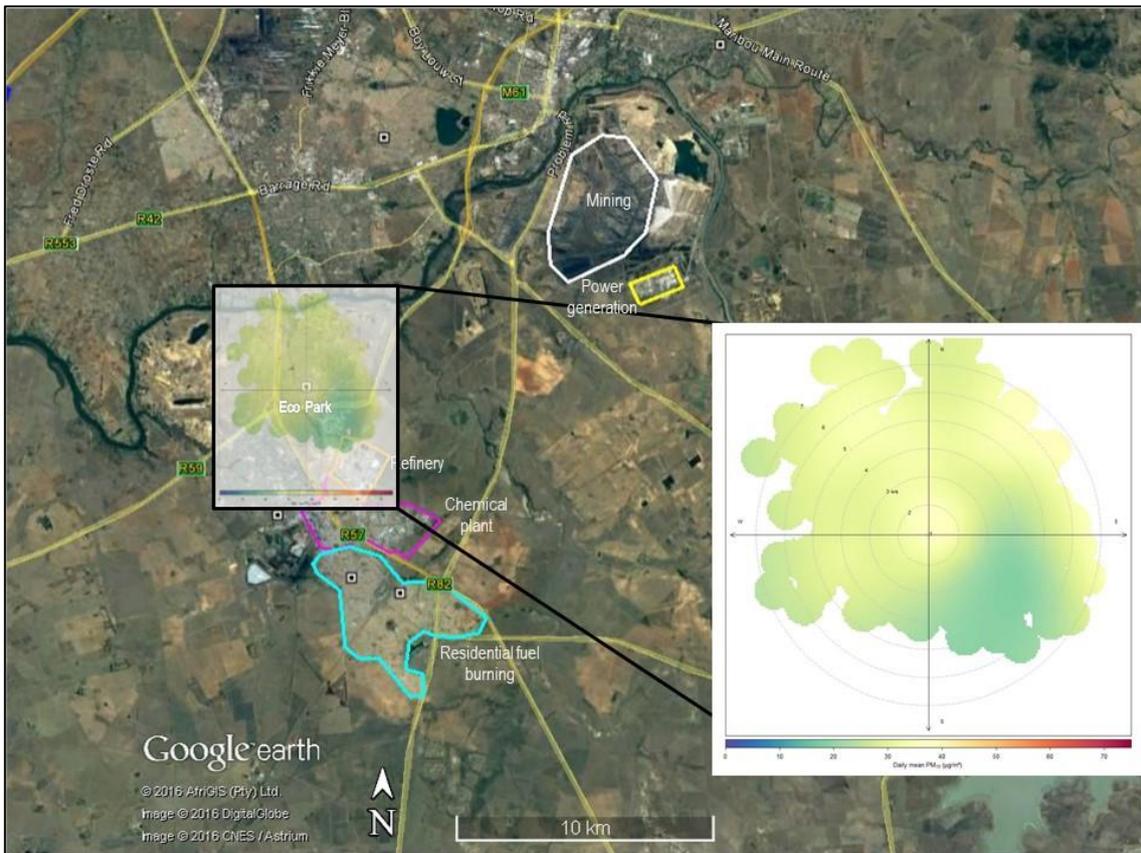


Figure 5-66: Polar plot of hourly median PM₁₀ concentration observations at Eco Park for 2015 to 2017

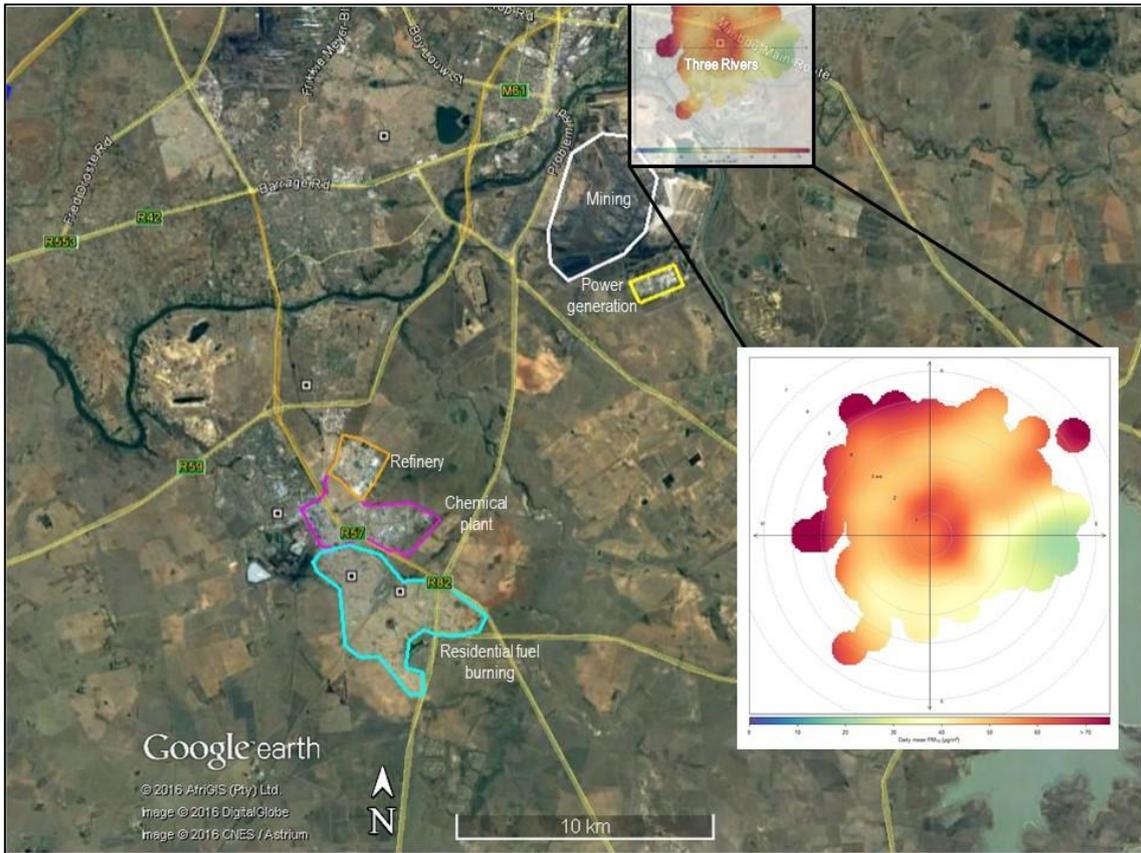


Figure 5-67: Polar plot of hourly median PM₁₀ concentration observations at Three Rivers for 2015 to 2017

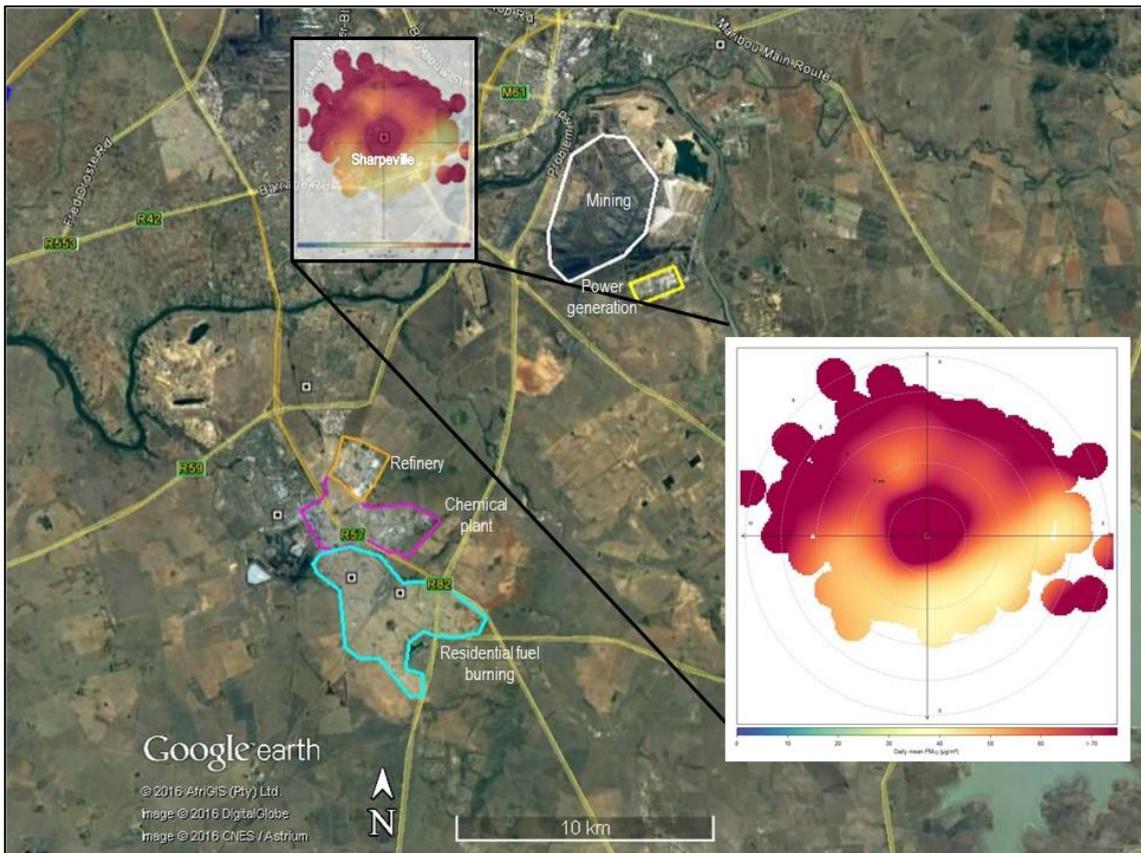


Figure 5-68: Polar plot of hourly median PM₁₀ concentration observations at Sharpeville for 2015 to 2017

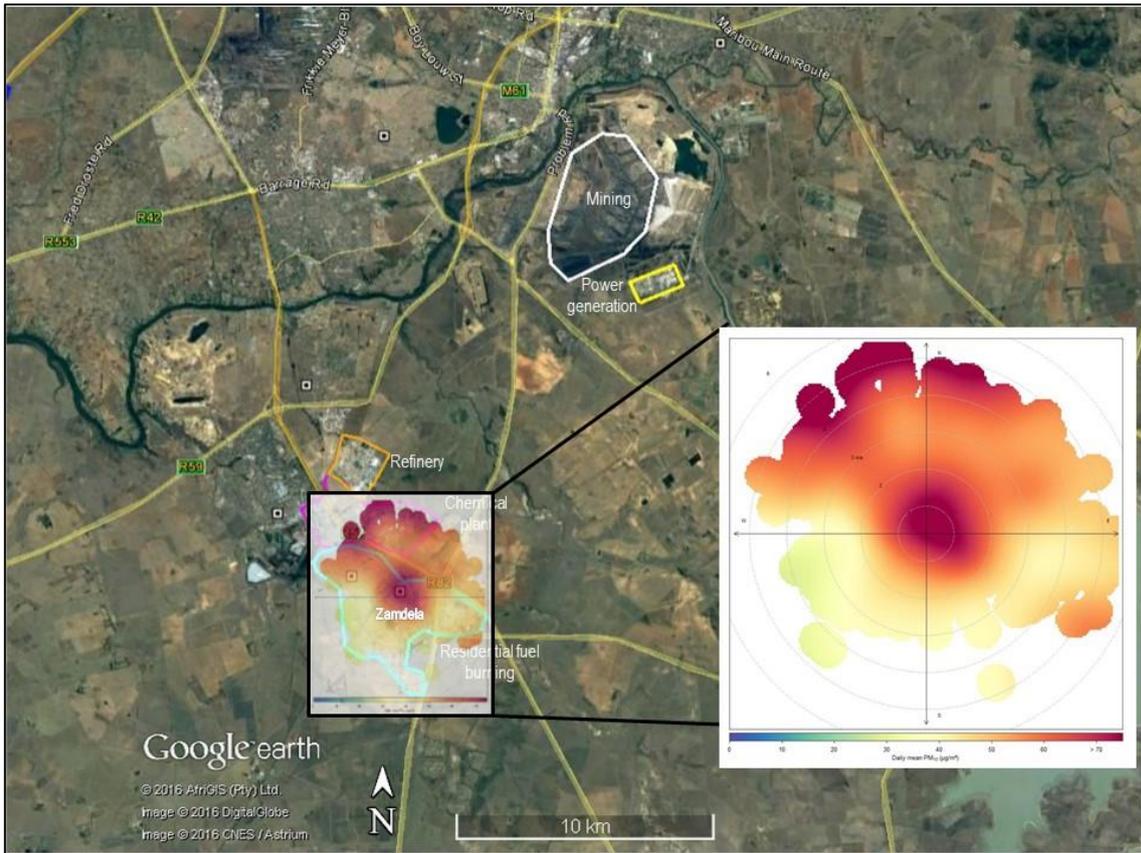


Figure 5-69: Polar plot of hourly median PM₁₀ concentration observations at Zamdela for 2015 to 2017

5.1.6.2 Model Validation

Ambient concentrations of NO₂, SO₂, and PM₁₀ measured by Sasol and the DEA in Sasolburg help provide an understanding of existing ambient air concentrations as well as providing a means of verifying the dispersion modelling. Since the aim of the investigation is to illustrate the change in ground level concentrations from the current levels (i.e. baseline emission scenario) to those levels resulting from the introduction of the required emission limits (i.e. new plant emission standards), the intention was not to comprehensively include all air emissions within Sasolburg. Unaccounted emissions include those from unintended leaks within the plant (fugitive emissions) and small vents, as well as air emissions from other industries, emissions from activities occurring within the communities, and biomass burning (especially during winter season), as well as long-range transport into the modelling domain. However, information about community activities, such as the amount of traffic within the community and the amount of fuel used for heating is often difficult to estimate.

These emissions, when combined, may potentially add up to be a significant portion of the observed concentrations in the modelling domain. In terms of the current investigation, the portion of air quality due to air emission sources that is not included in the model's emissions inventory constitutes the background concentration.

Discrepancies between predicted and observed concentrations may also be as a result of process emission variations and may include upset emissions and shutdowns. These conditions could result in significant under-estimating or over-estimating the air concentrations. In order to accommodate these upset emission conditions, a time varying emissions database would be required as input into the model.

A summary of the predicted concentrations (Sasol (SO) and Natref) and their comparison with observations are given in Appendix G. In order to establish model performance under average emission conditions, it is not uncommon to use a certain percentile of predicted and observed concentrations for comparison. Although these may range from a 90th to 99.9th percentile, it was decided to use the DEA NAAQS for guidance. For criteria pollutants SO₂, NO₂ and PM₁₀, the NAAQS requires compliance with the 99th percentile. As hourly averages, this allows exceedances of the limit value of 88 hours (SO₂ and NO₂) or 4 days (SO₂ and PM₁₀) per year. Estimated short-term (hourly or daily) background concentrations (not associated with the emissions included in the simulations) used the observed concentration value when simulated concentrations from SO indicate very small contributions (0.1 µg/m³).

The performance evaluation was completed using the fractional bias method. Fractional bias is one of the evaluation methods recommended by the U.S. EPA for determining dispersion model performance (U.S. EPA 1992). Fractional bias provides a comparison of the means and standard deviation of both modelled and monitored concentrations for any given number of locations.

In this assessment, the background concentrations were added to the simulated concentrations prior to the calculation of the fractional bias. The 99th percentile (with background concentration) was compared to the same ranked monitored concentrations.

Table 5-17 Table 5-18 summarises the comparisons between simulated (SO and Natref) and observed SO₂ concentrations at the monitoring stations in the study area. As shown in the table of the observed peak concentrations, 72% and 37% could not be accounted for at Leitrim and AJ Jacobs (the two closest monitoring stations to SO). The difference between simulated and observation increases significantly when considering long-term comparisons (i.e. 50th percentile and annual average) at these 2 stations, clearly illustrating the contribution of emission sources not included in the dispersion model's emissions inventory.

The performance evaluation was completed using the fractional bias method. Fractional bias is one of the evaluation methods recommended by the U.S. EPA for determining dispersion model performance (U.S. EPA 1992). Fractional bias provides a

comparison of the means and standard deviation of both modelled and monitored concentrations for any given number of locations.

In this assessment, the background concentrations were added to the simulated concentrations prior to the calculation of the fractional bias. The 99th percentile (with background concentration) was compared to the same ranked monitored concentrations.

Table 5-17: Comparison of predicted and observed SO₂ concentrations at monitoring station in Sasolburg

Description	SO ₂ concentration (µg/m ³)			Unaccounted Fraction*
	Simulated	Observed	Unaccounted	
Leitrim				
Peak	182	650	467	0.7
99th Percentile	67	187	120	0.6
90th Percentile	22	77	55	0.7
50th Percentile	0.01	24	24	1.0
Annual Average	4	35	31	0.9
AJ Jacobs				
Peak	422	666	244	0.4
99th Percentile	170	304	134	0.4
90th Percentile	8	135	127	0.9
50th Percentile	0.00	55	55	1.0
Annual Average	6	68	61	0.9
Eco Park				
Peak	214	872	658	0.8
99th Percentile	44	244	200	0.8
90th Percentile	1	79	78	1.0
50th Percentile	0.00	31	31	1.0
Annual Average	1	42	41	1.0
Three Rivers				
Peak	31	535	504	0.9
99th Percentile	11	138	127	0.9
90th Percentile	0.5	32	32	1.0
50th Percentile	0.00	9	9	1.0
Annual Average	0.3	16	16	1.0
Sharpeville				
Peak	47	642	595	0.9
99th Percentile	14	148	134	0.9
90th Percentile	0.6	40	40	1.0
50th Percentile	0.00	9	9	1.0
Annual Average	0.4	18	18	1.0
Zamdela				
Peak	301	473	172	0.4
99th Percentile	98	175	76	0.4
90th Percentile	31	50	19	0.4
50th Percentile	0.05	9	9	1.0
Annual Average	7	21	14	0.7

* unaccounted fraction as a percentage of observed concentration

In Figure 5-70, the fractional bias is plotted with the means on the X-axis and the standard deviations on the Y-axis. The box on the plot encloses the area of the graph where the model predictions are within a fractional bias between -2 and +2; indicating an acceptable correlation. The U.S. EPA states that predictions within a factor of two are a reasonable performance target for

a model before it is used for refined regulatory analysis (U.S. EPA 1992). Data points appearing on the left half of the plot indicate an over-prediction and those on the right half of the plot represent under-predictions.

The fractional bias of the means was less than 0.67, clearly showing good model performance at AJ Jacobs and Zamdela. At Three Rivers, Sharpeville, Leitrim and Eco Park the fractional bias of the means was less than 2, indicating an acceptable correlation.

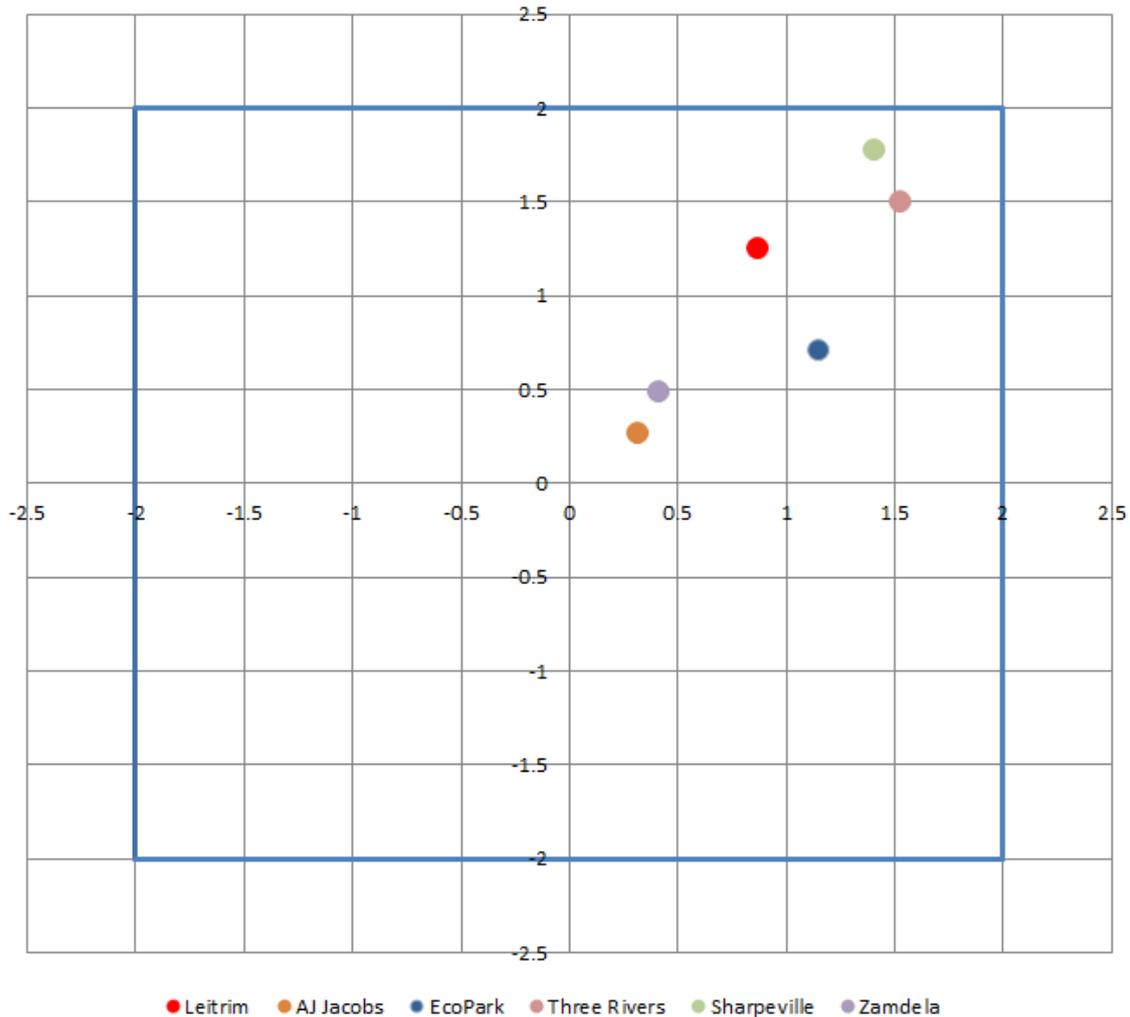


Figure 5-70: Fractional bias of means and standard deviation for SO₂

The same calculations and comparisons were repeated for NO₂ simulations and observations. The CALPUFF simulations were specifically for NO_x and the formation of HNO₃ and other nitrates using the MESOPUFF II chemical transformation mechanism, as discussed in Section 5.1.4.3.

Table 5-19 summarises of comparisons between simulated and observed NO₂ concentrations at the monitoring stations in the study area. For Zamdela, AJ Jacobs and Leitrim higher concentrations were simulated than the observed peak and 99th percentile concentrations. This may be due to the rather simplistic methodology of applying a constant conversion rate from NO_x to NO₂ (Section 5.1.4.3). As shown in Appendix E, the conversion ratio at high concentration levels (i.e. closer to the point of emission) generally varies between 14% and 27% for NO_x concentrations above 188 µg/m³. In this investigation, a NO₂ conservative ratio of not less than 40% was adopted for high concentrations of NO_x. Concentrations similar to the observed peak would be simulated if the lower conversions of 27% were used instead.

As for SO₂, the difference between simulated and observation NO₂ concentrations increases significantly when considering long-term comparisons (i.e. 50th percentile and annual average), clearly illustrating the contribution of emission sources not included in the dispersion model's emissions inventory.

Table 5-18: Comparison of predicted and observed NO₂ concentrations at monitoring stations in Sasolburg

Description	NO ₂ concentration (µg/m ³)			Unaccounted Fraction*
	Simulated	Observed	Unaccounted	
Leitrim				
Peak	133	145	12	0.08
99th Percentile	58	77	19	0.25
90th Percentile	23	43	21	0.48
50th Percentile	0.01	17	17	1.00
Annual Average	7	21	14	0.66
AJ Jacobs				
Peak	255	139	0	0.00
99th Percentile	111	78	0	0.00
90th Percentile	16	47	31	0.65
50th Percentile	0.00	19	19	1.00
Annual Average	8	23	15	0.65
Eco Park				
Peak	136	532	396	0.74
99th Percentile	44	85	41	0.49
90th Percentile	2	51	49	0.97
50th Percentile	0.00	15	15	1.00
Annual Average	2	21	20	0.92
Three Rivers				
Peak	51	168	117	0.70
99th Percentile	13	97	84	0.87
90th Percentile	0.6	57	57	0.99
50th Percentile	0.00	23	23	1.00
Annual Average	0.5	28	28	0.98
Sharpeville				
Peak	79	208	129	0.62
99th Percentile	18	106	87	0.83
90th Percentile	0.8	64	64	0.99
50th Percentile	0.00	22	22	1.00
Annual Average	0.8	30	29	0.97
Zamdela				
Peak	203	170	0	0.00
99th Percentile	62	105	43	0.41
90th Percentile	38	64	26	0.41
50th Percentile	0.08	23	23	1.00
Annual Average	10	30	19	0.65

* unaccounted fraction as a percentage of observed concentration