EXTERNAL PEER REVIEW OF ATMOSPHERIC IMPACT REPORTS IN SUPPORT OF SASOL'S AND NATREF'S APPLICATION FOR POSTPONEMENT AND EXEMPTION FROM CERTAIN REQUIREMENTS FOR THE NATIONAL ENVIRONMENTAL MANAGAMENT: AIR QUALITY ACT NO. 39 OF 2004 – MINIMUM EMISSIONS STANDARDS

JANUARY 2017

BACKGROUND TO EXTERNAL PEER REVIEW

- Sasol and Natref are required to comply with the Minimum Emission Standards (MES), published in terms of the National Environmental Management: Air Quality Act NEM:AQA). In terms of the MES, existing plans are required to comply by 1 April 2015 with existing plant standards, and by 1 April 2020 with stricter new plant standards.

- Paragraph 11 of Section 21of the Act allows for applications for postponing the deadlines for compliance with the Minimum Emission Standards if certain requirements are satisfied. Postponements of up to five years may be granted. Sasol and Natref previously requested a postponement of the compliance deadlines for certain activities in 2014, and the requested postponement was granted in February 2015. However, for some activities the postponement was granted for a period of only three years. Sasol and Natref now intends to submit applications for exemption or extension of compliance deadlines for certain activities for which compliance may not be possible or practicable within the prescribed timeframe.

- Sasol's applications will include independently compiled Atmospheric Impact Reports (AIR) to establish an objective analysis of the impact of not meeting the promulgated standards on ambient air quality.

- Airshed Planning Professionals (Pty) Ltd was the independent air quality specialist appointed to prepare atmospheric impact assessments as prescribed by the AIR Regulations, which provide for an assessment of the potential air quality risks caused by the emissions for which postponement or exemption is sought from the MES, on the basis of the South African National Ambient Air Quality Standards.

- E^{x}ponent was appointed to independently peer review the dispersion modelling methodology employed in the AIR.

- This document incorporates the dispersion modelling study plan, the peer reviewer findings, the response to the findings and is divided in the following parts:
    I. Part A – Airshed plan of study for the dispersion modelling for Sasol and Natref
    II. Part B – Peer review report
    III. Part C – Airshed response to peer review report

PART A

PLAN OF STUDY REPORT
In support of
An Air Quality Impact Study for Sasol to Serve as Motivation and Postponement Applications from Minimum Emission Standards

Project done on behalf of **Sasol Technology (Pty) Ltd.**

Report No: 16SAS01 | **Date:** September 2016

Address: 480 Smuts Drive, Halfway Gardens | **Postal:** P O Box 5260, Halfway House, 1685
Tel: +27 (0)11 805 1940 | **Fax:** +27 (0)11 805 7010
www.airshed.co.za

Report Details

Report No.	16SAS01
Status	Rev 1
Report Title	PLAN OF STUDY REPORT: In Support of an Air Quality Impact Study for Sasol to Serve as Motivation and Postponement Applications from Minimum Emission Standards
Date	September 2016
Client	Sasol Technology (Pty) Ltd
Prepared by	Reneé von Gruenewaldt (Pr. Sci. Nat.). MSc (University of Pretoria)
Notice	Airshed Planning Professionals (Pty) Ltd is a consulting company located in Midrand, South Africa, specialising in all aspects of air quality, ranging from nearby neighbourhood concerns to regional air pollution impacts as well as noise impact assessments. The company originated in 1990 as Environmental Management Services, which amalgamated with its sister company, Matrix Environmental Consultants, in 2003.
Declaration	Airshed is an independent consulting firm with no interest in the project other than to fulfil the contract between the client and the consultant for delivery of specialised services as stipulated in the terms of reference.
Copyright Warning	Unless otherwise noted, the copyright in all text and other matter (including the manner of presentation) is the exclusive property of Airshed Planning Professionals (Pty) Ltd. It is a criminal offence to reproduce and/or use, without written consent, any matter, technical procedure and/or technique contained in this document.

Revision Record

Revision Number	Date	Reason for Revision
Rev 1	26 September 2016	Incorporation of client comments

Checklist Regarding Air Dispersion Modelling Regulations: Plan of Study

Plan of Study Criteria	Reference
Facilities and modellers information	
Project identification information • Applicant details • Facility identification • Physical address of facility • Atmospheric Emissions License reference number (if applicable) • Environmental authorization reference number (EIA reference where applicable) • Modelling contractor(s), when applicable	Section 1
Project background • Purpose(s) and objectives of the air dispersion modelling under consideration. • General descriptive narrative of the plant process (es) and • Proposed new source or modification.	Section 1
Project location **Detailed scaled layout plan of proposed project area** • including the following • UTM coordinates on horizontal and vertical axis • Property lines, including fence lines • Roads and railroads within the proposed modelling domain • Location and dimensions of buildings and/or structures (on or off property) which could influence dispersion	Section 1.2

Area map(s)
• Map of adjacent area (10 km radius from proposed source) indicating the following
    ○ UTM coordinates on horizontal and vertical axis
    ○ Nearby known pollution sources
    ○ Schools, hospitals and old age homes within 10km of facility boundary
    ○ Topographic features
    ○ Any proposed or existing off-site or on-site meteorological monitoring stations
    ○ Roads and railroads
• Regional map that includes the following
    ○ Latitude/ Longitude on horizontal and vertical axis
    ○ Modelled facility
    ○ Topography features within 50 km
    ○ Known pollution sources within 50 km
    ○ Any proposed off-site meteorological monitoring stations
	Figure 1-1 and Figure 1-2 in a 5km radius.
	Figure 1-3 and Figure 1-4 in 50km by 50km modelling domain.

Land use determination in modelling domain • Urban • Rural/ Agricultural	Section 2.4.1.1
Elevation data (DEM) and resolution	Section 2.4.1.2
Emission characterisation	
Emission unit characteristics • Include fugitive & secondary emissions when applicable • Emission unit descriptions and capacities (including proposed emission controls) • New structures or modifications to existing structures	Section 2.4.2.2 Full list of sources and parameters will be included in the AIR
Operating scenarios for emission units • Operating condition applicable to the study	Section 2.4.2.2 Full list of sources and

Plan of Study Criteria	Reference
○ Upset conditions ○ Normal ○ Start-up ○ Standby ○ Shutdown	parameters will be included in the AIR
Proposed emissions and source parameter table (s) • List all identifiable emissions • Include parameter table(s) for each operating scenario of each emission unit, which may include, but not be limited to the following: ○ Operating scenario(s) ○ Source location (UTM Coordinates) ○ Point source parameters ○ Area source parameters ○ Volume source parameters ○ Include proposed emissions (and supporting calculations) for all identifiable emissions	Section 2.4.2.2 Full list of sources and parameters will be included in the AIR
Meteorological data	
Surface data discussions must include: • Off-site ○ Source of data ○ Description of station (location, tower height, etc.) ○ Period of record ○ Demonstrate temporal and spatial representativeness ○ Seasonal wind- rose(s) ○ 3-year of representative off-site data ○ Evaluate if off-site data complies with regulatory Code ○ of Practice ○ Program and version used to process data ○ Method used to replace missing hours ○ Method used to handle calm periods • On-site ○ Description of station (location, tower height, etc.) ○ Period of record ○ Demonstrate spatial representativeness ○ Minimum 1-year of representative on-site data ○ Evaluate if off-site data complies with regulatory the • Code of Practice ○ Program and version used to process data ○ Method used to replace missing hours ○ Method used to handle calm periods	Section 2.4.1.3
Discuss proposed upper air data • Discuss proposed upper air data from the most representative station. • Explain why it is "most representative".	Section 2.4.1.3
Ambient impact analysis and ambient levels	
Standards Levels • National Ambient Air Quality Standards	Section 3
Background Concentrations • Specify background values to be used including supporting documentation.	Section 4

Plan of Study Criteria	Reference
Modelling Procedures	
Proposed Model • Assessment level proposed and justification • Dispersion model proposed • Supporting models and input programs • Version of models and input programs	Section 2.4
Proposed emissions to be modelled • Pollutants • Scenarios and emissions that will be modelled • Conversion factor utilized for converting NO_x to NO_2 (if applicable)	Section 2.4.2.2 Section 2.4.2.3
Proposed Settings • Recommended settings to be utilized within model • Terrain settings (simple flat/ simple elevated/ complex) • Land characteristics (Bowen ratio. surface albedo, surface roughness)	Section 2.4
Proposed Grid Receptors • Property line resolution • Fine grid resolution • Medium grid resolution(s) • Course grid resolution • Hot spot resolution and size	Section 2.4.2.1

Table of Contents

List of Tables

List of Figures

PLAN OF STUDY REPORT
In support of
An Air Quality Impact Study for Sasol to Serve as Motivation and Postponement Applications from Minimum Emission Standards

1 PROJECT DESCRIPTION

Sasol's operations at the Sasolburg Facility (Infrachem, including the joint venture partner, Natref) and the Secunda Facility (Synfuels) are required to comply with the Minimum Emission 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. These standards require the refinery operations to comply with more lenient "existing plant" limits by 1 April 2015, and with more stringent "new plant" limits by 1 April 2020.

Technical investigations were conducted by Sasol to establish feasibility and practicality of improving its existing process plants operations in order to comply with the standards as set out in the Minimum Emission Standards. Guided by the technical investigations, Sasol requested postponement to comply with the Minimum Emission Standards in 2014. This was granted in February 2015, however for certain of the activities only a three year postponement was granted. Based on this as well as information associated with current roadmaps, Sasol intends to request an extension of the original postponement granted for the three year period to allow for the implementation of technical solutions. In support of the submissions and to fulfil the requirements for these applications stipulated in the Air Quality Act and the Minimum Emission Standards, air quality studies are required to substantiate the motivations for the extension.

The facility in Secunda, Sasol Synfuels, produces syngas from coal by gasifying the coal at a temperature of 1300°C, using two types of reactors (circulating fluidised bed and Sasol Advanced Synthol™ reactors). The syngas is subsequently converted to produce components for making synthetic fuels as well as a number of downstream chemicals. Gas water and tar oil streams emanating from the gasification process are refined to produce ammonia and various grades of coke respectively.

At the Sasolburg facility, natural gas is reformed in two auto thermal reformers (ATRs) with natural gas and oxygen at high temperature to produce synthetic gas (syngas). Sasol Infrachem produces ammonia from reformed gas and converts some of this ammonia into nitric acid and ammonium nitrate-based explosives and fertilisers for Sasol Nitro. Syngas is used by Sasol Wax to produce linear hydrocarbon waxes and paraffins. Sasol Solvents converts some of the Sasolburg syngas into methanol and butanol.

At the Natref Refinery in Sasolburg, imported crude oil is converted into "white products" such as petrol and diesel.

Whilst the main air pollutants from the Sasolburg and Secunda operations include sulfur dioxide (SO_2) and oxides of nitrogen (NO_x), other pollutants to consider include particulate matter (PM), volatile organic compounds (VOCs) (of primary importance – benzene), ammonia (NH_3), hydrochloric acid (HCl), hydrogen fluoride (HF), dioxins/furans and metals.

1.1 Scope of Work

Airshed Planning Professionals (Pty) Ltd (hereafter referred to as Airshed) was appointed by Sasol to provide independent and competent services for the compilation of an Atmospheric Impact Report as set out in the Regulations and detailing the results of the dispersion model runs. The tasks to be undertaken consist of:

1) Review of emissions inventory for the identified point sources and identification of any gaps in the emissions inventory. Where possible, it is preferable that gaps be estimated using an agreed emission estimation technique. No emission factors may be used without the written consent from Sasol that the emission factors are deemed acceptable. Should measurements be required, Sasol will source the required information. Additional sources could be added when new information becomes available.
2) Prepare meteorological input files for use in one or more dispersion models to cover the required modelling domain. The Employer will provide surface meteorological data and ambient air quality data from the Sasol ambient air quality monitoring stations. Surface meteorological data for three years (2013-2015), as required by the Dispersion Modeling Regulations for Level 3 Assessments, is available for ambient air quality monitoring stations.
3) Preparation of one or more dispersion models set up with the Employer's emissions inventory capable of running various scenarios for each of the point sources as specified by Sasol, in conjunction with Sasol's Research and Development Department. All dispersion models should comply with the requirements of the Dispersion Modelling Regulations.
4) Validate the dispersion model based on an acceptable and agreed approach. The validation methodology must be agreed between Sasol and Airshed.
5) Conduct a baseline assessment.
6) It is anticipated that sources applying for postponement will require 3 modelling scenarios, additional to the baseline modelling scenario, per component per point source to be modelled, in order to establish the impacts of the various limits. i.e:
    a. Compliance scenario – modelling must be conducted based on the legislative requirement as stipulated within the Listed Activities and Minimum Emission Standards (for both 2015 and/or 2020 standards as indicated).
    b. Alternative scenario – the actual Sasol proposed limit values, where applicable and if different from the other emission scenarios.
7) Comparison of dispersion modelling results with the applicable South African ambient air quality standards.
8) The inclusion of discrete receptor points at sensitive receptors in the model, as agreed with Sasol. Such discrete receptors must include, but is not limited to, all residential areas within the modelling domain, especially primary schools and hospitals/clinics. Biographical information at each discreet receptor must be included and classified as per Sasol's requirements.
9) A report detailing the methodology used and model setup must be compiled for purposes of an external peer review, which the Employer will contract independently.
10) Interactions with prospective peer reviewer to provide all necessary inputs into the compilation of a peer review document in support of the Employer's postponement applications and addressing of any matters raised during the peer review process.
11) Interaction with the Sasol representative for purposes of communicating the dispersion modelling: setup; parameterisation and results.

12) Interactions with prospective Environmental Assessment Practitioner (EAP) to provide all necessary inputs into the EAP's compilation of documentation in support of Sasol's postponement applications. Airshed will attend all Public Participation meetings scheduled by the EAP to address any queries pertaining to the dispersion model.

1.2 Study Area

The two study areas include the Sasolburg and Natref operations and the Secunda operations, as shown in Figure 1-1 and Figure 1-2 respectively. The sensitive receptors as well as ambient monitoring stations for Sasolburg and Secunda are provided in Figure 1-3 and Figure 1-4.

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 equilibriums between the photochemical reactions of oxides of nitrogen, carbon monoxide and ozone.

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 EPAs 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 source. 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 1-1.

Table 1-1: 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%
C1	Commercial	Less than 15%
R2	Dense/multi-family	Less than 30%
R3	Multi-family, two storey	Less than 35%

According to this classification scheme, Sasolburg and Secunda are both classified as urban.

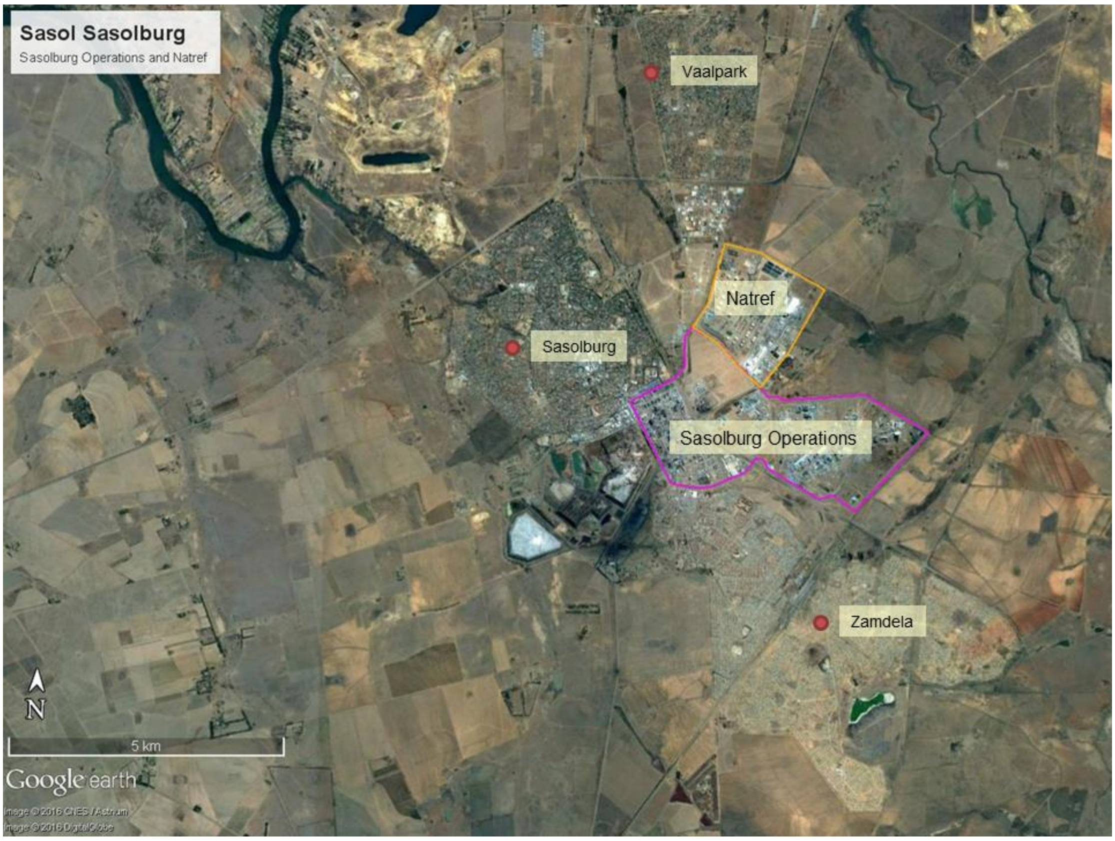

Figure 1-1: Locations of the study area centres at Sasolburg

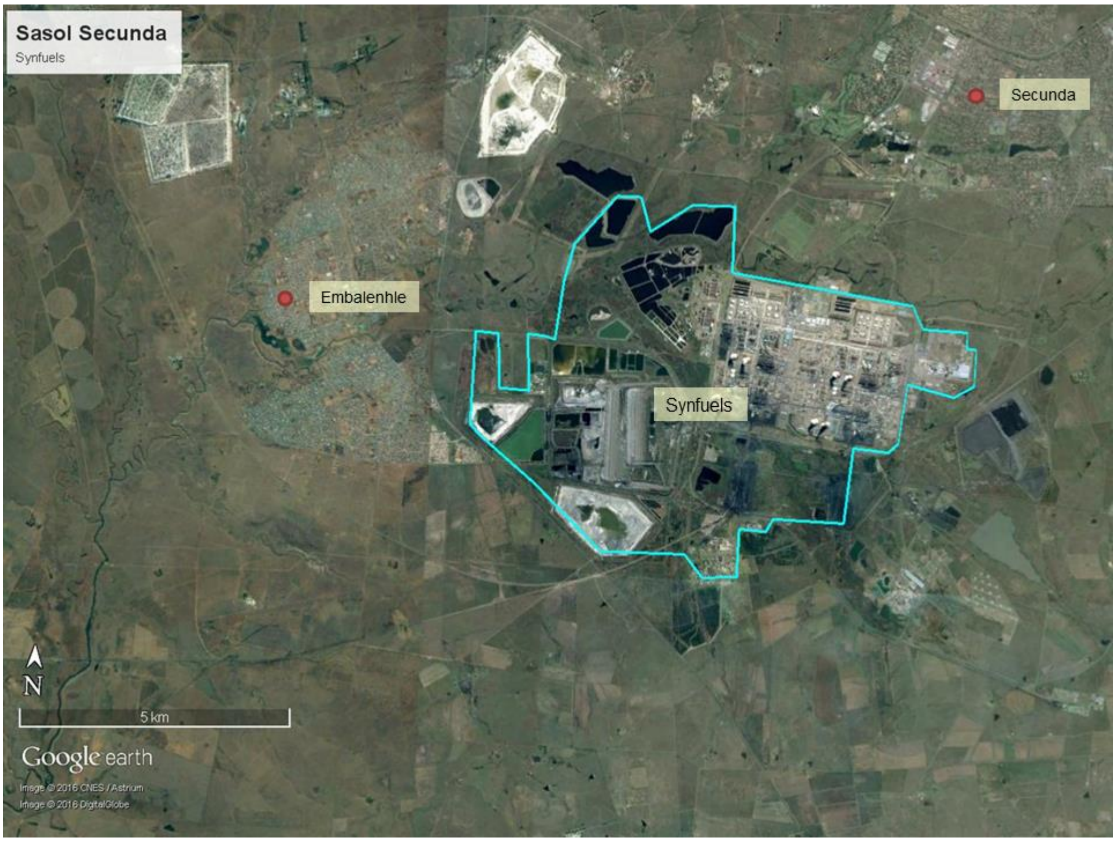

Figure 1-2: Locations of the study area centres at Secunda

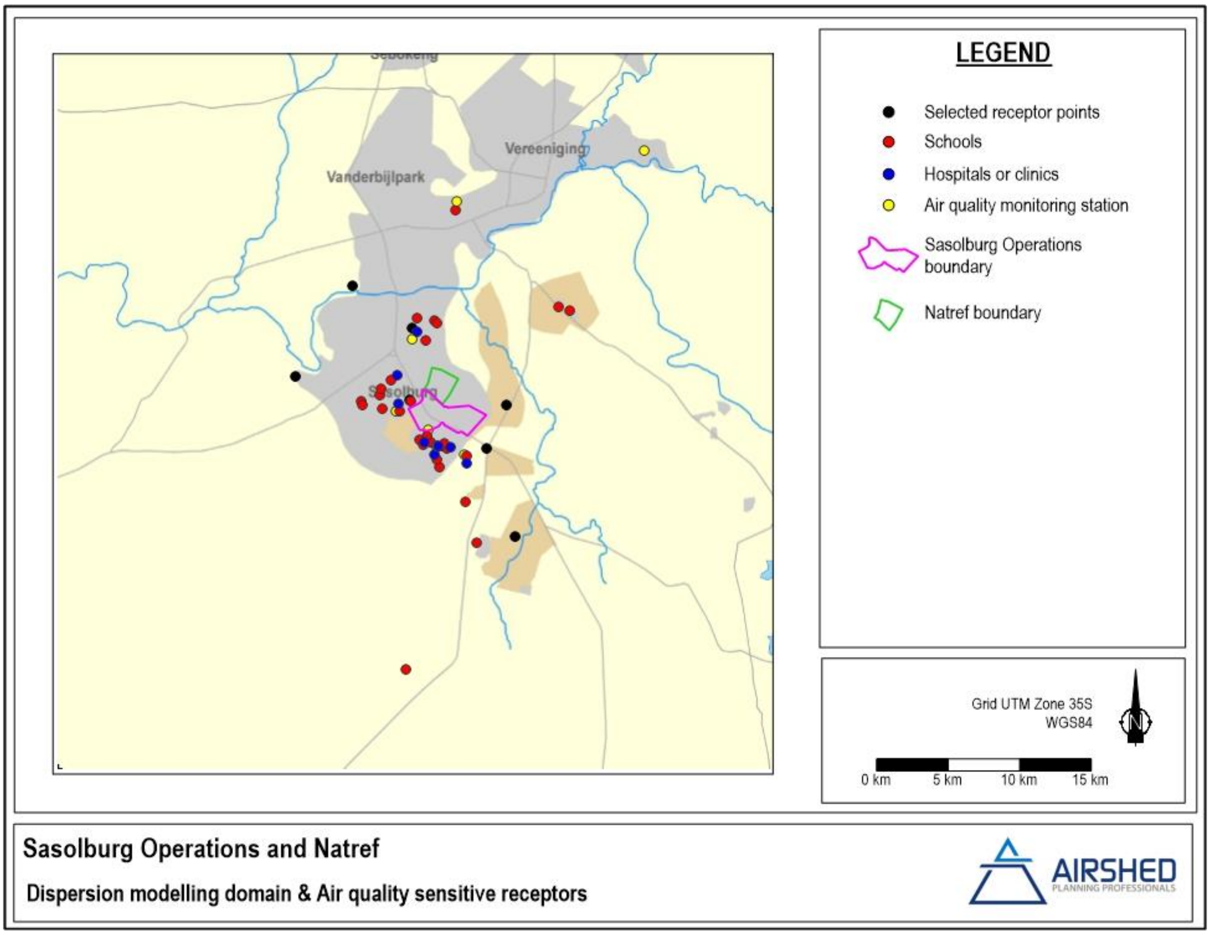

Figure 1-3: Identified sensitive receptors within the Sasolburg study area

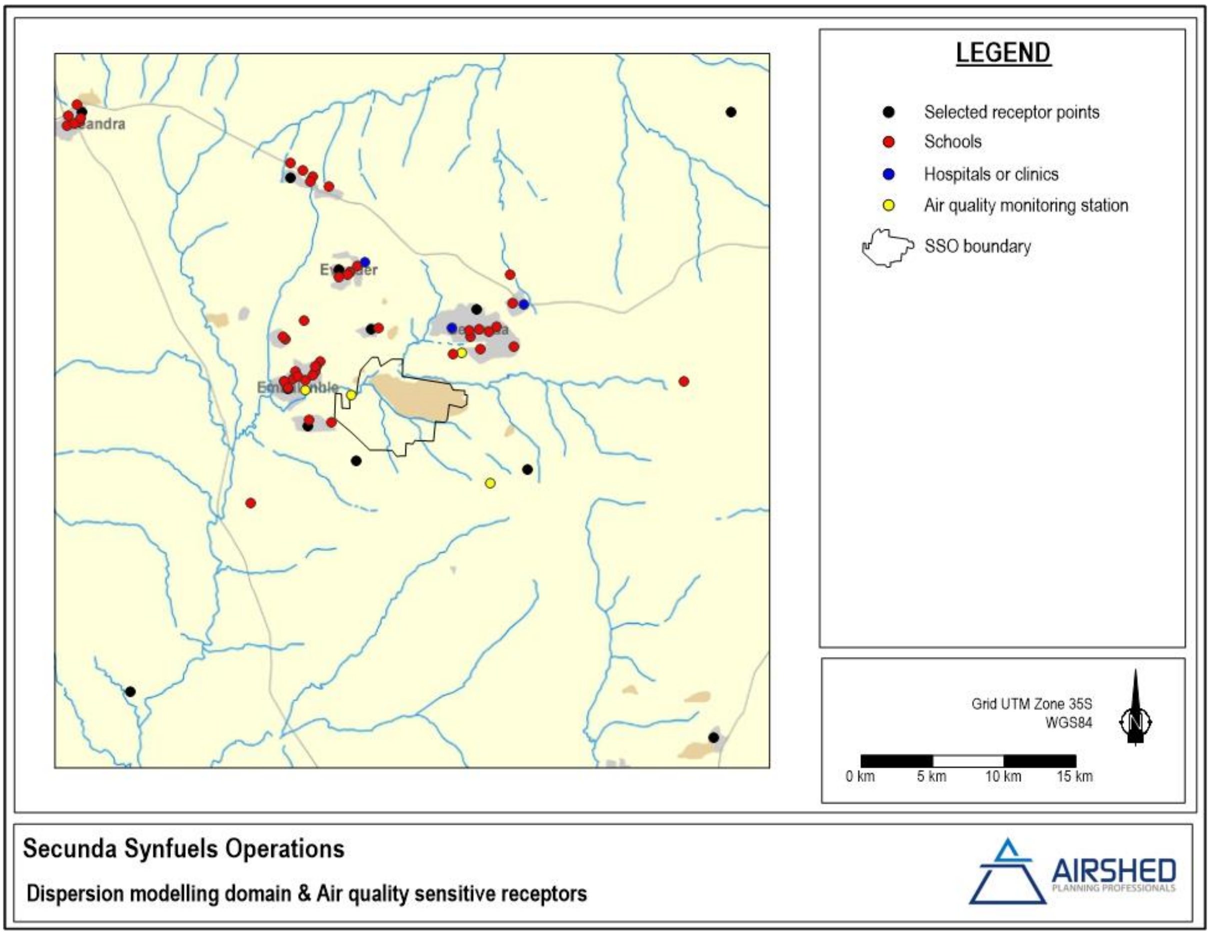

Figure 1-4: Identified sensitive receptors within the Secunda study area

2 MODELLING PROCEDURES

2.1 Competencies for Performing Air Dispersion Modelling

All modelling tasks will be performed by competent personnel. These personnel would include at least one principal to manage and direct the project as well as to verify the modelling results. The latter function requires a thorough knowledge of both the meteorological parameters that influence the atmospheric dispersion processes and the atmospheric chemical transformations that some pollutants may undergo during the dispersion process. The principal investigator will have a minimum of 10 years' experience in atmospheric dispersion modelling and its application to real-life simulations.

The project team will also include senior and junior staff, each with respectively lower technical responsibilities. Senior staff has at least three years applicable experience.

Table 2-1 is a summary of competency requirements. Apart from the necessary technical skills required for the calculations, personnel competency also include the correct attitude, behaviour, motive and other personal characteristic that are essential to perform the assigned job on time and with the required diligence as deemed necessary for the successful completion of the project.

Table 2-1: Competencies for Performing Air Dispersion Modelling

Competency	Task, Knowledge and Experience
Context	Communication with field workers, technicians, laboratories, engineers and scientists and project managers during the process is important to the success of the model
	Familiar with terminology, principles and interactions
	Record keeping is important to support the accountability of the model - Understanding of data collection methods and technologies

Knowledge	Meteorology:
	• Obtain, review and interpret meteorological data
	• Understanding of meteorological impacts on pollutants
	• Ability to identify and describe soil, water, drainage and terrain conditions
	  ○ Understanding of their interaction
	  ○ Familiarity with surface roughness`
	• Ability to identify good and bad data points/sets
	• Understanding of how to deal with incomplete/missing meteorological data

	Atmospheric Dispersion models • Select appropriate dispersion model • Prepare and execute dispersion model • Understanding of model input parameters • Interpret results of model
	Chemical and physical interactions of atmospheric pollutants • Familiarity with fate and transport of pollutants in air • Interaction of primary pollutants with other substances (natural or industrial) to form secondary pollutants
	Information relevant to the model • Identify potential pollution (emission) sources and rates • Gather physical information on sources such as location, stack height and diameter • Gather operating information on sources such as mass flow rates, stack top temperature, velocity or volumetric flow rate • Calculate emission rates based on collected information • Identify land use (urban/rural) • Identify land cover/terrain characteristics • Identify the receptor grid/site
	Legislation, regulations and guidelines in regards to National Environment Management: Air Quality Act (Act No 39 of 2004), including • Minimum Emissions Standards (Section 21 of Act) • National Ambient Air Quality Standards • Air Dispersion Modelling Guideline • Atmospheric Impact Report (AIR)
Abilities	Ability to read and understand map information
	Ability to prepare reports and documents as necessary
	Ability to review reports to ensure accuracy, clarity and completeness
	Communication skills
	Team skills

2.2 Regulations Regarding Air Dispersion Modelling

The recommended regulatory models for South Africa (as provided in the Regulations Regarding Air Dispersion Modelling– Gazette No 37804; published 11 July 2014) are provided in Appendix A.

2.3 Proposed Model

Due to the sensitive nature of the study, the more complex US EPAs CALPUFF model is considered to be an appropriate model for the purpose of this assessment as it well suited to simulate dispersion from a complex array of point sources at the Sasol Sasolburg and Secunda facility.

Since the dispersion model formulation in CALPUFF is based on a Lagrangian Gaussian Puff model, it is well suited for modelling terrain when used in conjunction with CALMET. The latter code includes a diagnostic wind field model which contains treatment of slope flows, valley flows, terrain blocking effects and kinematic effects.

The puff formulation 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 grossly over-estimates the plume travel distance.

2.4 Modelling Information

2.4.1 CALMET Model

2.4.1.1 Land Use

Lambert Azimuthal land use/land cover data is used in the CALMET model.

2.4.1.2 Elevation Data

Elevation data used in the CALMET model is obtained from the Shuttle Radar Topography Mission (SRTM) dataset at horizontal resolution of three arc-seconds (90 m).

2.4.1.3 Meteorology

The Weather Research and Forecasting (WRF) Model and surface field observations from monitoring stations operated by Sasol (i.e. Leitrum, Eco Park, AJ Jacobs and Sasol 1 Fence Line in Sasolburg and Secunda Club, Bosjesspruit, and Embalenhle in Secunda) for the meteorological period 2013, 2014 and 2015. 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 kilometers.

The WRF data was obtained from Lakes Environmental (Canada), and was prepared for a modelling domain of 200 km (East-West) by 200 km (North-South). The meteorological information was supplied on a horizontal grid spacing of 4 km.

Table 2-2: Ambient monitoring stations operated by Sasol

Station Name	Latitude	Longitude
Bosjesspruit	-26.605833	29.210833
Secunda Club	-26.523333	29.189667
Grootvlei	-26.801000	28.495833
Embalenhle	-26.551667	29.112500
Rosebank	-26.148667	28.038167
Springs Girls High School	-26.300333	28.441333
Eco Park	-26.777619	27.837317
Sasol One Fence Line	-26.834722	27.848611
Leitrim	-26.850278	27.874167

Station Name	Latitude	Longitude
AJ Jacobs	-26.818056	27.848611

2.4.1.4 Grid Resolution and Model Domain Size

The CALMET model domain selected for the Sasol Secunda Complex included an area of 200 km by 200 km. The horizontal grid resolution is 1 km with 11 vertical levels, viz. 20m, 40m, 80m, 120m, 200m, 300m, 600m, 1000m, 1500m, 2500m and 3500m.

2.4.1.5 Model Control Options

A summary of the model control options for CALMET is provided in Table 2-3. The option of Partial Observations was selected, which used both WRF data as well as Sasol's surface meteorological station data.

2.4.2 CALPUFF Model

2.4.2.1 Grid Resolution and Model Domain Size

The model domain selected for the point sources at the Sasol Sasolburg complex included an area of 50 km by 50 km. This area was selected based on the assessment undertaken for the Vaal Triangle Air-shed Priority Area and the predicted area of impact around Sasolburg. The horizontal grid resolution is 200 m.

The model domain selected for the point sources at the Sasol Secunda Complex included an area of 50 km by 50 km. The horizontal grid resolution is 200 m.

Table 2-3: CALMET model control options

Run Type	Description of Run Type	Ease of Use and Representativeness	Data availability	Advantages	Disadvantages
No Observations	•Prognostic model data, such as WRF to drive CALMET. •No surface or upper air observations input at all.	•Relatively simple to implement in model •Representative of regional meteorological conditions	WRF data (Lakes Environmental) for 2013, 2014 and 2015 at 4km resolution for 200km by 200km study area (Secunda + Sasolburg)	•Simple to implement •Full spatial and temporal variability •No overwater data required •Cloud cover has spatial distribution •Eliminates need for complicated 7 user-input site-specific variables •Ideal as screening run as gives very good estimate	Resolution of prognostic data may potentially be too coarse to be representative of local conditions
Partial Observations	•Prognostic model data, such as MM5 to drive CALMET PLUS •One or more surface stations	•More difficult to implement than only prognostic (MM5) data. •Require 7 site-specific model parameters to be specified. •Difficulty in dealing with missing data. •Potential disagreement between prognostic and surface observations. •Very representative and considered 'refined modelling'	• WRF data (Lakes Environmental) for 2013, 2014 and 2015 at 4km resolution for 200km by 200km study area (Secunda + Sasolburg) •Sasol operated surface meteorological weather stations (4 Sasolburg[1] and 3 Secunda[2])	•Full spatial and temporal variability •No overwater data required •Refined model run as using combined approach of numerical model and observations. •Ability to incorporate surface representative observation data when WRF data is too coarse to fully pick up local effects.	•Surface data, especially winds may be different to that in the WRF data file •User must include 7 site-specific variables •Data preparation and missing data
Observations Only	CALMET driven solely by surface, upper air and optional overwater and precipitation stations	•Require 7 site-specific model parameters to be specified. Difficulty in dealing with missing data. •Considered representative if sufficient observation stations and site specific choice of parameters by the modeller.	•Sasol operated surface meteorological weather stations (4 Sasolburg and 3 Secunda) •Closest upper air monitoring station is at OR Tambo International Airport (twice-daily soundings only)	Very good if upper air and surface stations are located close to the facility and if upper air data are recorded at sunrise and sunset.	•Upper air data typically 12 hourly, poor spatial and temporal resolution •Model has to interpolate between 12 hour soundings •Soundings at incorrect time of the day. •User has to deal with missing surface and upper air data

[1] Sasol 1 Fence Line (WS, WD, TEMP, RH,AMB PRESS, SOL RAD, RAIN); AJ Jacobs (WS, WD,SO_2, NO_2, PM_{10}, $PM_{2.5}$); Leitrum (WS, WD, TEMP, AMB PRESS, SO_2, O_3, NO_2, PM_{10}, $PM_{2.5}$) and Eco Park (WS, WD, TEMP, RH,AMB PRESS, SOL RAD, RAIN, SO_2, O_3, NO_2, PM_{10}, $PM_{2.5}$)

[2] Sasol Club (WS, WD, TEMP, NO_2, SO_2, H_2S, O_3, PM_{10}, $PM_{2.5}$, CO, VOC); Bosjesspruit (WS, WD, TEMP, NO_2, SO_2, H_2S) and Embalenhle (WS, WD, TEMP, NO_2, SO_2, H_2S, O_3, PM_{10}, $PM_{2.5}$, CO)

2.4.2.2 Source Information

All source information for the Sasol Sasolburg complex and Sasol Secunda complex is to be provided by Sasol.
The three main scenarios to be assessed are as follows:

- Baseline – modelling based on the current emissions inventory;
- Future – modelling based on the legislative requirement as stipulated within the Listed Activities and Minimum Emission Standards (for both 2015 and 2020 standards).
- Actual – modelling based on actual Sasol proposed reductions, where applicable and different from the other 3 emission scenarios.

2.4.2.3 Model Control Options

A summary of the model control options for CALPUFF is provided in Table 2-4.

Since the Sasolburg and Secunda study areas are classified as urban (Section 1.2), the MESOPUFF II chemical transformation scheme is selected. The disadvantage of the scheme, however, is that NO_2 formation has to be determined using an external method. The South African NAAQS stipulates the regulation of NO_2; however, emissions of nitrogen oxides (NO_x) must be modelled in order to estimate total NO_2 concentrations. The concentration of NO in the Sasol stack exhausts are typically >98%, but reacts fairly rapidly with background ozone in the plume to form NO_2. This reaction occurs at night.

Since the MESOPUFF II scheme does not distinguish or simulate the conversion from NO to NO_2, the predicted NO_x concentration must be equated into NO_2 using a conversion factor. Estimation of this conversion normally follows a tiered approach, as discussed in the DEA Modelling Guideline, 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 NO_2 concentrations by assuming a total conversion of NO to NO_2. If the maximum NO_x concentrations are less than the NAAQS for NO_2, then no further refinement of the conversion factor is required. If the maximum NO_x concentrations are greater than the NAAQS for NO_2, or if a more "realistic" estimate of NO_2 is desired, proceed to the second tier level.
>
> Tier 2: Ambient Ratio Method (ARM) - Multiply NO_x by a national ratio of NO_2/NO. = 0.80
>
> Assume a wide area quasi-equilibrium state and multiply the Tier 1 empirical estimate NO_x by a ratio of NO_2/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 NO_2 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/NO_2 ratio is not expected, then the NO/NO_2 ratio based on the monitoring data can be applied to derive NO_2 as an alternative to the national ratio of 0.80.

The second version of the Tier 2 approach will be used to estimate the NO_2 formation. As a starting basis, the NO_2/NO_x conversion factors described by Scire and Borissova (2011) as given in Table 2-5, will be employed. Observed NO_2/NO_x ratios at the Sasolburg and Secunda monitoring stations will also be analysed and compared to the factors in the table.

Table 2-4: CALPUFF model control options

Run Type	Description of Run Type	Ease of Use and Representativeness	Data availability	Advantages	Disadvantages
Sampling Function Puff	This sampling scheme employs radically symmetric Gaussian puffs and is suitable for far field.				
Sampling Function Slug	This sampling scheme uses a non-circular puff (a "slug), elongated in the direction of the wind during release, to eliminate the need for frequent releases of puffs. Used for near field during rapidly-varying meteorological conditions.				Takes a very long time to run.
Dispersion coefficients MDISP = 1	• Dispersion coefficients are computed from measured values of turbulence, sigma-v and sigma-w.	• The user must provide an external PROFILE.DAT file containing these parameters, and select a backup method out of options 2, 3 and 4 below in case of missing data.	• This measured data is not available in South Africa	• Very good if data is available.	• These measured parameters are not readily available in South Africa.
Dispersion coefficients MDISP = 2	• Dispersion coefficients are computed from internally-calculated sigma-v, sigma-w using micrometeorological variables (u*, w*, L, etc.).	• This option can simulate AERMOD-type dispersion when the user also selects the use of PDF method for dispersion in the convective boundary layer (MPDF = 1). Note that when simulating AERMOD-type dispersion, the input meteorological data must be from CALMET and cannot be ISC-type ASCII format data. The user should also be aware that under this option the CALPUFF model will be more sensitive to the appropriateness of the	• The data is obtained from MM5 input information.	• Based on improved theoretical work and is an improvement over Pasquill-Gifford.	• The coefficients are derived from other parameters.

Run Type	Description of Run Type	Ease of Use and Representativeness	Data availability	Advantages	Disadvantages
		land use characterization.			
Dispersion coefficients MDISP = 3	• Pasquill-Gifford (PG) dispersion coefficients for rural areas (computed using the ISCST3 multi-segment approximation) and McElroy-Pooler (MP) coefficients in urban areas.	• The current default selection is MDISP = 3, which is ISC-type dispersion. Given the demonstrated improved characterization of dispersion provided by AERMOD, and EPA's intention to replace ISC with AERMOD, use of AERMOD-like dispersion (MDISP = 2, and MPDF = 1) is also acceptable, but likely will be of most benefit for short-range complex flow applications.		• Simple to use if you don't have detailed meteorological information. This option can be run using fairly basic meteorological data.	• Based on discreet classification scheme (not continuous function). Based on field experiments done elsewhere, may or may not be representative of Highveld area. Previous projects done using this scheme however have provided good correlation over this area.
Dispersion coefficients MDISP = 4	• Same as MDISP = 3, except PG coefficients are computed using the MESOPUFF II equations				
Dispersion coefficients MDISP = 5	• CTDM sigmas are used for stable and neutral conditions. For unstable conditions, sigmas are computed as in MDISP=3 described above.	• When selecting this option, the user must provide an external PROFILE.DAT file, and select a backup method out of options 2, 3 and 4 above in case of missing data.			
Chemical transformation RIVAD	• Pseudo-first-order chemical mechanism for SO_2, SO_4^{2-}, NO, NO_2, HNO_3, and NO_3^- (RIVAD/ARM3 method)	• RIVAD is a 6-species scheme wherein NO and NO_2 are treated separately. • In the RIVAD scheme the conversion of SO_2 to sulfates is not RH-dependent. • The conversion of NO_x to nitrates is	• In order to use the RIVAD scheme, the user must divide the NO_x emissions into NO and NO_2 for each source. • Two options are specified for the ozone concentrations: (1) hourly ozone concentrations	• In several tests conducted to date, the results have shown no significant differences between the RIVAD and MESOPUFF II options.	• User has to input the NO and NO_2 emissions which are not always known for all sources. • User has to input the ozone concentrations which are not always known.

Run Type	Description of Run Type	Ease of Use and Representativeness	Data availability	Advantages	Disadvantages
		RH-dependent.	from a network of stations, or (2) a single user defined ozone value. • The background ammonia concentrations required for the HNO_3 /NH_4NO_3 equilibrium calculation can be user-specified or a default value will be used.		• The model is restricted to rural conditions.
Chemical transformation MESOPUFF II	• Pseudo-first-order chemical mechanism for SO_2, SO_4^{2-}, NO_x, HNO_3, and NO_3 - (MESOPUFF II method)	• MESOPUFF II is a 5-species scheme in which all emissions of nitrogen oxides are simply input as NO_x. • In the MESOPUFF II scheme, the conversion of SO_2 to sulfates is dependent on relative humidity (RH), with an enhanced conversion rate at high RH. • The conversion of NO_x to nitrates is RH-dependent.	• The MESOPUFF II scheme assumes an immediate conversion of all NO to NO_2. • Two options are specified for the ozone concentrations: (1) hourly ozone concentrations from a network of stations, or (2) a single user defined ozone value. • The background ammonia concentrations required for the HNO_3 /NH_4NO_3 equilibrium calculation can be user-specified or a default value will be used.	• In several tests conducted to date, the results have shown no significant differences between the RIVAD and MESOPUFF II options for sulphate and nitrate formation. • The model is applicable to both urban and rural conditions.	• User has to input the ozone concentrations which are not always known. • NO to NO2 conversion.is not included. In model.
User-specified diurnal cycles of transformation rates					
No chemical conversion					

Table 2-5: Recommended NO_2/NO_x conversion ratios for short and long-term NO_x concentration predictions (Scire and Borissova 2011)

Bin	Concentration (µg/m³)			NO_2/NO_x Ratios		
	Min	Max	Centre	Bin Average	1-Hour Max (1)	Annual Average
1	0	19	9	0.798	0.9938	0.798
2	19	38	28	0.813	0.9922	0.813
3	38	75	56	0.7306	0.9844	0.7306
4	75	113	94	0.5544	0.9094	0.625
5	113	150	132	0.437	0.7477	0.54
6	150	188	169	0.3553	0.6085	0.47
7	188	235	212	0.3013	0.4976	0.4
8	235	282	259	0.2559	0.4173	0.35
9	282	329	306	0.2276	0.3543	0.31
10	329	376	353	0.2081	0.3056	0.28
11	376	423	400	0.1852	0.2684	0.25
12	423	470	447	0.1809	0.2404	0.23
13	470	517	494	0.1767	0.2194	0.2194
14	517	564	541	0.1546	0.2035	0.2035
15	564	611	588	0.1524	0.1912	0.1912
16	611	658	635	0.1476	0.1813	0.1813
17	658	705	682	0.1402	0.1726	0.1726
18	705	752	729	0.1363	0.1645	0.1645
19	752	846	799	0.1422	0.1527	0.1527
20	846	940	893	0.1223	0.1506	0.1506
21	940	1128	1034	0.1087	0.1474	0.1474
22	1128	1316	1222	0.111	0.1432	0.1432
23	1316	1504	1410	0.1112	0.139	0.139
24	1504	1786	1645	0.1165	0.1337	0.1337

Note (1) as a conservative approach, ratios below 0.4 may be limited to 0.4 as a minimum.

3 LEGAL CRITERIA

Modelled concentrations will be assessed against National Ambient Air Quality Standards (Table 3-1).

Table 3-1: National Ambient Air Quality Standards

Pollutant	Averaging Period	Concentration (µg/m³)	Frequency of Exceedance	Compliance Date
Benzene (C_6H_6)	1 year	10	0	Immediate till 31 December 2014
	1 year	5	0	1 January 2015
Carbon Monoxide (CO)	1 hour	30000	88	Immediate
	8 hour(a)	10000	11	Immediate

Pollutant	Averaging Period	Concentration (µg/m³)	Frequency of Exceedance	Compliance Date
Nitrogen Dioxide (NO_2)	1 hour	200	88	Immediate
	1 year	40	0	Immediate
Ozone (O_3)	8 hour(b)	120	11	Immediate
$PM_{2.5}$	24 hour	65	4	Immediate till 31 December 2015
	24 hour	40	4	1 January 2016 till 31 December 2029
	24 hour	25	4	1 January 2030
	1 year	25	0	Immediate till 31 December 2015
	1 year	20	0	1 January 2016 till 31 December 2029
	1 year	15	0	1 January 2030
PM_{10}	24 hour	120	4	Immediate till 31 December 2014
	24 hour	75	4	1 January 2015
	1 year	50	0	Immediate till 31 December 2014
	1 year	40	0	1 January 2015
Sulphur 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.

4 Ambient Background Levels

Ambient concentrations of NO_2, SO_2, PM_{10}, $PM_{2.5}$, H_2S and VOC measured at the Sasol operations will provide an understanding of existing ambient concentrations.

Background concentrations are an essential part of the total air quality concentration to be assessed in determining air emission source impacts. In terms of the dispersion modelling exercise, the background concentration constitutes the portion of the air quality due to air emission sources that are not included in the model's emissions inventory. Background air quality includes pollutant concentrations due to the following:

- natural sources (including biomass burning);
- nearby sources that are unidentified in the inventory; and
- long-range transport into the modelling domain.

Typically, monitored air quality data are used to establish background concentrations.

The possibility of under-estimating or over-estimating the air emissions from the modelled sources also exist. This may occur, for example, during upset emissions or shutdowns.

Furthermore, to improve the prediction of air quality concentrations, emissions from activities occurring within the communities themselves must also be considered. 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.

To estimate the background concentrations not associated with the emission included in the simulations, the methodology below will be adopted.

- For **short-term** (1-hour and 24-hour) predicted averaging periods, the 99th percentile value from the cumulative frequency distribution of the monitoring data will be used.
- For the **annual** predicted averaging period (long-term), the observed concentration is used at the percentile where the modelled concentration becomes zero, but not less than the 50th percentile of the cumulative frequency distribution of the monitoring data will be used.

5 Management of Uncertainty

5.1 Simulation Uncertainty

As with any form of mathematical simulations, there are uncertainties associated with a model's capability to predict concentrations accurately. An accepted dispersion model (i.e., CALPUFF) was selected for the analysis to minimize some of these uncertainties.

It is widely understood and accepted that uncertainties, whether reducible (random) or irreducible (systematic), arise because of the inherent randomness in physical systems, modelling idealizations, experimental variability, measurement inaccuracy, etc., and cannot be ignored. This fact complicates the already difficult process of model validation by creating an unsure target—a situation in which neither the simulated nor the observed behaviour of the system is known with certainty. The following sections describe the methods that will be adopted in the study. These methods were selected to produce more conservative results, whilst still maintaining a realistic approach.

5.1.1 Validation of Predictions

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

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

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

A rigorous V&V programme will not be completed as part of the study; however, regular sanity checks on model results and comparisons with observations would be done. An attempt would also be made to quantify the level of agreement between observed data and model prediction, as well as the predictive accuracy of the model once the necessary adjustments have been made (such as including the estimated background concentrations).

A performance evaluation of CALPUFF will be conducted by comparing the modelling results of emission sources in the region for the years 2013, 2014 and 2015 to the Sasol monitoring data collected over the same time period. In particular, the predicted SO_2 and NO_2 concentrations in Sasolburg and SO_2, NO_2 and H_2S in Secunda will be compared to available monitoring data.

The performance evaluation will be 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, both short- and long-term fractional bias will be computed. With the short-term fractional bias the maximum 88 predicted concentrations (i.e. the 99^{th} percentile) will be compared to the same ranked monitored concentrations. The long-term fractional bias will be based on the annual mean predicted and observed concentrations and standard deviations.

The fractional bias values will be plotted on a graph with the means (FBmeans) on the X-axis and the standard deviations (FBstdev) on the Y-axis. A box will be placed on the plot enclosing the area of the graph where the model predictions are within a factor of two (corresponding to a fractional bias of between -0.67 and +0.67). 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.

5.1.2 Scenario Simulations

Since the focus of the study will be to illustrate the relative changes with the introduction of different emission conditions (i.e. emission rates, exit gas temperatures and velocities), whilst maintaining the same stack heights and diameters, it is expected that the model errors would mostly be carried amongst the different modelling scenarios.

The predicted concentration differences from scenario to scenario will be provided as percentage increase or decrease. However, these percentages need to also include concentrations attributable to other sources not accommodated in the model (CBackground). The change in concentration from any of the future scenarios (CFuture Scenario) compared to the baseline scenario (CBaseline Scenario) will therefore be provided as follows:

$$\frac{C_{Future\ Scenario} - C_{Baseline\ Scenario}}{C_{Baseline\ Scenario} + C_{Background}}$$

The background concentration in this expression will be the long-term value rather than the short-term value. If the short-term background concentration were to be used instead (i.e. a higher value), the comparison would be less optimistic since the denominator would be larger and the fraction therefore smaller. This offers a more conservative approach.

5.1.3 NO_2 Conversion Rates

The conversion of NO_2 from NO was discussed in Section 2.3.2.2. The modelled NO_x concentrations would be converted to NO_2 by using the NO_2/NO_x conversion factors described by Scire and Borissova (2011) (Table 2-5) as default. In addition, NO_2/NO_x ratios observed at the monitoring stations in Sasolburg and Secunda would also be analysed and compared to the factors in the table. As a conservative measure, the higher of the observed and Scire & Borrisova ratios will be used in the calculation. Furthermore, due to the added uncertainty in the transformation of NO to NO_2, the NO_2/NO_x factor will not be less than 0.4.

5.2 Emission Inventory Uncertainty

In addition to the dispersion model the uncertainty associated with the emissions inventory needs to be accommodated in the results. The emissions data for the Sasol and Natref activities will be therefore also be required to include an estimate of the uncertainty. Whilst this may take on a number of forms, the minimum requirement would be that the upper and lower values (range) or percentage variation be included in the emissions inventory.

No attempt will be made to estimate the emissions from non-industrial activities within regional communities. Instead, the community contribution of a particular compound would be discussed qualitatively, where necessary to explain differences in predicted and observational concentrations.

6 References

Scire, J. and Borissova M (2011). *An Empirical Method for Modeling Short-Term and Annual NO2 Concentrations in Regulatory Models*, TRC Energy & Environment Conference (EUEC), Phoenix, Arizona.

U.S. EPA (1992). *Protocol for Determining the Best Performing Model.* U.S. Environmental Protection Agency. Research Triangle Park, 2 NC. EPA-454/R-92-025.

7 APPENDIX A – DRAFT REGULATIONS REGARDING AIR DISPERSION MODELLING

7.1 SCREEN3

SCREEN3 is the recommended tool to calculate screening-level impact estimates for stationary sources in simple terrain, i.e., Level 1 assessments. Simple terrain is defined as that in which terrain elevations are lower in elevation than the top of the stack height of the source being evaluated in the modelling analysis. SCREEN3 is a Gaussian plume model which provides maximum ground-level concentrations for point, area, flare, and volume sources (US EPA 1992). The model is a single source model and impacts from multiple SCREEN3 model runs can be summed to conservatively estimate the impact from several sources. SCREEN3 calculates 1-hour concentration estimates in simple terrain areas and 24-hour concentration estimates in complex terrain. These modelled estimates should be converted to the averaging period of each applicable national ambient air quality standards.

SCREEN3 incorporates source related factors and meteorological factors to estimate pollutant concentration from continuous sources. The model assumed that the pollutant does not undergo any chemical reactions, and that no other removal processes (wet or dry deposition) act on the plume during its transportation. SCREEN3 examines a range of stability classes and wind speeds to identify the combination of wind speed and stability that results in the maximum ground level concentrations - the "worst case" meteorological conditions. Except for those sources employing the Schulman-Scire downwash algorithm, stack tip downwash is estimated following Briggs equations. Building downwash effects are estimated for the cavity recirculation and wake (near and far) regions. Sources subject to aerodynamic turbulence induced by nearby buildings and structures should use the building downwash options. Dispersion coefficients are estimated from the Pasquill-Gifford (rural) and McElroy-Pooler (urban) methods based on the Industrial Source Complex (ISC3) formulations. The dispersion coefficients are adjusted to account for the effects of buoyancy induced dispersion. The model can also estimate maximum concentrations from inversion breakup and shoreline fumigations (US EPA 1992).

SCREEN3 is recommended for use on:

- Single point, area, volume sources.
- Single building effects on point source.
- Building wake cavity concentrations.
- Flare releases.
- Transport distances of less than 50 km in simple terrain.

7.2 AERSCREEN

AERSCREEN is a screening-level air quality model based on AERMOD (US EPA 2004) used for Level 1 assessments. The model consists of two main components: 1) the MAKEMET program which generates a site-specific matrix of meteorological conditions for input to the AERMOD model; and 2) the AERSCREEN command-prompt interface program. AERSCREEN interfaces with MAKEMET for generating the meteorological matrix, but also interfaces with AERMAP and BPIPPRM to automate the processing of terrain and building information respectively, and interfaces with the AERMOD model utilising the SCREEN option to perform the modelling runs. AERSCREEN interfaces with version 09292 and later versions of AERMOD and will not work with earlier versions of AERMOD. The AERSCREEN program also includes averaging time factors for worst-case 3-hr, 8-hr, 24-hr and annual averages. AERSCREEN is intended to produce concentration estimates that are equal to or greater to estimates produced by AERMOD with a fully developed set of meteorological and terrain data, but the degree of conservatism will vary depending on the application. Details on AERSCREEN can be found elsewhere (US EPA 2011).

AERSCREEN is recommended for use on:

- Single point, area, volume sources.
- Single building effects on point source.
- Building wake cavity concentrations.
- Flare releases.
- Transport distances of less than 50 km in simple terrain.

A number of regulatory guidelines in other countries are opting to use AERSCREEN instead of SCREEN3. However, for South Africa, AERSCREEN is still marginally used, while SCREEN3 is the most commonly used model in the country. As such, this guideline is recommending both screening models to accommodate all users.

7.3 AERMOD

AERMOD (AERMOD Version 11353 or later version) is the recommended model for more sophisticated near-source applications in all terrain types (where near-source is defined as less than 50km from source). The model can mostly be applied to Level 2 assessments.

AERMOD is a steady-state plume dispersion model for simulating transport and dispersion from point, area, or volume sources based on an up-to-date characterization of the atmospheric boundary layer. The model can be applied to rural and urban areas, flat and complex terrain, surface and elevated releases, and multiple sources, including, point, area and volume sources. In the stable boundary layer (SBL), AERMOD assumes the concentration distribution to be Gaussian in both the vertical and horizontal. In the convective boundary layer (CBL), the horizontal distribution is also assumed to be Gaussian, but the vertical distribution is described by a bi-Gaussian probability density function (pdf) of the vertical velocity. The transport and dispersion of a plume in the CBL is characterised as the superposition of three modelled plumes; the direct plume (from the stack), the indirect plume, and the penetrated plume. The indirect plume accounts for the lofting of a buoyant plume near the top of the boundary layer, and the penetrated plume accounts for the portion of a plume that, due to its buoyancy, penetrates above. AERMOD is applicable to primary pollutants and continuous releases of toxic and hazardous waste pollutants. Chemical transformation of pollutants is treated by simple exponential decay.

This Guideline recommends meteorological fields generated by the meteorological pre-processor AERMET as the preferred mode of running AERMOD. AERMET uses standard meteorological measurements and surface parameters representative of the modelling domain to compute boundary layer parameters used to estimate profiles of wind, turbulence and temperature used by AERMOD.

AERMOD incorporates Plume Rise Model Enhancements (PRIME) building downwash algorithms which provide a more realistic handling of building downwash effects. PRIME algorithms were designed to address two fundamental features associated with building downwash; enhanced plume dispersion coefficients due to the turbulent wake; and to reduce plume rise caused by a combination of the descending streamlines in the lee of the building and the increased entrainment in the wake.

AERMOD is suitable for a wide range of near field applications in both simple and complex terrain. The evaluation results for AERMOD, particularly for complex terrain applications, suggest that the model represents significant improvements compared to previously recommended models, and has even outperformed the more complex CTDMPLUS model on several databases (US EPA 2005).

AERMOD has been designed to handle light wind conditions (wind speeds less than 1m/s) well, and also incorporates an approach for treatment of horizontal meander that can be significant under such conditions. The model can also accept multiple levels of site-specific wind measurements and will determine the transport direction for each source based on the wind direction from the vertical profile appropriate for the individual plume.

AERMOD is recommended for use on:

- Sources in an industrial complex (single or multiple point, area, line, volume sources) with no buildings or single or multiple buildings with building downwash.
- Gas and particle depositions.
- Constant or time-varying emissions.
- Rural or urban areas.
- Transport distances over which steady-state assumptions are appropriate, less than 50 km (depends on terrain).
- Concentration estimates for all terrain locations, except in lee areas.

7.4 CALPUFF

CALPUFF Version 6.42 is the recommended model for dispersion applications requiring detailed description of physical and chemical atmospheric processes, typically associated with Level 3 assessments for distances greater than 50 km. The continuing evolution of this model will necessitate updates to these guidelines. CALPUFF is a multi-layer, multi-species non-steady-state puff dispersion modelling system that simulates the effects of time- and space-varying meteorological conditions on pollutant transport, transformation, and removal. The model can simulate emissions at downward distances ranging from tens of metres up to 300 km for multiple point, volume, area and/or line sources with constant or variable emission rates. CALPUFF includes algorithms for near-field effects such as stack tip downwash, building downwash, transitional buoyant and momentum plume rise, rain cap effects and partial plume penetration into elevated temperature inversions. To solve the many computational difficulties in applying a puff model in the near source-fields, CALPUFF includes two accurate and computationally efficient puff sampling routines. An elongated puff (slug) routine is applied in the near-field during rapidly varying meteorological conditions, otherwise an integrated puff approach is used. For building downwash effects, CALPUFF contains options for the user to specify the Huber-Snyder or Schulman-Scire routines for all stacks or on a stack-by-stack preference. The model includes algorithms, subgrid scale terrain and coastal interactions effects, and terrain impingement as well as longer range effects such as pollutant removal due to wet scavenging and dry deposition, chemical transformation, vertical wind shear effects, overwater transport, plume fumigation, and visibility effects of particulate matter concentrations.

CALPUFF can use different forms of meteorological input data (surface, profile, or gridded); however, this Guideline recommends 3D meteorological fields generated by CALMET as the preferred mode of running CALPUFF. The meteorological input data should be fully characterised with time-and-space-varying three dimensional winds and meteorological conditions using CALMET. Data used by CALMET can be from single station surface and upper air observations, 3D prognostic model outputs (e.g. from models such as MM5, ETA, TAPM, Unified Model, WRF). The prognostic model outputs can be used in combination with or without station observations.

Plume rise algorithms in CALPUFF model are generalised for a variety of source types. CALPUFF contains an option for puff splitting algorithm that allows vertical wind shear effects across individual puffs to be simulated. Estimates of horizontal plume dispersion are provided from turbulence-based dispersion coefficients based on measured or computed coefficients. The model provides several options for calculating these dispersion coefficients from the use of (i) turbulence measurements (σv and σw) (ii) similarity theory to estimate σv and σw, (iii) Pasquill-Gifford (rural) and McElroy-Pooler (urban) dispersion coefficients.

CALPUFF can fully treat stagnant conditions, wind reversals such as those experienced in land-sea breezes, mountain-valley breezes and in very rugged terrain. Water bodies and coastal lines present spatial changes to meteorological and dispersion conditions due to the abrupt change in surface properties between land and water bodies. CALMET contains overwater and overland boundary layer algorithms that allows for the effects on plume transportation, dispersion and deposition to be simulated in CALPUFF. The model includes a subgrid scale complex terrain algorithm for terrain impingement. Plume impingement on subgrid scale hills is evaluated using a dividing streamline to determine which material of the plume is deflected around the hills or advected over the hills.

CALPUFF treats primary pollutants and simulates secondary pollutant formation using a parameterised, quasi-linear chemical conversion mechanism based on five species. Pollutants treated include sulphur dioxide (SO_2), sulphates (SO_4^{2-}), nitrogen oxides (NO., nitrogen oxides = nitric oxide + nitrogen dioxide i.e., NO + NO_2), nitric acid (HNO_3), aerosol nitrates (NO^{3-}), ammonia (NH_3), particulate matter (both PM_{10} and $PM_{2.5}$), toxic pollutants and others pollutant species that are either inert or subject to quasi-linear chemical reactions. A resistance-based dry deposition scheme is included for deposition of both gasses and particulate matter. Wet deposition is treated using a scavenging coefficient approach with removal rate as a function of precipitation type and intensity. CALPUFF Version 6.42 contains new options for gas-phase chemistry, aqueous phase chemistry and aerosol chemistry based on ISORROPIA chemical module used in models such as CMAQ. However, to these options have not been evaluated enough to be acceptable.

CALPUFF is currently the recommended model for most long-range (i.e. > 50 km) modelling applications. The model is used for major projects nationally, and it already has a measure of acceptance and public credibility worldwide. CALPUFF could have a distinct advantage over the use of a steady-state plume models such as AERMOD for near field impact analyses. One type of application where CALPUFF may be better than AERMOD is when there are strong localised influences on the wind field, such as valley channelling, upslope / downslope flows, and coastal areas. CALPUFF also has the ability to simulate spatial and temporal variations of concentration fields better than steady-state plume models like AERMOD. This may be an important advantage for risk-based assessments in which the accurate prediction of average exposure levels across the population in an area is more important than the prediction of the maximum concentration in any one location. The other type of application where CALPUFF could provide some advantage over the steady-state plume models is with stagnation conditions. Stagnation conditions may be especially important given the potential for a build-up of excessively high concentrations over time.

CALPUFF is recommended for use for:

- Long-range transport distances between 50 and 300 km.
- Complex, non-steady-state meteorological conditions where transport distances are less than 50 km, on a case-by-case basis including:
- inhomogeneous winds
- inversion breakup fumigation
- shoreline fumigation
- stagnation conditions.
- No buildings, single or multiple buildings.
- Availability of detailed meteorological and geophysical inputs.
- Deposition and light extinction where long-range transport distances are greater than 50 km.
- Secondary formation of particulate matter in long-range transport distances greater than 50km.

- Multiple source (point, area, volume) and buildings.

7.5 SCIPUFF

Like CALPUFF, SCIPUFF is another recommended model for Level 3 assessments requiring detailed description of physical and chemical atmospheric processes, typically associated with Level 3 assessments. SCIPUFF is a Lagrangian puff dispersion model that uses a collection of Gaussian puffs to represent an arbitrary, three-dimensional, time-dependent concentration field. The turbulent diffusion parameterization is based on modern turbulence closure theory, specifically the second-order closure model of Donaldson (1973) and Lewellen (1977), which provides a direct relationship between the predicted dispersion rates and the measurable turbulent velocity statistics of the wind field. In addition to the average concentration value, the closure model also provides a prediction of the statistical variance in the concentration field resulting from the random fluctuations in the wind field. The closure approach also provides a direct representation for the effect of averaging time (Sykes and Gabruk 1997).

SCIPUFF is appropriate for modelling both short and long range (greater than 50km) transport, steady or non-steady state emissions of primary pollutants (gases or particles), buoyant or neutral sources using time dependent meteorological data (surface, profile, or gridded). Shear distortion, complex terrain, linear chemical transformations, gravitational settling and deposition are treated. In addition to the mean concentration, dose and deposition, SCIPUFF provides an estimate of the probability levels of the predicted values. SCIPUFF has been extensively validated and compares favourably against comparison with CALPUFF and AERMOD (Lee, Peltier et al. 2009). These validation studies started as early as 1988 (Sykes, Lewellen et al. 1988) and (Sykes, Parker et al. 1993).

SCIPUFF contain pre-processors that work in similar manner to those used in the CALPUFF air dispersion modelling system. It contains a geophysical processor, named SCIGEO, which prepares the terrain and land cover properties to be used by the meteorological processor (SCIMET). One additional advantage of SCIMET is that unlike CALMET is does not require guessing "radius of influence" such as RMAX1, RMAX2, RMAX3, R1, R2, and TERRAD. Therefore, SCIMET facilitate the creation of the three-dimensional wind fields by the modeller and reduces uncertainties on the review process by the regulatory agency. The SCIPUFF modelling system input files were designed by SAGE and Lakes Environmental to be almost identical to the AERMOD modelling system. This way, SCIMET input files are almost identical to AERMET input formats, as well as the data format for SCIPUFF is almost identical to the ones for AERMOD (with all the keywords, including CO, SO, RE, and OU pathways).

Recent updates to SCIPUFF are currently being implemented in order to integrate SCICHEM and SCIPUFF into a single dispersion model with a more complex and realistic representation of gas, aqueous and aerosol chemistry and transformation. While this work is still in the testing stages at the time these guidelines are being finalized, this model holds promise for providing a superior treatment of pollutant concentrations when chemical transformations are important to characterize.

Exponent®

Atmospheric Sciences

Review of the Sasol Atmospheric Impact Report

Exponent®

Review of the Sasol Atmospheric Impact Report

Prepared for

Sasol Limited (Pty) Ltd.
Sasol Place, 50 Katherine Street, Sandton, 2090, South Africa
PO Box 5486, Johannesburg, 2000

Prepared by

Exponent
1 Mill and Main Place, Suite 150
Maynard, MA 01754
United States of America

January 2017

1605982.000 - 9140

Contents

List of Figures

List of Tables

Acronyms and Abbreviations

AIR	Atmospheric Impact Report
Airshed	Airshed Planning Professionals (Pty) Ltd.
ARM	Ambient Ratio Method
AQIS	Air Quality Impact Study
CMAQ	Community Multiscale Air Quality Model
CO	Carbon monoxide
deg	degrees
DEA	Department of Environmental Affairs
GEP	Good Engineering Practice
g/kg	grams per kilogram
GUI	Graphical User Interface
IOA	Index of Agreement
km	kilometer
LCC	Lambert Conic Conformal
m	meter
m/s	meters per second
NCEI	National Center for Environmental Information
NO_2	Nitrogen Dioxide
NO_3	Nitrates
NO_x	Oxides of Nitrogen
PBL	Planetary Boundary Layer
ppb	parts per billion
PDF	Probability Density Function
PM	Particulate Matter
PM_{10}	Particulate Matter with diameter $\leq$ 10 microns
PRIME	Plume Rise Model Enhancements
RH	relative humidity

RMSE	Root Mean Square Error
SO_4	Sulfates
U.S. EPA	United States Environmental Protection Agency
UTC	Coordinated Universal Time
UTM	Universal Transverse Mercator
WRF	Weather Research and Forecasting Model
YSU	Yonsei University

Limitations

This report summarizes work performed to date and presents the findings resulting from that work. The findings presented herein are made to a reasonable degree of scientific certainty and are based on the material provided to Exponent by the client or by Airshed Planning Professionals (Pty) Ltd. of South Africa during the period November 18, 2016 through January 26, 2017.

Exponent reserves the right to supplement this report and to expand or modify opinions based on review of any additional material that becomes available.

1 Introduction

Sasol Limited (Pty) Ltd. owns and operates several industrial facilities in South Africa. These include the Secunda Synfuels Operations, a petrochemical facility located in Secunda in the Province of Mpumalanga; Sasol Sasolburg Operations, a petrochemical facility located in Sasolburg in the Province of the Free State; and the Natref Facility, an oil refinery located in Sasolburg in the Province of the Free State. These facilities are subject to Minimum Emission Standards pursuant to Section 21 of the National Environmental Management: Air Quality Act (Act No. 39 of 2004), hereafter referred to as the Act. Paragraphs 8 and 9 of Part 2 of Section 21 of the Act require that existing plants comply with the Minimum Emission Standards for existing plants by April 1, 2015 and with Minimum Emission Standards for new plants by April 1, 2020.

Paragraph 11 of Section 21of the Act allows for applications for postponing the deadlines for compliance with the Minimum Emission Standards if certain requirements are satisfied. Postponements of up to five years may be granted. Sasol previously requested a postponement of the compliance deadlines for certain activities in 2014, and the requested postponement was granted in February 2015. However, for some activities the postponement was granted for a period of only three years. Sasol now intends to submit applications for exemption or extension of compliance deadlines for certain activities for which compliance may not be possible or practicable within the prescribed timeframe.

Subparagraph 12(a) of Section 21 of the Act requires that an Atmospheric Impact Report (AIR) as contemplated in Section 30 of the Act be included as part of an application for postponement of or exemption from deadlines for compliance with the Minimum Emission Standards. Air quality dispersion modeling for this purpose is being conducted by Airshed Planning Professionals (Pty) Ltd. of South Africa (Airshed), and Airshed is preparing AIRs to support the applications. Airshed's study includes modeling of the Secunda facility, the Sasolburg facility, and the Natref facility.

Exponent has been retained by Sasol to conduct a peer review of the methodology used in the air quality impact studies (AQIS) conducted by Airshed. The scope of the Exponent peer review includes review and comments on the following:

- Modeling techniques used in the AQIS and their appropriateness for the applications;
- Prognostic meteorological data incorporated in the modeling;
- CALMET, CALPUFF, and CALPOPST switch settings and model options;
- Any obvious information gaps, omissions, or inaccuracies;
- Key assumptions and uncertainties.

Basic information on the project and various regulatory documents were provided on November 18, 2016. This information included the South African National Framework for Air Quality Management, the Air Quality Act, Minimum Emission Standards, Ambient Air Quality Standards, and the Code of Practice for Air Dispersion Modelling in Air Quality Management in South Africa (2014). An initial set of modeling files was provided to Exponent on November 21, 2016, and some replacement copies of gridded land use and terrain additional modeling files were provided on December 12, 2016. Exponent was provided access to separate draft AIRs for the Secunda, Sasolburg, and Natref facilities on December 19, 2016. Although it appears that a fairly complete set of modeling files was provided for the Secunda facility, only a partial set of files were provided for the Sasolburg and Natref facilities. Consequently, our review of modeling files focused on those provided for the Secunda facility. It is our understanding that modeling files for the other sites were set up in a consistent manner. Additional material concerning the Lakes Environmental WRF modeling was provided on January 26, 2017.

The information used in our review was limited to the data provided in the documents, the modeling files described above, and additional meteorological data that we obtained. Note that our review did not include consideration or evaluation of the emissions data, source configuration data, the ambient background air quality data, or the comparison of predicted concentrations to National Ambient Air Quality Standards or to other ambient limits.

1.1 Summary of Major Comments

The list below summarizes the most important comments from the peer review of the report and the modeling data files provided. Additional informational comments or comments of a less significant nature are provided in the main body of the report.

- CALPUFF:
  - Gridded receptors were included in the modeling with a resolution of 200 meters. This resolution is less than what is required for near-field modeling by the Code of Practice.

  - When building downwash effects are included in the modeling, the ISC building downwash method (MBDW=1) was used. We recommend that a building downwash analysis be conducted for point sources below Good Engineering Practice (GEP) height using the BPIP-PRIME processor and that the Plume Rise Model Enhancements (PRIME) building downwash method (MBDW=2) be used to evaluate building downwash effects.

  - The AQIS modeling included wet and dry deposition. This would be expected to yield more accurate and reliable results because it accounts for material removed from the plume by deposition on ground and vegetation surfaces. However, the Code of Practice states that deposition should not be included in modeling studies for licensing unless deposition fluxes are of importance.

  - Non-default options have been selected that control the number of puffs produced during a time step. These non-default values will limit the number of puffs produced by the model and may result in less robust calculations of airborne concentrations.

- WRF summary:
  - The 4 km resolution for terrain used in WRF captures the key broad-scale terrain features within the CALMET modeling domain.

  - The vertical and spatial resolution of the WRF data is suitable to reasonably represent the meteorology of the modeling region.

  - Some of the computed performance statistics for wind speed are outside of the benchmark ranges. Wind speeds predicted by WRF for locations in the eastern portion of the modeling domain near the Secunda facility show a significant positive bias. These over-predictions of wind speed when used for air dispersion modeling could result in under-prediction or over-prediction in airborne concentrations.

  - Some of the computed performance statistics for wind direction are outside of benchmark ranges. Differences in wind roses of predicted and observed winds are also apparent by inspection. This suggests that there may be some degradation in WRF model performance with respect to the wind fields. The differences that we observe are not unusual or out of character for prognostic modeling and should be acceptable for use in the modeling studies.

  - The WRF model performance measures for temperature and specific humidity demonstrate that the temperature and specific humidity fields are suitable for use in these analyses.

- CALMET Summary:
  - The overall land use and terrain elevations look reasonable and representative of the characteristics of the modeling domain.

  - The selected CALMET options are reasonable for this application.

- The surface stations on the western portion of the CALMET domain are clustered very close together and show considerable variability with respect to wind speed and direction. We recommend that a single station representative of the area be selected for use to avoid or minimize the effects of differences in meteorological measurements among these stations.

2 Choice of Modeling Techniques

The methodology being used in the air quality impact study is a Level 3 assessment as defined in the Code of Practice. A Level 3 analysis uses sophisticated modeling techniques in cases where a detailed understanding of the time and space variation of impacts is required. The Code of Practice states that Level 3 assessments may be used to "evaluate air quality consequences under a permitting or environmental assessment process for large industrial developments that have considerable social, economic and environmental consequences."

Level 3 analyses include consideration of variable wind and turbulence fields, causality effects, curved trajectories, recirculation, stagnation/calm wind conditions, fumigation, and chemical transformation. This type of modeling requires more detailed meteorological and geophysical data than that required by Level 1 or Level 2 assessments.

Airshed selected the CALPUFF model (Scire et al., 2000) as the Level 3 model for use in AQIS. CALPUFF is one of the models recommended in the Code of Practice. CALPUFF is well suited for the types of industrial sources and areas of interest in this study. CALPUFF is capable of providing estimates of cumulative impacts from a variety of sources spread over a relative large area (50 km x 50 km). The model contains algorithms for assessing near-field effects such as building downwash, transitional plume rise, momentum rise, as well as far-field effects including chemical transformation and deposition processes. Version 6.42 of CALPUFF incorporates advanced chemistry including ISORROPIA aerosol chemistry and aqueous phase oxidation of SO_2, techniques that are used in photochemical models such as CMAQ. When combined with three-dimensional meteorological data from a numerical weather prediction model (the Weather Research and Forecasting mesoscale model (WRF) in this study) and surface-based meteorological observations, the data requirements for a proper assessment with CALPUFF are met.

The draft Airshed AIR for the Sasol Secunda facility provides a detailed justification for the use of the CALPUFF model for this study. Exponent agrees that the selection of the CALPUFF model is appropriate for this application and consistent with the regulatory guidance for a Level 3 assessment.

The use of Level 1 or Level 2 assessment techniques for this application would be less appropriate. Steady-state Gaussian plume models such as AERMOD make assumptions that limit their applicability to near-field impacts with relatively simple flow conditions. Gaussian plume models assume that steady-state conditions exist during each time step, which results in straight-line trajectories that extend to infinity for each hour. This also results in a lack of causality effects (i.e., neglecting the time it takes after emissions leave the stack to reach downwind receptors), limited ability to treat low-wind speed conditions, the lack of pollutant memory from one hour to the next (i.e., does not treat stagnation, recirculation or pollutant build-up), and the use of a single meteorological station to represent conditions throughout the modeling domain (i.e., assumed homogeneous wind and dispersion conditions during each hour for all sources). Such models are still useful for screening analyses for short distances with relatively simple wind conditions and homogeneous dispersion. Although steady-state plume models provide a conservative estimate of impacts in most cases, they are clearly less suitable for use for this application compared to Level 3 assessment techniques that were used.

3 WRF Meteorological Data

3.1 WRF Model Setup

The Weather Research and Forecast (WRF) model grid resolution in the analysis is 4 km with 34 vertical levels using a Lambert Conformal grid with an origin at 26.7262 degrees South and 28.5142 East. Standard parallels are at 27.2299 degrees South and 26.2299 degrees South. The original model simulations used 69 x 69 grid cells, and the 3D.DAT files contained 55 x 55 grid cells.

The WRF data set used in the assessments was generated by Lakes Environmental. Some documentation regarding the WRF data set was provided to Exponent on January 26, 2017. The configuration used appears to be typical and appropriate for this type of application. The Lakes Environmental documentation does not indicate whether grid analysis or observation nudging was applied in their WRF simulations, although this generally is done.

The use of 34 vertical layers is reasonable. In the current application, the centers of the five lowest layers are at about 11 meters, 35 meters, 61 meters, 91 meters, and 124 meters above the surface. These lowest layers are sufficient to define 10-meter level winds and the vertical temperature profiles.

Figure 1 shows the WRF domain terrain at 4 km resolution and the CALMET domain terrain at 1 km resolution. Comparison of these two terrain fields shows that the 4 km resolution terrain captures the key broad-scale terrain features within the CALMET modeling domain. The CALMET domain is slightly smaller than the WRF domain, and some additional detail is apparent in the depiction of terrain features at a grid resolution of 1 km.

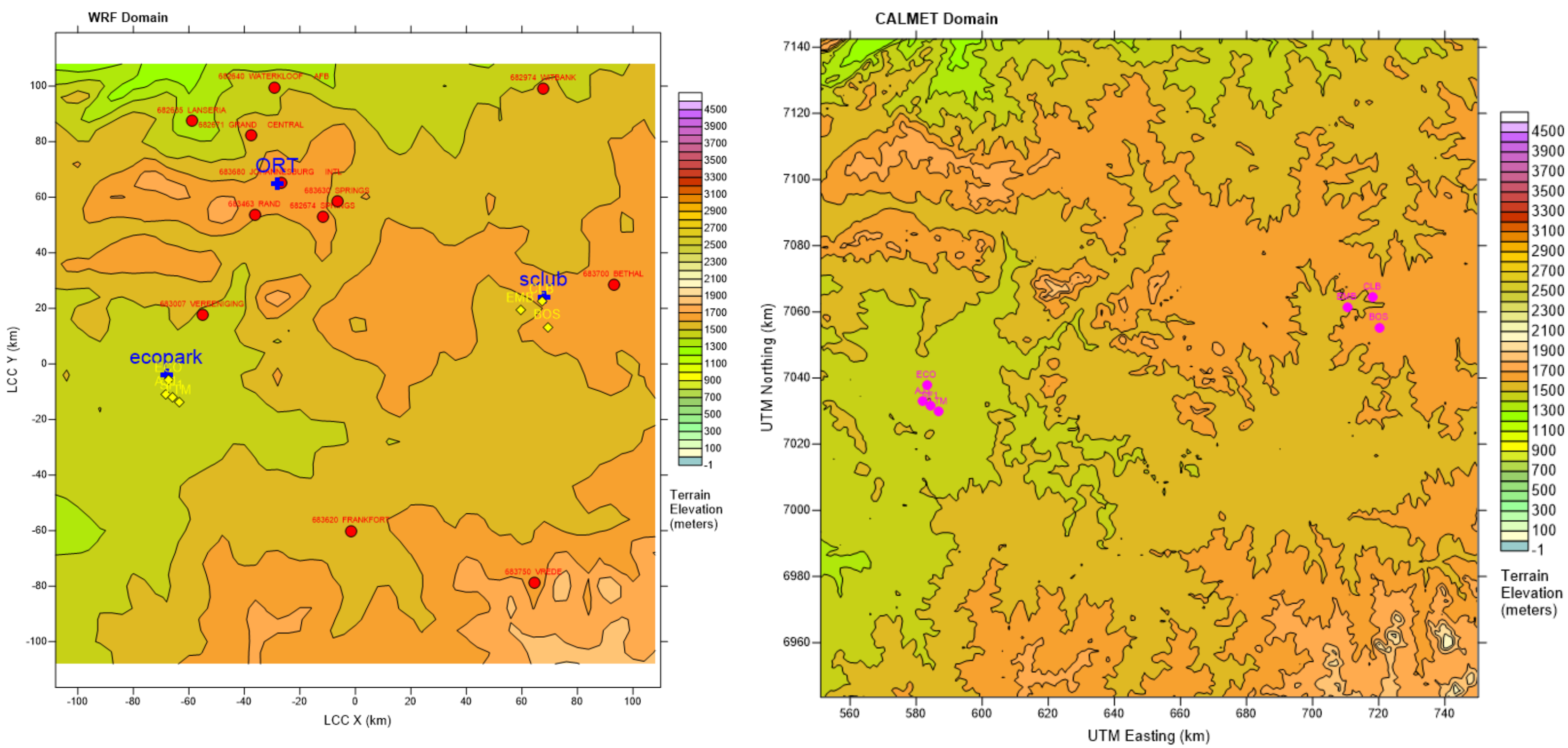

Figure 1 Terrain contour analysis for WRF 4-km terrain (left) and CALMET 1-km terrain (right).

3.2 WRF Evaluation

Airshed conducted an evaluation of the WRF data based on comparisons of WRF predictions and observations at a single station (OR Tambo) for the entire 3-year modeling period (2013-2015) and concluded that modeled values of wind speed, wind direction, temperature, and specific humidity satisfied or was sufficiently close to the performance benchmarks. This station is located in the northwestern portion of the domain near Johannesburg. As part of our review and assessment of the WRF data, Exponent conducted further evaluations involving an analysis of individual years of data and two additional stations, Sasol Secunda Club and Sasol Sasolburg Ecopark, for which data were provided to us. These additional stations are located in the western and eastern portions of the domain, respectively. Their locations are shown in Figure 1.

Table 1 shows generally accepted benchmarks for average WRF performance over an annual period for wind speed, wind direction, temperature, and specific humidity.[1] These benchmarks are not intended as pass/fail criteria but provide a method of characterizing the mesoscale model performance relative to available observational data.

Table 1 Benchmarks for WRF Model Evaluation

	Wind Speed	Wind Direction	Temperature	Specific Humidity
IOA	≥ 0.6	-	≥ 0.8	≥ 0.6
RMSE	≤ 2 m/s	-	-	-
Mean Bias	≤ ±0.5 m/s	≤ ±10 deg	≤ ±0.5 K	≤ ±1 g/kg
Gross Error	-	≤ 30 deg	≤ 2 K	≤ 2 g/kg

The following sections include an evaluation of wind speed and direction, temperature, and specific humidity. The performance statistics for temperature and specific humidity are within expected ranges for this type of application. However, the wind speeds predicted by WRF

[1] See Emery (2001), Tesche et. al. (2001), and Wilmott (1981) for information on performance benchmarks.

exhibit a positive bias relative to observed winds in the eastern portion of the domain. Therefore, we have some concerns about whether the WRF wind speeds adequately represent the winds in this region. Wind speeds with a bias high can result in over-stated dilution when used for dispersion modeling and under-prediction of concentrations. Conversely in situations involving downwash, higher wind speeds can increase ground level concentrations in the near field. In this application the observations from surface stations have been included in the CALMET generated wind fields, which will help to align the wind fields near the stations with the observations. There is still some risk of generating unrealistic or converging flows where there is significant disagreement between the WRF fields and observations. This issue is discussed in further detail in the CALMET section.

3.2.1 Wind Speed and Direction

The performance statistics for wind speed and direction for each year in the 3-year modeling period (2013-2015) are provided in

Table 2. The values are averaged over the three stations considered in each year.

For wind speed, the index of agreement (IOA) for the mean satisfies the benchmark ($\geq$ 0.6). However, the wind speed from WRF clearly shows a tendency for a positive bias (i.e., WRF wind speeds tend to exceed observed values) that falls outside the performance benchmark range in 2013 and 2015. The root mean square error (RMSE) for wind speed and direction meet the benchmark values in all three years. However, the gross error of wind direction falls outside the benchmark range in all three years.

Time series of daily average predicted and observed wind speeds were constructed for individual stations to further explore the extent of the wind speed bias. The resulting time series are presented in Figure 2, with OR Tambo shown in the top section, Sasol Sasolburg Ecopark in the middle, and Sasol Secunda Club in the bottom section. The time series for WRF predicted wind speeds at OR Tambo and at Sasol Sasolburg Ecopark showed good agreement with observations with little bias. However, the 10-meter wind speeds predicted by WRF at Sasol Secunda Club are consistently higher than the observed data.

Table 2 Statistics of WRF model performance for wind speed and wind direction

2013

	Wind Speed				Wind Direction	
	IOA	Mean Bias	Gross Error	RMSE	Mean Bias	Gross Error
	-	m/s	m/s	m/s	deg	deg
Benchmark	≥ 0.6	≤ ±0.5		≤ 2	≤ ±10	≤ 30
Mean	0.64	0.53	1.43	1.81	-6.38	39.53
Daily Minimum	0.30	-0.81	0.67	0.85	-38.34	12.21
Daily Maximum	0.95	2.22	3.06	3.86	9.1	58.8

2014

	Wind Speed				Wind Direction	
	IOA	Mean Bias	Gross Error	RMSE	Mean Bias	Gross Error
	-	m/s	m/s	m/s	deg	deg
Benchmark	≥ 0.6	≤ ±0.5		≤ 2	≤ ±10	≤ 30
Mean	0.63	0.49	1.37	1.74	-7.86	39.87
Daily Minimum	0.14	-0.53	0.77	1.06	-44.71	16.06
Daily Maximum	0.92	2.00	2.70	3.69	38.84	123.30

2015

	Wind Speed				Wind Direction	
	IOA	Mean Bias	Gross Error	RMSE	Mean Bias	Gross Error
	-	m/s	m/s	m/s	deg	deg
Benchmark	≥ 0.6	≤ ±0.5		≤ 2	≤ ±10	≤ 30
Mean	0.61	0.68	1.50	1.91	-9.02	42.50
Daily Minimum	0.24	-0.65	0.66	0.88	-47.80	13.51
Daily Maximum	0.95	2.24	2.78	3.47	31.17	103.58

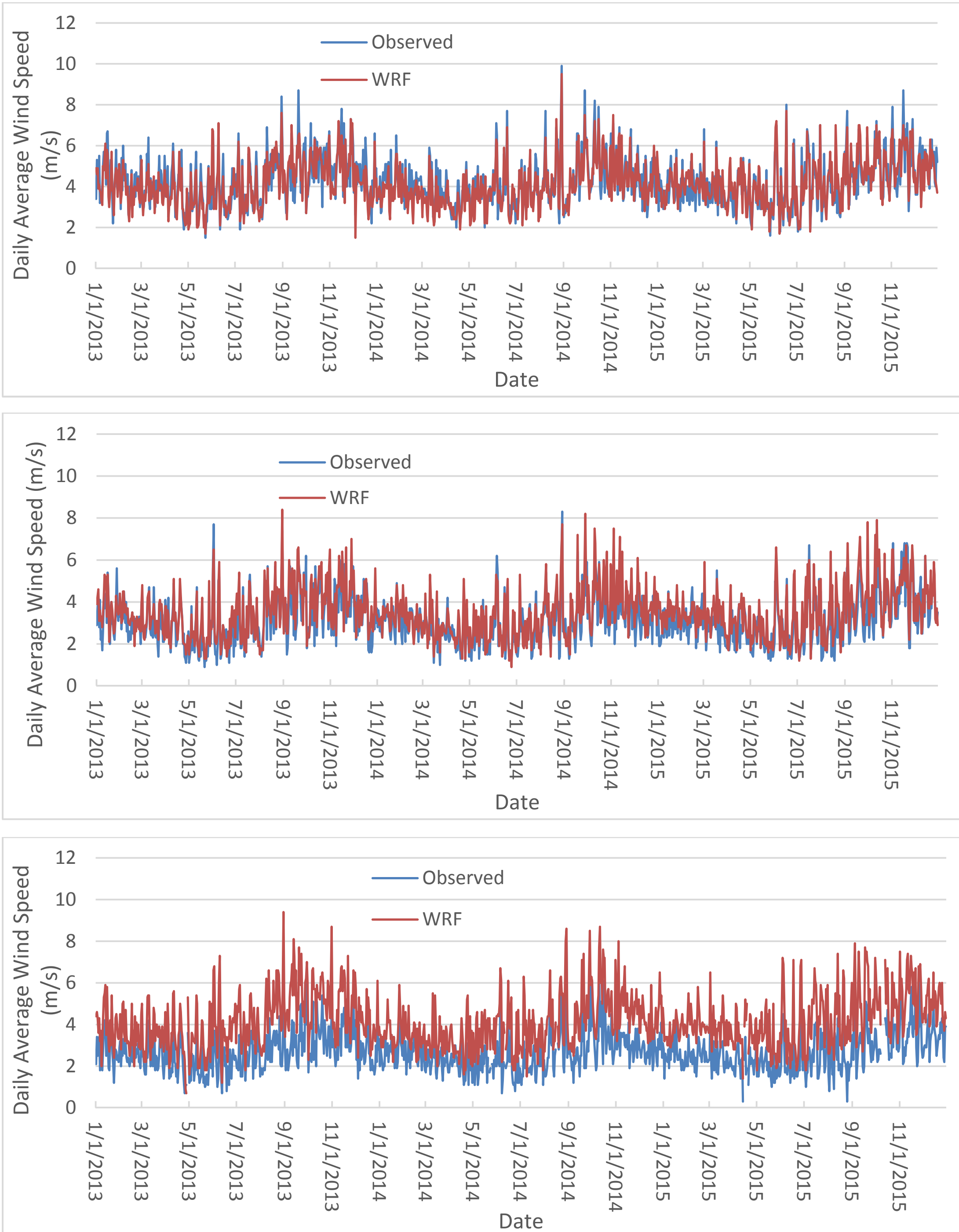

Figure 2 Time series of WRF predicted and observed daily average wind speed at OR Tambo (top), Sasol Sasolburg Ecopark (middle), and Sasol Secunda Club (bottom) for 2013-2015.

In order to determine whether this wind speed bias was limited to Sasol Secunda Club or was more widespread, Exponent examined two additional stations in the eastern region of the domain from the SURF.DAT file used for the CALMET modeling. These stations are labeled Bossjespruit and Embalanhle and are located within about 10 km of Sasol Secunda Club. Figure 3 shows time series for Bossjespruit and Embalanhle for predicted and observed daily averaged winds. The wind speeds predicted by WRF at the Bossjespruit and Embalanhle locations also show a clear positive wind speed bias. This positive wind bias at Sasol Secunda Club and at Bossjespruit and Embalanhle suggests that WRF may be overpredicting the observed surface level winds over at least some portions of the eastern part of the WRF domain. We note, however, that there may be some data quality issues at some of these stations, as discussed later in the CALMET section. This overprediction of wind speed was not observed at some other stations examined, such as OR Tambo and Sasol Sasolburg Ecopark, and thus may be limited to the eastern portion of the domain and therefore may be more of a potential concern for the modeling involving the Secunda facility.

Figure 4 through Figure 6 show wind roses predicted by WRF and actually observed for the period 2013-2015 for the locations of the three primary stations used in the analysis (Sasol Sasolburg Ecopark, OR Tambo, and Sasol Secunda Club). There are some noticeable differences in the predicted and observed wind directions at OR Tambo and Sasol Sasolburg Ecopark. However, the wind speed distributions are similar. At Sasol Secunda Club, the predicted and observed wind roses show more similar wind direction distributions, but the high wind speed bias from WRF is clearly evident.

The overestimation of wind speed is not uncommon in WRF and is often associated with excessive boundary layer mixing. Some optional algorithms for the Yonsei University (YSU) planetary boundary layer (PBL) scheme have been introduced into the WRF model to account for the effects of sub-grid scale terrain features and their effect on surface drag. We do not know if any of these algorithms were implemented in the generation of the WRF data by Lakes Environmental. The overestimation of wind speeds in this case could also be due to issues associated with the siting of the meteorological stations. These stations could be measuring highly localized wind features that were not resolved by the 4 km resolution WRF grid.

However, the positive wind bias shown at three stations in the region suggests a larger scale cause or issue.

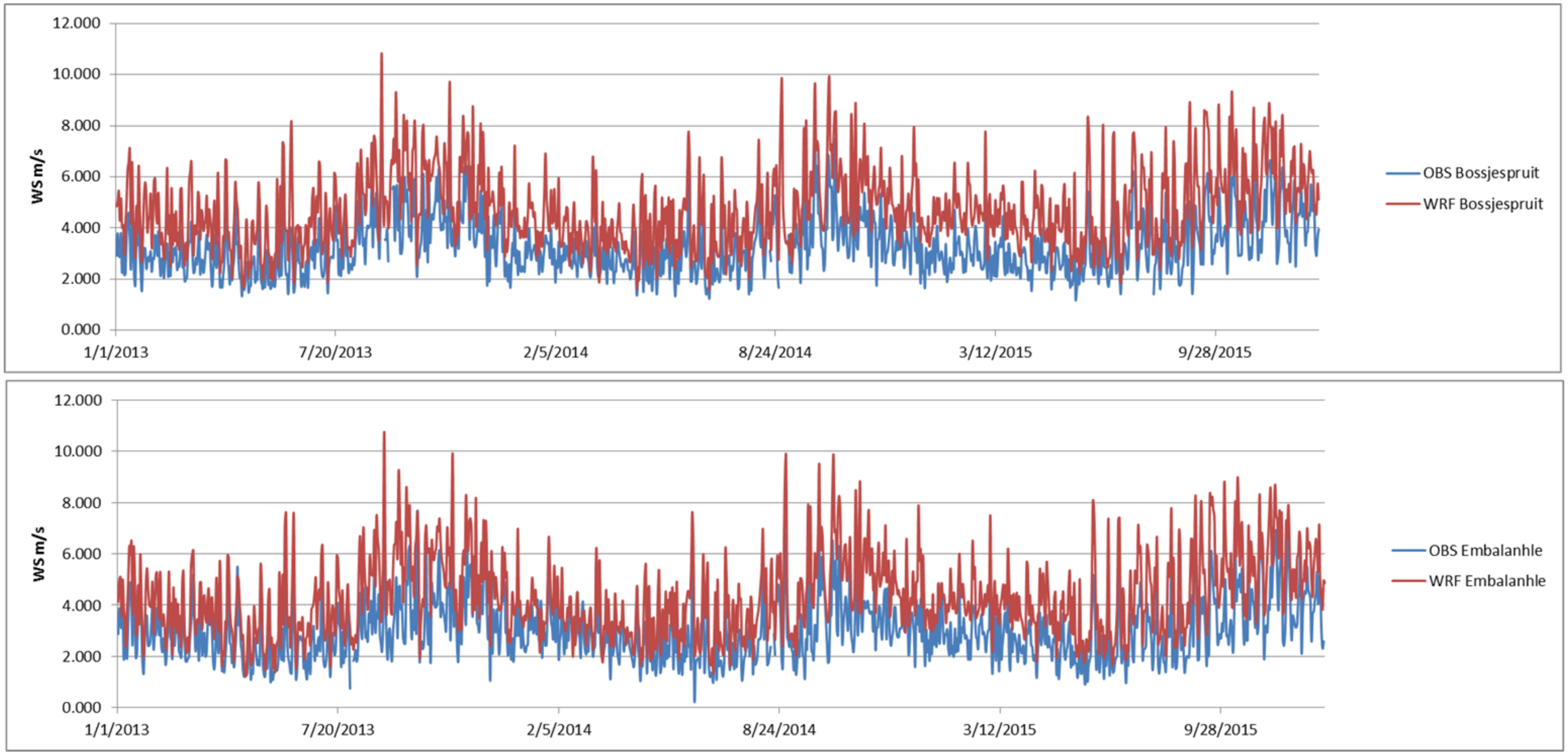

Figure 3 Time series of WRF predicted and observed daily average wind speed at Bossjespruit and Embalanhle for 2013-2015.

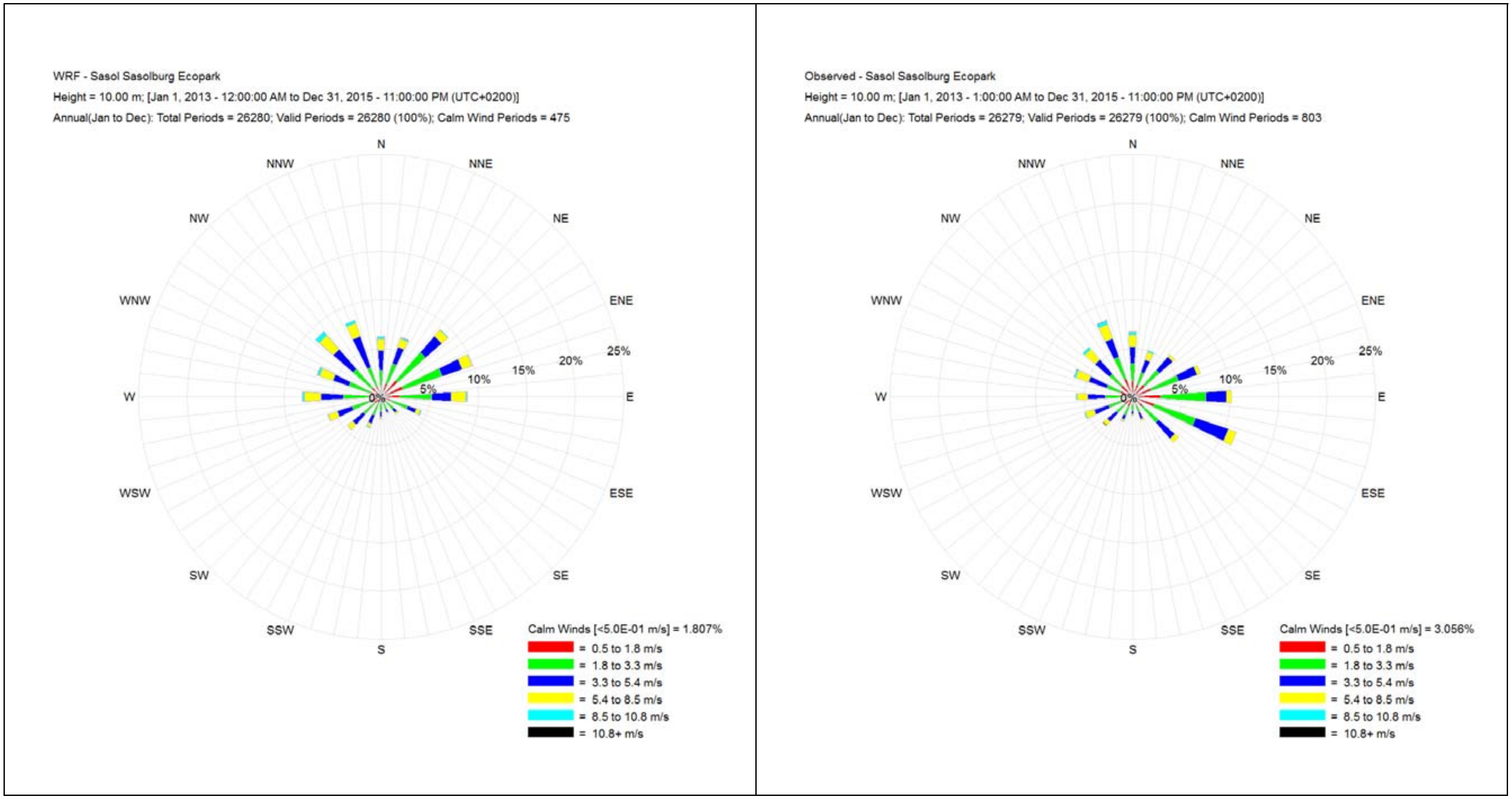

Figure 4 WRF Predicted versus Observed Wind Roses for Sasol Sasolburg Ecopark.

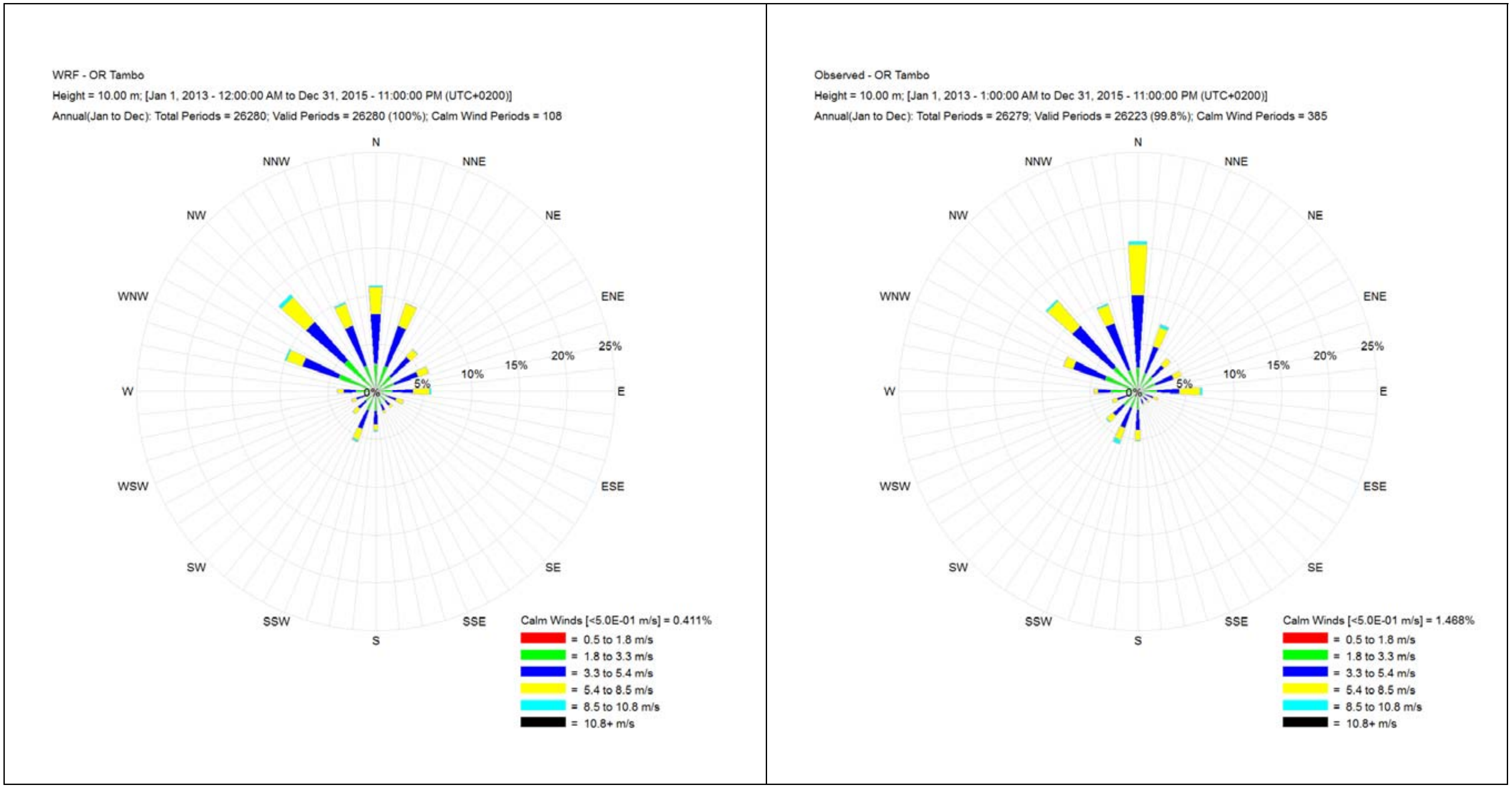

Figure 5 WRF Predicted versus Observed Wind Roses for OR Tambo

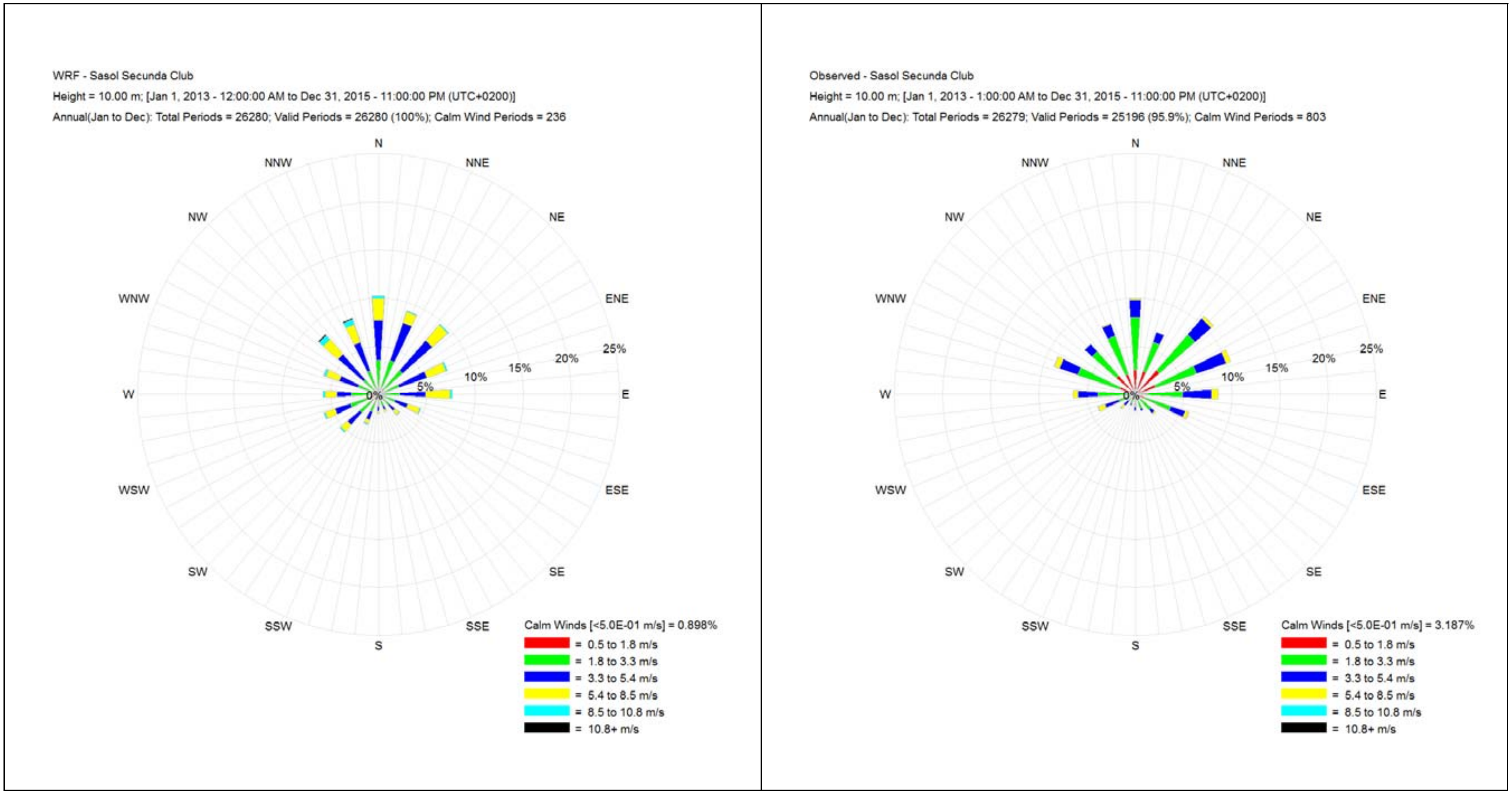

Figure 6 WRF Predicted versus Observed Wind Roses for Sasol Secunda Club

3.2.2 Temperature

The performance statistics for temperature for each year in the 3-year modeling period (2013-2015) are provided in Table 3. The values are averaged over the three stations considered in each year. Performance statistics are within the benchmark values for all parameters and all years. Figure 7 shows a time series of predicted and observed daily average temperatures for each of the three years. The agreement between WRF and the observations is good. There are no identified issues with the use of the WRF predicted temperature fields for dispersion modeling.

3.2.3 Specific Humidity

The performance statistics for specific humidity for each year in the 3-year modeling period (2013-2015) are provided in Table 4. The values are averaged over the three stations considered in each year. The IOA for specific humidity is slightly outside the benchmark range value in 2014. For all other years and parameters performance statistics are within the benchmark values. Figure 8 shows a time series of predicted and observed daily specific humidity for each of the three years. The agreement between WRF and the observations is good. There are no identified issues with the use of the WRF predicted specific humidity fields for dispersion modeling.

Table 3 Statistics of WRF model performance for temperature for 2013-2015

2013

	IOA	Mean Bias	Gross Error	RMSE
	-	K	K	K
Benchmark	≥ 0.8	≤ ±0.5	≤ 2	-
Mean	0.93	-0.49	1.83	2.31
Daily Minimum	0.53	-4.53	0.78	1.07
Daily Maximum	0.99	2.25	5.10	7.65

2014

	IOA	Mean Bias	Gross Error	RMSE
	-	K	K	K
Benchmark	≥ 0.8	≤ ±0.5	≤ 2	-
Mean	0.92	-0.35	1.81	2.27
Daily Minimum	0.34	-3.25	0.90	1.12
Daily Maximum	0.98	3.89	4.05	5.29

2015

	IOA	Mean Bias	Gross Error	RMSE
	-	K	K	K
Benchmark	≥ 0.8	≤ ±0.5	≤ 2	-
Mean	0.93	-0.21	1.89	2.37
Daily Minimum	0.61	-2.35	0.81	1.10
Daily Maximum	0.99	2.21	3.53	4.80

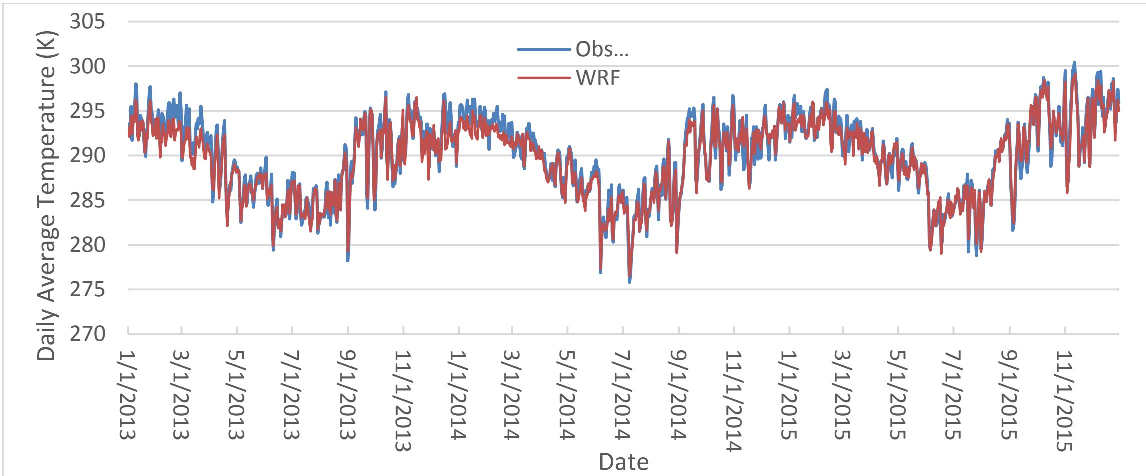

Figure 7 Time series of WRF predicted and observed daily temperature for 2013-2015.

Table 4 Statistics of WRF model performance for specific humidity for 2013-2015.

2013

	IOA	Mean Bias	Gross Error	RMSE
	-	g/kg	g/kg	g/kg
Benchmark	≥ 0.6	≤ ±1	≤ 2	-
Mean	0.61	-0.22	1.04	1.34
Daily Minimum	0.15	-7.97	0.19	0.22
Daily Maximum	0.96	1.95	8.35	12.60

2014

	IOA	Mean Bias	Gross Error	RMSE
	-	g/kg	g/kg	g/kg
Benchmark	≥ 0.6	≤ ±1	≤ 2	-
Mean	0.58	-0.44	1.01	1.25
Daily Minimum	0.13	-2.80	0.23	0.31
Daily Maximum	0.94	1.35	2.96	4.80

2015

	IOA	Mean Bias	Gross Error	RMSE
	-	g/kg	g/kg	g/kg
Benchmark	≥ 0.6	≤ ±1	≤ 2	-
Mean	0.60	-0.54	1.19	1.47
Daily Minimum	0.12	-4.43	0.22	0.26
Daily Maximum	0.96	1.89	4.43	4.95

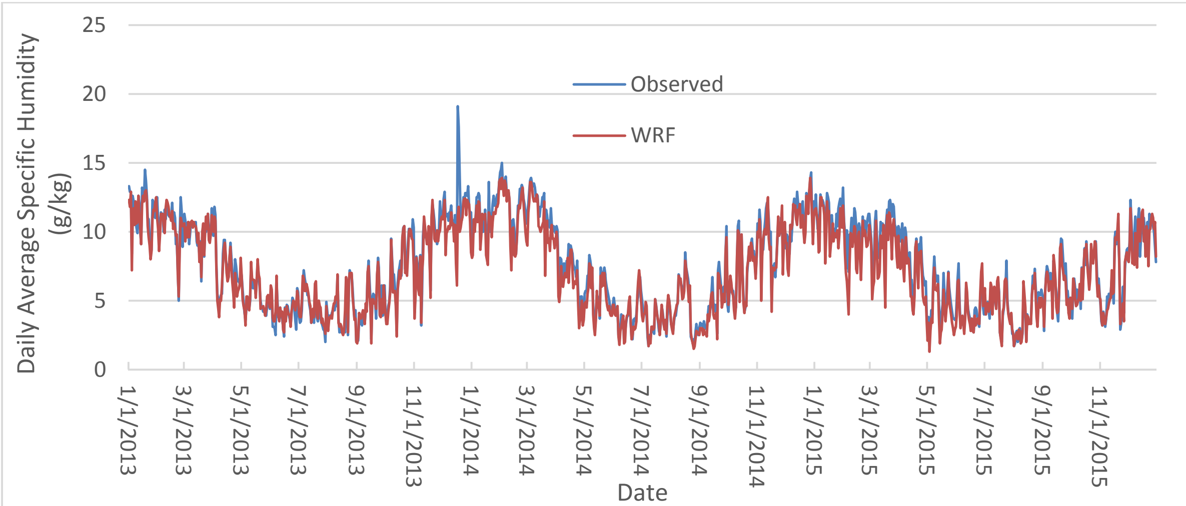

Figure 8 Time series of WRF predicted and observed daily average specific humidity (for 2013-2015.

4 CALMET Modeling Options

This section discusses the CALMET model option settings in the CALMET.INP file provided to us and the options chosen for the AQIS for Secunda. We provide recommendations for alternative options where appropriate.

A single CALMET.INP file was provided covering the 3-year period January 1, 2013 to December, 31 2015. This file includes 7 surface meteorological stations. As stated in the AIR, CALMET version v6.334 (level 110421) was used. Use of this version of CALMET is consistent with requirements in the Code of Practice.

We note that Version 6.5.0 of the CALMET model was released in June 2015. Version 6.5.0 represents an update of the prior Version 6.334 code. Version 6.5.0 fixes known coding errors in the prior Version 6.334 CALMET code. Since Version 6.334 contains some known bugs, we recommend that Version 6.5.0 be used for modeling studies. We recommend that the South African Department of Environmental Affairs (DEA) be consulted to determine if they would accept use of the current updated version of the CALMET model code (Version 6.5.0) for future modeling analyses.

4.1 Geophysical Data File

4.1.1 Land use Categories

As a first step, Exponent created the terrain elevation and land use gridded files from the CALMET output file in order to review the terrestrial data used in the CALMET simulations.

Figure 9 is a plot displaying the terrain contours and land use categories over the entire CALMET domain. The plot is consistent with similar plots contained in the various AIRs. Figure 9 also shows the locations of the surface stations used in the CALMET simulations.

Our review indicates that the overall land use and terrain elevations are reasonable and representative for the modeling domain.

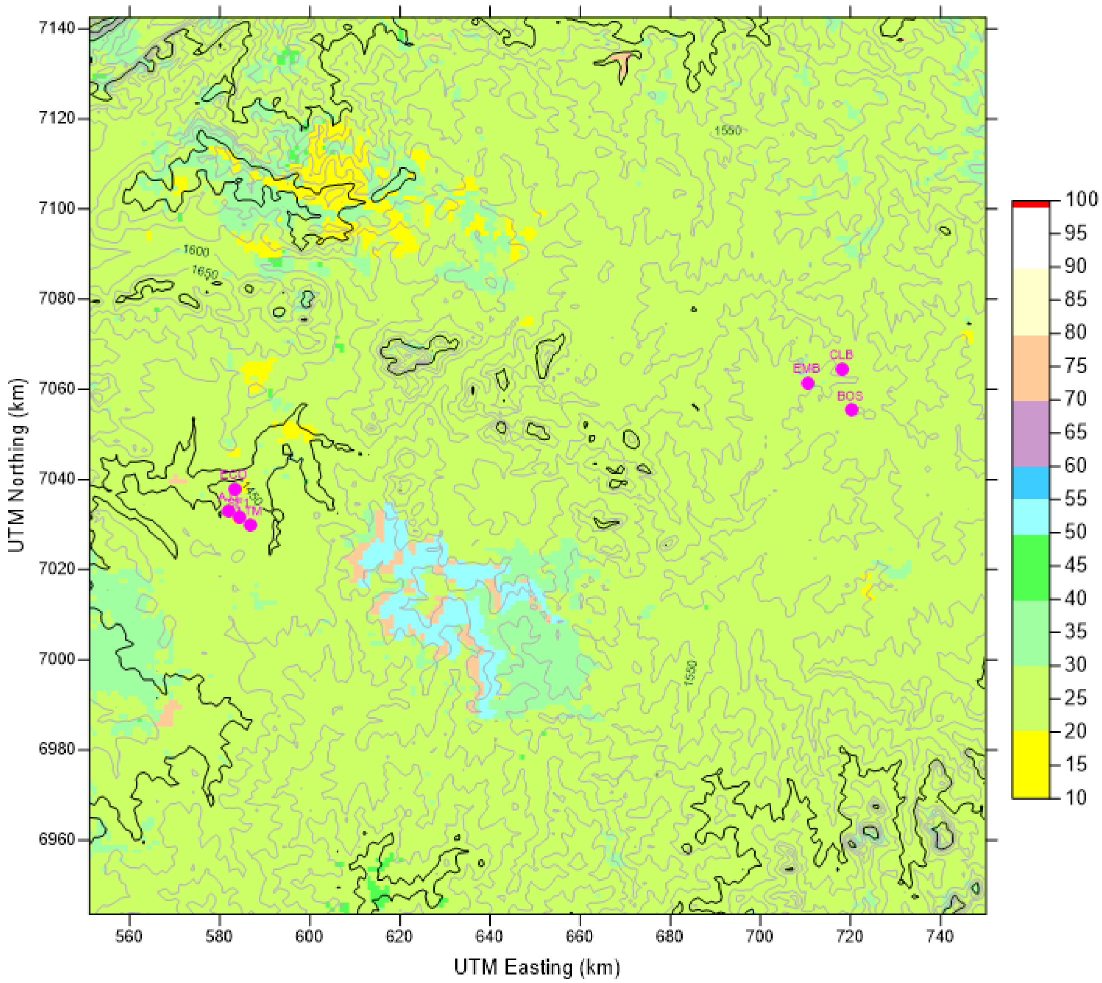

Figure 9 Terrain and land use for the CALMET modeling domain. Surface stations used in the CALMET simulations are shown by the pink circles.

4.2 CALMET Options

The following information was obtained from review of the CALMET.INP file:

- CALMET was run in the hybrid mode (NOOBS=1) using:
  - Surface observations (surface data in SURFACE.DAT, 7 stations)
  - Prognostic data (from WRF runs)
- The entire 3-year period (January 1, 2013 through December 31, 2015) was modeled in a single run.
- The time zone was set as UTC+0200.
- Time step for prognostic data (ISTEPPGS) set to 3600s
- The winds from WRF/3D.DAT are used as initial guess fields (IPROG=14)
- A UTM projection was selected (Zone 35 South) with WGS-84 datum.
- A 200 km x 200 km grid with a resolution of 1 km and a south west corner at X= 550.600 km, Y=6943.000 km was used.
- 11 vertical levels were defined (cell faces at: 0m, 20m, 40m, 80m, 120m, 200m, 300m, 600m, 1000m, 1500m, 2500m, and 3500m)
- Upper air data was provided from WRF
- Precipitation from WRF was selected
- Cloud information from WRF was chosen (clouds computed from the MM5toGrads algorithm (ICLOUD=4))

For a domain of this size, the use of UTM coordinates is satisfactory. Map distortion with UTM coordinates increases as the size of the modeling domain increases. For future consideration if appropriate in other analyses, the use of Lambert Conic Conformal (LCC) coordinates in mid-latitudes is preferred for domains on the scale of 200 km to 300 km or larger.

The CALMET options that were selected are reasonable overall for this application. Later in this section we recommend a few minor changes as refinements on technical grounds, but these items are not critical.

Table 5 lists those values used in CALMET that differ from their default values. The use of non-default values is not necessarily an issue, since the model is intended to allow for customization for site-specific conditions. In these cases all non-default values are associated with the use of prognostic data, a suitable choice for this application.

Table 5 Summary of CALMET Options Selected That Differ from Default Values

Variable	Description	Default Value	AIR Value	Comments
NOOBS	No observation mode	0 (observations only)	1 (surface observations and MM5 for upper air)	Suitable choice
ICLOUD	Cloud data options – Optional use of gridded cloud fields	0 (gridded clouds not used)	4 (Gridded cloud cover) MM5toGrads Algorithm	Suitable choice for NOOBS=1
IPROG	Use gridded prognostic wind field model output fields as input to the diagnostic wind field model	0 (no)	14 (yes, use winds from MM5/3D.DAT file as initial guess field)	Suitable option for NOOBS=1
IRHPROG	3D relative humidity from observations or from prognostic data	0 (Use RH from surf.dat file)	1 (Use prognostic RH)	Suitable option for NOOBS=1
ITPROG	3D temperature from observations or from prognostic data	0 (Use surface and upper air stations)	2 (MM5/3D.DAT for surface and upper air data)	Suitable for NOOBS=1

Figure 9 shows the locations of the seven surface stations used in the CALMET simulations. The stations on the western side of the domain are clustered very close together. We recommend that only one station representative of the area be chosen to avoid the effects that may be introduced by differences in meteorological measurements among these stations. Averaging among these stations could cause unrealistic perturbations in the predicted winds near these stations if the measurements (particularly wind direction) differ from station to station. These types of perturbations can also happen when surface observations differ from the WRF predicted fields.

During our examination of the SURF.DAT file we noted two items of potential concern. First, several stations in the SURF.DAT file contained wind speed data reported only to the nearest whole number m/s. This level of resolution is not, in our experience, typical. Next, we noted that there were significant differences in wind speed and wind direction among the four stations located near Sasol Sasolburg Ecopark. Given the close proximity of these stations to each other and the absence of significant terrain features in the area, this degree of variability is larger than we would expect and should be considered when reviewing modeling results.

4.3 CALMET Wind Fields

Figure 10 shows layer 1 wind fields from WRF and CALMET for September 11, 2013 at 3:00 am local time for a portion of modeling domain around the Secunda region. The WRF wind field is shown on the left, and the CALMET wind field is shown on the right. Although the overall wind fields are similar, there are notable differences in wind direction in the region near the three surface stations. These differences are due to the insertion of observations from these stations to the first guess CALMET field. This can occur if the observed winds are not adequately resolved by the mesoscale model data. The quality of the surface measurements and instrument siting issues can also play a role in causing differences of this sort. For example, if an observation station measures a highly localized flow, such as flow around an obstacle, the flow will not likely be resolved in the mesoscale model data (i.e., the WRF data).

The phenomenon shown in Figure 10 is offered as an example of what can occur when observations are used. We did not attempt to determine how frequently or how widespread this may be in the data set used in the modeling.

We recommend that wind fields be examined if the CALPUFF simulations produce unusually large concentrations to determine if the impacts might result from anomalous wind perturbations that can arise due to differences in model wind fields and observational data and/or differences among nearby observational stations.

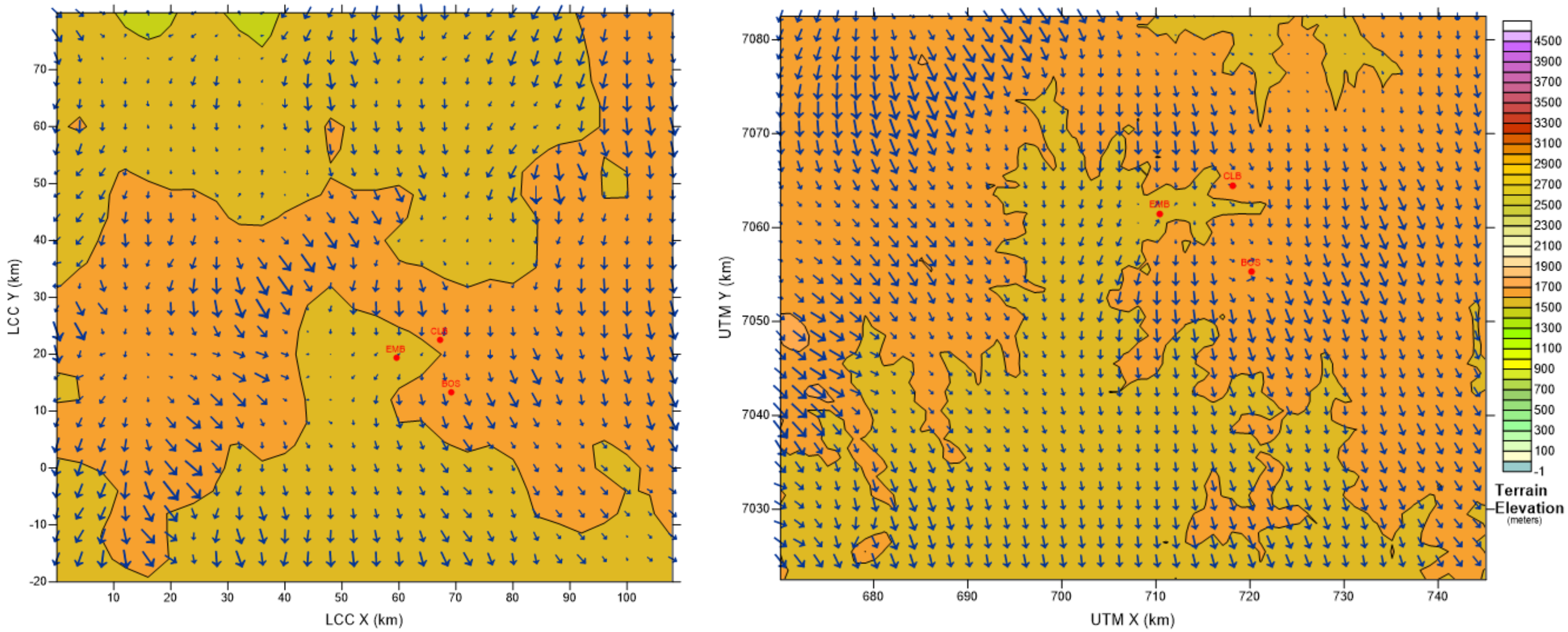

Figure 10 WRF layer 1 wind field (left) and CALMET layer 1 wind field (right) for September 11, 2013 at 300 am local time.

5 CALPUFF Model Options

CALPUFF version 6.42 (level 110325) was used for the air quality impact studies described in the AIRs. Use of this version of CALPUFF is consistent with requirements in the Code of Practice.

We note that Version 7.2.1 of the CALPUFF model was released in June 2015. Version 7.2.1 represents an update of the prior Version 6.42 code. Version 7.2.1 implements some new modeling options such as the ability to model roadways and flares and also fixes known coding errors in the prior Version 6.42 CALPUFF code. Since Version 6.42 contains some known bugs, we recommend that Version 7.2.1 be used for modeling studies. We recommend that the South African Department of Environmental Affairs (DEA) be consulted to determine if they would accept use of the current updated version of the CALPUFF model code (Version 7.2.1) for future modeling analyses.

A 3-year period (January 1, 2013 to December 31, 2015, (UTC+0200)) was executed in a single model run. The model input files specified an end time of December 31, hour 23. Version 6 and 7 of the CALPUFF code include explicit start and end times. As a result of using hour 23 as the end time, the run stops at 11:00 pm on December 31st and is one hour short of the full 3-year period. Completion of all 8760 hours during year 2015 would require an end time of Jan 1, 2016, hour 0. The impact of this one missing hour at the end of the meteorological dataset on the final results would be expected to be extremely small and it is noted here mainly for future reference.

Consistent with the CALMET runs, the projection is UTM-35 South, WGS84 datum. The modeling used default options for most variables with exceptions noted in Table 6 below. More details are provided in the following sections that discuss recommendations that differ from the present model setup.

Table 6 Summary of CALPUFF Options Selected that differ from Default Values

Variable	Description	Default Value	AIR Value	Comments
METRUN	Option to run all periods found in the met. file	0	1	Appropriate
NSPEC	Number of chemical species	5	7	Appropriate for MESOPUFF chemistry (5) plus 2 inert species of PM and CO.
MRESTART	Control flag for restart file	0	2	Appropriate
MDISP	Method used to compute dispersion coefficients	3	2	Appropriate
MPDF	PDF used for dispersion under convective conditions?	0	1	Appropriate when MDISP=2
MREG	Test options specified to see if they conform to regulatory values?	1	0	Appropriate for non-USEPA application
MXNEW	Maximum number of slugs/puffs release from one source during one time step	99	25	May not result in robust calculation of pollutant concentrations. See discussion in Section 2.4
MXSAM	Maximum number of sampling steps for one puff/slug during one time step	99	10	May not result in robust calculation of pollutant concentrations. See discussion in Section 2.4

5.1 Gridded Receptors

The computational grid specified in the CALPUFF modeling file covers a 50 km x 50 km square region. The gridded receptors are defined using a sampling grid which covers the same range with MESHDN set to 5 (200-meter spacing). Sampling grid receptor elevations are computed within CALPUFF based on the original CALMET 1 km resolution terrain data. This resolution will limit the precision of the elevation estimates, especially in areas of complex terrain. The use of discrete receptors would allow calculation of higher resolution terrain elevations directly from the original digital elevation model files.

Predicted concentrations in the draft AIRs are only presented at a limited number of discrete receptors representing sensitive locations. It appears that the gridded receptors are being used exclusively for producing contour plots. If the gridded receptors are to be used in the future for determining peak concentrations at locations other than the specified sensitive receptors, the uniform 200m spacing used for the gridded receptors does not satisfy the recommended receptor grid spacing listed in the Code of Practice. In order to ensure that peak impacts are resolved while maintaining a reasonable number of receptors, the Code of Practice recommends the use of nested Cartesian grids with higher resolution near the source and decreasing resolution further away. The suggested grid resolutions are summarized in Table 7.

Table 7 Receptor Spacing Recommended in Code of Practice

Resolution	Location
50m	General area of maximum impact, property boundary, and in steep terrain
100m	5 km from the facility of interest
250m	10 km from the facility of interest
1,000m	Beyond 10 km from the facility of interest

The use of receptors spaced at 200m intervals may not be adequate to locate and resolve peak impacts in the near field. Additional receptors with a finer spacing might be needed for this purpose. We also note that a resolution of less than 50m might be needed along property boundaries to locate maximum impacts. Nested grids centered on the facility or on a point of peak impact can be implemented using discrete receptors with terrain elevations calculated with the TERREL processor. Discrete receptors along the property boundary can also be implemented using discrete receptors. Flagpole receptor heights for discrete receptors should be set at ground level (0.0 meters).

In summary, the gridded receptors spaced at 200m intervals may not adequately determine peak concentrations. If peak concentrations are needed at locations other than the discrete sensitive receptors identified in the AIRs, then additional modeling with higher receptor density may be needed.

5.2 Building Downwash

The CALPUFF modeling analyses included building downwash effects for some sources. In cases where building downwash was modeled, the option MBDW=1 was selected, indicating that ISC model downwash algorithms were used. Building information is provided in Subgroup 13c in CALPUFF and includes the variables HEIGHT, WIDTH, LENGTH, XBADJ, and YBADJ. The variables LENGTH, XBADJ, and YBADJ are provided by the BPIPRM preprocessor, and these variables are required for running the PRIME downwash algorithm whose use is identified as the preferred option in the Code of Practice. Even though values for LENGTH, XBADJ, AND YBADJ were provided in Subgroup 13c, the specification of MBDW=1 means that these values were ignored and that the less refined ISC downwash option was used by CALPUFF. In order to use recommended PRIME downwash algorithm, MBDW should be set equal to 2.

The draft AIR for Secunda describes screening modeling that was conducted to justify limiting the number of stacks for which building downwash effects were included in the CALPUFF modeling analyses. The screening modeling was conducted using ScreenView, a Lakes Environmental GUI for the EPA screening program SCREEN3. SCREEN3 is based on ISC3, an earlier generation plume model that was later replaced by AERMOD. The draft AIR states that ScreenView (SCREEN3) includes the same building downwash scheme as CALPUFF. Although SCREEN3 does allow the user to select either the ISC or Schulman-Scire downwash algorithms, it does not contain the PRIME downwash algorithm that is recommended by the Code of Practice for use in CALPUFF. We note that the use of the PRIME downwash algorithm is also preferred on technical grounds. The screening analysis that was conducted to justify limiting the number of stacks for which building downwash effects were included in the CALPUFF analyses used a screening model that is not consistent with the recommended building downwash option in CALPUFF. A screening analysis using the PRIME downwash algorithm could be implemented using AERSCREEN, the screening version of AERMOD. However, predicted impacts at the specified discrete receptors may not be affected to a large extent by the particular downwash algorithm employed, if any, since the discrete receptors are fairly distant from the modeled sources. However, impacts predicted in the near field would be more likely to be affected by building downwash effects and by the selection of a particular downwash algorithm.

5.3 Deposition

Wet and dry deposition were calculated for all sources reviewed. Deposition accounts for material that is removed from the plume due to deposition on ground or vegetation surfaces. For wet deposition, only the scavenging coefficients for liquid precipitation are specified in CALPUFF as listed below:

Scavenging coefficients in the CALPUFF control file are:

```
!  SO2 =    3.0E-05,      0.0E00 !
!  SO4 =    1.0E-04,      0.0E00 !
! HNO3 =    6.0E-05,      0.0E00 !
!  NO3 =    1.0E-04,      0.0E00 !
! PM10 =    1.0E-04,      0.0E00 !
```

These coefficients are appropriate for liquid precipitation but not for frozen precipitation. Although frozen precipitation such as snow or hail may not typically occur often within this domain, the default scavenging coefficients for frozen precipitations should be included in the CALPUFF control file. The default frozen precipitation coefficients are $3x10^{-5}$ for the particulate species SO_4, NO_3 and PM_{10}.

Although inclusion of deposition in the modeling would be expected to provide more accurate results, the Code of Practice states ***"Unless deposition fluxes are of importance to the***

modelling study, pollutant deposition must not be modelled in licensing applications.” Accounting for deposition will deplete pollutant mass from the plume and provide a more refined analysis of final airborne concentrations. An application where deposition is not included will be conservative. Given the language in the Code of Practice, the AIR should justify the use of plume depletion and discuss why it is appropriate for this evaluation.

5.4 Model Sampling Step and Puff Limits

CALPUFF is structured to emit pollutants in a series of puffs, with the total emissions over an hour divided among ‘n’ separate puffs. The model time step (3600 sec, equal to one hour, in this application) is also divided into smaller sampling steps. Proper transport and dispersion of the plume requires the transport distance of an individual puff to be small enough to allow the puff to react to local meteorology and land use so that the puffs passing any particular point can be sampled in a manner consistent with a continuous plume. CALPUFF includes several parameters that control the frequency with which puffs are generated by the model. These values are included in input group 12 and are summarized in Table 8.

Table 8 Puff Parameter Values Used in CALPUFF

Variable Name	Description	Default Value	Modeled Value
XMXLEN	Maximum length of a slug (meteorological grid units)	1.0	1.0
XSAMLEN	Maximum travel distance of a puff/slug (in grid units) during one sampling step	1.0	1.0
MXNEW	Maximum Number of slugs/puffs released from one source during one time step	99	25
MXSAM	Maximum Number of sampling steps for one puff/slug during one time step	99	10

XSAMLEN will limit the puff transport distance to be no more than one meteorological grid cell (1 km in this application) during a sampling step. The values of MXNEW and MXSAM serve as caps on the total number of puffs released during a time step. The default values are large enough that they generally will not limit the number of puffs being generated. However, the non-default values selected in this case are much smaller and will result in transport distances greater than 1 km during certain meteorological conditions. We recommend use of the default values for these parameters in order to ensure sufficient resolution for the released puffs.

Sensitivity tests have been performed in order to estimate the impact of the selected non-default values for these variables (MXNEW and MXSAM). Two stacks were modeled, one 30 meters tall and the other 250 meters tall. A 6-month period (January – June 2013) was modeled using the default values of these variables and the alternate values that were used by AirShed. Concentrations were predicted at the 51 discrete receptors representing sensitive locations. The maximum 1-hour concentrations and the 44th ranked 1-hour (comparable to an 88th rank value when modeling a full year) concentrations from each simulation were compared to assess the effect of the different variable values.

Figure 11 and Figure 12 provide scatter plots comparing the concentrations predicted for the default and alternate variable values. Figure 11 provides results for the modeled 30 meter stack, and Figure 12 provides results for the modeled 250 meter stack.

Based on these tests, we conclude that the use of the non-default variables produce only slightly degraded results. The comparisons for the 44th ranked values show less variability than those for the maximum values. For each stack, there is no consistent bias, either high or low, in the concentrations.

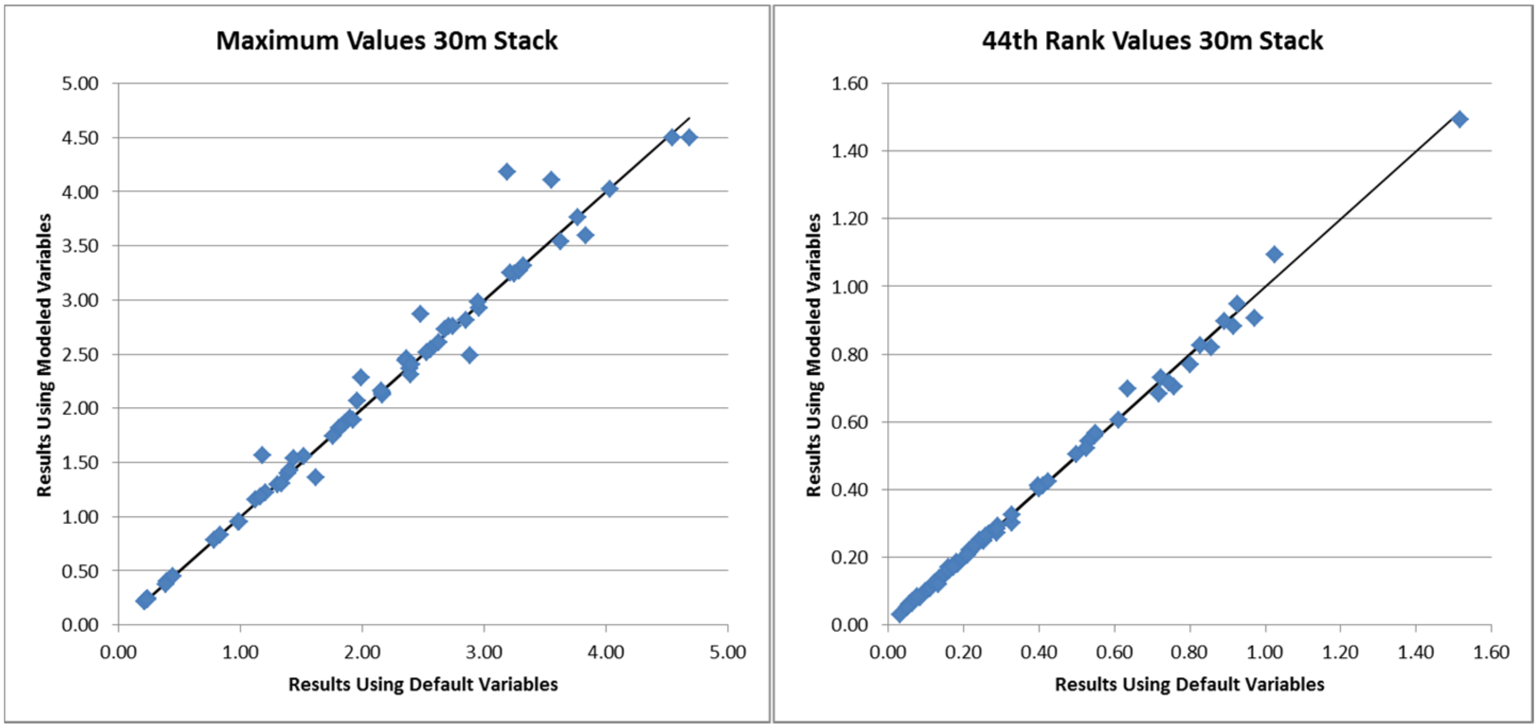

Figure 11 Comparison of results when using modeled and default values of MXNEW and MXSAM for a 30 meter stack.

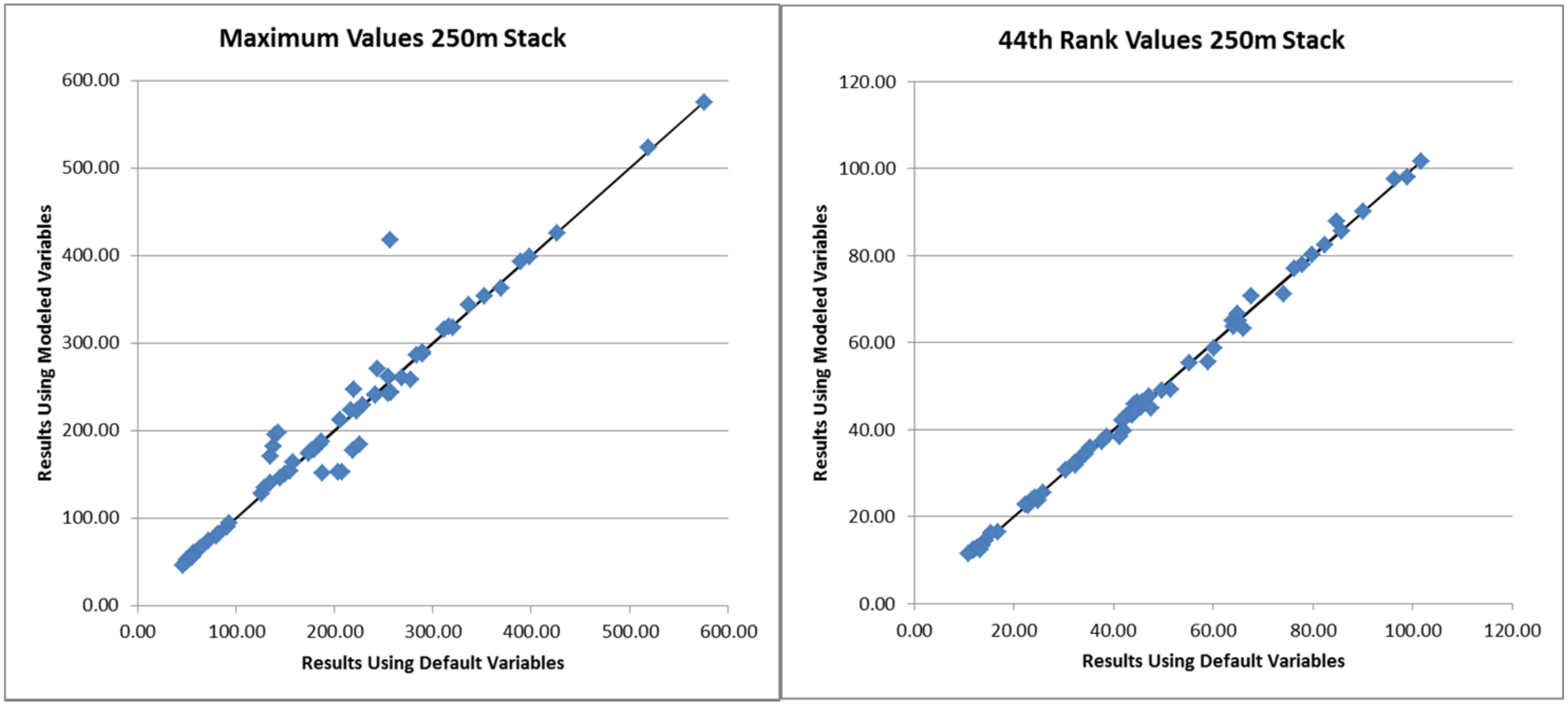

Figure 12 Comparison of results when using modeled and default values of MXNEW and MXSAM for a 250 meter stack.

6 CALPOST Options

The provided CALPOST.INP files were reviewed to determine the CALPOST model option settings that were used. As stated in the AIR, CALPOST version 6.292 was used. A newer version of the CALPOST code (7.1.0) was released in June 2015. This newer version should be considered for future modeling, but the only updates involved changes to ensure compatibility with the newly release CALPUFF version (7.2.1). There were no substantive changes to the code which would affect modeled results.

6.1 NO_2 Concentrations

The CALPOST input files specify NO2CALC=1, meaning that a fixed NO_2/NO_x ratio was used in the modeling. The specification of RNO2NOX=1.0 means that the NO2/NOx ratio used in the modeling was equal to 1.0. The use of full NO_x to NO_2 conversion is a Tier 1 technique, as described in the Code of Practice, and would be expected to overestimate NO_2 concentrations.

The draft AIR states that a more refined analysis employing the Ambient Ratio Method (ARM) was used to determine NO_2 concentrations. ARM is an acceptable refinement that is allowed by the Code of Practice. ARM can be implemented in CALPOST either by setting NO2CALC=1 and specifying the NO_2/NO_x ratio other than 1.0 or by setting NO2CALC=2 and defining separate bins with NO_2/NO_x ratios that depend on predicted concentration.

Appendix F of the AIR describes the use of NO_2/NO_x ratios defined for various bins with ratios extracted from Scire and Borissova (2011). The AIR describes the technique as "the second version of the DEA Tier 2 option." While the use of NO_2/NO_x ratios that vary with predicted NO_x concentrations is supportable on technical and scientific grounds, it is not clear that the Code of Practice explicitly allows for this technique. Rather, the Code of Practice describes either using default conversion ratios or defining site-specific ratios based on ambient monitoring. We recommend that the discussion regarding the acceptability of the selected technique be expanded.

In any case, based on the specified option setting for NO2CALC in CALPOST, it is evident that the CALPOST runs used a constant NO_2/NO_x ratio of 1.0. We assume that the ARM method calculations must have been applied in a separate, external, post-processing step. These calculations were not provided, so we are not able to confirm their accuracy.

7 Uncertainties

Appendix I of the AIR identifies the primary areas of uncertainty relevant to this modeling study. Specifically it reviews the uncertainties present in the observed meteorological data, modeled WRF fields, and the source emissions data. Appendix I discusses the steps taken to ensure that the model inputs are representative of conditions at the site and consistent with best practices. These three data elements represent the most important sources of uncertainty in the model inputs and are well described in the AIR. The data used in the AQIS appear to be sufficient and representative for regulatory air dispersion modeling purposes, and the uncertainties therein are typical for this type of evaluation.

The AIR also notes that uncertainty in the model results also includes uncertainty based on the use of computational models to represent atmospheric processes that are, by their nature, highly chaotic and variable. In order to assess the reliability of the complete modeling process, the AIR included a comparison of modeled concentrations with monitored values using the fractional bias method, a method recommended by USEPA for model evaluation. The modeled values used in this comparison included a component for background air quality concentrations. Including background in the comparison is appropriate in this context.

The fractional bias analysis demonstrated the modeled results to be within a factor of two of the observations and showed performance which is generally considered acceptable for regulatory purposes. This was true even though the comparison made at the monitor would be matching concentrations in space, but not in time, which is a test more stringent than generally required of regulatory models.

Exponent did not review the background air quality data, analysis, or the fractional bias calculations presented in the AIR. The files necessary to conduct these reviews were not provided to us, and these tasks were beyond the scope of the requested services.

8 References

Atmospheric Impact Report: Sasol Secunda Synfuels Operations. Report No. 16SAS03, Rev. 0, December 2016.

Atmospheric Impact Report: Sasol Sasolburg Operations. Report No. 16SAS01, Rev. 0, December 2016.

Atmospheric Impact Report: Natref. Report No. 16SAS02, Rev. 0, December 2016.

Emery, C., E. Tai, and G. Yarwood, 2001: Enhanced meteorological modeling and performance evaluation for two Texas ozone episodes. ENVIRON International Corporation, Novato, CA.

Lakes Environmental Software, 2015. Lakes Environmental WRF Modeling.

Scire, J.S. and M. Borissova, 2011: An Empirical Method for Modeling Short-Term and Annual NO2 Concentrations in Regulatory Models. Energy & Environment Conference (EUEC), Phoenix, Arizona. February 2011.

Scire, J.S., F.R. Robe, M.E. Fernau and R.J. Yamartino, 2000: A User's Guide for the CALMET Meteorological Model. (Version 5.0). Earth Tech., Inc. Concord, MA.

Scire, J.S., D.G. Strimaitis and R.J. Yamartino, 2000: A User's Guide for the CALPUFF Dispersion Model. (Version 5.0). Earth Tech, Inc., Concord, MA.

Tesche, T. W., D.E. McNally, C.A. Emery, E. Tai. 2001: Evaluation of the MM5 Model Over the Midwestern U.S. for Three 8-hour Oxidant Episodes, Prepared for the Kansas City Ozone Technical Workgroup. Alpine Geophysics, LLC, Ft. Wright, KY and ENVIRON International Corp., Novato, CA.

Wilmott, C.J., 1981: On the validation of models, *Phys. Geogr.*, 2, 168-194.

AIRSHED PLANNING PROFESSIONALS

Tel: +27 (0)11 805 1940
Fax: +27 (0)11 805 7010

Address: 480 Smuts Drive, Halfway Gardens
Postal: P O Box 5260, Halfway House, 1685

PART C

19 January 2017

Attention: Avishkar Ramandh

Subject: Response to Comments Raised by Independent Peer Review of the Dispersion Modelling Methodology Used in Support of the Sasol Atmospheric Impact Reports

An independent peer review of the dispersion modelling methodology used in support of the Sasol Atmospheric Impact Reports was undertaken in November 2016 to January 2017. Responses to comments raised have been provided below.

I trust this meets with your consideration. Should there be any further concerns, please do not hesitate to contact us.

Yours sincerely,

Ms Reneé von Gruenewaldt | Dr Terri Bird | Dr Lucian Burger

Response to Comments Outlined in the Peer Review

1. WRF DATA

Comment:

"No documentation is provided regarding the data that were used for initial and lateral boundary conditions. No details of the model configuration and model nest(s) in the mother domain(s) were provided. The WRF data set used in the assessments was generated by Lakes Environmental. No documentation was provided in the AIRs for the selection of or rationale for model settings used in generating the WRF data. We recommend that additional information be provided regarding these items."

Response:

The model settings as provided by a third-party contractor (Lakes Environmental Software) are provided in Annexure 1.

2. CALMET

Comment:

"The surface stations on the western portion of the CALMET domain are clustered very close together and show considerable variability with respect to wind speed and direction. We recommend that a single station representative of the area be selected for use to avoid or minimize the effects of differences in meteorological measurements among these stations."

Response:

The data for the surface stations was checked for invalid and spurious information before being included into CALMET. Although varying wind fields was noted at the surface stations, there was no indication that the data was invalid. It is likely that the readings are different due to local effects that may be of importance close to receptors. All surface stations were therefore included in the modelling to take these local effects into account

3. CALPUFF

Comment:

"Gridded receptors were included in the modelling with a resolution of 200 meters. This resolution is less than what is required for near-field modelling by the Code of Practice."

Response:

The Code of Practice recommends the use of a multi-tier grids to capture maximum impacts in the model (Table 1). For this study a Cartesian grid of equal spacing was selected (200m resolution) in order to adequately display contour plots of the results. The resolution of the Cartesian grid was selected based on detail required to display contours for the entire modelling domain (50 km north-south and 50 km east-west) and computation time. In order to capture maximum concentrations at sensitive receptors within the modelling domain, schools, hospitals and clinics were modelled as receptor points. The approach thus captures maximum concentrations at sensitive receptors and provides a high resolution for the entire domain for contour purposes.

Table 1: Recommended grid spacing for receptor grids

Resolution	Receptor Spacing
50 m	General area of maximum impact, property boundary and over steep terrain
100 m	5 km from the facility of interest
250 m	10 km from the facility of interest
1 000 m	Beyond 10 km from the facility of interest

Comment:

"When building downwash effects are included in the modelling, the ISC building downwash method (MBDW=1) was used. We recommend that a building downwash analysis be conducted for point sources below Good Engineering Practice (GEP) height using the BPIP-PRIME processor and that the Plume Rise Model Enhancements (PRIME) building downwash method (MBDW=2) be used to evaluate building downwash effects."

Response:

The ISC building downwash method is the default setting in CALPUFF. Based on this recommendation, a sensitivity analysis was subsequently conducted using CALPUFF in which a comparison was made between the ISC building downwash method, PRIME building downwash method and no building downwash. The findings showed that the ISC building downwash provided conservatively higher concentrations downwind, with the PRIME building downwash method more in line with results when modelled with no building downwash (Figure 1 and Figure 2). The final results at the nearby receptors were henceforth corrected with PRIME.

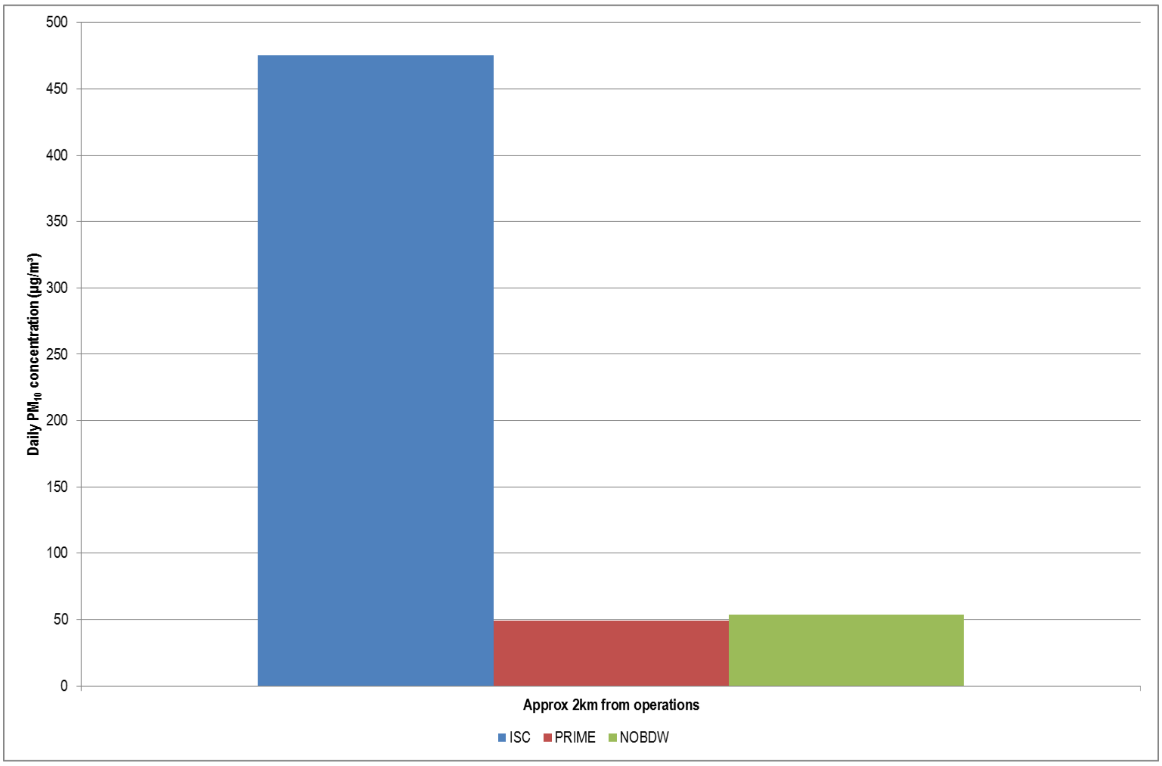

Figure 1: 99th percentile daily PM concentration approximately 2 km from source or three building downwash schemes

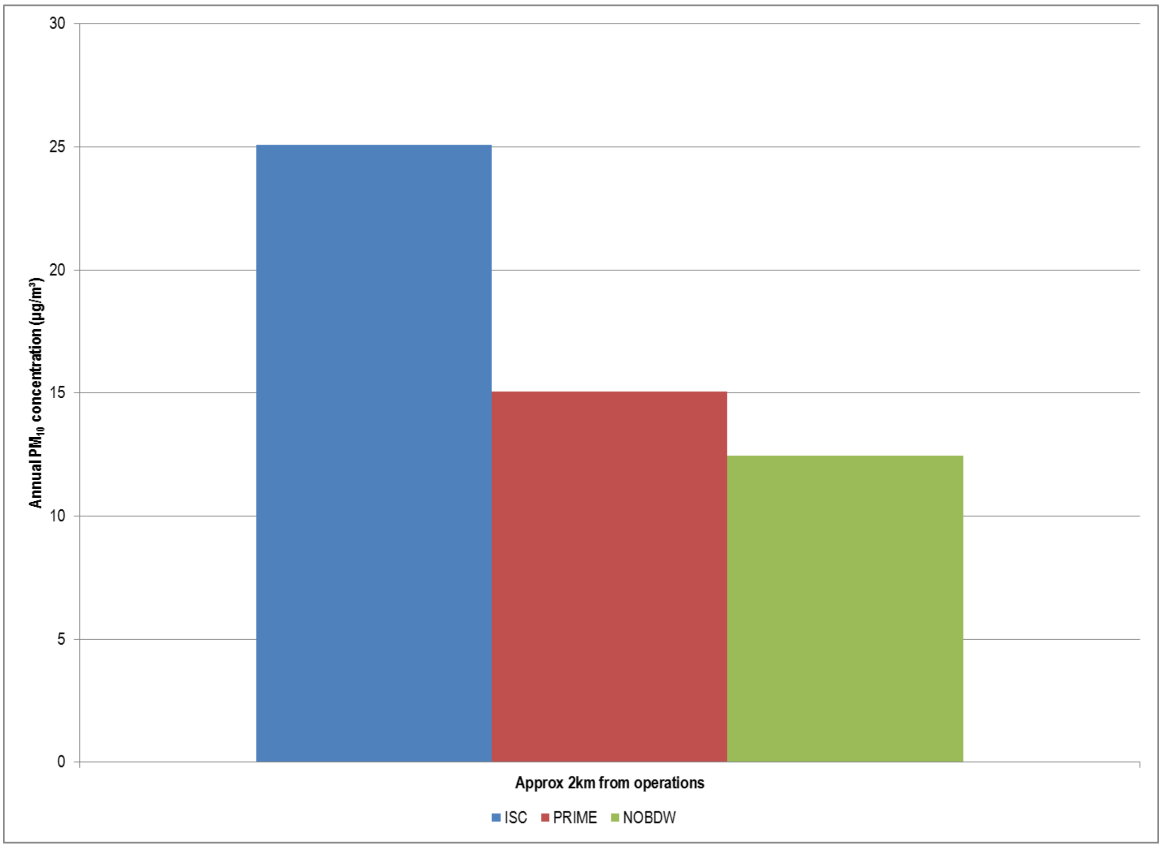

Figure2: Annual average PM concentration approximately 2 km from source for three building downwash schemes

Comment:

"The AQIS modelling included wet and dry deposition. This would be expected to yield more accurate and reliable results because it accounts for material removed from the plume by deposition on ground and vegetation surfaces. However, the Code of Practice states that deposition should not be included in modelling studies for licensing unless deposition fluxes are of importance."

Response:

The understanding of deposition was of importance to the study and hence the decision to include the deposition option in the CALPUFF model in the model.

Comment:

"Non-default options have been selected that control the number of puffs produced during a time step. These non-default values will limit the number of puffs produced by the model and may result in less robust calculations of airborne concentrations."

Response:

Due to the complexity of the model setup (e.g. number of sources, grid resolution, chemical transformation scheme, building downwash, and deposition). the number of puffs had to be reduced from default values to allow for reasonable run times of the dispersion model.

Comment:

"Only the scavenging coefficients for liquid precipitation are specified in CALPUFF…Although frozen precipitation such as snow or hail may not typically occur often within this domain, the default scavenging coefficients for frozen precipitations are recommended to be included in the control file, which are $3x10^{-5}$ *for* SO_4*,* NO_3 *and* PM_{10}*."*

Response:

Comment noted.

ANNEXURE 1: WRF MODELLING AT LAKES ENVIRONMENTAL

LAKES ENVIRONMENTAL WRF MODELING

DRAFT

1 Introduction

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

2 WRF Description

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

3 WRF Processing Specifications

3.1 Input of Meteorological Data

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

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

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

3.2 Nested Grids Domains

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

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

Table 1. WRF Nested Domain Grids

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

E-mail: info@webLakes.com
Web: www.webLakes.com

3.3 WRF Physics Options

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

Table 2. Physics Options Used for WRF Modeling

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

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

http://www2.mmm.ucar.edu/wrf/users/wrfv3.5/phys_references.html

3.4 Additional WRF Modeling Information

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

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

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

3.5 WRF Output for AERMET

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

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

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

Table 3. Files Generated by MMIF

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

E-mail: info@webLakes.com
Web: www.webLakes.com

3.6 WRF Output for CALMET

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

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

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

Table 4. Variables Available in 3D.DAT File

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

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

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

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

3.7 WRF Output for CALPUFF

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

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

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

E-mail: info@webLakes.com
Web: www.webLakes.com

4 Additional Information

If you require any further information, please contact us at support@webLakes.com. When contacting us, please provide the met data order number.

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

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