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

14 APRIL 2014

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.
- While most of Sasol's and Natref's processes will be able to comply with the future MES, there are selected activities for which Sasol and Natref will either be unable to comply within the stipulated compliance timeframes, or the specified emission limits at all.
- For these specific cases Sasol and Natref intend to apply either for a postponement or exemption to meet specific MES. In accordance with the provisions the NEM:AQA, 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 Atmospheric Impact Report (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 (not included in this report – please see Sasol Exemption & Postponement Motivation Documents Annexure B for a copy of this report)
    II. Part B - Airshed plan of study for the dispersion modelling for Natref
    III. Part C – Peer review report
    IV. Part D – Airshed response to peer review report

PART B

PLAN OF STUDY REPORT

In support of

An air quality impact study for Natref for postponement and exemption applications from minimum emission standards

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1 PROJECT DESCRIPTION

Sasol and Total South Africa are joint owners of the National Petroleum Refiners of South Africa (Natref) refinery in Sasolburg. Natref is 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) in March 2010, but which were amended in Government Notice No. 893 in November 2013. These standards require the refinery operations to comply with "existing plant" limits by 1 April 2015, and with more stringent "new plant" limits by 1 April 2020. Natref intends submitting an application for extension of the compliance timeframes in some cases, and an application for exemption from the Minimum Emission Standards in other cases. 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 postponement and exemptions.

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

The main air pollutants from Natref include sulfur dioxide (SO_2) and oxides of nitrogen (NOx), as well as particulate matter (PM)

1.1 Scope of Work

Airshed Planning Professionals (Pty) Ltd (hereafter referred to as Airshed) was appointed by Sasol on behalf of Natref to provide independent and competent services for the compilation of an Atmospheric Impact Report as set out in the Draft 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 Natref that the emission factors are deemed acceptable. Should measurements be required, Natref will source the required information. Additional sources could be added when new information becomes available.
2) It has been identified by Natref that the following point sources should be included within the Scope of Work:

Point source	Components
Natref refinery	
Main stack	Sulphur dioxide
	Particulate matter
	Oxides of nitrogen

3) Prepare meteorological input files for use in one or more dispersion models to cover the Natref site. Sasol will provide surface meteorological data and ambient air quality data from the Sasol ambient air quality monitoring stations in Sasolburg. Surface meteorological data for three years, as required by the draft Dispersion Modelling Guidelines for Level 3 Assessments, is available for ambient air quality monitoring stations situated in Sasolburg.
4) Preparation of one or more dispersion models set up with Natref's emissions inventory capable of running various scenarios for each of the point sources as specified by Natref, in conjunction with Sasol Technology's Research and Development Department. The intent is to model delta impacts of the various emission scenarios against an acceptable emissions baseline, for instance the Vaal Triangle priority areas DEA-approved baselines.
5) Airshed will validate the dispersion model based on an acceptable and agreed approach. The validation methodology must be agreed between Sasol and Airshed. It is anticipated that each point source identified above will require 3 scenarios per component per point source to be modelled, in order to establish the delta impacts against the DEA-approved baselines. i.e.:
    a) Current baseline – modelling is conducted based on the current inventory and impacts
    b) Compliance with MES – modelling must be conducted based on the legislative requirement as stipulated within the Listed Activities and Minimum Emission Standards (for both 2015 existing plant standards and 2020 new plant standards).
    c) Alternative emissions limits – the actual Natref proposed alternative emissions limits, where applicable and different from the other emission scenarios.
6) Comparison of dispersion modelling results with the National Ambient Air Quality Standards (NAAQS).
7) A report detailing the methodology used and model setup must be compiled for purposes of a peer review, which Sasol will contract independently.
8) Interactions with Environmental Assessment Practitioner (EAP) to provide all necessary inputs into the EAP's compilation of documentation in support of Natref's postponement and exemption 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 study area includes Sasolburg, where Natref is located, as shown in Figure 1-1. Figure 1-1 also illustrates the location of Sasol's other operations in Secunda, Ekandustria and Sasolburg.

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.

Figure 1-1: Locations of the Sasol study area centres at Sasolburg, Secunda and Ekandustria and Natref study area in Sasolburg

It can be appreciated that the definition of urban and rural conditions for the dispersion coefficients and wind profiles, on the one hand, and chemical reactions on the other, may not be the same. Nonetheless, it was decided to use the US Environmental protection Agency's (US 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 stack. Areas typically defined as rural include residences with grass lawns and trees, large estates, metropolitan parks and golf courses, agricultural areas, undeveloped land and water surfaces. An area is defined as urban if it has less than 35% vegetation coverage or the area falls into one of the use types in Table 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 is classified as urban.

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 the 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
	  o Understanding of their interaction
	  o 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

Competency	Task, Knowledge and Experience
	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 Draft Regulations Regarding Air Dispersion Modelling

The recommended regulatory models for South Africa (as provided in the draft regulations regarding air dispersion modelling guideline – Gazette No 35981 published 14 December 2012) are provided in Appendix A.

2.3 Sasolburg Site

2.3.1 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 Sasolburg site. It is also able to simulate secondary pollutant formation, such as sulphates and nitrates, using a parameterised, quasi-linear chemical conversion mechanism.

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.

2.3.2 Modelling Information

2.3.2.1 CALMET Model

Land Use

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

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).

Meteorology

The three-dimensional meteorological data will be calculated using PSU/NCAR mesoscale model (known as MM5) and surface field observations from monitoring stations operated by Sasol (i.e. Leitrim, AJ Jacobs and Sasol 1) in Sasolburg for the meteorological period 2010, 2011 and 2012. MM5 is a limited-area, non-hydrostatic, terrain-following sigma-coordinate model designed to simulate or predict mesoscale atmospheric circulation. The model is supported by several pre- and post-processing programs, which are referred to collectively as the MM5 modelling system.

The MM5 data was obtained from Lakes Environmental (Canada), and was prepared for a modelling domain of 300 km (East-West) by 300 km (North-South). The meteorological information was supplied on a horizontal grid spacing of 12 km.

Table 2-2: Ambient monitoring stations operated by Sasol in Sasolburg

Station Name	Latitude	Longitude
Sasol One Fence Line	-26.834722	27.848611
Leitrim	-26.850278	27.874167
AJ Jacobs	-26.818056	27.848611

Grid Resolution and Model Domain Size

The CALMET model domain selected for the Natref facility in Sasolburg included an area of 300 km by 300 km. The horizontal grid resolution is 1 km with 10 vertical levels, *viz.* 20m, 40m, 80m, 160m, 300m, 600m, 1000m, 1500m, 2200m and 3500m.

Model Control Options

A summary of the model control options for CALMET is provided in Table 2-2. The option of *Partial Observations* was selected, which used both MM5 data as well as Sasol's surface meteorological station data.

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 MM5 to drive CALMET. •No surface or upper air observations input at all.	•Relatively simple to implement in model •Representative of regional meteorological conditions	MM5 data (Lakes Environmental) for 2010, 2011 and 2012 at 12km resolution for 300km by 300km study area (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	•More difficult to implement than only prognostic (MM5) data. •Require 7 site-specific model parameters to be specified.	•MM5 data (Lakes Environmental) for 2010, 2011 and 2012 at 12km resolution for 300km by 300km study area	•Full spatial and temporal variability •No overwater data required •Refined model run as using combined approach of	•Surface data, especially winds may be different to that in the MM5 data file •User must include 7

Run Type	Description of Run Type	Ease of Use and Representativeness	Data availability	Advantages	Disadvantages
	PLUS •One or more surface stations	•Difficulty in dealing with missing data. •Potential disagreement between prognostic and surface observations. •Very representative and considered 'refined modelling'	(Sasolburg) •Sasol operated surface meteorological weather stations (3 Sasolburg[1])	numerical model and observations. •Ability to incorporate surface representative observation data when MM5 data is too coarse to fully pick up local effects.	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	•Sasol operated surface meteorological weather stations (3 Sasolburg) •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

[1] Steam Station 1 (WS, WD, TEMP, RH,AMB PRESS, SOL RAD, RAIN); AJ Jacobs (WS, WD,SO_2, NO_2, PM_{10}) and Leitrum (WS, WD,SO_2, NO_2, PM_{10})

Run Type	Description of Run Type	Ease of Use and Representativeness	Data availability	Advantages	Disadvantages
		and site specific choice of parameters by the modeller.			time of the day. •User has to deal with missing surface and upper air data

2.3.2.2 CALPUFF Model

Grid Resolution and Model Domain Size

The model domain selected for the point sources at Natref 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.

Source Information

All source information for the refinery is to be provided by Natref.

The three main scenarios to be assessed are as follows:

- *Current baseline* – modelling based on the current emissions inventory;
- *Compliance with MES* – modelling based on the legislative requirement as stipulated within the Listed Activities and Minimum Emissions Standards (for both 2015 existing plant standards and 2020 new plant standards).
- *Alternative emissions limit* – modelling based on Natref's proposed alternative emissions limits, where applicable and different from the other emission scenarios.

Model Control Options

A summary of the model control options for CALPUFF is provided in Table 2-3.

Since the study area is 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 (NOx) must be modelled in order to estimate total NO_2 concentrations. The concentration of NO in Natref's stack exhausts are typically >98%, but reacts fairly rapidly with background ozone in the plume to form NO_2. This reaction occurs at night.

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	• Dispersion coefficients are computed from	• This option can simulate AERMOD-type dispersion	• The data is obtained from MM5 input	• Based on improved theoretical work and is an	• The coefficients are derived from other

Run Type	Description of Run Type	Ease of Use and Representativeness	Data availability	Advantages	Disadvantages
coefficients MDISP = 2	internally-calculated sigma-v, sigma-w using micrometeorological variables (u*, w*, L, etc.).	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 land use characterization.	information.	improvement over Pasquill-Gifford.	parameters.
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

Run Type	Description of Run Type	Ease of Use and Representativeness	Data availability	Advantages	Disadvantages
					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 RH-dependent.	• 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 from a network of stations, or (2) a single	• 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. • The model is restricted

Run Type	Description of Run Type	Ease of Use and Representativeness	Data availability	Advantages	Disadvantages
			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.		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 NO_2 conversion is not included in model.

Run Type	Description of Run Type	Ease of Use and Representativeness	Data availability	Advantages	Disadvantages
User-specified diurnal cycles of transformation rates					
No chemical conversion					

Since the MESOPUFF II scheme does not distinguish or simulate the conversion from NO to NO_2, the predicted NOx 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 NO2 concentrations by assuming a total conversion of NO to NO_2. If the maximum NOx concentrations are less than the NAAQS for NO_2, then no further refinement of the conversion factor is required. If the maximum NOx 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 NOx by a national ratio of NO2/NO. = 0.80

Assume a wide area quasi-equilibrium state and multiply the Tier 1 empirical estimate NOx by a ratio of NO_2/NOx = 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/NOx conversion factors described by Scire and Borissova (2011) as given in Table 2-5, will be employed. Observed NO_2/NOx ratios at the Sasolburg monitoring stations will also be analysed and compared to the factors in the table.

Table 2-5: Recommended NO2/NOx conversation ratios for short and long-term NOx concentration predictions (Scire and Borissova 2011)

Bin	Concentration (µg/m³)			NO_2/NOx 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

Bin	Concentration (µg/m³)			NO_2/NOx Ratios		
	Min	Max	Centre	Bin Average	1-Hour Max [1]	Annual Average
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
Lead (Pb)	1 year	0.5	0	Immediate
Nitrogen Dioxide (NO_2)	1 hour	200	88	Immediate
	1 year	40	0	Immediate
Ozone (O_3)	8 hour[(b)]	120	11	Immediate
$PM_{2.5}$	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 and PM_{10} measured in the vicinity of Natref's 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.

Although all major air emission sources from Natref would be included in the dispersion simulations, a number of small emitters may have been excluded, and when combined, may potentially add up to be a significant portion. It is therefore expected that the observed pollutant concentration levels would be higher than the predicted 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 99^{th} 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 50^{th} 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 2010, 2011 and 2012 to the monitoring data collected over the same time period. In particular, the predicted SO_2 and NO_2 concentrations in Sasolburg 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 99th 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 (FB_{means}) on the X-axis and the standard deviations (FB_{stdev}) 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 ($C_{Background}$). The change in concentration from any of the future scenarios ($C_{Future\ Scenario}$) compared to the baseline scenario ($C_{Baseline\ Scenario}$) 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 NOx concentrations would be converted to NO_2 by using the NO_2/NOx conversion factors described by Scire and Borissova (2011) (Table 2-5) as default. In addition, NO_2/NOx ratios observed at the monitoring stations in Sasolburg 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/NOx 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 Natref's activities will 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.

APPENDIX A – DRAFT REGULATIONS REGARDING AIR DISPERSION MODELLING

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.

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.

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.

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 (σ_v and σ_w) (ii) similarity theory to estimate σ_v and σ_w, (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.

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

PART C

Review of the Sasol Atmospheric Impact Report

April 11, 2014

Exponent

Review of the Sasol Atmospheric Impact Report

April 11, 2014

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Contents

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
DEA	Department of Environmental Affairs
GEP	Good Engineering Practice
GUI	Graphical User Interface
km	kilometer
MM5	Mesoscale Model Version 5
m	meter
µg	microgram
mb	millibar
MRF	Medium Range Forecast
PBL	Planetary Boundary Layer
PDF	Probability Density Function
PM	Particulate Matter
PRIME	Plume Rise Model Enhancements
RH	relative humidity
U.S. EPA	United States Environmental Protection Agency
UTC	Coordinated Universal Time
UTM	Universal Transverse Mercator
WRF	Weather Research and Forecasting Model

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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 by the client during the period January 30, 2014 through April 10, 2014. Exponent reserves the right to supplement this report and to expand or modify opinions based on review of additional material as it becomes available through any additional work or review of additional work performed by others.

1 Introduction

Sasol Limited (Pty) Ltd. owns and operates facilities in South Africa at Secunda in the Province of Mpumalanga and at Sasolburg in the Province of the Free State. The company is required to comply with certain Minimum Emission Standards that are part of the South African regulatory framework. For existing facilities, compliance with the Minimum Emission Standards is required by April 1, 2015 and for new plants by April 1, 2020 by Section 21 of the National Environment Management: Air Quality Act (Act No. 39 of 2004).

Air quality dispersion modeling is being conducted by Airshed Planning Professionals (Pty) Ltd. of South Africa (Airshed), and an Atmospheric Impact Report (AIR) is being prepared. The AIR is required to document the basis for Sasol's application pursuant to Section 59 of the Air Quality Act for a postponement of the Minimum Emission Standards in cases where compliance with the relevant standards can ultimately be achieved but not within the prescribed timeframe. For other emissions sources where compliance with the minimum standards is not achievable due to technical, environmental, resource, or capacity constraints, an exemption will be applied for in accordance with the Air Quality Act.

Exponent, Inc. has been retained to conduct a peer review of the methodology used in the air quality impact study (AQIS) by Airshed. Airshed's study includes modeling of the Secunda facility, the Sasolburg facility, the Natref joint venture refinery and the Ekandustria site. The scope of the Exponent review includes a review and comments on the following:

- Modeling techniques used in the AQIS and their appropriateness for this application;
- Background air quality data used in the study;
- Prognostic meteorological data and observational data;
- CALMET, CALPUFF, CALPOPST switch settings and model options;
- Model validation techniques and any obvious information gaps, omissions or inaccuracies;
- Alternative viewpoints; and
- Key assumptions and uncertainties.

Background information on the project was provided January 30, 2014 including the South African National Framework for Air Quality Management, the Air Quality Act, Minimum Emission Standards, Ambient Air Quality Standards and draft modeling guidelines. An initial set of modeling files was provided to Exponent on February 27, 2014 and additional modeling files submitted on March 11, March 20, April 8 and April 10, 2014. A draft AIR for the Sasol Secunda Facility (Synfuels) dated February 2014 was provided to Exponent on February 28. A second draft Secunda AIR was provided on April 8. A draft modeling report on the Ekandustria site based on the AERMOD model was provided on April 7. Documents for the other facilities were not available for this review. Draft documents with Airshed's

preliminary response to comments were provided on April 9 and April 11. The information used in the review was limited to the data provided in these documents and the modeling files described above.

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. Following the description of the comments is a ranking of the significant of the main comments.

1. CTGPROC:
    a. Landuse processing has strings of gaps of missing landuse due to the resolution of the landuse data used. The CTGPROC input variable MESHGLAZ should be changed from 1 to 2 to eliminate the missing data crossing the domain. A new geophysical (GEO.DAT) file should be created after this change.
2. MAKEGEO:
    a. The soil heat flux parameter for landuse category 11 (Residential) should be 0.25 instead of 1.0
3. CALMET:
    a. There are discrepancies in the CALMET input files (CALMET.INP) regarding the number of surface stations used in the modeling (9 stations) vs. 2 stations found in the binary CALMET data file (ALLMET.DAT). The CALMET input files provided may be obsolete due to a decision to use only two stations. It is recommended the justification for the use of two stations be included in the report.
4. CALPUFF:
    a. Building downwash effects are not included in the modeling. It is recommended 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, except for any large or long buildings, where the ISC building downwash method (MBDW=1) is recommended.
    b. It is recommended that the Probability Density Function (PDF) be used with the turbulence-based dispersion coefficients (MDISP=2). The PDF is especially important for tall stack dispersion under convective conditions, which is a consideration in this application with both tall stacks and common convective atmospheric conditions.
    c. Wet deposition is used in an inconsistent manner in the modeling. This option is used for some of the sources but not for others. A consistent approach to the treatment of wet deposition is recommended, i.e., using it for all sources or turning the option off. Ignoring wet deposition will produce more conservative (higher) concentration estimates during periods of precipitation. However, it is likely including deposition effects will be

more accurate. Dry deposition is not modeled. Consideration should be given to include both wet and dry deposition. Not including deposition is discretionary as it will produce conservative air quality impacts.

d. There were some discrepancies in the concentrations provided in the draft Secunda reports vs those in the modeling files. Through an exchange of files and an explanation of the summary data provided in the second draft Secunda AIR, the discrepancies have been resolved (see Section 6 for details). The clarifications and corrections discussed should be reflected in the final AIR document.

e. When using the chemical conversion module to predict NO_x concentrations, it is preferred that the actual emission rates be used because of a non-linearity in the conversion rate equations. That is, the conversion rate depends somewhat on the NO_x concentrations in the puff, so the use of actual NO_x emissions will better characterize the chemical process. In practice, the non-linearity is relatively weak, but nonetheless, the recommendation is to avoid postprocessing scaling NO_x concentrations for emission rates.

5. POSTUTIL:

   a. The calculation of total particulate matter (PM) concentrations by summing primary PM and secondary PM (ammonium sulfate and ammonium nitrate) in the POSTUTIL processor requires the application of a molecular weight adjustment of 1.375 to change sulfate (weighed as SO_4 in the model) to $(NH_4)_2SO_4$ and 1.29 to change nitrate (weighed as NO_3 in the model) to NH_4NO_3.

6. CALPOST:

   a. The CALPOST input files provided do not show the application of the ambient ratio method, which applies NO_2/NO_x ratios as a function of NO_x concentrations to compute NO_2 concentrations from NO_x concentrations. The CALPOST files indicate NO2CALC=1, RNO2NOX=1.0, which would produce no scaling. We believe these files are not the final versions used in the draft Secunda report, but because of Item 4e above, we have not been able to confirm the calculations of NO_2 using the ambient ratio method.

Table 1. Ranking of Significance of Summary Comments

Significance		
High	Medium	Low
• Use PDF option (CALPUFF) • Include molecular weight adjustments in computing particle mass (POSTUTIL) • Updates to summary tables in AIR to reflect reconciliation of differences noted, including computation of NO_2 using ambient ratio method. (Report)	• Land use meshing factor (CTGPROC)	• Update soil parameter (MAKEGEO) • Consistent treatment of wet/dry deposition (CALPUFF) • Avoid scaling of N species when using chemistry (CALPUFF) • Building downwash (in the Secunda application, tall stack emissions dominate and short stacks subject to downwash have low emissions) (CALPUFF)

2 Choice of Modeling Techniques

The methodology being used in the air quality impact study is a Level 3 assessment as defined by the draft Department of Environmental Affairs (DEA) document entitled *Regulations Regarding Air Dispersion Modelling* (Gazette No. 35981 published on December 14, 2012). A Level 3 analysis uses more sophisticated modeling techniques in complex meteorological cases where a detailed understanding of the time and space variation of impacts is required. The guidance indicates that Level 3 studies are 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 inclnde 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 the air quality impact study. CALPUFF is one of the models recommended in the draft *Regulations Regarding Air Dispersion Modelling*. CALPUFF is well suited for the types of industrial sources and areas of interest in this study. CALPUFF is capable of providing 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 includes 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 (Mesoscale Model Version 5 (MM5) 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.

Steady-state Gaussian plume models such as AERMOD make assumptions that limit their applicability to near-field impacts with relatively simple flow conditions. The simplifying assumptions of plume models include that steady-state conditions exist during each time step, which results in straight-line trajectories that reach infinity each hour, lack of causality effects (i.e., neglecting the time it takes after emissions leave the stack to reach receptors than may be 5 km, 10 km or more from the source), 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. In most cases, steady-state plume models provide a conservative estimate of impacts. However, there are cases, including dispersion from tall stacks in simple terrain (Strimaitis, 2009) that show significant plume model underpredictions (close to a factor of two) in the Kincaid SF_6 tracer dataset by both AERMOD and the ISCST3 models.

3 Background Air Quality Data

Background concentrations are defined as concentrations due to sources not included explicitly in the air quality model. The sources that contribute to background concentrations include:

- Emissions from distant industrial facilities,
- Local and distant mobile sources (cars and trucks) including tailpipe emissions and emissions due to road dust, tire wear, etc.,
- Fugitive emissions from various leaks from valves and vents as well as fires from biomass burning, biogenic sources and wind erosion.

Especially for secondary particulate matter formed through chemical reactions of SO_2, NO_x or biogenic emissions, long range transport can be a significant source of PM_{10} and $PM_{2.5}$. Wintertime biomass fires can also be a major source of primary particulate matter as well as NO_x in South Africa.

Section 5.1.5.2 of the draft Secunda AIR discusses an estimation procedure for the short-term and long-term background concentrations which are presented in Table 5-12. The draft modeling guidance (DEA, 2012) does not provide specific recommendations on the approach to be used for assessing background concentrations. The AIR computes short-term background concentrations of SO_2 and NO_2 based on the 99th percentile monitored values for each year. For the annual average background, the observed hourly concentration at the percentile when the modeled concentration becomes zero (or 50th percentile, whichever is higher) was used to determine long-term (annual) background. The Draft Regulations Regarding Air Dispersion Modeling (DEA, 2012) does not discuss this methodology used in the AIR.

The information provided in the draft report was not sufficient to reproduce the calculations of the background values using the methodology described in the report. The methodology is different from the United States Environmental Protection Agency (U.S. EPA) procedures which involve three tiers of conservatism (Level 1 background is highly conservative and Level 3 is more refined). The Level 3 U.S. EPA methodology involves the use of wind direction to compute hours that are unaffected by modeled sources to determine hourly background values. It is not clear if the monitoring network is sufficient to obtain a Level 3 background estimation. However, the methodology used in the AIR is difficult to assess because we have been unable to reproduce the background values reported in the tables. In addition, the reliability of the method based on the 50th percentile hourly concentration (or the percentile for where the modeled concentration becomes zero) is untested.

4 MM5 Meteorological Data

4.1 MM5 Model Setup

Model grid resolution is 12 km with 18 vertical levels using a Lambert Conformal grid with an origin at 26.41 degrees South and 29.00 East. Standard parallels are at 30.00 degrees South and 60.00 degrees south. MM5 was configured with the Dudhia simple-ice microphysics, the Medium Range Forecast (MRF) Planetary Boundary Layer (PBL) scheme, and the multi-layer soil model. Analysis nudging is performed but no observation nudging. It is not stated in the AIR what data was used for initial and lateral boundary conditions or for the analysis nudging. Nor are the details of the model configuration and model nest(s) in the mother domain(s) provided. The MM5 data was generated by a third-party contractor. There is no report or documentation for this South African application of MM5 on the rationale for the model settings and no evaluation of the MM5 model performance relative to observations. Normally an evaluation of the MM5 modeling is conducted by the modeler conducting the simulations and referenced in the air quality dispersion modeling report. The software tools for conducting a quantitative evaluation of the MM5 or Weather Research and Forecasting (WRF) model is provided in the CALPRO Plus Graphical User Interface (GUI) in the CALTOOLS suite of utilities. An example of the type of analysis produced by the Meteorological Evaluation module is shown in Tables 2 and 3. The first table shows generally accepted benchmarks for average MM5 performance over an annual period for wind speed, wind direction, temperature and humidity. Table 3 is an example of actual model performance for MM5 simulations conducted in Europe for the year 2006. Often, this type of quantitative analysis is supplemented by qualitative analyses such as wind roses including seasonal and diurnal variations and vector plots.

4.2 Evaluation

Terrain contour analysis, for terrain used in the CALMET simulations at a resolution of 1 km grid compared to the 12 km resolution, shows that the 12 km resolution terrain captures the key broad-scale terrain features within the CALMET modeling domain. As one would expect, some details of the terrain features are lost in the 12 km resolution of the MM5 terrain. Figure 1 shows a comparison of the 1 km CALMET terrain and the 12 km MM5 terrain. Overall, the 12 km MM5 grid appears to be reasonable for use in the CALMET simulations. The lack of any qualitative or quantitative model evaluation of the MM5 dataset is a limitation of the dataset.

Use of only 18 vertical levels is much coarser than most MM5 simulations. Normally a minimum of 30 layers and often 40 or more layers are used. In the current application, the first layer is about 14 meters thick, the second layer is about 20 meters, the third layer is about 70 meters and the fourth layer increases to about 100 meters thick. Accordingly, the lowest layers are adequate to define 10 meter level winds, but the resolution quickly reduces with height. The proper vertical resolution is even more

important for determining the temperature structure of the atmosphere, which is a significant factor in boundary layer processes affecting plume dispersion, missing heights and boundary layer turbulence parameterizations. Coarse vertical resolution may limit the ability of MM5 to properly resolve elevated temperature inversions, cloud layers affecting surface radiation fluxes, precipitation and many other variables important for air quality modeling.

Table 2. Benchmarks for MM5 Model Evaluation

	Wind Speed	Wind Direction	Temperature	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

Table 3. Example of Evaluation Results for European MM5 Simulations for 2006

	Wind Speed	Wind Direction	Temperature	Humidity
IOA	0.85	-	0.97	0.90
RMSE	1.81 m/s	-	-	-
Mean Bias	0.13 m/s	2.25 deg	-0.38K	0.28 g/kg
Gross Error	-	27.5 deg	1.93K	1.25 g/kg

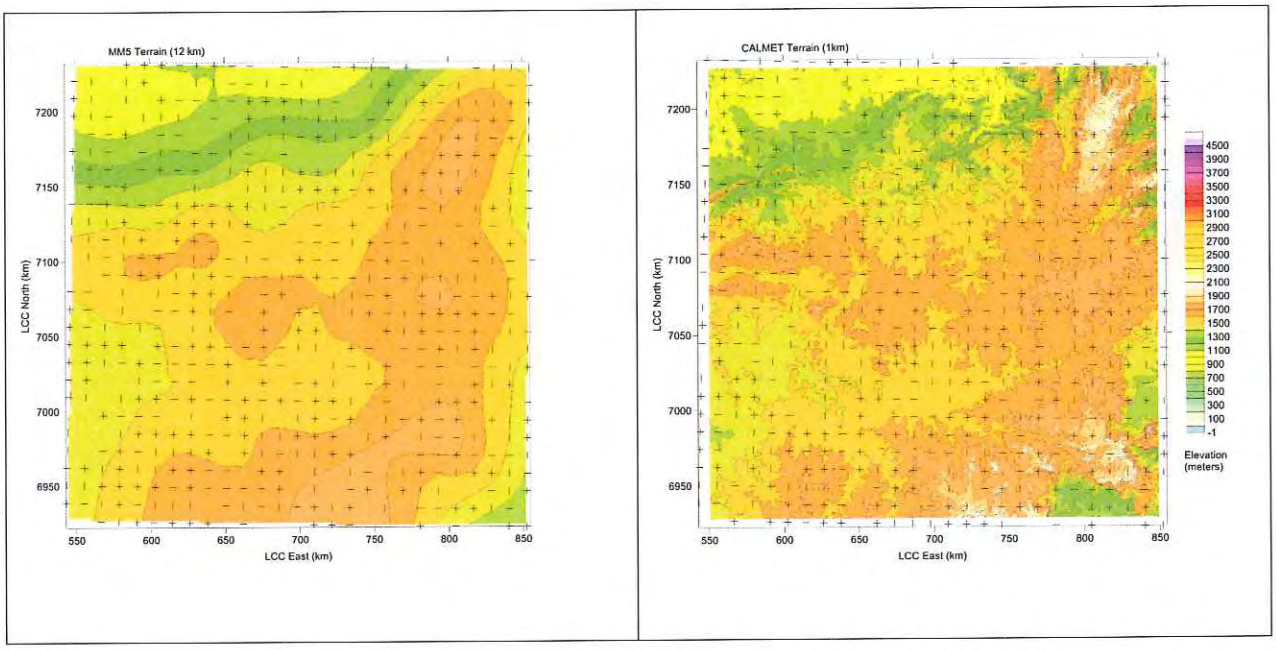

Figure 1. Terrain contour analysis for MM5 12-km terrain (left) and CALMET 1-km terrain (right).

5 CALMET Modeling Options

CALMET model option settings in the CALMET.INP file provided and options chosen for the AIR are discussed in this section. Alternative recommendations are proposed where appropriate. Note that initially one CALMET.INP file was provided covering the 3-year period January 2010 to December 2012. This file includes 9 meteorological stations, which is inconsistent with the CALMET output file (ALLMET.DAT) that was also provided in the same directory. It was determined during the review that the 9-station CALMET files do not represent the final CALMET configuration. Subsequently, CALMET.INP files with two surface stations were provided reflecting the way CALMET was run in its final configuration.

In the AIR, CALMET version v6.334 (level 110421) is used, as stated in the report and as read from the CALPOST extraction of the CALMET information recorded in the CALPUFF concentration files.

5.1 Geophysical Data File

a. Landuse Categories

As a first step, the GEO.DAT file was reprocessed to investigate and review the landuse data, terrain contour data, and associated parameters which are essential and imported into a CALMET run.

A plot displaying the terrain contours and landuse categories over the entire CALMET domain and the location of the CALPUFF computational domain (as shown in Figure 2) are not provided in the Secunda report. This kind of plot allows the validation of the landuse and terrain data after their preparation and before they are input in CALMET. Figure 2 shows that there are some errors for some of the landuse categories, specifically those having a value allocated as 55 (ocean or missing values). The pattern displayed by these missing values (in the shape of parallel blue curved lines), is misleading for it does not correspond to "real" water landuse but rather the missing values. These lines appear clearly on Figure 2 (full domain), Figure 3 (zoom-in on CALPUFF computational domain for Natref/ Sasolburg) and Figure 4 (zoom-in on CALPUFF computational domain for Secunda).

The cells were filled with missing values because both domain resolutions (CALMET domain and the raw dataset domain) are 1-km but with different map projections. As a result, CTGPROC does not always find a valid land use type when a CALMET domain cell is at the border of four cells of the raw dataset. This can be corrected by changing the mesh density factor (MESHGLAZ) for USGS Global (Lambert Azimuthal) in CTGPROC to 2 (See Figure 5 displaying corrected land use categories).

b. MAKEGEO Landuse Parameters

In MAKEGEO, the soil heat flux parameter for Input Category 11 (urban/residential landuse) is set to 1.0 but should be 0.25 according to the CALMET User's Guide (Scire et al., 2000). This is probably not a critical error, but it should be fixed in any rerun of MAKEGEO. It is therefore recommended that the correct soil heat flux parameter (0.25) for Input Category 11 be used in the reruns of MAKEGEO and CALMET/CALPUFF. The urban/residential category has the correct default values of surface roughness (zo=0.5m) and Bowen ratio (1.0) which are lower than other urban subcategories and leaf area index (LAI=1.0) which is higher than other urban subcategories.

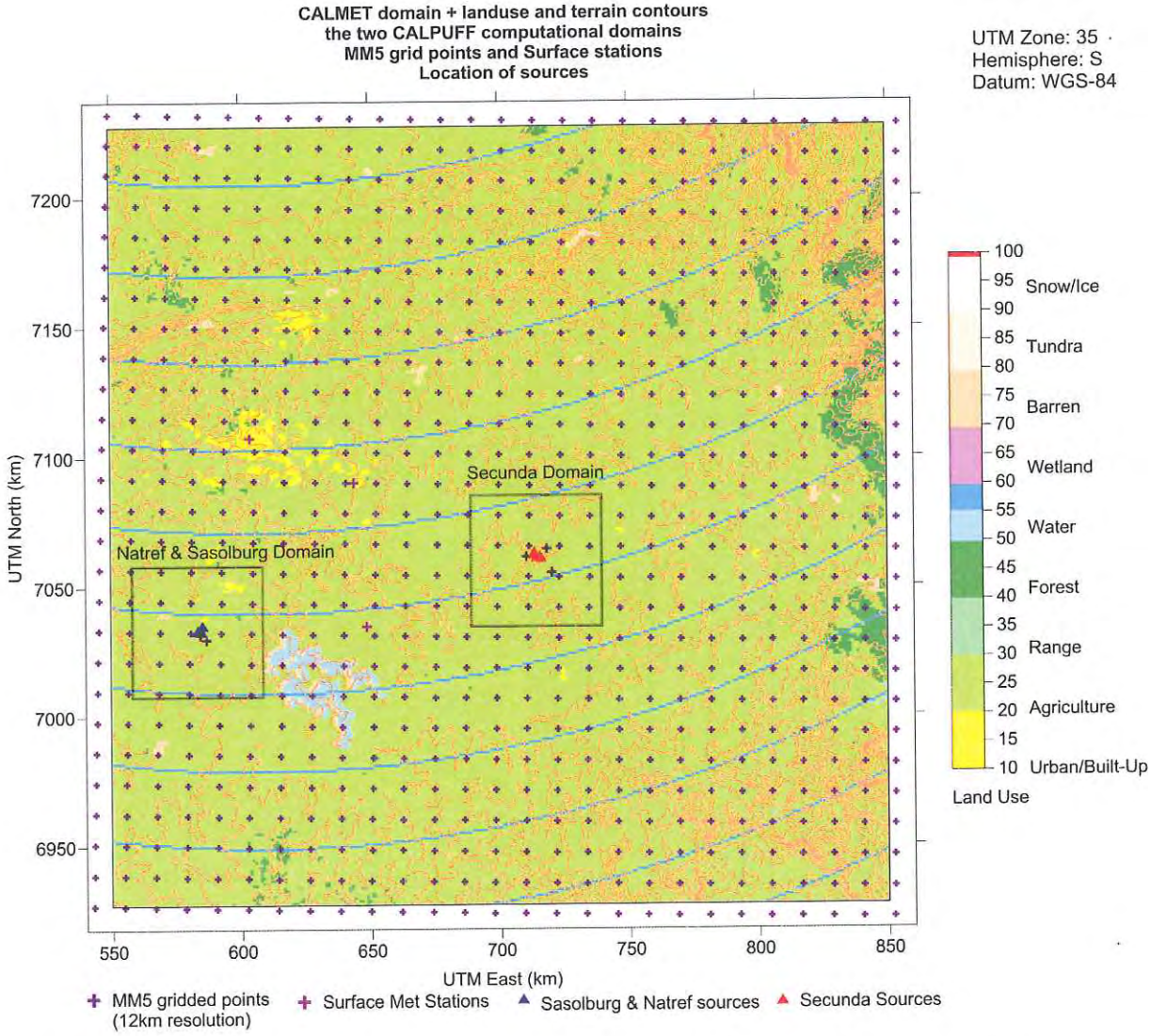

Figure 2. Land use categories, terrain contours and meteorological MM5 grid points and surface stations locations displayed on 300 x 300 km CALMET domain (1-km resolution).

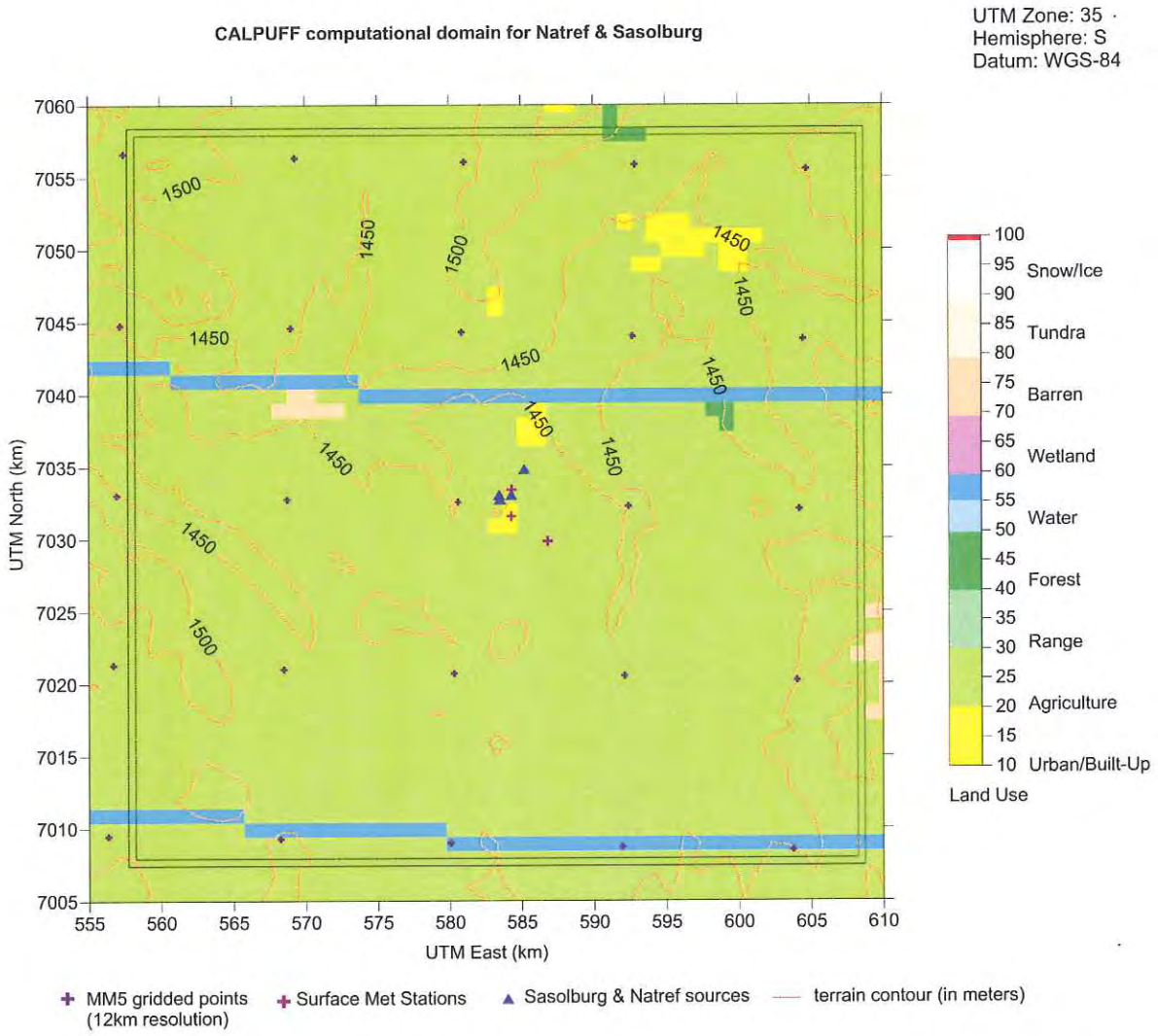

Figure 3. Zoom-in of Natref and Sasolburg 50 x 50 km CALPUFF computational domain, showing relatively flat terrain at 1450 – 1500 meters ASL and two large bands of missing landuse categories (shown as "water", shown in blue) which need to be corrected.

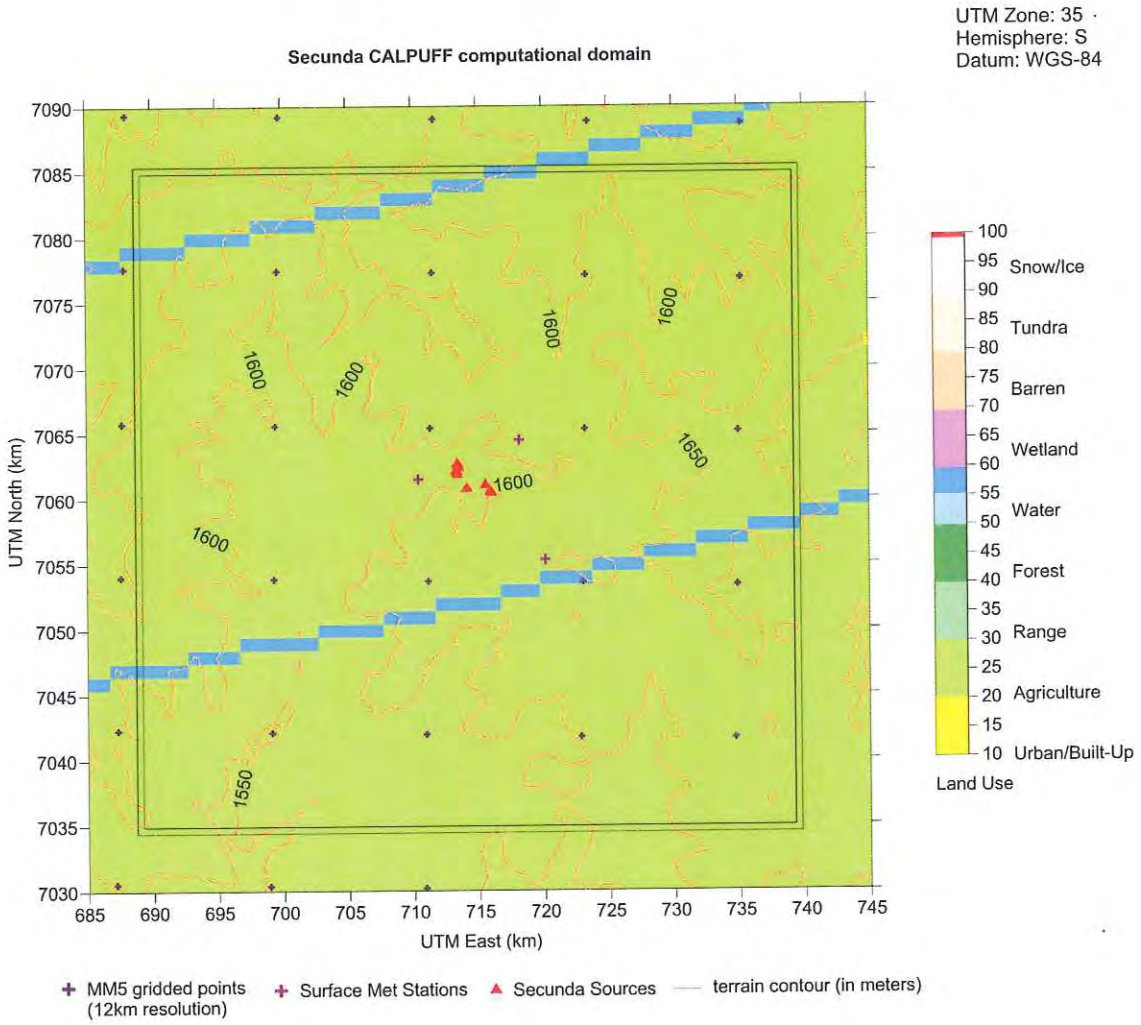

Figure 4. Zoom-in of Secunda facility 50 x 50 km CALPUFF computational domain, showing relatively flat terrain at 1550 – 1600 meters ASL and two large bands of missing landuse categories (shown as "water", shown in blue) which needs to be corrected).

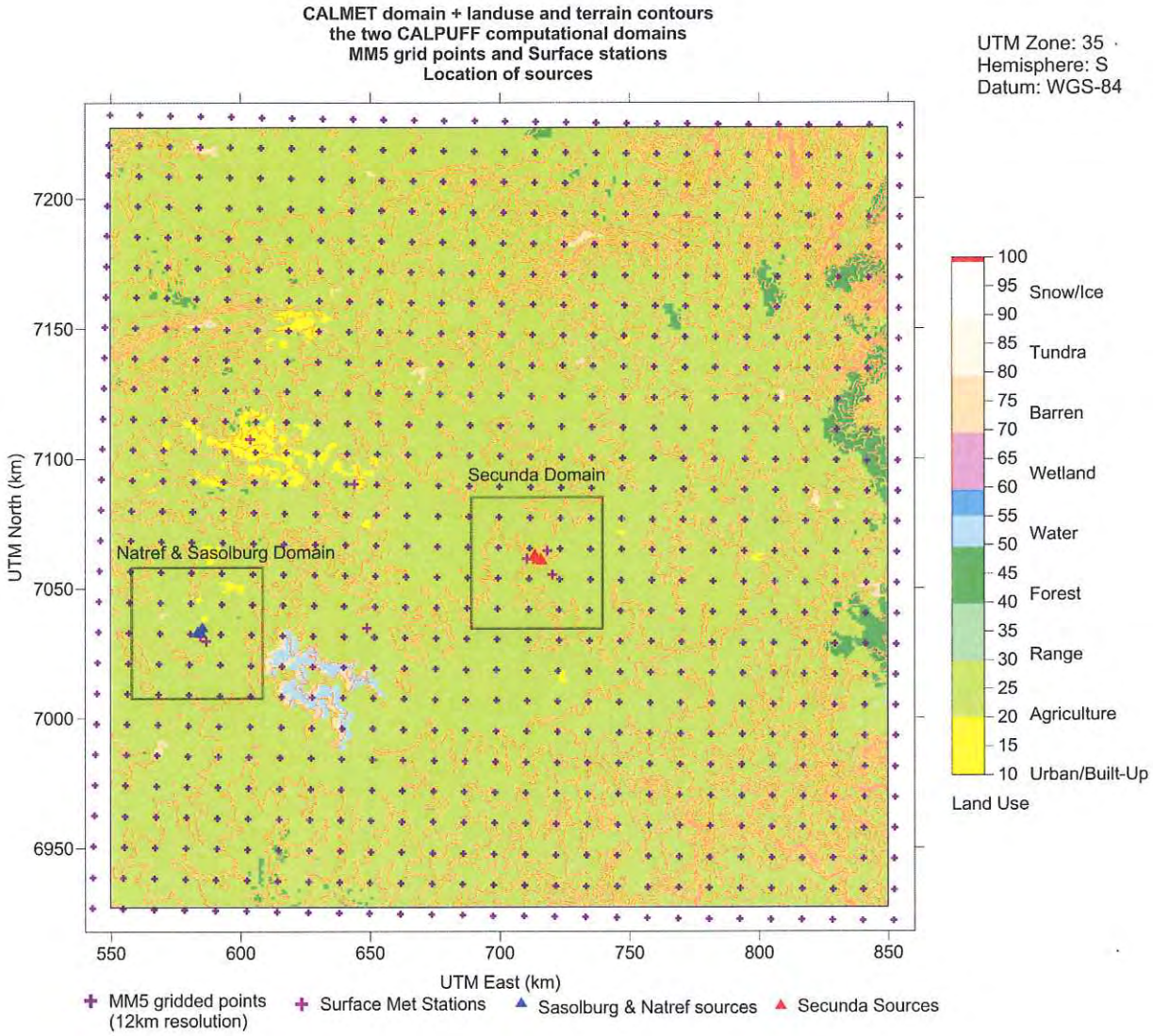

Figure 5. Same as Figure 2 but with landuse categories correct (MESHGLAZ = 2 in CTGPROC).

5.2 CALMET Options

From the revised CALMET.INP file provided, the following information was obtained:

- CALMET was run in hybrid mode (NOOBS=1) using:
  - Surface observations (surface data in SASOL.DAT, 2 stations)
  - Prognostic data (from MM5 runs)
- Three years were run in one single run (from January 1 2010 to December 31 2012).
- The time zone is set as UTC+0200. Time steps of prognostic data = 3600s (ISTEPPGS)
- The winds from MM5/3D.DAT are used as initial guess fields (IPROG=14)
- The projection chosen is UTM-35 South, datum WGS-84 for a grid of 300 x 300 km with a resolution of 1 km, and a south west corner: X= 549.718km; Y=6927.413km.
- 10 levels in the vertical (0,20,40,80,160,300,600,1000,1500,2200,3500)
- Upper air data provided from MM5
- Precipitation from MM5 is chosen, Cloud information from MM5 is chosen (cloud computed from RH at 850 mb)

For a domain size of this size, the use of UTM coordinates is marginal. Map distortion with UTM coordinates becomes larger as the size of the modeling domain increases. Normally somewhere in the range of 200 km to 300 km or larger, the use of Lambert Conic Conformal (LCC) coordinates in mid-latitudes would be used rather than UTM projection. This is not considered a major issue, but is noted for future consideration.

CALMET options chosen for the Secunda AIR are reasonable overall for this application. There are several changes that are recommended, however, they are not considered critical items but rather recommended refinements. Table 4 lists those values used in CALMET that are different from their default values. The use of non-default values is not necessarily an issue as the model is intended to allow customization for site-specific conditions.

The main comments on the options selected are provided below:

- IOBR=1; use O'Brien procedure for adjustment of the vertical velocity. Generally the O'Brian procedure is turned off. The basis for the use of it in this application is not discussed in the AIR.
- The following input options identify which meteorological parameters MM5 provides to CALMET. These selections are reasonable given the application and data sources used in the simulations.
  - 2D temperature from MM5 (ISURFT=-1)
  - 2D spatially varying lapse rate from MM5 (IUPT=-1)
  - 3D initial guess field for upper air (IUPWND = -1, which is not used as NOOBS=1)
  - Overwater lapse rates used in convective mixing height is assumed neutral as no sea.dat (ITWPROG = 0, which will not have an impact as the domain is basically all inland, after correction to CTGPROC landuse problem noted above);
  - 3D RH from MM5 (IRHPROG= 1);

- The multi-layer option (ICLOUD=4) option is generally recommended ("MM5toGrads" algorithm) rather than the Teixera algorithm when using clouds based on MM5 data. The Teixera option ICLOUD=3) uses a single layer (850 mb) to determine the cloud amount, while the MM5toGrads option uses multiple layers and is considered more accurate.
- MNMDAV=1 grid cell (1 km). This variable controls the amount of smoothing done for the spatial interpolation of mixing heights. Using one grid cell of smoothing with the fine-scale (1 km) grid may produce unrealistically large spatial variations in mixing heights. A larger smoothing radius of ~3 km is recommended (MNMDAV=3).
- The CALMET 3-D temperature is determined using data from surface stations and from the MM5 model above (ITPROG=1). Given that there are only two surface stations, the use of the spatial variable MM5 temperature field is recommended (ITPROG=2) rather than the two isolated surface measurements. This would be consistent with the use of MM5 for other 3-D scalar meteorological variables.
- JWAT1 = JWAT2 = 999, which is fine as only small water bodies on the domain (will be the case after correction of CTGPROC issue noted above).

As seen on Figure 3 and Figure 4, which are zoom-in plots of the two CALPUFF computational domains, the terrain contours are around 1450-1500 meters for Natref/Sasolburg and around 1550-1600 meters for Secunda. The terrain in both domains is relatively flat terrain. Although more complex terrain contours are present in the northern part of the domain, they are not in the primary area of interest.

The extraction of data from the meteorological stations into the SASOL.DAT surface data file cannot be commented on since the data from the raw meteorological stations are not available. A time zone of 0 is indicated but it cannot be confirmed that the surface meteorological data provided correspond to that time zone.

Three meteorological stations are listed in the Secunda report with a location provided in latitude and longitude (assuming the datum to be WGS-84): The coordinates in UTM-35 (datum WGS-84) for the three stations: (1) station Bosjesspruit (BOS), (2) station Secunda Club (CLB), and (3) station Langverwacht (LVW) were checked and are correct with an uncertainty of 0.001 km.

A discrepancy was noted between the CALMET.INP and the CALMET control input file recorded in the CALMET output ALLMET.DAT regarding the number of surface stations (9 vs 2) but that has been resolved as the 9-station run was replaced with the 2-station run in the final simulations.

5.3 CALMET Wind Fields

Figure 6 shows an example CALMET layer 1 wind vector plot from the CALMET data file for May 15, 2010 at 0500 local time. This plot shows nothing unusual in the Layer 1 winds. The spatial variations in the wind field over parts of the domain are due to terrain effects which would be expected during this part of the diurnal cycle. Figure 7 shows a second plot on February 2, 2011 at 0500 local time. This plot shows less terrain effects and a smoother wind field. A circulation is evident over the western part of the domain at this time. Overall no apparent problems are indicated in these CALMET wind fields.

Figure **8** shows a plot of mixing heights from CALMET on February 5, 2010. This plot shows a significant banding structure in the mixing height field. This feature is due to the missing landuse data which uses a water landuse category as the default value (also shown in Figure 2, Figure 3 and Figure 4). This is correctable by changing the CTGPROC meshing factor (MESHGLAZ) and creating a new GEO.DAT file.

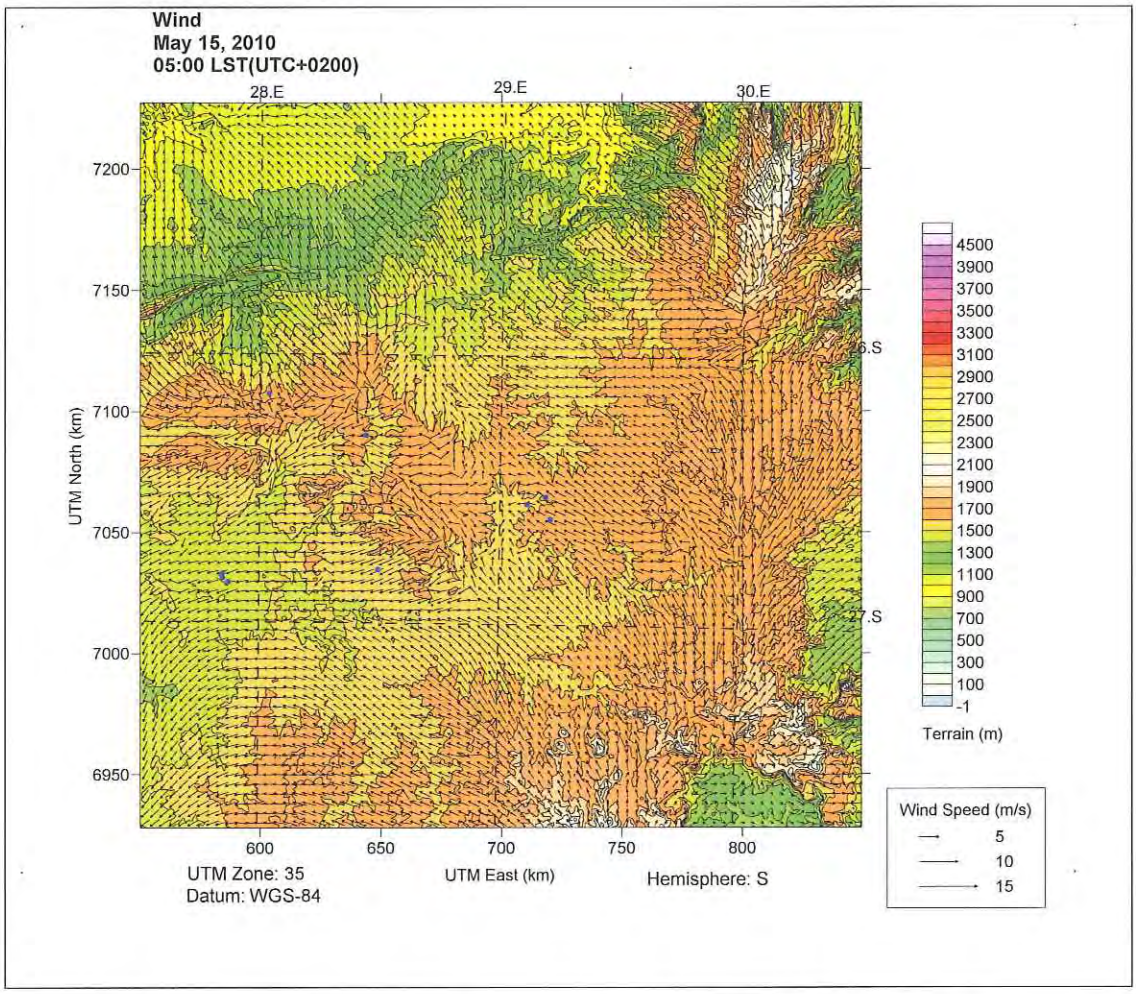

Figure 6. CALMET Layer 1 wind vectors on May 15, 2010 at 0500 Local Standard Time.

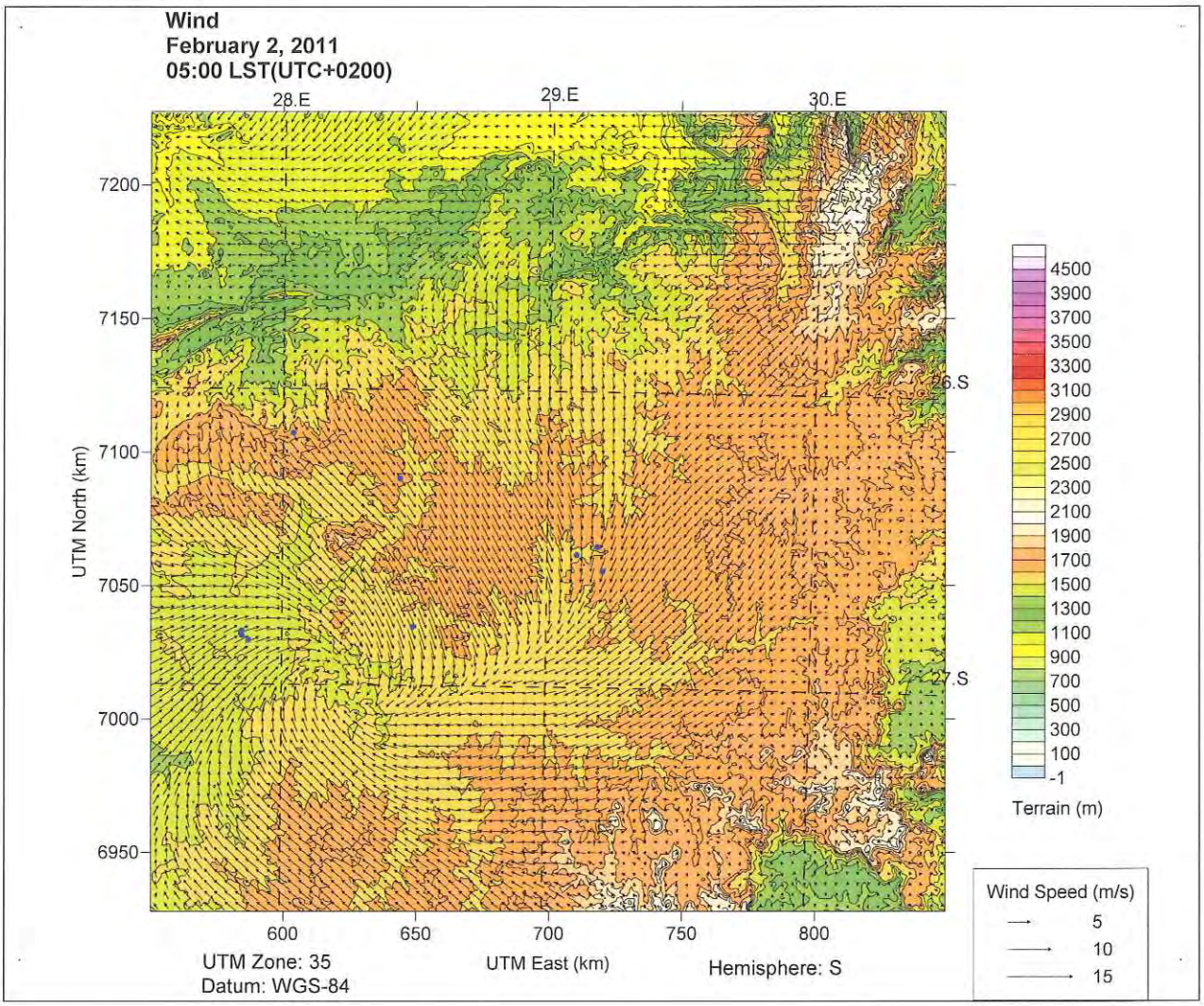

Figure 7. CALMET Layer 1 wind vector plot for February 2, 2011 at 0500 Local Standard Time.

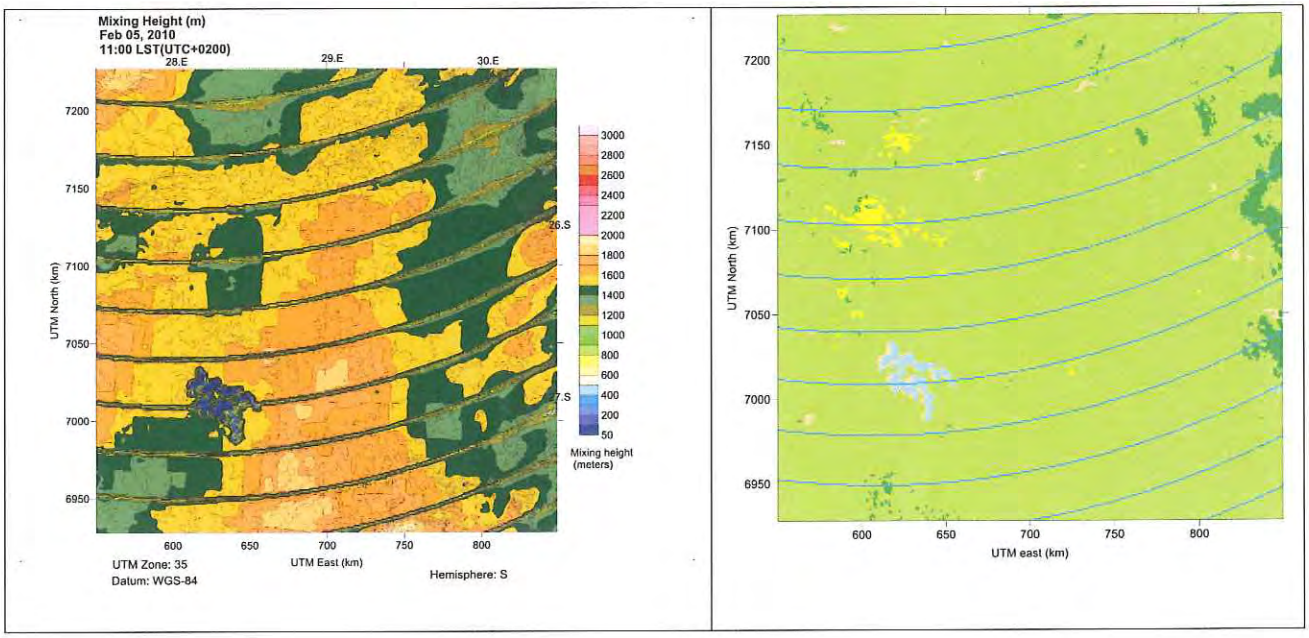

Figure 8. CALMET mixing heights on February 5, 2010 (left) compared with the CALMET landuse categories plot (right).

Table 4. Summary of CALMET Options Selected as Different 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 – Gridded cloud fields or not	0 (gridded clouds not used)	3 (Gridded cloud cover from Prognostic Rel. Humidity at 850mb [Teixera])	The multi-layer option (ICLOUD=4) option is generally recommended (MM5toGrads algorithm) rather than the Teixera algorithm (ICLOUD=3)
IOBR	Use O'Brien procedure for adjustment of the vertical velocity	0 (NO)	1 (YES)	Generally, the O'Brien procedure is not used in CALMET
IEXTRP	Extrapolate surface wind observations to upper layers	-4 (similarity theory used except layer 1 data at upper air stations are ignored)	4 (similarity theory used)	Since no upper air stations are used in the run, both options (-4 and +4) are equivalent.
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
IRHPROG	3D relative humidity from observations or from prognostic data	0 (Use RH from surf.dat file)	1 (Use prognostic RH)	Suitable option
ITPROG	3D temperature from observations or from prognostic data	0 (Use surface and upper air stations)	1 (Use surface stations for surface and MM5/3D.DAT for upper air data)	Recommend using ITPROG=2 because of the relative poor coverage of the surface observational network (i.e., only two surface stations are used).

6 CALPUFF Model Options

CALPUFF version 6.42 (level 110325) was used as stated in the report and found in the record of the CALPUFF output files. This was the most appropriate version of the model for use at the time of the study.

The CALPUFF model option settings are determined from CALPUFF.INP files. Three sets of input files were provided: Natref (1 file), Sasolburg (10 files) and Secunda (19 files). Each file contains the source information for one stack. A check was conducted to evaluate whether all files contain the same model settings and switches. The options were found to be consistent except for the following:

- The chemistry option is active or inactive depending on the pollutant modeled (this is as expected).
- In runs for a couple of sources, wet deposition is computed while most of the runs do not account for wet deposition (discussed later in the report).
- The discrete receptors differed in some of the files (discussed later in the report).
- The CALPUFF computational domain and gridded receptor differ between Natref/Sasolburg and Secunda.

Three years were run in one single run from January 1 2010 to December 31 2012 (UTC+0200). The projection as in CALMET run is UTM-35 South, WGS84 datum.

When the chemistry option is selected:

- Six chemical species SO_2, SO_4, NO_x, HNO_3, NO_3, PM_{10} are modeled, but only SO_2, NO_x and PM_{10} are emitted
- The MESOPUFF-II scheme for chemical transformation is chosen.
- Only concentrations are output from the runs while deposition fluxes are not stored.

6.1 Gridded Receptors

The computational grid is I=9 to 59; J=81 to 131. The gridded receptors covered the same grid with a MESHDN of 5 (200-meter spaced). An alternative option would be to use discrete receptors on a 200-m spaced grid to allow the calculation of the elevation with TERREL and select peak elevation for each receptor. In the gridded receptors option in CALPUFF, elevation is computed from gridded terrain data of 1 km provided in CALMET, whereas the discrete receptors allow point values of elevation to be assigned to each receptor. *The impact of this comment on results would be minimal as the terrain is rather flat (50 meter variations on the computational domain).*

6.2 Dispersion Methods

Turbulence-based dispersion (MDISP=2) was chosen for the dispersion coefficient method but the Probability Density Function (PDF) option was not used. The PDF option has been found in various model evaluation studies to be important for tall stack dispersion under convective conditions. These conditions are likely to be important in this application with both tall stacks present and frequent, highly convective conditions expected. When the turbulence based dispersion option is used (MDISP=2) which is the recommended setting for CALPUFF, the use of the PDF algorithm is also recommended. There is a discussion in Appendix D (page 156) of the Secunda report commenting on CALPUFF Model Control Options. It states that "*when using MPDF=1,* the *CALPUFF model will be more sensitive to the appropriateness of the land use characterization*". The PDF algorithm treats the effects of updrafts and downdrafts that can vertically displace an elevated plume by a significant amount over short periods of time.

A test run for the two steam stack sources of the Secunda facility was performed in order to estimate the impact the use of the PDF algorithm would have on the results. SO_2 concentrations and NO_x concentrations were extracted at 14 receptors (the receptors selected in the AIR as described in the results section of the first draft Secunda report (Table 5-23)). The concentrations were ranked by gridded receptors and discrete receptors separately. The discrete receptors correspond to the three monitoring stations. For a comparison of the results from the run of the two steam stacks using CALPUFF options MPDF=0 (PDF off) or MPDF=1 (PDF on), Rank 1, 2 and 4 are displayed in Table 5 for NO_x concentrations and Table 6 for SO_2 concentrations respectively. It demonstrates using the PDF algorithm produces larger concentrations for all three ranks selected and for the two pollutants. The considerable increase in predicted concentration using MPDF=1 confirms a significant sensitivity to the results due to the PDF option. Use of the PDF algorithm is recommended and it is considered a critical change.

Table 5. Hourly NO_x concentrations at Rank 1, 2 and 4 over the 3-year period and the 13 gridded receptors selected (top of table) and the 3 discrete receptors, corresponding to the 3 monitoring stations (bottom of table) – results for CALPUFF PDF option off (MPDF=0) and on (MPDF=1) are displayed

Receptors	Rank	NO_x Concentration (MPDF=0) ($\mu g/m^3$)	NO_x Concentration (MPDF=1) ($\mu g/m^3$)
Gridded	1	476.8	1047.6
Gridded	2	416.7	796.8
Gridded	4	384.1	618.1
Discrete	1	514.2	834.3
Discrete	2	416.5	811.9
Discrete	4	371.3	734.7

Table 6. Hourly SO_2 concentrations at Rank 1, 2 and 4 over the 3-year period and the 13 gridded receptors selected (top of table) and the 3 discrete receptors, corresponding to the 3 monitoring stations (bottom of table) – results for CALPUFF option MPDF=0 and MPDF=1 are displayed

Receptors	Rank	SO_2 Concentration (MPDF=0) ($\mu g/m^3$)	SO_2 Concentration (MPDF=1) ($\mu g/m^3$)
Gridded	1	783.1	1540.1
Gridded	2	768.5	1249.2
Gridded	4	634.4	938.8
Discrete	1	810.7	1289.9
Discrete	2	671.6	1240.8
Discrete	4	620.4	1109.9

6.3 Stack Parameters

The CALPUFF input files contained different emission rates from those reported in the first draft Secunda AIR. We used scaling factors to adjust the concentrations in order to reflect the emission rates believed used in the modeling, but were not able to reproduce the reported results in the first draft report. Table 7 contains a summary of the emission rates in the provided CALPUFF.INP files compared to two scenarios in the first draft Secunda AIR. For the largest emitting sources the emission rates in the CALPUFF files do not match those listed in the report, indicating that scaling of the concentrations in postprocessing steps may have been done. The files provided do not include the scaling operations, so several tests have been done to compute the scaling factors and apply them. The scaled factors are shown in Table 8 along with emission rates provided in several spreadsheets.

Table 9 and 10 show the results of the scaled concentrations compared to the values in the first draft Secunda AIR. Also shown are the computed maximum 1-hour average and annual concentrations from time series files provided to Exponent for review.

As part of the process to reconcile the differences noted above, new modeling files and time series output from the model were provided by Airshed on April 8, 2014 for the two main stacks (MainE and MainW) along with a second draft Secunda AIR. The results of SO_2 tests are shown in Tables 11. In these files, the SO_2 emission rates of 2899.2 g/s and 2578.7 g/s for MainE and MainW, respectively. The results of the Exponent simulation with deposition and the PDF option match the results from Airshed for this same run based on the time series file provided by Airshed. The results in the second draft Secunda AIR did not match the files, but it was noted by Airshed that the draft report contains the 2nd highest SO_2 concentration, not the highest. The report will be updated to use the maximum value (or the use of the 2nd highest will be noted). The annual SO_2 concentration is considered a match when rounded to the same number of significant digits. As a result of this analysis, the discrepancies in the SO_2 results are considered resolved.

The NO_2 predictions using the April 8 modeling files are shown in Table 12. These runs are based on NO_x emission rates of 1940.0 g/s (MainE) and 1725.6 g/s (MainW). The 1-hour and annual NO_x results from this run (Column 2 of Table 12) match the results in the time series file (TSF) (Column 4) provided by Airshed on April 8, 2014. However, there are differences in the NO_2 concentrations computed by Exponent using the Ambient Ratio Method (ARM) in CALPOST vs those reported in the second draft Secunda AIR. It has been clarified that Airshed used a different approach in applying the ARM, using a spreadsheet to compute NO_2 concentrations from NO_x predictions from the model, rather than the option in CALPOST to do this. From an inspection of the Airshed spreadsheet provided on April 10, the formulas apply the Scire and Borissova (2011) short-term NO_2/NO_x ratios up to NO_x concentrations of 150 ppb (~282 $\mu g/m^3$) and apply a constant ratio of 0.4 for higher concentrations (See Figure 9). This will lead to more conservative (higher) predicted NO_2 concentrations in the Airshed results since the short-term ratios used in the AIR do not fall below 0.4. In the Secunda AIR, no ARM adjustment has been applied to the annual average NO_x concentration, which is also a conservative assumption.

Table 7. Source emissions for Scenario 1 and 2a provided for Sasol Secunda facility (From Table 5-22 of the 1st draft Secunda AIR) compared with source emissions from the CALPUFF input files provided to Exponent on Feb 27, 2014.

Source Group	Source Name	Data in CALPUFF Input Files - Feb 27, 2014			Scenario 1 – Baseline Emissions			Scenario 2a – Compliance with Existing Plant Standards		
		PMs (g/s)	SO_2 (g/s)	NO_x (g/s)	PMs (g/s)	SO_2 (g/s)	NO_x (g/s)	PMs (g/s)	SO_2 (g/s)	NO_x (g/s)
Steam Stations	Main Stack East	***138.48***	***5730.6***	***3834.7***	70.06	2899.19	1939.08	166.81	5838.42	1834.89
	Main Stack West	***123.18***	***5097.2***	***3410.8***	62.32	2578.74	1725.55	148.37	5193.09	1632.08
Sulfur Recovery	Sulfur Recovery East									
	Sulfur Recovery West									
HOW Incinerators	HOW West	1.6194	0.059375	7.3112	1.62	0.06	7.31	0.54	1.09	4.34
	HOW East	0.60846	0.12445	6.8347	0.61	0.12	6.83	0.45	0.90	3.59
Biosludge Incinerators	Biosludge East	1.3992	0.074488	1.9467	1.40	0.07	1.95	0.43	0.87	3.48
		1.1558	0.39675	1.9815	1.16	0.40	1.98	0.42	0.83	3.32
	Biosludge West	0.29634	0.10189	0.26029	0.30	0.10	0.26	0.35	0.71	2.83
		1.169	0.032593	4.3942	1.17	0.03	4.39	0.39	0.78	3.13
WSA	WSA		10.67	**18.479**		10.67			10.67	
Rectisol	Rectisol East									
	Rectisol West									
SCC	SCC	10.5999			10.60			4.87		

Table 8. Comparison of emission rates from the provided CALPUFF input files and spreadsheets.

Source	Emission Rates				
	Baseline –Draft Secunda AIR[1]	Baseline to Airshed Spreadsheet[2]	CALPUFF Input Files	Copy of Baseline-Airshed[3]	Exponent Estimated Scaling Factors[4]
	(g/s)	(g/s)	(g/s)	(g/s)	
SO_2					
BWSA	10.67	10.67	10.67	10.67	1.0
MainE	2899.19	2899.19	5730.6	5730.6	0.5059
MainW	2578.74	2578.74	5097.2	5097.2	0.5059
HowW	0.06	0.06	0.06	0.06	1.0
HowE	0.12	0.12	0.12	0.12	1.0
SLGE1	0.07	0.07	0.07	0.07	1.0
SLGE2	0.40	0.40	0.40	0.40	1.0
SLGW1	0.10	0.10	0.10	0.10	1.0
SLGW2	0.03	0.03	0.03	0.03	1.0
NO_x					
BWSA	10.67	10.67	18.48	no NO_x	1.0
MainE	2899.19	2899.19	3834.7	no NO_x	0.5057
MainW	2578.74	2578.74	3410.8	no NO_x	0.5059
HowW	0.06	0.06	7.31	no NO_x	1.0
HowE	0.12	0.12	6.83	no NO_x	1.0
SLGE1	0.07	0.07	1.95	no NO_x	1.0
SLGE2	0.40	0.40	1.98	no NO_x	1.0
SLGW1	0.10	0.10	0.26	no NO_x	1.0
SLGW2	0.03	0.03	4.39	no NO_x	1.0

[1] Emissions taken from Table 5-22 on page 87 of the draft report "SC_13STL01_rev1.1.docx", Baseline emissions.
[2] Emission rates from spreadsheet "Baseline to Airshed NO NO2 NOx Corrected-splitted (Feb).xlsx"
[3] Emission rates from spreadsheet "Copy of Baseline to Airshed NO NO2 NOx corrected – splitted"
[4]Scaling factors are computed as a ratio of the emissions from the baseline-draft report and the emissions within the CALPUFF input files.

Table 9. Summary of Modeled SO_2 Concentrations vs. 1st Draft Secunda AIR

	Exponent		Sasol Results	
Year	No Scaling[1]	After Scaling[2] ($\mu g/m^3$)	1st Draft Report[3] ($\mu g/m^3$)	From Time Series[1,4] ($\mu g/m^3$)
1-hour Max				
2010	671.9	340.1	416.8	
2011	597.3	302.6	447.3	
2012	811.7	411.2	490.9	
Max	811.7	411.2	490.9	1240.9[5]
Annual				
2010	5.92	4.7	3.7	
2011	6.89	3.5	4.1	
2012	7.26	3.7	5.5	
Max	7.26	4.7	5.5	7.8

Table 10. Summary of Modeled NO_2 Concentrations vs. 1st Draft Secunda AIR

	Exponent		Sasol Results	
Year	No Scaling[1]	After Scaling[2] ($\mu g/m^3$)	1st Draft Report[3] ($\mu g/m^3$)	From Time Series[1,4] ($\mu g/m^3$)
1-hour Max				
2010	416.8	211.0	112.8	
2011	366.5	185.7	119.1	
2012	516.2	262.5	125.9	
Max	516.2	262.5	125.9	516.2
Annual				
2010	5.9	3.3	1.9	
2011	4.3	2.4	2.1	
2012	4.4	2.4	2.7	
Max	5.9	3.3	2.7	4.88

[1] Concentrations are based on emissions from the CALPUFF input files with no additional scaling. Predicted NO_x concentrations are generated using NO_2/NO_x ratios from the Sasol CALPOST input files.
[2] Scaling factors were applied to the emissions from the main stacks to adjust the emissions to the baseline values in Table 5-22 of the Sasol AIR.
[3] The draft AIR is the document "SC_13STL01_rev1.1.docx" with predicted concentrations taken from Appendix G Table G-1.
[4] Concentrations computed from output time series concentration data from the original CALPOST runs generated by Sasol.
[5] The concentration of 1240.9 does not agree with the value to 811.7. This was traced to an inconsistency in the time series data for the HOW source group provided by Sasol. When CALSUM and then CALSUM were rerun the time series data files did not match that provided by Sasol. Other time series data files for the main stacks, the SLG stacks and BWSA stacks were in agreement.

Table 11. Summary of SO_2 Concentrations for Secunda Main stacks (MAIN East and West Stack Only), except for last column which includes the total concentrations from all 19 Secunda stacks.

	(1) Exponent Run April 2014 4/8/14 Rerun of Main stacks only	(2) Sasol TSF Files April 2014 Computed from TSF data provided on 4/8/14	(3) 2nd Sasol Draft Report April 8, 2014 TOTAL CONC (Main stacks + other sources)
PDF option: Deposition:	PDF With Dep. µg/m^3	PDF With Dep. µg/m^3	PDF With Dep. µg/m^3
1-hour Max			
2010	627.55	-	605.03
2011	488.18	-	485.50
2012	652.03	-	576.90
Max	652.03	652.03	605.03
Annual			
2010	6.05	-	6.1
2011	4.53	-	4.5
2012	4.56	-	4.6
3-yr average	5.05	5.05	5.1

Table 12. Summary of NO_x or NO_2 Concentrations for Secunda Main stacks (MAIN East and West Stack Only), except for last column which includes the total concentrations from all 19 Secunda stacks.

	(1) Exponent Run April 2014 4/8/14 Rerun of Main stacks only	(2) Exponent Run April 2014 4/8/14 Rerun of Main stacks only	(3) Exponent Run April 2014 4/8/14 Rerun of Main stacks only	(4) Sasol TSF Files April 2014 Computed from TSF data provided on April 8, 2014	(5) Sasol Draft Report v1.2 Rec. April 2014 TOTAL CONC (Main stacks + other sources)
NO_2 or NO_x: PDF option: Deposition:	NO_x (no ARM) No PDF No Dep. µg/m^3	NO_x (no ARM) PDF With Dep. µg/m^3	NO_2 (with ARM in CALPOST) PDF With Dep. µg/m^3	NO_x (no ARM) PDF With Dep. µg/m^3	NO_2 (with ARM in spreadsheet) PDF With Dep. µg/m^3
1-hour Max					
2010	205.84	407.61	108.75	-	156.3
2011	184.53	326.14	108.80	-	129.4
2012	256.76	417.23	108.81	-	153.7
Max	256.76	417.23	108.81	417.23	156.3
Annual					
2010	2.67	3.71	3.25	-	3.6
2011	1.91	2.68	2.38	-	2.7
2012	1.94	2.63	2.36	-	2.7
3-yr average	2.17	3.01	2.67	3.01	3.0

[1]ARM = Ambient Ratio Method used to estimate NO_2 conc. from predicted NO_x conc. using empirical NO_2/NO_x ratios

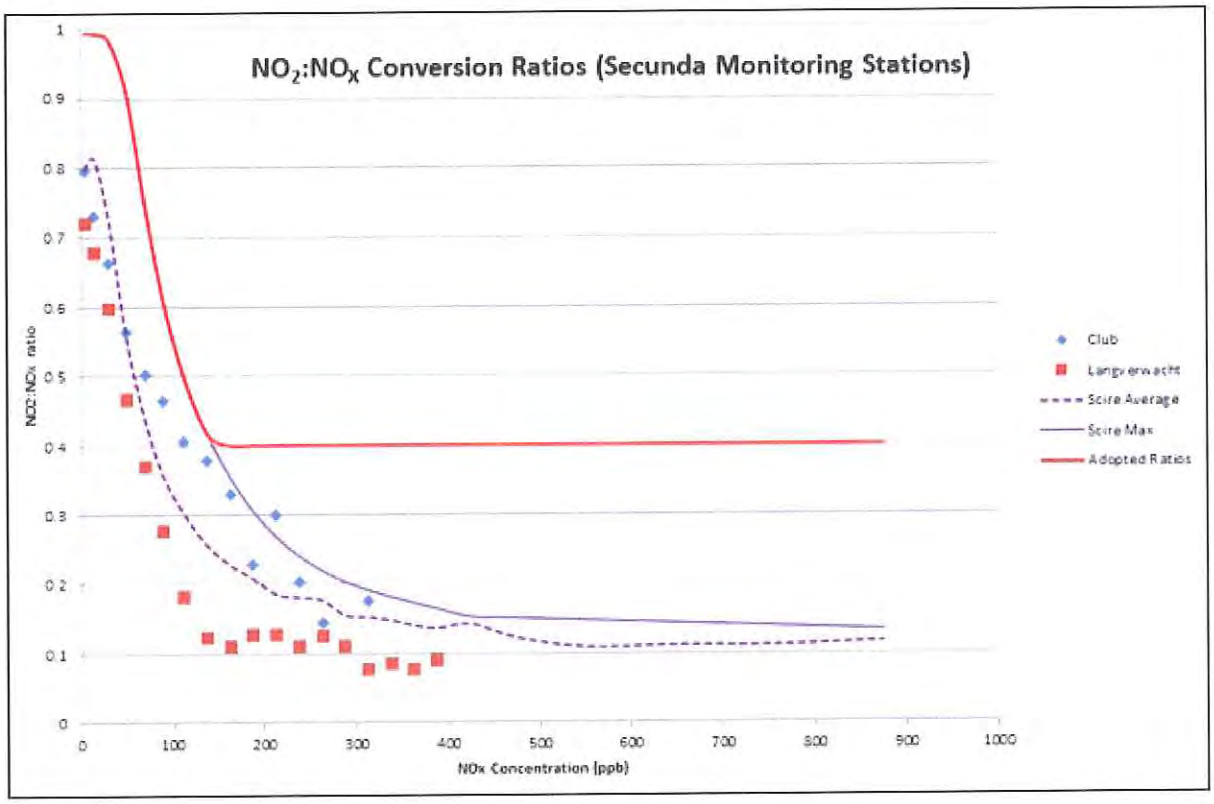

Figure 9. NO_2/NO_x conversion ratios used by Airshed for the Secunda monitoring stations (from Figure E-1, 2nd draft Secunda AIR).

6.4 Ozone Monthly Averages

For Secunda, there are two ozone stations in the SECUNO3.DAT file. The file includes 1,857 missing hours out of the 26,304 hours (over 3 years) at one station and 1,738 missing hours out of 26,304 hours at the other station. This represents missing hours of 7.0% and 6.6% respectively. The missing hours do not seem to occur during the same hours for the hours checked. Therefore, hourly values from the ozone.dat file from the other station (this is not clear as it seems hours were missing from both stations- do you mean from the control station) will be used. The monthly average ozone data in the control file will be used only for hours with all of the hourly ozone data missing, which is infrequently.

However, for NATREF and SASOLBURG, there is only one ozone station in the SASOLO3.DAT file and it includes 4,963 missing hours out of 26,303 hours (over 3 years), which represents 18.9 % of the hours. For those missing hours, the monthly averages entered in the CALPUFF control file will be used. The monthly averages of hourly ozone data seem to have been calculated including all hours instead of daylight hours only. Because ozone is used as a surrogate for daytime OH radicals in the atmosphere when using the MESOPUFF chemical transformation algorithm, it is best to use daytime ozone only in computing the monthly ozone averages that serve as a backup when hourly ozone data is missing. At night, ozone concentrations are not used by the chemistry, but rather, a small nighttime conversion rate reflecting heterogeneous reactions is used.

A new calculation of the ozone monthly averages to include only the daylight hours is expected to have little effect on the Secunda concentration predictions and could have a slight effect on the NATREF and SASOLBURG concentration predictions for pollutants involving chemical transformation. This change although recommended, is not considered a critical item.

6.5 Discrete Receptors for Sasolburg CALPUFF runs

The discrete receptors have a height above ground set at 3 meters for B6930.INP, B6990.INP, UB6930.INP while they are set at 2 meters for all other sources (B6993.INP, SS1A.INP, SS1B.INP, SS1C.INP and SS2.INP, UB6990.INP, UB6993.INP). We did not have sufficient information to confirm the measurement height of the monitored data. However, it is recommended the measurement heights be confirmed. It is not likely that a small change in measurement height would alter any conclusions from the study.

6.6 Sensitive Receptors Chosen for Secunda Facility Results

Three discrete receptors are provided in CALPUFF.INP files for the Secunda facility. The 11 other sensitive receptors are extracted from the gridded receptors at the location of a sensitive area, (e.g. residential area) and receptors with predicted maximum impacts. However, it is not stated which pollutant was used to decide which receptor to select with a maximum prediction. Also, only two

receptors with maximum predictions were chosen in the entire area. Note also that there is an inconsistency between discrete receptors and gridded receptors since the height above ground for the discrete receptors is set at 3 meters while the gridded receptors are always assumed in the model to be at the ground (zero height).

6.7 Building Downwash

In Appendix B: A comparison of the study approach with the regulations prescribing the format of the atmospheric impact report (page 152 of the Secunda report), it states that "*based on screening of nearby buildings and due to the height of release from the largest pollutant emitting sources (Steam stations), it is unlikely that building downwash would significantly influence the plume*". The authors of the report recognized that not taking into account the building downwash in the calculation is not in compliance with draft guidelines as stated in Appendix B. They discuss how sources that potentially might be subject to downwash have rather small emission rates for most pollutants compared to other large sources and that these large sources are unlikely to be influenced by building downwash. The argument that the peak emissions are from tall stacks unaffected by building downwash is likely valid for this application. However, it is generally preferred to include downwash effects for sources with sub-Good Engineering Practice (GEP) stack heights and allow the model to compute the overall impacts of the downwash effect.

6.8 Linearity and Chemical Scheme

In Section 5.1.1.2 page 24 of the Secunda report, it states that "*CALPUFF includes parameterized chemistry modules for the formation of secondary sulfate and nitrate from the oxidation of the emitted primary pollutants, SO_2 and NO_x. The conversion processes are assumed to be linearly dependent (first-order) on the relevant primary species concentrations*".

The MESOPUFF II chemistry mechanism is linear with respect to SO_2 conversion to sulfate. However, the rate equations contain a weak non-linearity in the conversion of NO_x to nitric acid (HNO_3) and other nitrogen products. The puff NO_x concentration appears in the denominator of the rate equation (see Eqns. 2-254 and 2-255) in the CALPUFF User's Guide as $[NOx]^{-0.33}$ or $[NOx]^{-0.12}$). Therefore, it is recommended when using chemical conversion with NO_x emissions that the intended source NO_x emission rates be used in the CALUFF simulation to more accurately define the conversion rates, and that postprocessing scaling not be done on the NO_x concentrations. As noted above, the non-linear effect is relatively weak due to the small magnitude of the exponent in the rate equation. It is not expected that this would change conclusions of the study.

From the files received (CALPUFF input files, POSTUTIL files, CALSUM files and CALPOST files) it is interpreted that only the actual / baseline case is computed. This does not explain how the two other cases will be calculated. WhileSO_2, SO_4 concentrations and all other pollutant concentrations not subject

to chemistry can be scaled as the chemical transformation process is linear, this is not the case for NO_x, NO_2 and NO_3. The chemical transformation for those species is not linear. When running CALPUFF, any chemical transformation of NO_x will have to be run separately for all scenarios. NO_x, NO_2 and NO_3 concentrations should not be scaled from the baseline run in order to calculate concentrations for other scenarios.

6.9 Wet Deposition

Wet deposition is calculated for only two of the sources: BWSA.INP and BSCC.INP (the two sulfuric acid plant sources). Only the scavenging coefficients for liquid precipitation are specified in CALPUFF for these two sources 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 correct 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 are recommended to be included in the control file, which are $3x10^{-5}$ for SO_4, NO_3 and PM_{10}.

Note: in Section 5.2 of the report, it is stated that the deposition fluxes due to the sources modeled are not included in the report as it was not specifically requested by the National Air Quality Officer. Since a cumulative impact including all sources is performed for results in Appendix G and is discussed in Section 5.1.5.2 of the model validation, an inconsistency in using wet deposition options for some sources and not for others might have an effect on the cumulative results. It is recommended that a consistent approach be used for all sources in the treatment of deposition. While not using any deposition option for predicting concentrations is conservative, it is important that deposition options be applied consistently for all sources.

6.10 NO_3 Predictions and NH_3 Background Concentrations

The computation of monthly averages of ammonia background was discussed in Section 2. Regarding the prediction of NO_3 in CALPUFF, as the monthly averages of ammonia background are used on a puff by puff basis for the repartitioning of NO_3 and HNO_3, ammonia could be double counted. A POSTUTIL run with the same monthly background averages of ammonia as used in CALPUFF could be processed

as a refinement to compute the NO_3/HNO_3 concentrations and provide a corrected estimation of the NO_3 concentrations. In the POSTUTIL process, there is also an option to have the ammonia concentrations from the local sources (if not already added to the background) taken into account in the process. The background ammonia is fairly high, so it is not expected that ammonium nitrate formation would be limited by the amount of available ammonia in this application.

6.10.1 Monitored Monthly Average Ammonia

The monthly averaged ambient background NH_3 concentrations used in the CALPUFF simulations were evaluated. This was done using monitored NH_3 data from the three monitoring stations Bosjesspruit, Secunda, and Langverwacht. Using the hourly NH_3 concentrations from the three monitors, 3-year monthly average NH_3 concentrations were computed and then averaged over all three monitors. The averages were weighted averages based on the number of valid observations for each month, year, and monitor. The monthly average NH3 concentrations were then compared to the monthly NH_3 concentrations from the CALPUFF input files. The monitor locations at Bosjesspruit, Secunda, and Langverwacht are shown in Figure 9 and these locations correspond to the meteorological monitoring stations. The results of the weighted average calculations are shown in Table 7. This shows the 3-year monthly average NH_3 concentrations compared to the values used in the CALPUFF simulations. For the Secunda CALPUFF values, the results computed using the hourly data match the values in the control file. The CALPUFF ammonia values used for the Sasolburg and Natref runs are different from the Secunda values. It is likely these data are from a different source. We did not have access to the NH_3 monitoring data used in the Sasolburg and Natref runs and therefore could not confirm the ammonia values used in the modeling for these facilities.

Table 13. Summary of Monthly Weighted Average Monitored NH_3 Concentrations

	3-Year Average NH_3 Concentration[1,2,3]				CALPUFF Monthly NH_3		
Month	Bosjesspruit (ppb)	Secunda (ppb)	Langverwacht (ppb)	NH_3 Average[1,2,4] (ppb)	Secunda (ppb)	Sasolburg (ppb)	Natref (ppb)
January	11.57	3.36	38.01	17.6	17.6	6.9	6.9
February	6.01	4.13	45.59	18.6	18.6	6.2	6.2
March	3.75	6.71	32.24	14.2	14.2	5.7	5.7
April	4.03	8.50	19.42	10.7	10.7	7.4	7.4
May	1.24	6.63	33.96	13.9	13.9	15.5	15.5
June	5.85	14.55	37.58	19.3	19.3	19.3	19.3
July	8.22	7.71	41.50	19.1	19.1	8.2	8.2
August	10.98	3.78	45.42	20.1	20.1	15.7	15.7
Septembe r	4.79	5.79	39.97	16.9	16.9	12.5	12.5
October	3.07	2.53	20.36	8.7	8.7	16.9	16.9
November	5.92	2.07	13.91	7.3	7.3	8.4	8.4
December	4.70	2.01	25.03	10.6	10.6	11.6	11.6

[1] Years: 2010-2012
[2] Units of ppb are assumed. The monitored data did not indicate units and there were no units conversions applied.
[3] Averages are weighted by number of valid observations
[4] Average values are over all three monitors

7 CALPOST Options

CALPOST model option settings reviewed are from the CALPOST.INP files provided. CALPOST version 6.292 is used as stated in the report. This is an appropriate version of the program to use in this study. Note that no list files were provided for any of the CALPOST runs.

7.1 General Comments

In All CALPOST runs A = 1 and B = 0 (which is not necessary), but should produce the same results as using A=B=0, which is the default to use if no background is added in the CALPOST run.

Note that for extraction of time series, all gridded receptors' concentrations are at ground level (0 meters) while discrete receptors are at a height of 2 meters or 3 meters, depending on the receptor.

The files provided (CALPUFF, CALPOST, POSTUTIL and CALSUM) seem to be only for the Baseline scenario. It is not clear how the other two scenarios were computed. A comment in the CALPUFF section mentioned that the process for calculating NO_x and NO_3 is not linear. A direct scaling by the ratio of emissions for a future scenario and baseline scenario is not accurate. It will affect results for NO_2 concentration and total PM (which includes ammonium nitrate).

The CALPOST.INP files associated with the unit emission scaled run are not provided. Only one set of time series for these runs are provided and it is not possible to specify to which species it corresponds as it is only for CO the generic species used in CALPOST.

7.2 Total PM Calculation

Total concentrations of particulate matter (PM) is computed as the sum of primary PM_{10} concentrations plus the contribution of concentrations from secondary PM, including ammonium nitrate and ammonium sulfate. The secondary PM is formed through chemical reactions in the atmosphere of primary (emitted) pollutants of SO_2 and NO_x.

The calculation in the POSTUTIL files reviewed is set up as total PM = sum of PM_{10} +SO_4 + NO_3. However, the secondary pollutants to be added are in the form of ammonium sulfate $(NH_4)_2SO_4$ and ammonium nitrate NH_4NO_3. To calculate ammonium sulfate and ammonium nitrate from SO_4 and NO_3 concentrations, they need to be scaled by a molecular mass ratio (the molecular mass of ammonium nitrate over nitrate for ammonium nitrate and the molecular mass ratio of ammonium sulfate over sulfate for ammonium sulfate) which is calculated as:

- NH_4NO_3 concentration = 80/62 x NO_3 = 1.29 x NO_3 concentration
- $(NH_4)_2SO_4$ concentration = 132/96 x SO_4 = 1.375 x SO_4 concentration

The computations of PM in the report are therefore underestimated, and should be recalculated using the molecular weight scaling.

7.3 NO_2 Concentrations

NO_x is extracted and used as NO_2 concentrations for comparison with NAAQS and observations from monitoring sites. The CALPOST input files provided indicate that the ambient ratio method of applying NO_2/NO_x ratios as a function of NO_x concentrations to the predicted NO_x concentrations to obtain NO_2 concentrations was not used (i.e., NO2CALC=2). The files reviewed indicate NO2CALC=1 (i.e., fixed NO_2/ NO_x ratio, with the ratio set to 1.0 RNO2NOX=1.0). This configuration will likely overestimate NO_2 concentrations. However, the draft Secunda AIR indicates that the ambient ratio method was used in the calculations, so the discrepancy in the files appears to be a matter of the latest files not being provided. However, as noted in Section 6, we have not been able to reproduce the concentrations in the AIR.

8 Model Validation Techniques

Uncertainties and Validation of the Model

The model was validated at the monitor using the performance evaluation called the fractional bias method (recommended by US EPA (1992), developing a diagram between means and standard deviation comparison of modelled and monitored concentrations. The conclusion was that the model predictions are within a factor of 2 of the observations (for SO_2 and H_2S and most of NO_2). NO_2 predictions for short-term at two of the monitoring stations were not within a factor of 2.

Pages 77-79 (Table 5-9 to 5-11) of the draft Secunda AIR, in the comparison of the predicted and observed concentrations on a short-term bases of SO_2 concentrations, it is discussed that if predicted peak is above the observed (Table 5-9) it does show it is due to Sasol facility, but if the predicted concentrations (Peak or 99^{th} percentile, Table 5-9 and 5-10) are below the observed concentrations it mentioned that it might be due to other sources. The differences between predicted and observed also increase for the comparison with the monitoring stations further away from the facility, which is discussed as potential sources of pollutant from other facilities than Sasol.

The above is one of the explanations of the discrepancies between predicted and observed. A second explanation could be due to the uncertainties in the predictions at the exact monitoring location. The uncertainty can be due to model uncertainty but also wind speed and wind direction uncertainty. The inclusion of a cluster of gridded receptors around the monitoring location and a comparison of the concentrations predicted by this cluster of receptors to the observations at the monitor might reduce the differences between predictions and observations and take into account the uncertainties due to the model and wind speed and wind direction.

Also, the choice of calculation (the reference of the method is missing in the report) of the background concentrations to be added to the prediction for comparison with the monitoring data might not be appropriate as the sources modeled might be double counted.

9 References

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PART D
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14 April 2014

Attention: Lauren Rota

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 April 2014. 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,

Dr Lucian Burger

Dr Terri Bird

Ms Reneé von Gruenewaldt

1. Response to the Main Comments Outlined in the Peer Review

1. CTGPROC

Comment:
"Land use processing has strings of gaps of missing land use due to the resolution of the land use data used. The CTGPROC input variable MESHGLAZ should be changed from 1 to 2 to eliminate the missing data crossing the domain."

Response:
Comment and the recommended correction of the default of mesh density factor to 2, is noted. This file will be re-run for sensitivity analysis.

2. MAKEGEO:

Comment:
"The soil heat flux parameter for land use category 11 (Residential) should be 0.25 instead of 1.0"

Response:
Comment is noted. This file will be re-run for sensitivity analysis.

3. CALMET

Comment:
"There are discrepancies in the CALMET input files (CALMET.INP) regarding the number of surface stations used in the modeling (9 stations) vs. 2 stations found in the binary CALMET data file (ALLMET.DAT). The CALMET input files provided may be obsolete due to a due to a decision to use only two stations."

Response:
An obsolete version of the CALMET input file was inadvertently sent to the peer reviewer referring to 9 stations, and the correct version (referring to 2 surface stations) was subsequently forwarded on 11 March 2014.

We note nine Sasol monitoring stations in modelling domain (300km x300km). Three stations are located at each of the complexes within a 5km radius. The other remaining three monitoring stations were located outside the Calpuff modelling domains. After data screening identified the lack of complete sets at all nine stations (as required for CALMET), a representative data set was compiled per complex. Secunda Club was used as the primary station for Secunda and supplemented with data from Bosjiesspruit and Langverwacht for the parameters of RH, and temperature, where missing. Similarly AJ Jacobs was the primary station for Sasolburg, supplemented by Fence Line and Leitrim stations.

4. CALPUFF

Comment:
"Building downwash effects are not included in the modelling."

Response:
Due to the majority of the air emissions being released from tall stacks that are not influenced by the nearby building structures, the correction for building downwash were not required.

Comment:
"It is recommended that the Probability Density Function (PDF) be used with the turbulence-based dispersion coefficients (MDISP=2)."

Response:
Comment noted and modelling has been redone to include the PDF option.

Comment:
"Wet deposition is used in an inconsistent manner in the modeling."

Response:
At the time of the original baseline modelling, deposition was not considered. This decision was also made knowing that the results would provide a more conservative estimate of the air concentrations.

However, subsequent modelling has included wet and dry deposition.

Comment:
"There were some discrepancies in the concentrations provided in the draft Secunda reports vs those in the modeling files. Through an exchange of files and an explanation of the summary data provided in the second draft Secunda AIR, the discrepancies have been resolved (see Section 6 for details). The clarifications and corrections discussed should be reflected in the final AIR document."

Response:
The AIRs have been updated to reflect the corrected data.

Comment:
"when using the chemical conversion module to predict NO_x concentrations, it is preferred that the actual emission rates be used because of a non-linearity in the conversion rate equations."

Response:
Linear scaling was abandoned in favour of re-running the model for altered or changed scenarios.

5. POSTUTIL

Comment:
"The calculation of total particulate matter (PM) concentrations by summing primary PM and secondary PM (ammonium sulfate and ammonium nitrate) in the POSTUTIL processor requires the application of a molecular weight adjustment of 1.375 to change sulfate (weighed as SO_4 in the model) to $(NH_4)_2SO_4$ and 1.29 to change nitrate (weighed as NO_3 in the model) to NH_4NO_3."

Response:
Comment noted and correction made.

6. CALPOST

Comment:
"The CALPOST input files provided do not show the application of the ambient ratio method, which applies NO_2/NO_x ratios as a function of NO_x concentrations to compute NO_2 concentrations from NO_x concentrations."

Response:
Ambient ratio method as recommended by the Peer Reviewer described by Scire and Borissova (2011) (Table E-1 in the AIRs) was used. This was done in individual spreadsheets and not in the post processing. Although the methodology was the same as given in Scire and Borissova, the NO_2/NO_x ratio was conservatively limited to a minimum of 40% conversion at high concentration levels. In the original methodology, this conversion could be lower than 20%.

2. Response to Additional Comments Outlined in the Peer Review

Section 3: Background Air Quality Data

Comment:
"The methodology is different from the U.S. EPA procedures which involve three tiers of conservatism (Level 1 background is highly conservative) and Level 3 is more refined. The Level 3 U.S. EPA methodology involves the use of wind direction to compute hours that are unaffected by modeled sources to determine hourly background values. It is not clear if the monitoring network is sufficient to obtain a Level 3 background estimation. However, the methodology used in the AIR is difficult to assess because we've been unable to reproduce the background values reported in the tables and the reliability of the method based on the 50th percentile hourly concentration (or the percentile for where the modeled concentration becomes zero) is untested."

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

However, as used in the current investigation, background concentrations could also incorporate the contributions from air emission sources present in the modelling domain, but which were not included in the dispersion simulations. For example, air emissions from vehicle tailpipes can significantly contribute to the local ambient NO_2 air concentrations. Similarly, domestic fuel burning is well-known for its contribution to airborne particulate air concentrations (PM_{10} and $PM_{2.5}$). Also, coal-fired power stations in and the near vicinity of the modelling domain are significant sources of SO_2 emission. Although most of the sources of air emissions within the Sasol operation were included in the simulations, there remains some that were excluded, for instance fugitive emissions. It is expected that all of these emissions that were not part of the simulation emissions inventory, would add to the background concentration level.

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

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

Section 4: MM5 Meteorological Data

Comment:
"It is not stated in the AIR what data was used as initial and lateral boundary conditions, the data was used for the analysis nudging, or the details of the model configuration and model nest(s) in the mother domain(s)."

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

Comment:
"...no evaluation of the MM5 model performance relative to observations."

Response:
A comparison of wind data was provided in the AIR (Section 5.1.5) and it was found that there is an acceptable agreement.

Further analysis will include comparisons of the temperature and relative humidity.

Comment:
Use of only 18 vertical levels is much coarser than most MM5 simulations.

Response:
Lakes Environmental Software confirms that using 30 to 40 layers is great for obtaining good representation above 1,000m. For air dispersion models, however, the focus is in the lowest layer of the atmosphere. Lakes Environmental analysed numerous cases when developing their service and found no magnitude change in both speed and direction when adding many layers. The additional data increased file size and processing time but didn't affect dispersion from tall stacks. Subsequently, Lakes Environmental stuck with 18 vertical levels.

Section 5: CALMET Options

Comment:
"CALMET options for the Secunda AIR are reasonable overall for this application. There are several changes that are recommended, however, they are not considered critical items but rather recommended refinements."

Response:
Recommended refinements of the CALMET model setup is noted for future applications.

Section 6: CALPUFF Model Options

Comment:
"Turbulence-based dispersion (MDISP=2) was chosen for the dispersion coefficient method but the Probability Density Function (PDF) option was not used. The PDF option has been found in various model evaluation studies to be important for tall stack dispersion under convective conditions. These conditions are likely to be important in this application with both tall stacks present and frequent, highly convective conditions expected."

Response:
Comment noted and modelling has been redone to include the PDF option.

Comment:
"The monthly averages of hourly ozone data seem to have been calculated including all hours instead of daylight hours only. Because ozone is used as a surrogate for daytime OH radicals in the atmosphere when using the MESOPUFF chemical transformation algorithm, it is best to use daytime ozone only in computing the monthly ozone averages that serve as a backup when hourly ozone data is missing. At night ozone concentrations are not used by the chemistry, but rather a small nighttime conversion rate reflecting heterogeneous reactions is used.

A new calculation of the ozone monthly averages to include only the daylight hours is expected to have little effect on the Secunda concentration predictions and could have a slight effect on the NATREF and SASOLBURG concentration predictions for pollutants involving chemical transformation. This change although recommended, is not considered a critical item."

Response:
Recommendation noted.

Comment:
"...it is not stated which pollutant was used to decide which receptor to select with a maximum in prediction"

Response:
The receptors were chosen based on SO_2 concentrations as this pollutant provides the highest emissions from the Infrachem and Synfuels complex. Simulations have since confirmed that these selected maximum points are representative of the maximum concentrations across all other pollutants simulated (with the exception of NO_2 due to time variant chemical transformation processes).

Comment:
"From the files received (CALPUFF input files, POSTUTIL files, CALSUM files and CALPOST files) it is interpreted that only the actual / baseline case is computed. It is not explained how the two other cases will be calculated."

Response:
The other scenarios were based on the same procedure. The only changes were to emission rates and if theoretical compliance scenarios resulted in stack parameters for example, temperature changes and stack heights (Section 5.1.7 in the AIRs).

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.

References

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.

ANNEXURE 1: MM5 MODELLING AT LAKES ENVIRONMENTAL

MM5 MODELING AT LAKES ENVIRONMENTAL

MM5 Meteorological Data for AERMOD and CALPUFF

1 Introduction

This document is designed to provide a brief description of MM5 modeling at Lakes Environmental. Our MM5 modeling focuses on generating high resolution meteorological data with the objective of gathering enough information to create AERMOD and CALPUFF meteorological input files.

For AERMOD, Lakes Environmental generates the surface met file in SAMSON format and the upper air met file in TD-6201 format from hourly MM5 results. These two files are input into the AERMET pre-processor to produce the .SFC and .PFL files required by AERMOD. For CALPUFF, Lakes Environmental generates CALMET.DAT meteorology files which can be processed by the CALMET meteorological model.

Lakes Environmental has chosen MM5 modeling options based on publications of studies for high resolution (small grids) evaluation runs. It is expected that a more precise analysis should be conducted by the U.S. EPA in the future.

1.1 What is MM5?

MM5 (5^{th}-generation Mesoscale Model) is a prognostic meteorology model developed by Pennsylvania State University and the U.S. National Center for Atmospheric Research (NCAR). The model is a limited-area, non-hydrostatic, terrain-following sigma-coordinate model designed to simulate or predict mesoscale and regional-scale atmospheric circulation. MM5 was primarily developed using FORTRAN coding, and is

still widely used as a community model even though formal development of the model has ended.

2 MM5 Modeling at Lakes Environmental

2.1 Input of Meteorological Data

MM5 cannot 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 take account of 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 NCEP (National Center for Environmental Protection).

Lakes Environmental has obtained NCEP Global Reanalysis data for input to MM5, from 1999 to 2008 (and beyond as further data becomes available). The NCEP reanalysis has a resolution of 2.5 degrees by 2.5 degrees for the entire globe, given every 6 hours. For further details on the Global Reanalysis data set, please refer to the NCAR data website at http://dss.ucar.edu/datasets/ds090.0/.

The reanalysis data incorporates global weather data. Figure 1 presents an example for the Great Lakes region of North America. The station numbers in the figure below show which weather stations were used for the reanalysis data. Note that these stations do *not* directly provide the data used for MM5 output; they serve as *input* into the MM5 model.

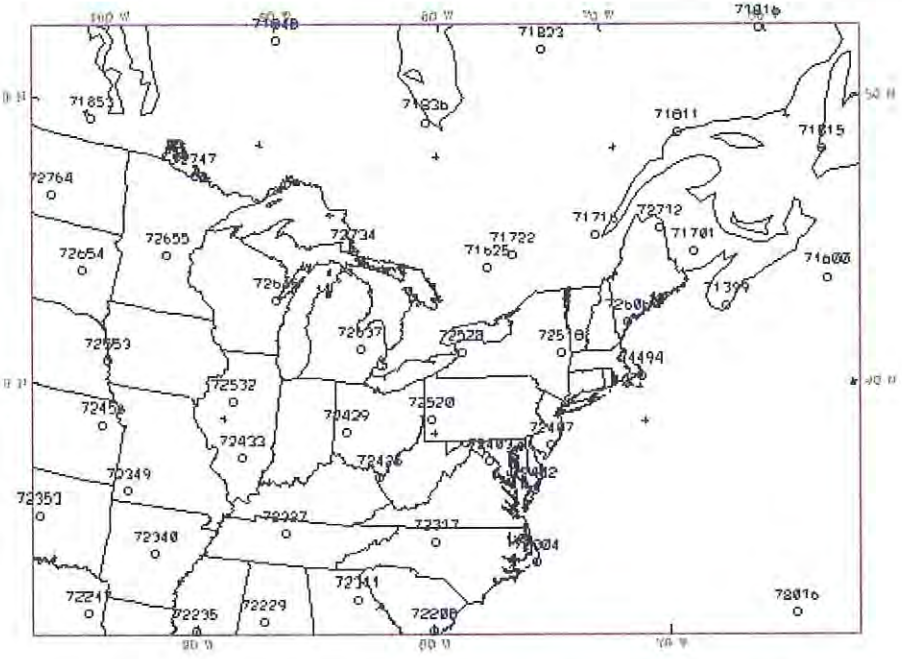

Figure 1: Sample MM5 domain with meteorological stations

2.1.1 Modeling Nested Grids Domain

MM5 uses a nested grid approach. In this way, an area of interest can 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 a 12km grid or a 4 km grid spacing at the highest resolution (internal) grid. MM5 data for the AERMOD model is available only in 12 km resolution, while MM5 data for the CALPUFF model is available at either 12 km or 4 km resolution.

Table 1 presents the grid dimensions and number of grid points that are commonly used in our MM5 runs when obtaining AERMOD meteorological formatted data files.

	NEST 1	NEST 2	NEST 3
Grid Points	23	31	31
Grid Size (km)	108	36	12

Table 1 - Sample MM5 with 12km nested internal grid.

Figure 2 presents an example of an MM5 domain used to generate AERMOD meteorological data for a source located in Southern Ontario, Canada. This domain contains a three level nest (with labels D01, D02, and D03). Data for use in AERMOD are extracted from the innermost domain (NEST 3) only; the other domains are used only to provide information to the innermost domain.

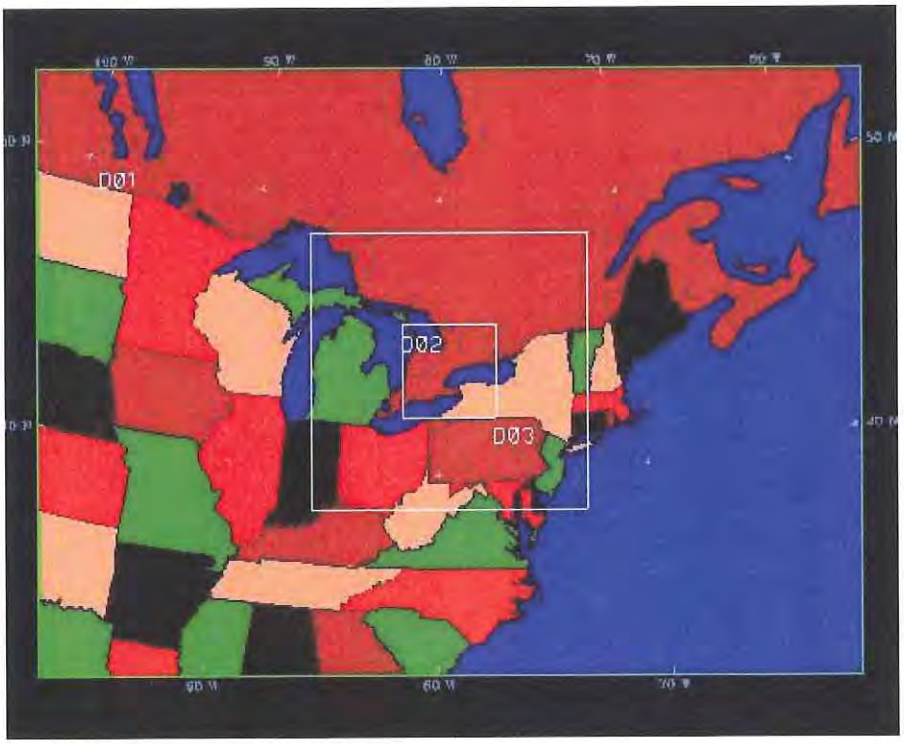

Figure 2 – An example of a nested MM5 domain.

2.1.2 MM5 Physics Options

The MM5 application provides many modeling options which can greatly affect the final output. In Table 2 below we have listed the physical options that we most commonly use; however, these options may change at our discretion. These options are the ones that many MM5 users have adopted when generating data for AERMOD and CALPUFF:

Physics Option	Option Chosen and Details
Cumulus Clouds	Kain-Fritsch 2 (Kain 2002, Kain and Fritsch 1993). Includes shallow convection. Uses a sophisticated cloud-mixing scheme to determine entrainment/detrainment. Predicts updraft and downdraft properties and detrains cloud and precipitation. Shear effects on precipitation efficiency are also considered.
Planetary boundary Layer (PBL)	MRF PBL (Hong and Pan, 1996) Suitable for high-resolution in PBL. Efficient scheme based on Troen-Mahrt representation of counter-gradient term and K profile in the well mixed PBL, as implemented in the NCEP MRF model. Vertical diffusion uses an implicit scheme to allow longer time steps.
Moisture Scheme (Microphysics)	Simple Ice/Dudhia (Dudhia, 1989). Adds ice phase processes to above without adding memory. No supercooled water and immediate melting of snow below freezing level.
Radiation Scheme	RRTM Longwave Scheme (Mlawer et al. 1997). Rapid Radiative Transfer Model - this is combined with the cloud-radiation shortwave scheme. It represents the effects of the detailed absorption spectrum taking into account water vapor, carbon dioxide and ozone. It is implemented in MM5 to also interact with the model cloud and precipitation fields.
Surface Scheme	Five-Layer Soil Model (Dudhia1996, MM5 workshop abstracts). Temperature predicted in 1, 2, 4, 8, 16 cm layers with fixed substrate below using vertical diffusion equation.

Table 2: Physics Options used for MM5 Modeling

2.1.3 Four-Dimensional Data Assimilation (FDDA)

Four-Dimensional Data Assimilation, or FDDA for short, is used in our MM5 modeling. Specifically, analysis or grid nudging is applied – Newtonian relaxation terms are added to the prognostic equations for wind, temperature, and water vapor. These terms relax the model value towards a given analysis. The model linearly interpolates the analyses in time to determine the value towards which the model relaxes its solution.

2.2 MM5 to CALMET and CALPUFF

2.2.1 Retrieval of MM5 Data: CALMM5

The CALPUFF model's MM5 processor *CALMM5* is currently employed to retrieve MM5 output grid point data and place it into a formatted text file. The CALMM5 file format contains the following output variables (for each sounding):

- Pressure (mb)
- Elevation (m)
- Temperature (K)
- Wind direction (deg)
- Wind speed (m/s)
- Vertical wind velocity (m/s)
- Relative humidity (%)
- Mixing ratio of vapor (g/kg)
- Mixing ratio of cloud water (g/kg)
- Mixing ratio of rain water (g/kg)
- Mixing ratio of ice water (g/kg)
- Mixing ratio of snow (g/kg)
- Mixing ratio of graupel (g/kg)

In addition, each sounding record also reports the following surface variables:

- Sea level pressure (hPa)
- Rainfall accumulation for the past hour (cm)
- Indicator of snow cover

The CALMM5 output forms a grid covering the modeling domain with the specified resolution of either 4 km or 12 km. The CALMM5 output can be used as direct input in CALMET.

2.3 MM5 to AERMOD and AERMET

2.3.1 Pseudo Stations

The CALMM5 output is used to create MM5 data ready for input into AERMET. Even though this MM5 data is intended for use in AERMOD, CALMM5 can provide appropriate output which can then be formatted to meet the requirements of AERMOD and AERMET. This is done by adding an extra step to create a pseudo meteorological station.

The grid cell that contains the desired site is extracted from the overall CALMM5 output grid. The MM5 sounding data is taken from this grid cell and used to create a pseudo station consisting of surface and upper air meteorological files. This is described in more detail in the following sections.

2.3.2 Psuedo Surface Report

The CALMM5 surface output data is formatted into a SAMSON met file. This file contains the following information:

- Date, hour (YYMMDDHH)
- Total cloud cover, opaque cloud cover (0-10) – derived by formula
- Ambient temperature (deg C)
- Dew point temperature (deg C)
- Relative humidity (%)
- Station pressure (mb)
- Wind direction (0-360 deg)
- Wind speed (m/s)
- Ceiling height (0-30450 m) - derived
- Present weather (09999, 99999:- unknown)
- Hourly precipitation rate (inches and hundredths)
- Global radiation (0-1415 Wh/m^2):- unknown

Certain parameters must be calculated from the CALMM5 output, as they are not directly available. The methods we use are all based on methods found in CALPUFF's meteorological processor; CALMET.

Cloud coverage

- Deduced using relative humidity at 850 hPa (or nearest available level) using the empirical equation (Teixeira, 2001):

$$a = \frac{0.2\left(-1+\sqrt{1+100(1-RH)}\right)}{1-RH}$$

- The above equation assumes a detrainment rate, $D=4\times10^{-6}$ s^{-1}, and an erosion coefficient, $K=1\times10^{-6}$ s^{-1}, as used in the ECMWF model
- For RH > 99%, a = 1

Cloud ceiling height

- The lowest height of non-zero cloud mixing ratio
- If a non-zero cloud mixing ratio is not found and cloud coverage > 0.2, then a default ceiling height of 8000 ft (i.e. 2438 m) is set. This is the same as the procedure used by CALMET.

2.3.3 Pseudo Upper Air Report

The CALMM5 upper air output data is formatted into a TD6201 file. Measurements are recorded twice daily at 00Z and 12Z. This file contains the following parameters:

- Station ID, latitude, longitude
- Year (YYYY), month, day, hour (UTC)
- Number of vertical levels
- Repeat number of vertical levels (currently, 18)
- Pressure
- Elevation
- Ambient temperature
- Relative humidity
- Wind direction
- Wind speed

All parameters in the upper air data file are obtained directly from the CALMM5 output.

3 Conclusion

Lakes Environmental currently uses the MM5 prognostic meteorological model to generate data for AERMET. The methodology currently in use adopts the U.S. EPA guidance and accepted models, such as MM5, CALMM5, CALMET, and AERMET. We continue to conduct various analyses on our current approach in order to improve our results, and to provide guidance on conditions when better use of direct data from MM5 or data processed through CALMM5 and AERMET would be more appropriate.

However, we re-iterate that the current approach should already be acceptable "as is" as it is based on accepted methods and software codes.

Note: This document describes the methods currently used in preparing AERMOD and ISC meteorological data from MM5 modeling; therefore, changes may occur at the meteorologist's discretion to fulfill our commitment to ongoing improvements.

4 Additional Information

This document is meant to provide a brief description of the MM5 model, how it is used at Lakes Environmental, and its application to AERMOD and CALPUFF.

For more information on MM5 at Lakes Environmental, please contact us at info@weblakes.com. For more detail on the MM5 model, please visit the MM5 Community Model Homepage at http://www.mmm.ucar.edu/mm5/mm5-home.html.

