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MODELLING THE DISPERSION OF SO_2 EMISSIONS FROM THE CHEVRON (Cape Town) OIL REFINERY USING THE US EPA DISPERSION MODELS AERMOD and CALPUFF.

Master of Technology Thesis
(Chemical Engineering)

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November 2013

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By
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Thesis submitted in partial fulfilment of the requirements for the degree Master of Technology: Chemical Engineering in the Faculty of Engineering at the Cape Peninsula University of Technology

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Bellville
Date submitted: Novemer 2013

Declaration

I, Khanyisa Siyakudumisa Mtiya, hereby declare that I have developed and written the enclosed theses by myself and have not used any sources or means without any appropriate referencing. Any thoughts and quotation that were inferred from such sources have been clearly acknowledged. This thesis was not submitted in the same or in a substantially same version, not even partially to any other academic institution to achieve academic grading. Furthermore, it represents my own opinions and not necessarily those of the Cape Peninsula University of Technology.

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Certification of Approval

We hereby declare that this thesis is from the student's own work and effort. All sources of information have been properly acknowledged. Furthermore, this thesis has been submitted with our approval.

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Signature: ……...

Date: …15 January 2014 …….

Dedications

In memory of my late father

Khululekile Conilius Mtiya

(1961 – 2012)

Enkosi Nokhala, Msuthu, Jiyana, Tiba ulalengoxolo.

Acknowledgements

My sincere appreciation and gratitude are due to the following people and organizations: The assistance of **Raoul Duesimi** of the Department of Land Affairs Cape Town (digital topography), **Gail Linnow** of the Regional Office-Western Cape at South African Weather Services (meteorological data application), **Musa Mkhwanazi** Scientist for Climate Information and **Colleen de Villiers** of the South African Weather Services (for meteorological data), **Judith St Leger, Borman Adele, Salie Nathmi, Fortuin Morne Victor,** and **Petersen Vernon John** of Chevron Refinery are gratefully acknowledged for all the refinery data, including annual stack emission data, as is **Michael T. Hammer,** Senior Product Specialist, of Lakes Environment for his valuable insight and generous help in the AERMOD and CALPUFF model operation and processing of Meteorological data. **Julie Swatson,** Senior Sales Associate of Lakes Environment for a free CALPUFF license for the duration of the study. **Michael Weston and Theo Fischer** from Escience Environment for his valuable insight and generous help in the AERMOD and CALPUFF model operation and processing of meteorological data. **Beverley Terry** of National Association of Clean Air (NACA) for the NACA presentation sponsorship. **Sally Benson,** Scientific Services in Cape Town, for providing air pollution data throughout the life of this project. **Prof. Daniel Ikhu-Omoregbe** Department of Chemical Engineering, Cape Peninsula University of Technology for his co-supervision.

Prof. Eugene K. Cairncross, Department of Chemical Engineering, Cape Peninsula University of Technology for his supervision, constant support and invaluable guidance throughout the research period.

Last but not least, I would like to thank my friends and family for their patience and moral support from the beginning to end of my study.

Thank you all. I would not have completed this study without your assistance.

Abstract

In South Africa, the Department of Environmental Affairs (DEA) under the National Environmental Management Act, 1998 (Act 107 of 1998) ("NEMA") sets out a series of environmental management principles that apply to the interpretation and application of all legislation that may affect the environment. Since 1998, various specific environmental statutes that fall under the NEMA framework have been promulgated, including the National Environmental Management: Air Quality Act, Act 39 of 2004 (NEM: AQA).NEM:AQA provides norms and standards for all technical aspects of air quality management. The National Framework (Sections 7 and 8 of NEM:AQA) must provide mechanisms, systems and procedures to promote holistic and integrated air quality management through pollution prevention and minimisation at source, and through impact management with respect to the receiving environment, from local scale to international issues.

Among other measures, the NEM:AQA (Section 9) requires the establishment of Ambient Air Quality Standards and Emission Standards. These standards were promulgated in December 2009 and March 2010 respectively. Air quality monitoring stations, which sample and analyse pollutant concentrations continuously, are a common method of assessing air quality in a region. But a few continuous monitors located in source given region or airshed are inadequate for assessing compliance with ambient air quality standards – they are only able to monitor concentrations at a fixed site, not through the entire region of impact. In contrast, the ambient air quality standards are applicable everywhere. Air quality models estimate ground level ambient concentrations throughout the modelling domain, and in principle (subject to proper validation) provide better estimates of area-wide concentrations and hence the basis for assessing compliance with air quality standards. The United States Environmental Protection Agency (US EPA) approved atmospheric air dispersion models AERMOD and CALPUFF were used in this thesis to predict the ground level concentrations of SO_2 emitted from Chevron Refinery (Cape Town), for the year 2010. The modelling is validated by comparing measured ambient concentrations with modelled concentrations.

The results showed AERMOD-modelled annual average values for 2010, based on refinery emissions only, are in good agreement with monitored values at the Table View and Bothasig sites, predicting the monitored values by -11% and +17% respectively. The 24-hr average values similarly are in good agreement with monitored values, on average over-predicting by 9% at Table View, although the fit of the day-to-day modelled vs monitored values is comparatively poor (R^2=0.32); at the Bothasig site the corresponding values are - 36% and R^2= 0.089.

The AERMOD-modelled isopleths imply that the 2010 annual average concentrations exceeded the South African Standard of 50 µg/m^3 in a small area in the immediate vicinity of the refinery. The hourly and 24-hourly average standard concentrations of 350µg/m^3 and 125µg/m^3 respectively are exceeded in significantly larger areas. The allowable exceedences for hourly and 24-hourly averages are also exceeded, implying that the hourly and 24-hourly standards were exceeded.

CALPUFF-modelled average values for 2010, based on refinery emissions only, are in comparatively poor agreement with monitored values at the Table View and Bothasig sites, under-predicting the monitored values by -20% and -61% respectively. Since the AERMOD-modelled concentrations are in far better agreement with monitored concentrations, only AERMOD was used for further analysis.

The Emission Standards promulgated in March 2010 included emission limit values for sulphur dioxide emitted from oil refineries. If the actual 2010 emission rates were adjusted downwards to match the emission standards (to be complied with from 1 April 2015), AERMOD modelling indicates that the annual, 24-hourly and hourly Ambient Air Quality Standards would not be exceeded. Based on this case study, the current Emission Standard for SO_2 emissions from existing crude oil refineries is therefore coherent with the Ambient Air Quality Standards.

Regulatory air dispersion modelling practices in South Africa are being standardised for model applications regulatory purposes and to ensure that dispersion modelling practices are undertaken in a compatible form to ensure that results from one dispersion model study can be compared directly to those from another. In this study both AERMOD and CALPUFF modelling complied with the draft South African guidelines for Air Quality Modelling, yet the CALPUFF-

modelled outputs differed significantly from the monitored values. This emphasizes the importance of the inclusion of modelling validation in guidelines for modelling for regulatory purposes. The 2012 draft regulation should be amended to make validation of regulatory dispersion modelling compulsory rather than optional as per the draft.

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Acronyms/ Abbreviations

1. AAQS	Ambient Air Quality Standards
2. ADMS	Atmospheric Dispersion Modeling System.
3. AERMOD	American Meteorological Society/ Environmental Protection Agency Regulatory Model.
4. AQMN	Air Quality Monitoring Networks.
5. ASG	Atmospheric Studies Group.
6. BPEO	Best Practicable Environmental Option
7. CALPUFF	CALifornia PUFF model.
8. CALPOST	CALifonia POST-processing program.
9. CALMET	CALifonia METeorological model.
10. CAMx	Comprehensive Air Quality Model with Extensions.
11. CBL	Convective Boundary Layer.
12. CTIA	Cape Town International Airport.
13. DEM	Digital Elevation Model.
14. EMIs	Environmental Management Inspectors.
15. EHP	Environmental Health Practitioner.
16. FCCU	Fluid Catalytic Cracking Unit.
17. FGR	Flue Gas Recirculation.
18. GPM	Gaussian Plume Model.
19. HVG	Heavy Vacuum Gas Oil.
20. ISC3	Industrial Source Complex.
21. ISCST3	Industrial Source Complex - Short Term.
22. LULC	Land use and land cover.
23. NAAQS	National Ambient Air Quality Standards.
24. NEAF	National Environmental Advisory Forum.
25. PBL	Planetary Boundary Layer.
26. SAPIA	South African Petroleum Association.

27. SAWS	South Africa Weather Service.
28. SAAAQS	South African Ambient Air Quality Standards.
29. SAAQIS	South African Air Quality Information System.
30. SANAS	South African National Accreditation System.
31. SO_2	Sulphur Dioxide.
32. SO_3	Sulphur Trioxide.
33. SO_x	Oxides of sulphur (sulphur dioxide and sulphur trioxide).
34. NO_2	Nitrogen Dioxide.
35. NO_x	Oxides of Nitrogen (Nitrogen dioxide and Nitrogen trioxide).
36. SWS	Sour Water Strippers.
37. USGS	United States Geological Survey.
38. SRU	Sulphur Recovery Unit.
39. US EPA	United States Environmental Protection Agency.
40. UTM	Universal Transverse Mercator.
41. WHO	World Health Organization.

Glossary of terms

1. ADMS	An advanced atmospheric pollution dispersion model for calculating concentrations of atmospheric pollutants emitted both continuously from point, line, volume and area sources, or intermittently from point sources.
2. AERMOD	Gaussian steady state air pollution dispersion model that has single point meteorology.
3. AERMIC	American Meteorological Society/Environmental Protection Agency Regulatory Model Improvement Committee.
4. AERMAP	AERmod MAPing program.
5. AERMET	AERMod METeorological pre-processor.
6. AERSURFACE	AERMOD SURface characteristics pre-processor.
7. AMBIENT AIR	The air of the surrounding environment; outdoor air.
8. AIR QUALITY	A measure of exposure to air.
9. AP-42	A compilation of emission factors and process descriptions for a broad range of emission sources. EPA Document Number AP-42, Compilation of Air Pollutant Emission Factors, Environmental protection Agency, Research Triangle Park, North Carolina. Current information on AP-42 is available on the USEPA website.
10. BACKGROUND CONCENTRATION	Concentration already present and due to natural or other anthropogenic sources.
11. CALPUFF	Transport and dispersion processor, a non-steady-state puff dispersion model that simulates dispersion and transport processes of pollutant(s) along the dispersion path.
12. CALMET	Meteorological processor that develops hourly wind and temperature fields in the three-dimensional gridded modelling domain.

13. CALPOST	Postprocessor used to process the files from CALPUFF to produce a summary of the simulation results.
14. DEA	Department of Environmental Affairs.
15. Convective Boundary Layer	The lower tropospheric layer in contact with the ground heated by the sun and swept by the wind.
16. COMPLEX TERRAIN	Terrain exceeding the height of the stack being modelled
17. EMISSION FACTOR	Representative value, relating the quantity of a pollutant to a specific activity resulting in the release of the pollutant to atmosphere.
18. NEM	National Environmental Management
19. Monin-Obhukov Length	Used to describe the effects of buoyancy on turbulent flows, particularly in the lower tenth of the atmospheric boundary layer.
20. Planetary Boundary Layer	The layer where the earth's surface interacts with the large scale. atmospheric flow
21. SIMPLE TERRAIN	An area where surrounding terrain heights are all lower in elevation than the top of the stack of the source.

Chapter 1: Overview

1.1 Introduction

Since 1965, the approach to air pollution control in South Africa was informed and driven by the Atmospheric Pollution Prevention Act (APPA) (Act No. 45 of 1965). The Act did not set targets or standards that would permit the achievement of an environment that is not harmful to health or well-being. Clean air is essential for the good quality of life and it is important to consider the effects of pollutants (SO_2) on the human health. Because the APPA Act suffered from many shortcomings, the National Environmental Management: Air Quality Act, Act 39 of 2004 (NEM: AQA) amended the legislative framework for environmental management in South Africa. Its purpose is to provide for cooperative environmental governance, and it defines principles for decision-making on matters affecting the environment. The NEM: AQA has further provides for the establishment of the National Environmental Advisory Forum (NEAF) as a body to encourage stakeholder participation and develop management methods that include the guidance and perspectives of stakeholders within the NEAF. The NEM: AQA provides government with the regulatory tools to implement the National Environmental Management Policy.

Air quality management in South Africa has rapidly evolved from the control of a few contaminants emitted from industrial stacks to a complex network of management approaches to address a host of new, inter-related air quality issues. The NEM: AQA represents a distinct shift from exclusively source-based air pollution control to holistic and integrated effects-based air quality management. Among other measures, the NEM:AQA (Clause 9) requires the establishment of AAQ Sand Emission Standards. The Minister, by notice in the Gazette (1) must identify substances or mixtures of substances in ambient air which, through ambient concentrations, bioaccumulation, deposition or in any other way, present a threat to health, well-being or the environment or which the Minister reasonably believes present such a threat; and (2) must, in respect of each of those substances or mixtures of substances, establish national standards for ambient air quality, including the permissible amount or concentration of each such substance or mixture of substances in ambient air; and (3) may, in respect of each of

those substances or mixtures of substances, establish national standards for emissions from point, non-point or mobile sources (NEM:AQA, 2005).

NEM:AQA also requires (Clause 7.1) the minister to establish a national framework for achieving the object of the Act, within two years of the date on which the section took effect, by notice in the Gazette. The National Framework must provide mechanisms, systems and procedures to promote holistic and integrated air quality management through pollution prevention and minimisation at source, and through impact management with respect to the receiving environment from local scale to international issues. The implementation of the National Framework is dependent on a combination of both process/governance and technical mechanisms/measures.

The National Framework, in terms of Section 7(3) of the AQA: binds all organs of state in all spheres of government; and may assign and delineate responsibilities for the implementation of the AQA amongst the different spheres of government; and different organs of state. According to Section 8 of the AQA, with respect to national monitoring and information standards, the National Framework must establish national standards for (1) municipalities to monitor ambient air quality; and point, non-point and mobile sources, (2) provinces to monitor: ambient air quality; and the performance of municipalities in implementing the AQA. Ambient Air Quality Standards (Government Gazette 2009) and National Minimum Emission Standards for listed activities (Government Gazette 2010), including those for the Petroleum Industry, were promulgated under NEM:AQA, based on the procedures set out in the Framework.

The National Framework prescribes how both AAQS and ELs should be determined. AAQS are determined based on evidence of health impacts but ELs for LAs are based on Best Practicable Environmental Option (BPEO). BPEO entails a consideration of information provided in peer-reviewed local and international literature which is feasible and realistic to be measured in terms of its impact on the environment, where the environmental surroundings is influence human health and wellbeing. The methodologies and the basis for developing and setting these two standards do not therefore require a check to establish whether or not an emission limits even when applied to a single source in a given area is likely to result in the non-compliance with the ambient air quality standards.

In order to understand the complexities involved, decision makers are increasingly relying on atmospheric dispersion models as they simulate of the physics and chemistry governing the transport, dispersion and transformation of pollutants in the atmosphere and estimates downwind air pollution concentrations given information about the pollutant emissions and meteorology during the period of interest, an air pollutant is transported from a source to a potential receptor and provide a way to evaluate different emission control scenarios. In South Africa, the use of modelling to demonstrate compliance with air dispersion models is at an early stage (DEA, 2012). Dispersion modelling is the only established tool for evaluating the impacts of future developments and measurable answers to questions for environmentally sound and scientifically based and cost effective air quality management decisions.

The SO_2 emission limit for an existing Category 2 (Petroleum Industry) Listed Activity is 0.8kg/day/t of crude throughput (Government Gazette 2010, Category 2, sub-category 2.1). Compliance with this limit comes into effect on 01 April 2015. The AAQSs for $SO_2$for different averaging periods are 500 µg/m^3 for 10 minutes, 350 µg/m^3 for 1 hour, 125 µg/m^3 for 24 hour and 50 µg/m^3 for 1 year. The impact of total refinery emissions on ambient SO_2 concentrations, and hence compliance or otherwise with the national ambient air quality standards, depends on source emission characteristics, including number of stacks, stack heights, exit temperatures and velocities, meteorological conditions and local terrain. In addition, site-specific background pollution sources should be considered.

In this thesis a case study, namely air pollution modelling using the actual emission characteristics of the Chevron Refinery, situated in Milnerton, Cape Town, and local meteorology, is used to assess the coherence between the sulphur dioxide (SO_2) emission standard for the Petroleum Industry and the ambient SO_2 standards. That is, to assess whether the emission standard are coherence with ambient SO_2 standards. The Chevron refinery, with a regulated capacity to process 100 000 (SAPIA, 2011) barrels per day of crude oil, is located in Cape Town, 3km from Milnerton and 2km from Table View residential areas and 20km from the central business district.

The processing of sulphur-containing crude oil produces various products including liquefied petroleum gas (LPG), petrol, paraffin, diesel, and bunker fuels. Sulphur is an inherent component of crude oil. Sulphur dioxide is generated in a number of process units in a refinery, including various furnaces and boilers that use fuel gas, process gas and fuel oil. A refinery uses large quantities of energy to heat process streams, promote chemical reactions, provide steam, isolate and recover excess sulphur and generate power. This is usually accomplished by combustion of fuels, typically those generated on site such as refinery fuel gas and the coke deposited on cracking catalysts. Examples of combustion sources include furnaces, boilers, heaters, turbines and the catalytic cracker regenerator. Off gas from the overheads condensers is also burned in the heaters converting H_2S to SO_2.

Combustion emissions from the refinery are mainly released via nine point sources (eight stacks and one flare system). Flare systems in oil refineries are designed to provide safe disposal of gases/vapours released from process equipment. The steam assisted flare system uses fuel gas to burn any unprocessed hydrocarbons and H_2S from the entire refinery, generating SO_2 in the process. Unfortunately, the combustion process in these flares is intermittent and is less than 100% efficient, resulting in the emission of unburned hydrocarbons, carbon monoxide and soot. In addition, the high temperature of combustion would also result in formation carbon dioxide, NO_X and SO_X are emitted. These pollutants may have a severe influence on the industrial area and surrounding urban localities (Cairncross E.K, 2007), (Saqer S.S et al, 2008).The emission of these pollutants may result in significantly elevated ambient concentrations of these pollutants, with consequent health impacts to exposed communities. The SO_2 from all these sources is emitted to the atmosphere via stacks, including the flare stack, with different height, exit velocity and temperature characteristics.

There are two ambient air quality monitoring stations within 5 kilometres of the refinery. However monitored data are not an adequate measure of air quality in the zone of impact, especially with respect to hourly and daily short-term average concentrations. The location of the area of highest impact is dependent on the stack discharge characteristics – emission rate, height, exit velocity and temperature – which may vary in accord with refinery operating conditions. In addition, the more influential cause of short term variability is usually likely to be meteorological conditions – wind speed, wind diction, temperature and humidity. The precision of modelled outputs of even well-established and validated models such as the United States'

Environmental Protection Agency (US EPA) regulatory models AERMOD and CAPUFF (Cimorelli et al 2004), used in this study, are dependent on the accuracy of the input variables. Groschand Lee (Grosh T.G et al,1998) highlighted this sensitivity of modelled outputs by evaluating the effect on design concentration predictions from AERMOD, for a range of sources, of variations of the albedo, Bowen ratio, and surface roughness length individually and in combination over ranges of values and also evaluated the land use parameters that are characteristic of each of four types of ground covers (Grosh T.G et al,1998). Validation of predicted ambient concentrations against measured data is essential before model results can be used with confidence to assess air quality.

Lakes Environment's AERMOD View^{TM} and CALPUF View^{TM} were used with local meteorology (Cape Town International Airport and meteorological stations local to the refinery), reported daily SO_2 emissions and local terrain data as inputs to model the dispersion of SO_2 emitted by the Chevron Refinery (Milnerton). AERMOD is a steady state Gaussian plume model with features similar to ISCST3, but with additional capabilities, including the handling of complex local terrain. CALPUFF is an unsteady Langrangian Gaussian puff model which has the ability to model pollutant dispersion, chemical transformation, dry deposition, and wet deposition better than AERMOD. Modelling was done over a year to assess the effect of meteorological variability. Model-predicted ambient concentrations based on actual refinery emissions and are compared with corresponding monitored data from three local stations to validate the modelling. Emission rates are then compared with the regulated emission standard, and model-estimated ambient concentrations are compared with the 1 hour, 24 hour and annual average Air Quality Standards.

1.2 Objectives

The main objective of this study is to use air quality modelling to assess the coherence between the sulphur dioxide (SO_2) emission standard for the Petroleum Industry and the ambient SO_2 standards by comparing dispersion model-predicted ambient air concentrations of SO_2 in the vicinity of the source (Chevron Refinery) with the National Ambient Air Quality Standards and National Minimum Emission Standards for listed activities.

To accomplish this aim, the following sub-objectives must be achieved:

a) Validation of use of meteorology local to the refinery and Cape Town International Airport meteorology.

b) Using AERMOD View™ and CALPUFF View™, comparison between model-predicted ambient concentrations, based on actual refinery emissions data and local meteorology, with ambient data from the Bothasig and Table View monitoring stations and compare between modelled AERMOD and CALPUFF ambient concentrations.

c) Comparing modelled SO_2 concentrations based on current (2010) emission rates and the new South African Ambient Air Quality Standards.

1.3 Research design and methodology

This study uses Lakes Environment's AERMOD View™ and CALPUFF View™ which incorporate AERMET and CALMET respectively with local meteorology, reported daily SO_2 emissions, geophysical data, land use data and local terrain data as inputs, to model the dispersion of SO_2 emitted by the Chevron Refinery. Modelling was done over a year period (2010) to assess the effects of seasonal meteorological variability. To validate the modelling, model-predicted ambient concentrations based on actual refinery emissions were compared with corresponding monitored data from two local monitoring stations. To evaluate the coherence between Petroleum Industry (Oil Refining) Minimum Emission Standards and the Ambient Air Quality Standards, emission rates were adjusted to comply with the regulated emission standards, and model-estimated ambient concentrations were compared with the 1 hour, 24 hour and annual average Air Quality Standards.

1.4 Thesis Outline.

This research report is divided into four chapters:

Chapter 1 provides a background and introduction to the research topic, including an overview of relevant air quality legislation. **Chapter 2** provides the Literature Review relating to the legislative context, as well as the characteristics of urban air dispersions models, with dispersion modelling. **Chapter 3** looks at Gaussian air dispersion models in detail and basic mathematical algorithms and factors affecting the dispersion of pollutants in the atmosphere. **Chapter 4** describes the methodology used to model for outputs using AERMOD and CALPUFF air dispersion models in the study including how the emissions inventory and meteorological data were obtained and used. **Chapter 5** comprise of results and discussion of two modelling scenarios with maximum 1-hour; 24-hour and annual average concentrations presented in isoplaths, and tables of comparisons. **Chapter 6** incorporates conclusions and recommendations for the study.

Chapter 2: Literature Review.

2.1 Use of Dispersion Modelling in Air Quality Management

Air pollution models are routinely used in environmental impact assessments, risk analysis and emergency planning, and source apportionment studies. In highly polluted cities such as Athens, Los Angeles and Mexico, regional scale air quality models are used to forecast air pollution episodes. The results from these models may initiate compulsory shutdown of industries or vehicle restrictions. The various roles served by air pollution models, which cover a broad range of scales from local to global, lead to distinct modelling requirements. The use of Gaussian-plume type models for continuous releases, which are at the core of most U.S. Environmental Protection Agency (EPA) regulatory models, is highly recommended (Macdonald R, 2003).

The term “air pollution model” usually refers to a computer program, but in the past it has also included hand calculations or use of charts and tables from simple handbooks. A dispersion model is essentially a computational procedure for predicting concentrations downwind of a pollutant source, based on knowledge of the emissions characteristics (stack exit velocity, plume temperature, stack diameter, etc.), terrain (surface roughness, local topography, nearby buildings) and state of the atmosphere (wind speed, stability, mixing height, etc.). The basic problem is usually to predict the rate of spread of the pollutant cloud, and the consequent decrease in mean concentration. The model has to be able to predict rates of diffusion based on measurable meteorological variables such as wind speed, atmospheric turbulence, and thermodynamic effects. The algorithms at the core of air pollution models are based upon mathematical equations describing these various phenomena which, when combined with field data, can be used to predict concentration distributions downwind of a source.

Although the Gaussian plume model (GPM) is based upon many simplifying assumptions about the dispersion process, it is applied to a wide array of dispersion scenarios and some form of this model is adopted in most regulatory air pollution models for continuous releases. In order to extend the applicability of the GPM to realistic scenarios, the U.S. EPA models make use of several special algorithms or semi-empirical corrections to account for the various effects. These include the influence of atmospheric stability, plume trapping below elevated inversions,

fumigation, non-uniform wind profiles, dry or wet deposition, stack-tip downwash, buoyancy-induced dispersion, finite initial source dimensions, complex terrain and the influence of buildings.

Many of the algorithms in the advanced EPA models are based on simplified physical models of the various dispersion processes, combined with empirical data. The modifications to the basic GPM make extensive use of wind tunnel and measured field data. Because of strong peer reviews and model validations studies, the resulting model codes are quite robust and can be used in a wide variety of situations combining many separate effects. All of the EPA codes, such as SCREEN3, ISC3, AERMOD and CALPUFF, have been run through extensive physical audits, sensitivity analyses, and quality assurance studies using benchmark data in order to justify their use in environmental assessment (Macdonald R, 2003, US EPA, 2005).

2.2 Air Quality Management in South Africa.

In South Africa, the environment is governed by the National Environmental Management Act, 1998 (Act 107 of 1998) (NEMA). NEMA sets out a series of environmental management principles that apply to the interpretation and application of all legislation that may affect the environment. Since 1998, various specific environmental statutes that fall under the NEMA framework have been promulgated, including the Air Quality Act, 2004 (Act 39 of 2004) (AQA). Air Quality Act makes no provision for the compliance monitoring and enforcement of its own provisions. These provisions are located in NEMA as framework legislation, where provision is made for the statutory designation of Environmental Management Inspectors (EMIs) to monitor compliance with and enforce AQA(Fourie M, 2008).

The purpose of the National Framework, is to achieve the objectives of the AQA, and as such the National Framework provides a medium- to long-term plan of the practical implementation of the AQA. The National Framework must provide mechanisms, systems and procedures to promote holistic and integrated air quality management through pollution prevention and minimisation at source, and through impact management with respect to the receiving environment from local scale to international issues. The National Framework provides norms and standards for all technical aspects of air quality management.

The development of the National Framework was received from stakeholders during the public hearings for the Air Quality Bill and the public participation process conducted as an integral part of the development of this National Framework. Formal contributing projects to the National Framework include the (1) development of a South African Air Quality Information System (SAAQIS) (2) AQA Implementation for listed activities and minimum Emission Standards, (3) Air Quality Management Planning Implementation Manual Development, (4) Framework for Setting and Implementing National Ambient Air Quality Standards (SANS 69). According to Section 7(1) of the AQA, the Minister must establish a National Framework for achieving the above objectives of the Act (DEAT, 2007).

National Ambient Air Quality Standards (Government Gazette 2009) for SO_2, and National Minimum Emission Standards for listed activities (Government Gazette 2010), including those for the Petroleum Industry of existing Category 2 (Petroleum Industry) Listed Activity of 0.8kg/day/t of crude throughput (Government Gazette 2010, Category 2, sub-category 2.1).The AQA stipulates that emission standards must include the permissible amount, volume, emission rate or concentration of that substance or mixture of substances that may be emitted and the manner in which measurements must be carried out. This requirement in the AQA came about as a result of the manner in which emission standards have been historically specified within the APPA Registration Certificates.

The specification of a total mass as a permissible amount or a volume in a general national minimum emission standard intended to regulate a number of individual industries is problematic, unless it is specified on a per unit production or output basis. Emission standards must be expressed either as an emission concentration or a performance standard or, where appropriate, a combination of both, with the actual concentration or level of performance taken from BAT. Total masses of emissions permissible can be included in the AELs of Listed Activities. The AQA stipulates that the manner in which the measurement of emissions from Listed Activities is undertaken must be specified. For purposes of compliance monitoring, it is necessary to carry out measurement of emissions.

The emission monitoring required clearly depends on the nature of the source, the pollutant and the emission standard. Emission standards expressed as emission concentrations require direct stack monitoring. Continuous stack monitoring will be required in areas that are not in compliance with ambient air quality standards, especially within declared priority areas where the emissions from the stack significantly contribute to poor air quality in the area. Emission standards expressed as a performance standard (e.g. kg of pollutant per ton product) requires a combination of direct monitoring and product tonnage tracking methods (DEAT, 2007).Only EMIs can monitor compliance and enforce the AQA. Before the AQA was promulgated in 2004, the national legislation that governed South Africa's air quality was the Atmospheric Pollution Prevention Act (Act 45 of 1965) (APPA).

The APPA suffered from many shortcomings, including the absence of national air quality standards, and the absence of appropriate compliance and enforcement provisions. For example, under APPA, contravention of a condition of a permit was not a criminal offence, and no punitive action could therefore be taken against a permit holder that contravened its permit. In AQA new provisions have been made including a national air quality framework; the establishment of national, provincial and local ambient air quality and emission standards; declaration and management of priority areas for areas where air quality is of particular concern; listed activities that require an atmospheric emissions license; listing of controlled emitters and controlled fuels and a range of new criminal offences (Fourie M, 2008). An idealised AQMS is represented in the figure 1 below.

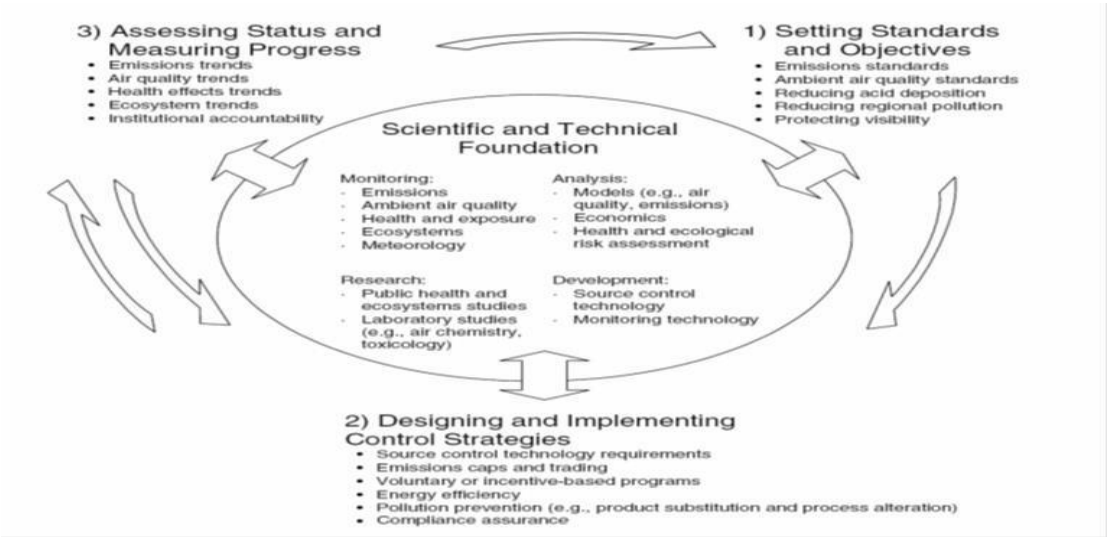


Figure 1: The air quality management cycle (National Research Council, 2004)

2.3 Air Dispersion Modelling Applications in South Africa

Air dispersion models have become powerful tools for assessing the consequences of ground level air pollutant concentrations (Sappurd A., et al 2010), although there have been comparatively few published modelling studies for South African sources.

Haripursad (Haripursad Y, 2007) used Calpuff to model five scenarios including a control run with actual emissions data at uMhlathuze Municipality in Durban; a worst-case run using permitted emissions data; and three emissions reduction scenarios using 25%, 50% and 75% reductions of the permitted data. The results of his modelling scenarios were compared with results of other modelling studies recently conducted in the uMhlathuze Municipality, as well as with the South African Ambient Air Quality Standards (SAAAQS) for SO_2.The results revealed that the permitted emissions scenario led to exceedances of the SAAAQS 1-hour and 24-hour average concentrations over most of the uMhlathuze Municipal area. The use of the permitted emissions values produced higher SO_2 concentrations over the study area than the control run that comprised current emissions values. The control scenario produced similar results to the scenario in which there was a 50% reduction in permitted emissions data and suggests that the industries are operating at half of their permitted levels of SO_2 emissions. The reduction of the permitted emission by 75% shows a significant decrease in the area exceeding the SAAAQS 1-hour standard, and compliance with the SAAAQS 24-hour and annual average standards.

Malusi (Malusi H. B, 2009) used AERMOD to examine the dispersion potential of stack and fugitive emissions at Anglo Gold Ashanti's sulphuric acid (H_2SO_4) plant located in Klerksdorp, North West province. Only SO_2 emissions stack emissions were considered in the model. Malusi modelled for 1-hour and 24-hour averaging periods and compared the results with the current South African ambient air quality standards for all averaging periods for the East Acid Plant. Malusi (Malusi H. B, 2009) noted that modelled SO_2 stack concentrations were within the 2009 South African ambient air quality standards for all averaging periods. As from Malusi AERMOD demonstrated a satisfactory performance to model stack emissions from the East Acid Plant. Malusi concluded that the model compared poorly with the monitored ambient air quality data partly due to the lack of comprehensive emission factors for fugitive sources.

Sowden et al (Sowden M et al., 2008) used the US-EPA's approved Emissions Processing System (EPS) to develop a temporally and spatially resolved emissions inventory for the City of Cape Town for use in the Dynamic Air Pollution Prediction System (DAPPS). The emission inventory for the DAPPS in the City of Cape Town was developed to support predictive photochemical modelling of air pollutants. The photochemical dispersion model that was employed in the DAPPS was the Comprehensive Air Quality Model with Extensions (CAMx). The modelling domain for the City of Cape Town was 70x105 km^2, with a horizontal grid resolution of 1x1 km^2. The FRAULEIN approach that was adapted considered six source types that include large point sources, small point sources, residential burning, motor vehicles, biogenic emissions and the airport. Based on the research there was reasonable level of confidence for the characterization of large point sources but the two biggest source contributors namely vehicle and biogenic emissions, needed some improvement (Sowden M et al., 2008).

2.4 Ambient Air Quality Standards and International Guide Line Values

The National Environmental Management: Air Quality Act, Act No. 39 of 2004 (AQA) represents a distinct shift from exclusively source-based air pollution control to holistic and integrated effects based air quality management. As part of the ongoing process of implementing the AQA, regulations for AAQS were recently (12/2009 and 03/2010 respectively) promulgated (Government Gazette, 2009 & 2010).

Table 1: South African National Ambient Air Quality Standards for Sulphur Dioxide (SO_2) (DEA, 2009).

Averaging Period	***Concentration***	***Frequency of Exceedence***	***Compliance Date***
10 minute	*500 µg/m^3 (191 ppb)*	*526*	*Immediate*
1 hour	*350 µg/m^3 (134 ppb)*	*88*	*Immediate*
24 hour	*125 µg/m^3 (48 ppb)*	*4*	*Immediate*
1 year	*50 µg/m^3 (19 ppb)*	*0*	*Immediate*

2.5 DEA Authorized Refinery Emission Levels

Due to the implementation of AQA, South Africa has introduced new refinery ambient air emissions, in order to set limits on theSO_2 emissions at refineries in such a way that they cannot exceed certain prescribed maximum values (DEA, 2004).The SO_2 emission limit for an existing Category 2 (Petroleum Industry) Listed Activity is 0.8kg/day/t of crude throughput (Government Gazette 2010, Category 2, sub-category 2.1), Table 2. This Act was promulgated on 31 March 2010, with refineries required to comply with this standard by 01 April 2015. As a result of such regulations, it is to know the effects of stack and flare emissions on ambient atmospheric conditions. To achieve this, consideration are given to air dispersion models because they take into account: sources of pollution in a given area, the amounts of pollutants emitted by each source, chemical reaction transformations, different meteorological conditions and topographical features (Abdul-Wahab et al., 2002).

Table 2: Category 2 Subcategory 2.1 Emission Standards for Sulphur Dioxide (SO_2) (DEA, 2010).

Substance	***Plant Status***	***Daily average kg SO_2/ton of crude oil throughput.***
SO_2	*Existing*	*0.8*
	New	*0.4*

2.6 Ambient Air Quality Monitoring.

The City of Cape Town has a well-established network of twelve (12) air quality monitoring stations located in the various parts within the metropolitan, the stations are well placed industrial, residential areas and also in high traffic hotspots, the sites are located in Khayelitsha, Somerset West, Goodwood, Molteno, Foreshore, Bellville South, Wallacedene, City Hall, Athlone, Tableview, Killarney and Bothasig. Some of the stations were commissioned twenty six (26) years ago with the oldest being City Hall and others in the nineties and are currently being managed in-house by officials from Scientific Services division, the stations are visited every week for routine maintenance work and also calibration checks are undertaken by the officials from the Scientific Services. The annual SANAS calibration is carried out by accredited laboratory. During the routine maintenance visits a zero and span checks are conducted on

various gas analysers. In some of the stations PM_{10}, SO_2, NO_x, O_3, CO, H_2S and BTEX are also measured. In addition meteorological parameters for wind speed and wind direction are also measured.

In 2011 an annual SANAS calibration survey was conducted. The main purpose of the baseline assessment was to assess the current status of all the government owned air quality monitoring networks, currently being operated by National, Provincial and Local Government Departments across the country in order to provide air quality data to the South African Air Quality Information System (SAAQIS). The survey consisted of the physical assessment of all the government owned air quality monitoring networks. In addition, the audit assessed the technical capabilities of the networks in accordance with South African National Accreditation System (SANAS) TR07-02, "Supplementary requirements for accreditation of continuous ambient air quality monitoring stations". Based on the audit findings some of the networks were not operating and being managed in accordance with the "SANAS TR07-02".

Of the ninety four (94) government-owned stations, only one (1) belonging to City of Cape Town was SANAS Accredited in terms of ISO 17025. Furthermore, the baseline audit assessed the number of networks providing air quality data to the South African Air Quality Information System (SAAQIS) and also those that are in the process. At that time, current status of infrastructure at the stations was assessed and whether the monitoring equipment complies with either US Environmental Protection Agency (EPA) or other International recognised standards. The most area of concerns raised during the survey was insufficient allocation of funds or in some other networks lack of funding was a major challenge, particularly in Local municipalities and also the capacity to operate the network was a big concern, most of the networks at local government level are currently being operated by Environmental Health Practitioner (EHP) who lack basic training from the equipment suppliers (DEA, 2011)

2.7 Review of applications of Air Dispersion Modelling to Industrial Point Source

Sabah (Sabah A.W., et al 2010) carried out a study to investigate the transport and dispersion patterns of SO_2 originating from Mina Al-Fahal refinery, in the Sultanate Oman by employing California Puff (CALPUFF) dispersion modelling system. The major goal of this study was to make a comparison of the results produced by this modelling system with a previous study which was conducted for the same area using Industrial Source Complex Short Term (ISCST) model.

In order to obtain the meteorological fields of the study area the CALPUFF modelling system was coupled with Weather Research and Forecasting (WRF), a prognostic meteorological model. The results indicated that the performance of the CALPUFF model were better than that of ISCST model, however a difference in magnitudes of predicted and measured concentrations an important role in distribution of SO_2 in and around the refinery. The land–sea interaction also influenced the predicted results of SO_2 found. This difference was reduced to using high-resolution terrain elevation data, site specific observational meteorological data and buoy data. The complex geography and variable wind regimes also played an important role in distribution of SO_2 in and around the refinery. They also discovered that land–sea interaction also influenced the predicted results.

Mete (Mete T., et al 2006) investigated the dispersion of SO_2 over Izmit Gulf where they simulated California Puff (CALPUFF) model for three air pollution cases, which occurred on January 28, February 12, and February 26, 1997. These days were generally characterized by dominant high-pressure systems – pressure values reaching 1032 mb, low wind speeds and sometimes calm conditions, and low temperatures with a minimum of 0°C. Hourly simulations during those critical cases were carried out and results revealed very high concentrations of SO2 transported to the downwind regions of Tüpraz and Gebze, and values sometimes exceeded 1,000 µg/m3. Night time and morning simulations associated with inversion produced considerably higher values of SO_2 than the afternoon simulations associated with breeze. Model verification was conducted by comparing the measured daily average values of eight stations with the model predicted values at the same receptor points. Results showed that the model well predicted the values at station Gebze in all three cases. The model sometimes underestimated and sometimes overestimated the concentrations at other receptor stations.

Abdul-Wahab (Abdul-Wahab S.A., et al 2002) investigated the use of the Industrial Source Complex Short Term (ISCST3) model at a refinery. The study was performed over a period of 21 days. The first objective of this study was to measure the atmospheric levels of SO_2 and then to compare their values with the international standard limits. The second objective was to evaluate the ISCST3 model by comparing the calculated and measured concentrations. The third objective was to demonstrate the effect of wind regimes on the dispersion of SO_2 and to determine the spatial distribution of SO_2 over the modelled area. The results showed that the levels of SO_2 were well below the ambient air quality standard. Based on isopleths for SO_2 distribution in the study area (as output from the ISCST3 model). It then concluded that no health risk were present in areas adjacent to the refinery.

Saqer (Saqer S.S., et al 2008) carried out an investigation to estimate the total emissions of SO_2, non methanated hydrocarbons (VOCs) and NO_X from flares in two petroleum refineries in Kuwait and to assess their impact on the air quality in industrial and suburban areas. AERMOD model was used to predict the ground level concentrations of major pollutants to indicate the quality of air and certify the adequacy of the model by comparing the measured values of selected receptors. It was found that (86%-98%) agreement between predicted and measured values depending on location of receptor. Further study is ongoing to consider all refineries in Kuwait and to measure the contribution of each source.

Zivorad (Zivorad R., et al 2005)carried out an investigation which was intended to compare the performance of different types of dispersion models (ISCST3, ISC-Prime, AERMOD and CALPUFF) relative to tritium air emissions from over 20 stacks in the Pickering Nuclear Power Generation Facility in Ontario, Canada and to provide recommendations as to the most appropriate dispersion model for predicting contaminant concentrations for both onsite and offsite the plant. This report provides an assessment of the ISCST3, ISC-Prime, AERMOD and CALPUFF models that were used by the United States Environmental Protection Agency to predict contaminant levels in air and in precipitation.

The ISCST3, ISC-Prime and AERMOD dispersion models performed in a similar manner, exhibiting a tendency towards under-estimation relative to the tritium air concentration measurements but well within a factor of two. The CALPUFF dispersion model exhibited the least bias between the predicted and observed data for both tritium in air and tritium in

precipitation measurements. Although the CALPUFF dispersion modelling system requires more data input and computer time (related to the simulation of dynamic wind conditions in complex terrain), CALPUFF would be the model of choice to simulate impacts in the vicinity and offsite of the industrial site.

2.8 Validation of Modelling Outputs.

Grosch and Lee (Grosh T.G et al, 1998) evaluated the effect on design concentration predictions from AERMOD, for a range of sources, of variations of the albedo, Bowen ratio, and surface roughness length individually and in combination over the ranges of values. The study was conducted for four sources (Surface Source, 35-meter Stack, 100-meter Stack and 200-meter Stack) ranging from a surface release with no plume rise to a 200 meter high stack with plume rise. Stack diameter, gas temperature, and gas exit velocity were set at values that might reasonably be used for a small, medium, and large boiler, respectively. The effects of variations of combinations of these parameters on design concentration predictions was evaluated by selecting the land use parameters that are characteristic of each of four types of ground cover.

The effects of changes in albedo, Bowen ratio, and surface roughness lengths, in combination and individually, on regulatory design concentrations predicted by AERMOD were sufficiently complex that it could not be accurately anticipated what effect any changes in those values will have on design concentrations for a given source configuration. The study showed that modelled design concentrations can vary substantially due to normal ranges of variations in the albedo, Bowen ratio, and surface roughness length. Changes in albedo, Bowen ratio, and surface roughness length can result in changes in design concentrations of factors of 1.5, 2.6, and 160, respectively. Changes in design concentrations can be even greater when these parameters are varied in combination. Groschand Lee (Grosh T.G et al,1998) concluded that it was reasonably accurate estimates of albedo, Bowen ratio, and surface roughness lengths were necessary for AERMOD to provide accurate results.

Chapter 3: Dispersion Modelling.

3.1 Atmospheric Dispersions Modelling.

Atmospheric dispersion models are a mathematical simulation of the physics and chemistry governing the transport, dispersion and transformation of pollutants in the atmosphere and estimates downwind air pollution concentrations given information about the pollutant emissions and meteorology during the period of interest, an air pollutant is transported from a source to a potential receptor.

The pollutant disperses into the surrounding air so that it arrives at a much lower concentration than it was on leaving the source. Atmospheric dispersion models are used to estimate how much reduction in concentration has occurred during the transportation of pollutant in the modelling domain. The concentration of an air pollutant at a given place is a function of a number of variables, including the realise rate of the pollutant released at the source, the distance of the receptor from the source, and the atmospheric conditions (Manatū MōTe Taiao, 2004).The processing of air dispersion modelling contains four stages (data input, dispersion calculations, deriving concentrations, and analysis). The accuracy and uncertainty of each stage must be known and evaluated to ensure a reliable assessment of the significance of any potential adverse effects.

The most important atmospheric conditions are wind speed, wind direction, and the vertical temperature characteristics of the local atmosphere. Most commonly the air temperature decreases with height, which results in an unstable atmosphere that tends to mix pollutants into the higher layers of the atmosphere, keeping pollution concentrations moderate or weak at ground level. If the vertical temperature pattern is inverted, such that the upper air is warmer than the lower air, then the atmosphere will be stable, with calm winds and potentially high pollution concentrations (Manatū MōTe Taiao, 2004).

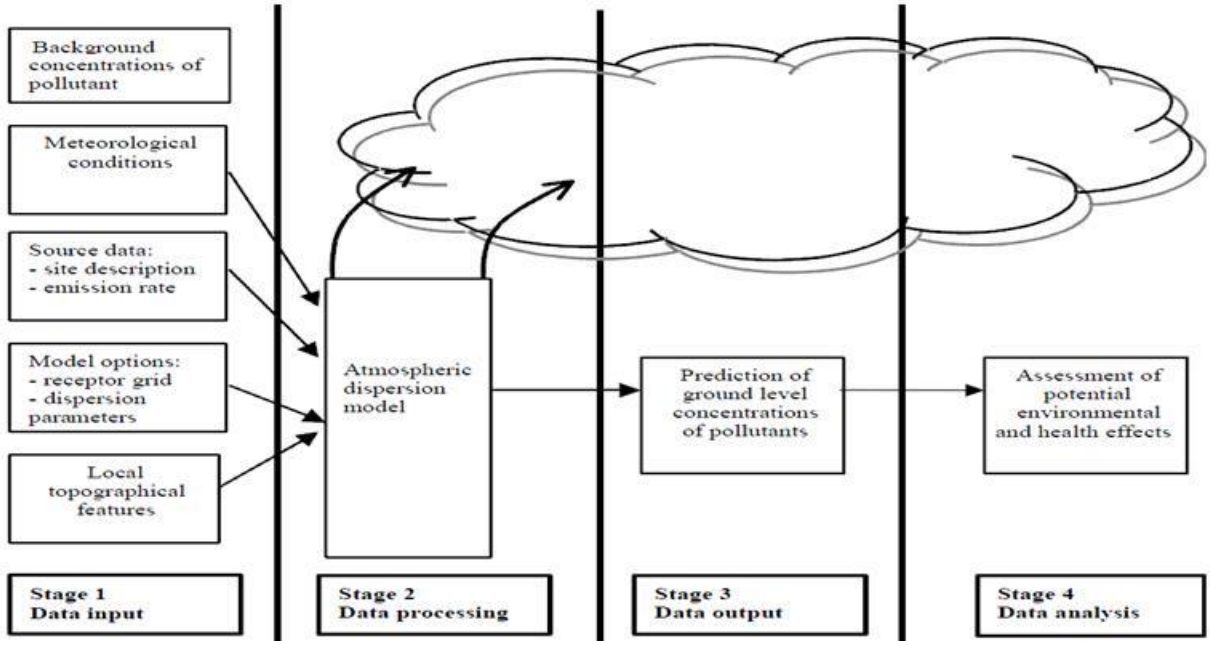


Figure 2: Overview of Air Dispersion modelling (ManatūMōTeTaiao, 2004).

3.1.1 Types of Dispersion Models

There are three general types of dispersion models that are the box, Lagrangian and Gaussian model. The box model is the simplest although some relatively complex models have been built on box model foundations. The Lagrangian and Gaussian models are more involved and complex models have been constructed using these models. In addition to these three types, some very complex models have been developed that attempt to solve the basic physical equations of motion of the air parcels without using the approximations of the box, Lagrangian and Guassian models. (1) Box models are based on the conservation of mass. The site is treated as a box into which pollutants are emitted and undergo chemical and physical processes. It requires the input of simple meteorology and emissions and the movement of pollutants in and out of the box is allowed. (2) Lagrangian models are similar to box models in that they define a region of air as a box containing an initial concentration of pollutants. The Lagrangian model then follows the trajectory of the box as it moves downwind.

The concentration is a product of a source term and a probability density function as the pollutant moves from point to point. Lagrangian models incorporate changes in concentration due to mean fluid velocity, turbulence of the wind components and molecular diffusion (Morawska L., et al 2010). (3) Gaussian type models are widely used in atmospheric dispersion modelling, in particular for regulatory purposes, and are often nested within Lagrangian models. Gaussian models are based on a Gaussian distribution of the plume in the vertical and horizontal directions under steady state conditions. The normal distribution of the plume is modified at greater distances due to the effects of turbulent reflection from the surface of the earth and at the boundary layer when the mixing height is low (Holmes NS, et al 2010).

3.1.2 Gaussian Dispersion models.

Gaussian models are the most widely used techniques for estimating the impact of non-reactive pollutants, or pollutants being treated as non-reactive. These models are based on the assumption that the plume concentration at each downwind distance has independent Gaussian distributions both in the horizontal and in the vertical axis, thus the Gaussian formula (below) will describe a three dimensional concentration field generated by a point source under stationary meteorological and emission conditions. The Gaussian dispersion equation for a point source, which is the basis for AERMOD and CALPUFF model, describes the three dimensional concentration field generated by a point source under meteorological and emission conditions (US EPA 2004b).

3.1.3 Assumptions in Gaussian Modelling (Turner D.B, 1931).

In order to estimate pollutants concentrations using equations presented in this chapter several assumptions are made.

a) Continuous Emissions

The emissions of pollutant in mass per time are taking place continuously and the rates of these emissions are not variable over time.

b) Conservation of Mass

During the transport of pollutants from source to receptor, the mass that is emitted from the source is assumed to remain in the atmosphere. None of the material is removed through

chemical reaction nor is lost at the ground surface through reaction, gravitational settling, or turbulent impaction. It is assumed that any of the released pollutant that is dispersed close to the ground surface by turbulent eddies is again dispersed away from the ground surface by other subsequent turbulent eddies. This called eddy reflection.

c) Steady-State Conditions

The meteorological conditions are assumed to persist unchanged with time, at least over the period of transport (travel time) from source to receptor. It is very easy to satisfy this assumption for close in receptors under usual conditions. However, for light wind conditions or receptors at great distances, this assumption may not be satisfied.

d) Crosswind and Vertical Concentration Distributions

It is assumed that the time averaged (over about an hour) concentration profiles at any distance in the crosswind direction, horizontal (perpendicular to the path of transport) are well represented by a Gaussian, or normal, distribution and, similarly, concentration profiles in the vertical direction (also perpendicular to the path of transport) are also well represented Gaussian, or normal, distribution (Turner D.B, 1931).

3.1.4 Gaussian Dispersion Equation Formulation (Turner D.B, 1931).

The Gaussian dispersion equation below estimates the concentration X at the receptor located at a distance x downwind, y crosswind and at a height z above the ground that results from an emission rate Q which occurs at an effective height H above the ground:

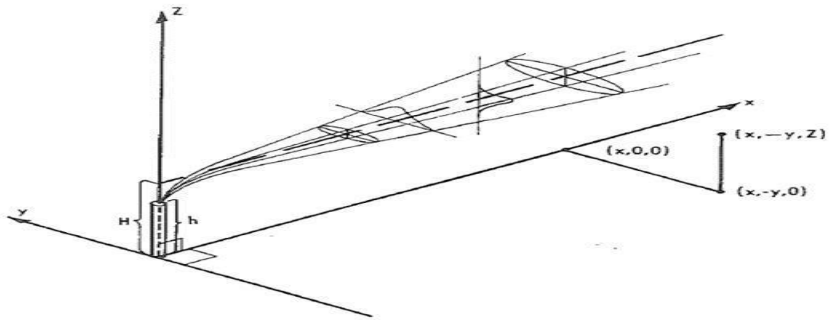


Figure 3: Coordinate system showing Gaussian distribution in the horizontal and vertical (Turner D.B, 1931)

The variables are:

X is the air pollution concentration (g/m^3) in mass per volume,

Q is the pollutant emission rate (g/s) in mass,

x , y , z are the distance (m) and,

H is the effective height (m) of the centreline of the pollutant plume.

The notation used X in the parentheses is to give the three coordinates of the receptor located according to the coordinate scheme described above. Following a semicolon, the effective height of emission of the source to the three coordinate axes. The equation is given in four separate factors which are multiplied times each other. These four factors represent the dependency upon emissions, or the source factor, and what occurs in the three dimensions parallel to the three coordinate axes.

$X_{(x,y,z,H)}$ = The product of the following four factors:

Emission factor Q

Downwind factor $\frac{1}{u}$ …….....……...……(1)

Crosswind factor $$\frac{1}{(2\mu)^{1/2}\sigma_y}\exp\left[-\frac{y^2}{2\sigma_y{}^2}\right]$$ …….....……...……(2)

Vertical factor $$\frac{1}{(2\mu)^{1/2}\sigma_y}\left\{\exp\left[-\frac{(H-z)^2}{2\sigma_z{}^2}\right]+\exp\left[-\frac{(H+z)^2}{2\sigma_z{}^2}\right]\right\}$$ .....(3)

Variables for the equation above are:

u Wind speed at the point of release, m/s

σ_y The standard deviation of the concentration distribution in the crosswind direction, m, at the downwind distance x.

σ_z The standard deviation of the concentration distribution in the crosswind direction ,m, at the downwind distance x.

μ The mathematical constant pi equal to 3.141

A brief explanation of the four terms above:

a) The concentrations at the receptor directly are proportional to the emission rate.
b) Parallel to the x axis, the concentration are inversely proportional to wind speed.
c) Parallel to the y axis, that is , crosswind, the concentrations are inversely proportional to the crosswind spreading, σ_y, of the plume ; the greater the downwind distance from the source, the greater the horizontal spreading, σ_y, the lower the concentration. The exponential involving the ratio of y to σ_y just corrects for how far off the center of the distribution the receptor is in terms of standard deviations. The receptor is y from the center since the crosswind distribution center is at $y = 0$, that is directly above the x-axis.

Parallel to the z axis, that is, vertical, the concentrations are inversely proportional to the vertical spreading of the plume, σ_z, the greater the downwind distance from the source, the greater the vertical dispersion and the lower how far the receptor height, z ,from the plume centreline in the vertical. The first term represents the direct distance, $H - z$, of the receptor from the plume centreline. The second term represents the eddy reflected distance of the receptor from the plume centreline, which is the distance from the centreline to the ground, H, plus the distance back up to the receptor, z, after eddy reflection (Turner D.B, 1931).

After multiplication of the four factors, the equation simplifies to:

$$X_{(x,y,z,H)} = \frac{Q}{2\mu u \sigma_y \sigma_z} \exp\left[-\frac{y^2}{2\sigma_y{}^2}\right]\left\{\exp\left[-\frac{(H-z)^2}{2\sigma_z{}^2}\right] + \exp\left[-\frac{(H+z)^2}{2\sigma_z{}^2}\right]\right\} \text{.....(4)}$$

3.2 Gaussian Model Restrictions.

One severe limitation of plume models with regards to modelling particle dispersion is that since the plume models use steady state approximations they do not take into account the time required for the pollutant to travel to the receptor. Therefore, aerosol dynamics must be calculated by post processing treatment of the results. Gaussian plume equation assumes that there is no interaction between plumes, which can become significant within urban environments. Gaussian equation is not able to calculate recirculation effects caused by multiple buildings or at intersections. Some further limitations of the Gaussian treatment means that Gaussian models are not designed to model the dispersion under calm or low wind conditions (wind velocities less than 0.5 m/s) or at sites close to the source (distances less than 100m). A further limitation is a result of the simplified treatment of turbulence and meteorology so they are best suited to calculating hourly (or longer) average pollutant concentrations. Since Gaussian plume equations assume a homogeneous wind field such as AERMOD, it is not recommended that they are used for far-field modelling as the meteorology is expected to change over such large distances, greater than 50km (Holmes N.S. et al, 2010).

3.3 Treatment of Mixing Height by Gaussian Dispersion Models.

Mixing height is one of the most important parameters required by Gaussian dispersion models as input data for forecasting the air quality. When pollutants are emitted into the atmospheric boundary layer, they dispersed horizontally and vertically because of the action of convection and mechanical turbulences until they become completely mixed. The depth of the mixed layer is defined as the mixing height, which determines the volume available for the dispersion of pollutants. The greater the depth of the mixed layer the larger the available volume to dilute the atmospheric pollutants.

The planetary boundary layer is in the lowest part of the troposphere where the air is influenced by the earth's surface and responds to surface forcing such as frictional drag, evapo-transpiration, heat transfer, pollutant emissions, and topography (Cooper D.I et al., 1994). Above the planetary boundary layer is the free atmosphere where the effects of friction from the earth's surface are negligible and the motion of air can be treated as an ideal fluid (Glickman T.S, 2000). The planetary boundary layer is the layer where the earth's surface interacts with the large scale atmospheric flow. Since substances emitted into this layer disperse gradually horizontally and vertically through the action of turbulence, and become completely mixed if sufficient time is given and in the absence of sinks or sources, this layer also called the mixing layer (Cooper D.I et al., 1994).

The planetary boundary layer height or mixing height is a key parameter in air pollution models determining the volume available for pollutants to dispersion and the structure of turbulence in the boundary layer (Glickman T.S, 2000). In spite of its importance there is no direct method available to determine the mixing height. The most common methods for determining the mixing height are utilization of radio-soundings, remote sounding systems and parameterization methods. All these methods have advantages and disadvantages and consider different related or assumed properties of the planetary boundary layer. It is relevant to identify and evaluate different techniques or methods in order to lower the inherent uncertainty involved in the determination of the mixing height (Khandokar A et al., 2000).

3.4 Survey of Atmospheric Dispersion Models.

Atmospheric dispersion modelling is a method of predicting the ambient impact of one or more sources of air pollutants. The algorithms used in the models are based both on the known physics of atmospheric processes, including meteorological processes and on pollutant emission processes. Such information is used by the model to mathematically simulate (or predict) the pollutant's downwind dispersion in order to derive estimates of concentration at a specified location (usually a receptor site). Some dispersion models may simulate the chemical transformations and removal processes that can occur along the transport path. The results of such analysis can for example be used by the regulatory authorities to determine if a new or

existing source of air pollutants complies with authorities' maximum ambient concentration limits (Boubel R.W et al., 1994; Oklahoma Department of Environmental Quality, 2006).

Dispersion models are important predictive tools that are used to simulate the way the atmosphere transports and diffuses chemical parameters from a source of pollution. The selection of an air dispersion model depends on many factors, such as, the nature of the pollutant (e.g., gaseous, particulate, reactive, inert), the characteristics of emission sources (point, area, volume, or line), emission source and receptor relationship, the meteorological and topographic complexities of the area, the complexity of the source distribution, the spatial scale and resolution required for the analysis, the level of detail and accuracy required for the analysis, and averaging times to be modelled. The technical decision of choosing a puff model or a plume model is based on considerations of pollutant transport distance and the potential for temporally spatially varying flow fields due to influences of complex terrain, non-uniform land use patterns, coastal effects, and stagnation conditions characterized by calm or very low wind speeds with variable wind directions. The models include: ISCST3, AERMOD, ASPEN, CALPUFF, UTM-TOX, and CAMx. For this study we have selected the CALPUFF and AERMOD model. Below, we describe each model and discuss its application to the Chevron Refinery evaluation and provide the basis for selection of the CALPUFF and AERMOD model for this study.

3.4.1 ASPEN

The Assessment System for Population Exposure Nationwide (ASPEN) was developed for the inhalation component of U.S. EPA's Cumulative Exposure Project. ASPEN includes an air dispersion module similar to the long-term average version of ISCLT2. It includes treatment of wet and dry deposition for particles, and simple treatment of chemical transformation. The concentrations estimated from ASPEN are designed to represent population-weighted averages over a size scale of census tracts or several square kilometers. ASPEN can utilize meteorological information from several locations, and includes a simplified treatment of secondary formation of gaseous air toxics. Although ASPEN has been used in an U.S. EPA's air toxic modelling, it lacks the capability to fully incorporate 3-dimensional wind fields. ASPEN emission releases are assumed to be straight lines, regardless of the patterns at downwind locations, and wind patterns in upper layers are derived from surface patterns based on

atmospheric stability and land use (urban or rural), rather than being independently estimated. In addition, ASPEN is a micro-scale model and it only can be used when there are distances of less than 50 km between the emission source and receptors(Hanna et al., 2008).

3.4.2 CAMx

CAMx is a multi-scale photochemical model designed to simulate primary and secondary pollutants over a large range of spatial scales from hundreds to thousands of kilometers using a flexible, nested grid structure. It is a 3-dimensional Eulerian (gridbased) dispersion and photochemical model. It is capable of treating the transport, dispersion, and chemical reaction and removal of a wide variety of gaseous and particulate pollutants. CAMx includes plume-in-grid algorithms for treating near-source, sub-grid scale dispersion. CAMx requires a gridded emission input (except for point sources). This means that area sources can be no smaller in size than a single grid cell. In addition, for area source emissions, CAMx treats the emission source as a ground level release(Walker J.I. et al., 2008).

3.4.3 UAM-TOX

The Urban Airshed Model for Toxics (UAM-TOX) is an enhanced version of U.S. EPA's UAM model. It is a three-dimensional grid model designed to simulate all-important physical and chemical processes that occur in the atmosphere. The model incorporates mathematical representations of the processes of transport, diffusion, chemical reaction and deposition. Because UAM-TOX is a grid based model, all emissions are characterized as being spread uniformly over a 3-dimensional grid cell. This characterization may result in a significant loss of spatial resolution information for the emission. In addition, UAM-TOX treats emission sources as ground level releases for area emission sources (Wagler J. et al., 2008).

3.4.4 ADMS

ADMS is an advanced steady state, Gaussian-like dispersion model capable of simulating continuous plumes and short duration puff releases. The model can be applied to point, line, area and volume sources and has a module applicable to motor vehicle emissions. Unlike other freely downloadable modes, it is a proprietary model and therefore needs to be licensed for commercial applications. Improvements to the model over ISCST3 are most evident in the

treatment of dispersion rate variations within the atmospheric boundary layer. In this regard it is similar to AERMOD. Verification of the model has been partially based upon the Kincaid and Indianapolis data bases, which were also used to verify AERMOD. ADMS compare well with AERMOD in the treatment of dispersion and complex effects, and provides a variety of other options that are unavailable in AERMOD (short term fluctuations for odours, condensed plume visibility, puff release, and special treatment for coastline area). ADMS is one of the few models classified as user friendly. Nonetheless, the potential costs involved for both software and training may limit accessibility of this model (Scaplen M. et al., 2008).

3.4.5 ISCST3

ISCST3 is a straight line trajectory model, based on a steady-state Gaussian plume algorithm. It is applicable for estimating ambient impacts from point, area, and volume sources to a distance of about 50 kilometres in a simple terrain. ISCST3 includes algorithms for addressing building downwash influences, dry and wet deposition. This model utilises hourly meteorological data that have been pre-processed using the PCRAMMET. This model can also be used as a screening model to determine whether more advanced modelling is required. The major advantages of ISCST3 over models like AERMOD and ADMS are its relative simplicity of use and its robust predictions (i.e., the same results can be obtained by different users for the same scenario). The amount of meteorological input data required by ISCST3 is relatively small, and the model can be run sequentially with routinely collected airport data. For a single meteorological condition for a passive pollutant, the meteorological data needed are a single wind speed, a wind direction, a stability class determination, and an assumed mixing depth. Terrain elevations at receptor points, building dimensions in addition to emissions and stack parameters are also needed. The disadvantages of ISCST3 are largely associated with the fact that an improved knowledge of the structure of the atmospheric boundary layer and resulting estimations of turbulent dispersion processes cannot be accommodated in this model (Gorge M. et al., 2008)

3.4.6 AERMOD

For two decades, the most commonly used model for air dispersion modelling was the U.S. EPA's Industrial Source Complex model (ISCST3). The ISCST3 model is a steady-state Gaussian plume model, which can be used to assess primary pollutant concentration and deposition from a wide variety of sources. It can be applied in urban or rural areas, and has optional features to account for settling and dry deposition of particles, reactive decay, and limited terrain elevations. The U.S. EPA established AERMOD as the regulatory model in 2005 (EPA, 2005), to replace ISCST3 (Industrial Source Complex model for Short Terms, version 3). AERMOD is an advanced Gaussian model that incorporates updated treatments of turbulence and dispersion in the planetary boundary layer for flow over flat and complex terrain. AERMOD adopts the ISCST3's input/output architecture, ensuring that the sources and atmospheric processes modelled by the ISCST3 can still be handled. Therefore, all the work done to implement ISCST3 (Turtos et al., 2007a) is a starting point for the implementation of AERMOD. Since a version that supports a free format for surface data is still pending, the program SD_Aermet (built within AERMET program) was developed to convert the surface data from Microsoft Excel to a format supported by AERMET.

AERMET estimates the mixing height in the Convective Boundary Layer, taking into account its dependence on both mechanical and convective processes. Monin–Obukhov Length describes the effects of buoyancy on turbulent flows, particularly in the lower tenth of the atmospheric boundary layer. The mixing height is calculated based on the following criteria:

a) During the day, when the Monin–Obukhov Length is negative, it is estimated as the larger of the convective or the mechanical mixing height.
b) During the night, when the Monin–Obukhov Length is positive, it is equal to the mechanical mixing height.

A problem emerges when trying to estimate the convective mixing height because upper air meteorological data are required. In other countries, upper air soundings are not available with the required frequency (twice daily) or they are not measured, using AERMET upper air estimator as an initial estimator is helpful for initial AERMET runs (Carbonell L.M.T et al.,2010). AERMET guarantees the use of the convective mixing height once adequate convection has been established even though the mechanical mixing height is calculated during all convective

conditions (EPA, 2004). Because AERMOD is designed for near-field and steady-state conditions, AERMOD has some inherent limitations for applications in complex terrain and for source – receptor distances exceeding roughly 50 km in all terrain situations. There are no considerations in AERMOD of underlying effects, the trajectory of the airflow is treated as straight-line, and it relies on spatially uniform meteorological conditions. AERMOD also has very limited capability for treating chemical transformation, and it is unsuitable for estimating secondary formation of the pollutants such as nitrate and sulphate PM. Because of the Gaussian plume model formulation, AERMOD can only consider wind data from a single location and it cannot directly simulate near stagnation conditions (i.e., very low wind speeds 0.5-0 m/s) (US EPA 2004).

AERMOD uses meteorological fields generated by the meteorological pre-processor AERMET. 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 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 model on several databases (US EPA, 2005).

$$X_{(x,y,z,H)} = \frac{Q}{2\mu u \sigma_y \sigma_z} \exp\left[-\frac{y^2}{2\sigma_y{}^2}\right]\left\{\exp\left[-\frac{(H-z)^2}{2\sigma_z{}^2}\right] + \exp\left[-\frac{(H+z)^2}{2\sigma_z{}^2}\right]\right\} \quad \text{.....(4)}$$

Figure 4: General Gaussian dispersion equation for a point source (US EPA, 2004).

AERMOD uses meteorological fields generated by the meteorological pre-processor AERMET. 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 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 model on several databases (US EPA, 2005).

3.4.7 CALPUFF

CALPUFF is the recommended US EPA model for dispersion applications requiring detailed description of physical and atmospheric chemistry. CALPUFF is a multi-layer, multi-species non-steady-state Lagrangian puff transport and dispersion model that advects Gaussian puffs of multiple pollutants from modelled sources and simulates the effects of time- and space-varying meteorological conditions on pollutant transport, transformation, and removal. The model can simulates 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. The model includes algorithms, sub-grid 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 (BART, 2005).

CALPUFF uses 3D meteorological fields generated by the meteorological pre-processor CALMET. CALMET can use data from single station surface and upper air observations and 3D prognostic model outputs. The prognostic model outputs can be used in combination with or without station observations.

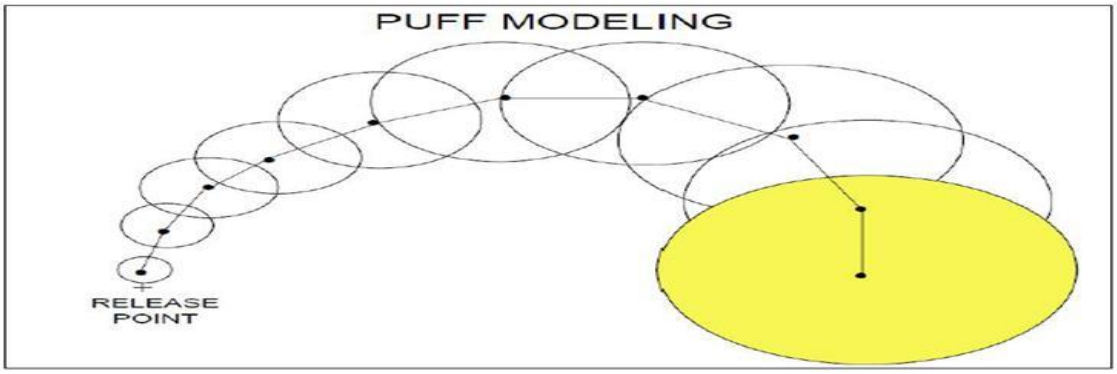


Figure 5: Gaussian puff distribution of pollutants from a point source (Earth Tech, 2005)

Basic equation for the contribution of a puff at a receptor is:

$$C = \frac{Q}{2\pi\sigma_x\sigma_y} g \exp\left[\frac{-d_a^2}{2\sigma_a^2}\right]\exp\left[\frac{-d_c^2}{2\sigma_y^2}\right] \quad \text{.....(1)}$$

$$g = \frac{2}{(2\mu)^{1/2}\sigma_z}\sum_{n=-\infty}^{\infty}\exp\left[\frac{-(H_e + 2nh)^2}{2\sigma_z^2}\right] \quad \text{.....(2)}$$

Where, C is the ground-level concentration (g/m^3),

Q is the pollutant mass (g) in the puff,

σ_x is the standard deviation (m) of the Gaussian distribution in the x-direction,

σ_y is the standard deviation (m) of the Gaussian distribution in the y-direction,

σ_z is the standard deviation (m) of the Gaussian distribution in the z-direction,

d_a is the distance (m) from the puff center to the receptor in the along-wind direction,

d_c is the distance (m) from the puff center to the receptor in the cross-wind direction,

g is the vertical term (m) of the Gaussian equation,

H is the effective height term (m) above the ground of the puff center, and

h is the mixed-layer height (m).

Figure 6: General Gaussian dispersion equation for a point source on a puff at a receptor (Earth Tech, 2000).

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. CALPUFF can also 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 (Egan B.A. et al., 2008).

CALPUFF uses CALMET for meteorological processing, which is a key component of the CALPUFF modelling system. Its primary purpose is to prepare meteorological inputs for running CALPUFF, consisting of 3-D wind fields, 2-D gridded derived boundary layer parameter fields (e.g. mixing height, friction velocity, Monin Obukhov length, etc.), and 2-D gridded fields of surface measurements and precipitation rates (for use in calculating wet deposition fluxes). CALMET also 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. Execution of the CALMET meteorological model requires establishment of the modelling domain (meteorological grid), pre-processing and quality assuring meteorological and geophysical input data, and determination of appropriate control file settings. Meteorological input data include surface, upper-air, and overwater data (Earth Tech, 2005).

Chapter 4: Methodology

Regulatory air dispersion modelling practices in South Africa have been operating in the absence of a standardised regulatory approach and do not have locally developed air quality models. This presents a number of challenges as (1) air dispersion models are used by industry, consultancies and all levels of government at the discretion of modellers; (2) assessments to estimate the impacts of proposed / existing regulated industries on ambient air quality vary in terms of quality; (3) different regulatory authorities have different requirements in respect to estimating the impacts of proposed / existing regulated industries on ambient air quality and (4) the choice of methodology used to estimate the impacts of proposed / existing regulated industries on ambient air quality may be improperly influenced by the desired outcome of estimates.

The recently (government gazette, 2012) published draft (Guideline to Air Dispersion Modelling for Air Quality Management in South Africa, 2012) regulations by the Department of Environmental Affairs seeks to regulate air dispersion modelling in South Africa (DEA, 2012). In the guideline AERMOD (AERMOD Version 6.4.0or 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) and CALPUFF Version 4.5.2 is the recommended model for dispersion applications requiring detailed description of physical and chemical atmospheric processes for distances greater than 50 km. In 2003, US EPA issued revisions to the Guidelines on Air Quality Models that recommended using the CALPUFF dispersion model to address far-field (> 50 km) air quality issues. The US EPA Air Quality Modelling Guidelines were revised again in 2005 to include AERMOD as the EPA-recommended dispersion model for near-source (< 50 km) air quality issues (US EPA, 2012).

4.1 Selection of CALPUFF and AERMOD for the Study

Of the models surveyed, ADMS, AERMOD and CALPUFF are all in principle capable of handling the required modelling features such as complex 3-D fields, a fine spatial resolution and elevated emission sources. Due to limited funds, the use of ADMS was not evaluated. AERMOD and CALPUFF were selected for this study.

4.1.1 CALPUF and AERMOD Model comparison

Differences between AERMOD and CALPUFF can be characterized as follows:

i. CALPUFF allows for variable and curved trajectories (i.e., relies on non-steady-state dispersion) whereas AERMOD assumes a straight a straight line trajectory (i.e, assumes steady-state dispersion).

ii. CALPUFF utilizes meteorological data that varies spatially and temporally.

iii. CALPUFF retains information on emissions from the previous hour to allow plumes to meander the modelling domain.

iv. CALPUFF can compute concentrations for calm or low wind speed meteorological observations.

v. CALPUFF allows for limited chemical transformation mechanisms (SO_2, SO_4, NO_X, HNO_3, and NO_3)

vi. CALPUFF is a more accurate and representative model than AERMOD especially in its treatment of meteorology and complex terrain. (Donaldson I et al., 2008).

4.1.2 AERMOD and CALPUFF Modelling assumptions

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 of the vertical velocity. Steady-state is assumed during each one hour modelling interval; emission rates are assumed to be constant and continuous. Furthermore, all of the pollutants released in the atmosphere remain in the atmosphere. Portions of the plume dispersing toward the ground are assumed to be dispersed back away from the ground by

turbulent eddies. No variations occur in wind speed or wind direction when transporting from the source to the receptor.

AERMOD Also assumes that there is no memory of the previous hour's emissions. Consequently, for each hour the plume is dispersed in the direction of the given hourly meteorology in a straight line. Although AERMOD is capable of estimating building downwash, these effects were assumed to be negligible in this model setup. Only SO_2 emissions from the Chevron Refinery were considered in the model. CALPUFF assumes variable/curved trajectories (i.e., relies on non-steady-state dispersion); meteorological conditions may be variable and are not assumed to be steady-state, it retains information of previous hours emissions, allows calm and low wind speed conditions (Elizabeth A.H. 2003).

Only dispersion of SO_2 emissions from the Chevron Refinery were considered in the modelling.

4.2 Applications of AERMOD and CALPUFF

The source data, meteorological data and site data are essential to run any air quality model. The data collected have to be converted to a form so that it is acceptable by the model to be used. The input data and related procedures constitute an integral part of the modelling. Apart from these data the receptor data and the air quality data are needed to study the impact of a source. A brief discussion is given below on the different classes of the data needed to run AERMOD and CALPUFF models. A typical AERMOD and CALPUFF interface uses the five pathways to develop an input file. These pathways are Control pathway, Source pathway, Receptor pathway, Meteorological pathway, Terrain Grid pathway, and Output pathway.

The Control pathway is used to specify the modelling scenario, and the overall control of the modelling run. Source pathway is used to define the sources of pollutant emissions. Receptor pathway is used to determine the air quality impact at specific locations. Meteorology pathway is used to define the atmospheric conditions of the area being modelled, which will be used to determine the distribution of air pollution impacts for the area. Terrain Grid pathway is the one where the user has the option of specifying gridded terrain data. Gridded terrain data is used in

calculating dry depletion in elevated or complex terrain. The Output pathway defines the type of output results necessary to meet the needs of air quality modelling analyses (US EPA, 2004).

4.3 Model Setup and Application.

In this study Lakes Environment's AERMOD View™ and CALPUFF View™ which incorporate AERMET and CALMET respectively (Jesse L et al, 2009 and 2012) with local meteorology, reported daily SO_2 emissions and local terrain data as inputs, to model the dispersion of SO_2 emitted by the Chevron Refinery. Modelling was done over a year period (2010) to assess the effects of seasonal meteorological variability.

To validate the modelling, model-predicted ambient concentrations based on actual refinery emissions were compared with corresponding monitored data from two local (Bothasig and Table View) monitoring stations. To evaluate the coherence between Petroleum Industry (Oil Refining), Minimum Emission Standards and the Ambient Air Quality Standards, emission rates were then adjusted to comply with the regulated emission standards, and model-estimated ambient concentrations were compared with the 1 hour, 24 hour and annual average Air Quality Standards.

4.3.1 Source Emission Data.

Air pollution in the Cape Peninsula is generated by several sources, including large industrial point sources, small point sources (mainly fossil-fuel fired boilers), petrol and diesel vehicle emissions and domestic fuel burning emissions (Sowden et al., 2008).The Chevron refinery is the largest single source of point SO_2 emissions in its immediate vicinity, although its contribution to total annual SO_2 emissions in the Peninsula is less than 35% (Sowden et al., 2008). All SO_2 emissions from the Chevron Refinery occur via stacks.

The Refinery measures and/ or calculates daily emission rates by stack and, along with other relevant data, reports these values to the City of Cape Town on a quarterly basis. These daily average emission values for 2010 were used to estimate hourly average emission rates by assuming that emission rates were constant for each 24-h period. Stack height and diameter, exit flue gas velocities and temperature data were obtained from the Atmospheric Impact Report

Chevron Cape Town Refinery by ERM Southern Africa (Pty) Ltd 2007 (Dreessen W.J et al, 2007) (Table 3). All data were converted to appropriate units.

4.3.2 Modelling Domain.

The CALMET/CALPUFF modelling system uses a grid system consisting of an array of horizontal grid cells and multiple vertical layers (figure 7). Three gridded domains need to be defined in the CALMET/CALPUFF model – meteorological, computational, and sampling. The meteorological gridded domain defines the extent over which land use, winds, and other meteorological variables are defined. The computational gridded domain defines the extent of the concentration calculations, and is required to be identical to or a subset of the meteorological domain. The sampling or receptor domain defines the extent over which receptors are arranged with a nesting factor. The AERMOD model has considerable flexibility in the specification of receptor locations (figure 7). AERMOD can specify multiple receptor networks in a single run, and may also mix cartesian grid receptor networks and polar grid receptor networks in the same run. This is useful for applications when coarse grid over the whole modelling domain, but a denser grid in the area of maximum expected impacts. There is also flexibility in specifying the location of the origin for polar receptors, other than the default origin at (0,0) in x,y, coordinates (US EPA, 2004).

Figure 7: Study area for CALPUFF (red boundary) and AERMOD (blue boundary) with receptor grid, location of refinery (R), monitoring stations (T, A, B) and surrounding communities.

4.3.3 Meteorological Data

South African meteorology data are mostly available in Microsoft Office Excel ™ formats for upper air and surface meteorological data. The Excel files were converted into relevant formats for each model. Hourly surface meteorological data used in this study were obtained from the South African Weather Service (SAWS); the City of Cape Town provided a comprehensive set of meteorological data from the Cape Town International Airport weather station, including wind speed and direction, surface temperature and pressure, relative humidity, cloud cover and upper air data. Limited surface data were also available from the Refinery, Bothasig and Table View meteorological stations. CALMET/AERMET require upper air sounding data which were only available from National Weather Service (NWS) stations for the Cape Town International Airport. Upper Air data required by CALMET/AERMET are standard TD6201 format data including wind speed, wind direction, temperature, pressure, and elevation.

CALMET/AERMET requires at least one valid record at any given hour for a given parameter such as wind speeds. When all records simultaneously missed relevant records, surrogate data were generated by CALMET/AERMET by interpolating values from the previous and/or subsequent record. If data were missing for a longer period such as a day, the missing data were filled by repeating the previous or subsequent day manually. The surface data were processed with the CALMET/AERMET pre-processor utility program, to create the SURF.DAT file for input to CALMET/AERMET. The upper air data were processed by the CALMET/AERMET pre-processor utility program, READ62, to create an upper air file the station (UPn.DAT). Refer to figure 8 below for AERMOD and CALPUFF model set up.

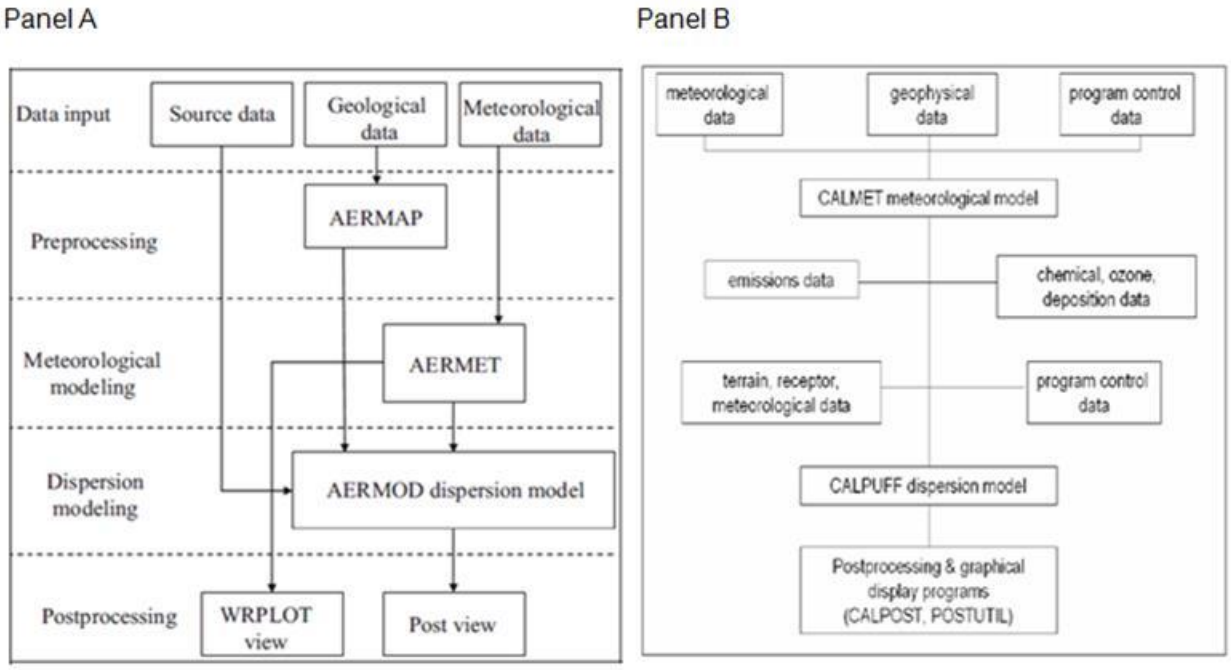


Figure 8: AERMOD (Panel A) and CALPUFF (Panel B) modelling system components (Seankiatiyuth K, 2011 and (BART, 2005)

4.3.4 Geophysical Data.

Geographical information requirements range from basic (for screening analyses) to advanced (for more sophisticated modelling). The AERMOD and CALPUFF models make use of complete three-dimensional geographic data with support for digital elevation model files and real-world spatial characterization of all model objects. MAKEGEO/AERMAP requires geophysical data in order to prepare the wind fields/wind rose and other meteorological parameters. The

geophysical data required include land use categories, terrain elevations, surface roughness length, albedo, Bowen ratio, soil heat flux parameter, vegetation leaf area index and anthropogenic heat flux. All these data are derived from terrain and land use data and processed into gridded fields within the modelling domain.

The coordinate system most commonly used for air dispersion modelling is the Universal Transverse Mercator (UTM) system which uses metres as its basic unit of measurement and allows for more precise definition of specific locations than latitude/longitude. The Digital Elevation Models (DEM) file obtained from Department of Land Affairs and extracted for the modelling domain grid using the utility program TERREL. MAKEGEO/AERMAP used Land-use data that was extracted from the United States Geological Survey (USGS) files and processed using utility programs CTGCOMP and CTGPROC. Terrain elevations and the corresponding land use parameters were assigned to each MAKEGEO/AERMAP grid cell for a GEO.DAT file for input using the MAKEGEO/AERMAP processor by interpolating the DEM and LULC data.

4.3.5 Terrain Data.

Terrain elevations can have a large impact on the air dispersion and deposition modelling results and therefore on the estimates of potential risk to human health and the environment. Terrain elevation is the elevation relative to the facility base elevation. Figure 9 describes the primary types of terrain. Although the consideration of a terrain type is dependent on the study area, the definitions below must be considered when determining the characteristics of the terrain for the modelling analysis. As illustrated in Figure 9 complex terrain is where terrain elevations for the surrounding area, are above the top of the stack being evaluated in the air modelling analysis and simple terrain is where terrain elevations for the surrounding area are not above the top of the stack being evaluated in the air modelling analysis (Environmental Protection Act, 2009).

Simple terrain can be divided into two categories:

Simple Flat Terrain: is used where terrain elevations are assumed not to exceed stack base elevation. If this option is used, then terrain height is considered to be 0.0 m.

Simple Elevated Terrain: as illustrated in Figure 9 is used where terrain elevations exceed stack base but are below stack height.

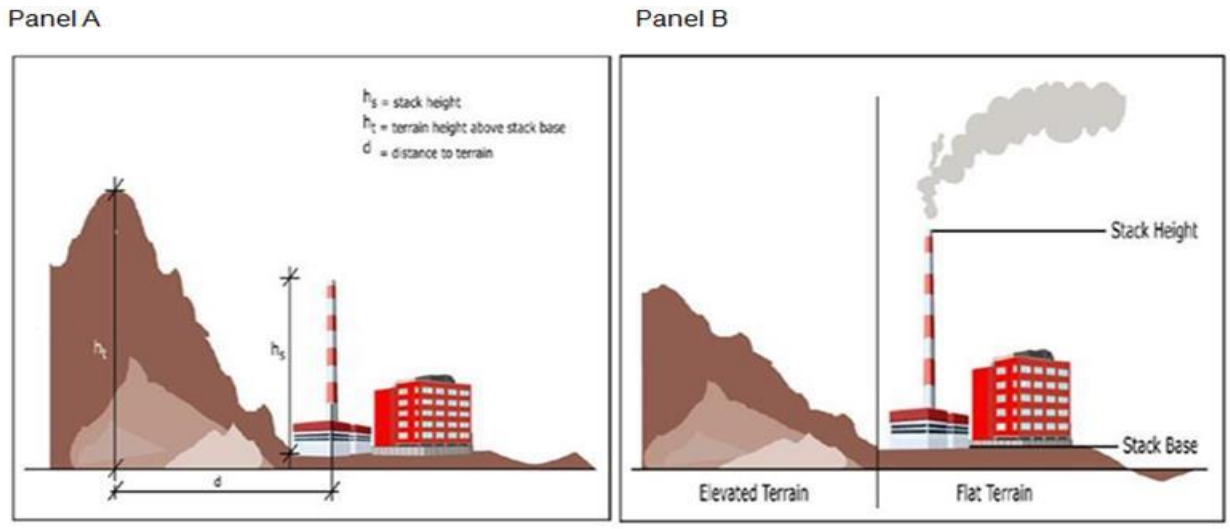


Figure 9: Complex (Panel A) and Simple (Panel B) Terrain (Environmental Protection Act, 2009).

4.3.6 Land Use and Land Cover Data.

Land use plays an important role in air dispersion modelling from meteorological data processing to defining modelling characteristics such as urban or rural conditions. Land use data can be obtained from digital and paper land-use maps. The maps provide an indication into the dominant land use types within an area of study, such as industrial, agricultural, forested and others. This information can then be used to determine dominant dispersion conditions and estimate values for the critical surface characteristics which are surface roughness length, albedo, and the Bowen ratio. In 2008 the US EPA released the AERSURFACE tool, part of the AERMOD modelling system, to assist users in the appropriate selection of surface characteristics for different land use categories in the vicinity of a facility or site. These characteristics are then input into AERMET which determines the appropriate dispersion parameters for each area/sector surrounding the site. The AERSURFACE tool is designed to use US Geological Survey (USGS) National Land Cover Data 1992 (NLCD92), which includes 21 separate land cover categories (US EPA, 2008).

Chapter 5: Results and Discussion

5.1 Stack Emission Rates

Chevron Refinery in Cape Town, Milnerton has the capacity to process 100 000 barrels/day of crude (SAPIA, 2011). Sulphur dioxide emissions from the refinery are released via nine point sources (eight stacks and one flare system stack). There are two general types of refinery emissions: hydrocarbons, and combustion products such as SOx, NOx and CO_2. Most of the major pieces of process equipment handling hydrocarbons at refineries do not emit any combustion products. However, the combustion sources such as heaters and boilers will typically emit air pollutants and greenhouse gases as well as small amounts of hydrocarbons due to incomplete combustion (Saqer S.S et al, 2008).

Daily emission rates (Table 1 in Appendix) were extracted from the four 2010 Chevron Quarterly Reports obtained from the City of Cape Town (CAPCO, 2010). Emission rates were assumed to be constant over each 24 hour period and converted from t/day to g/s emission rates for each hourly modelling run (Table 2&3 in Appendix). The 2010 daily emission rates includes the shutdown period (from 16th April to 4th May 2012 , 19 days duration). The average total (all stacks) emission rate for 2010 was 143 g/s (standard deviation = 49.6 g/s). Below is the summary of the refinery SO_2 point source emissions.

Table 3: Chevron Refinery hourly average SO_2 emission rates 2010, (Dreessen W.J et al, 2007)

Source	Unit	x-Coord.	y-Coord.	Stack Height	Stack Diameter	Temp.	Gas Exit Velocity	Base Elevation	Ave. SO_2 emission rate**
		(m)	(m)	(m)	(m)	(K)	(m/s)	(m)	(g/s)
Stack 1	2F-1	271328.8	6252297	60.96	2.68	677	10	14.3	7.61 (4.13)*
Stack 2	2F-201	271329.7	6252304	60.96	1.68	572	8	14.1	4.22 (2.10)
Stack 3	52F-201	271375.9	6252470	91.44	2.53	824	8	14.6	23.3 (22.2)
Stack 4	4F-1	271382	2652278	59.13	3.35	503	2	14.4	4.39 (4.71)
Stack 5	56F-201	271451.1	6252240	53.35	0.91	671	6	14.3	0.01 (0.04)
Stack 6	71F-1	271457.2	6252341	53.00	0.90	502	7	14.6	0.04 (0.20)
Stack 7	53F-201	271452.9	6252400	59.50	1.20	488	18	14.7	23.5 (9.75)
Stack 8	69F-4	271559.6	6252608	91.44	3.05	536	17	15.5	77.6 (32.4)
Flare 1	101F-1	271451.5	6253017	53.34	0.92	1273	20	14.0	2.30 (12.52)

*(..) standard deviation of daily mean values

** Average total emission rate: 143g/s, standard deviation 49.6 g/s.

5.2 Modelling Domain.

In this thesis, the modelling domain includes the Chevron Refinery, the Atlantic Ocean to the west of the refinery, high topography areas to the north east and south west with elevations in excess of 300 and 900 meters, and the nearby communities. The size of the modelling domain was, determined by considering that the domain should cover low and high topographical area, the Atlantic Ocean about 4km to the west of the refinery and communities nearby the refinery. The modelling domain shown is in Figure 19.The approximate Universal Transverse Mercator (UTM) coordinates of the facility are 261 to 284 km Easting and 6242 to 6263 km northing for AERMOD and 250 to 290 km Easting and 6235 to 6363 km northing for CALPUF (UTM Zone 34, Lo 21).

The selection of grid cell size reflects a compromise between the desire to define meteorological and geophysical variations on a very small scale, and the computer time and resources necessary to do so. To provide a more detailed estimate of localized impacts of the emissions on the nearby community to the refinery for complex terrain (sea-land, rolling mountains), non-uniform land-use characteristics, and water, we selected a grid cell size of 1 x 1 km for both AERMOD and CALPUFF meteorological modelling. The receptor grid, terrain contours, location of the City of Cape Town monitoring stations, populated areas and the refinery are shown in Figure 10.The following notation is used in Figure 9**:** R-Refinery, T, B and A -Table View, Bothasig and Cape Town International Airport (CTIA) monitoring stations respectively.

Figure 10: Study area for CALPUFF (red boundary) and AERMOD (blue boundary) with receptor grid, location of refinery (R), monitoring stations (T, A, B) and surrounding communities.

5.3 Meteorological Results

A comprehensive set of meteorological data is available for the Cape Town International Airport (Synop No 68816) but this station is about 14km from the refinery. The refinery operates a more limited meteorological station. Although the terrain between the airport and the Table View is generally flat, the refinery is located about 3.5km from the sea and 4 to 8km from hills (high point 400m) to the north-east, and 15 to 20 km from the Table Mountain range (high points 900-1000m) (Figures 10 and 11) to the south-west, features suspected to have a significant effect on the local wind vectors.

Figure 11: Chevron Refinery Site.

5.3.1 Surface data

To assess the validity of using CTIA meteorological surface data for modelling dispersion from the refinery we compared the wind vectors for the two locations during one month (March 2010). Figure 12 and 13 show that for the month of March 2010, daily wind direction at the Table View station (4km from the refinery) is poorly correlated (R^2 = 0.53) with CTIA (14km from the refinery) data, although there is negligible bias between the two stations (slope = 1.03). Wind speed is better correlated (R^2=0.63) but CTIA wind speeds are about 50% higher on average at the airport site (slope = 1.54) and there are significantly more low wind speed days at the Table View site compared with the airport site.

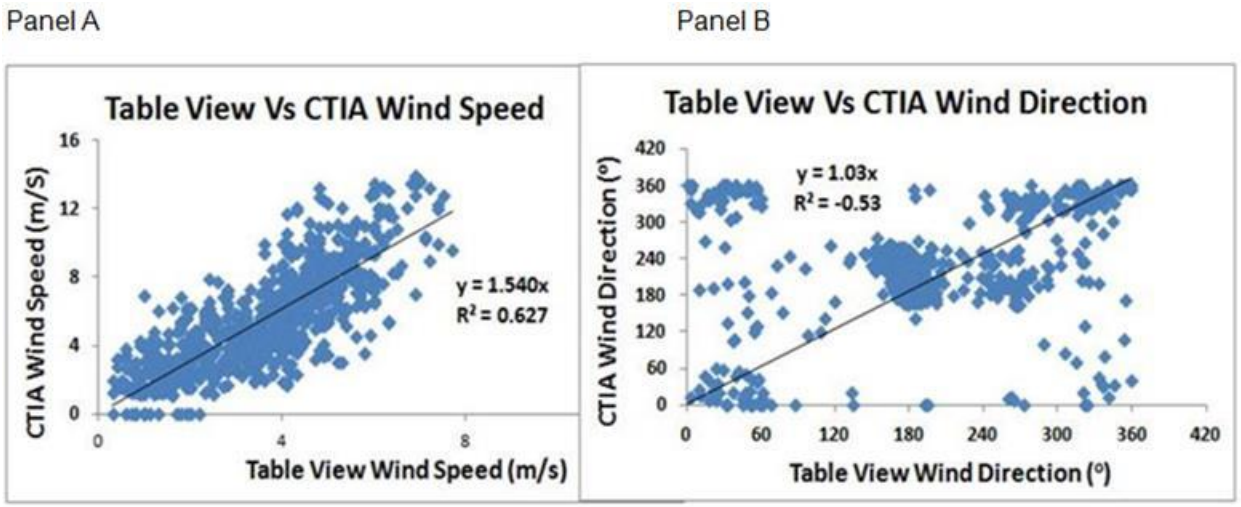


Figure 12: Comparison of hourly average wind vectors, CTIA (Panel A) vs Table View (Panel B), March 2010.

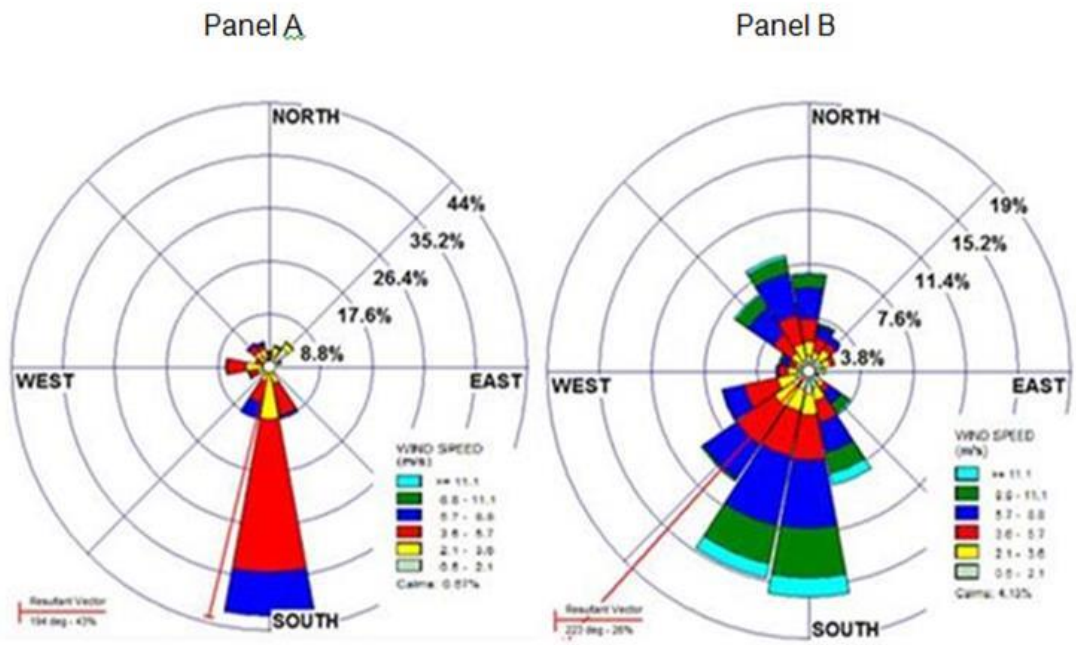


Figure 13: March 2010 AERMET wind rose for Table View (Panel A) and CTIA (Panel B).

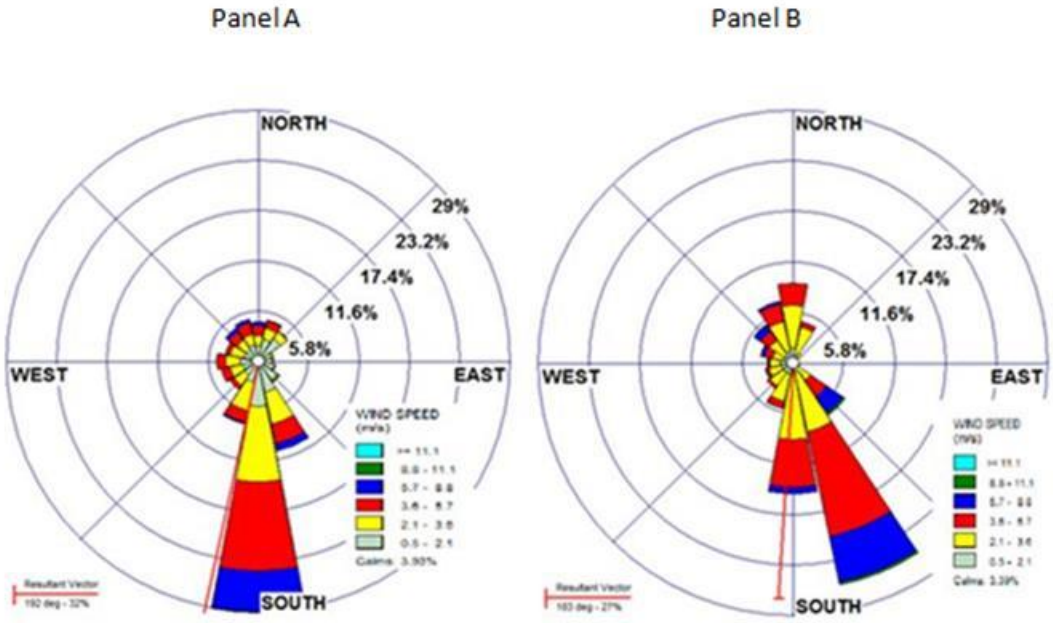


Figure 14: AERMET Annual wind rose for Table View (Panel A) and CTIA (Panel B), 2010.

Figure 12 shows that although the most frequently occurring wind direction is southerly in both cases, the frequency is about 42% for the Table View site, and about 16% for the CTIA site; for the south-south westerly component, the frequencies are about 9% and 15% respectively. As may be expected, the use of these two meteorological datasets, with all other input data identical, produced significantly different modelled isopleths (Figure 17). We therefore used local (Table View and Bothasig) wind speed and direction data combined with airport humidity, cloud cover and surface temperature, and pressure data for the plume and puff modelling.

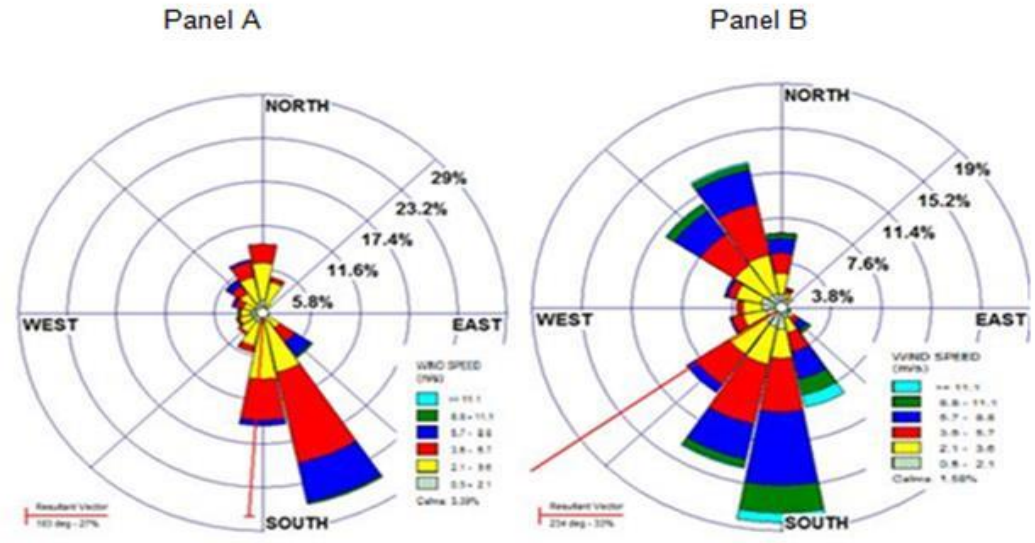


Figure 15: 2010 Annual wind roses for CTIA: CALMET (MM5) (Panel A) and surface data (Panel B).

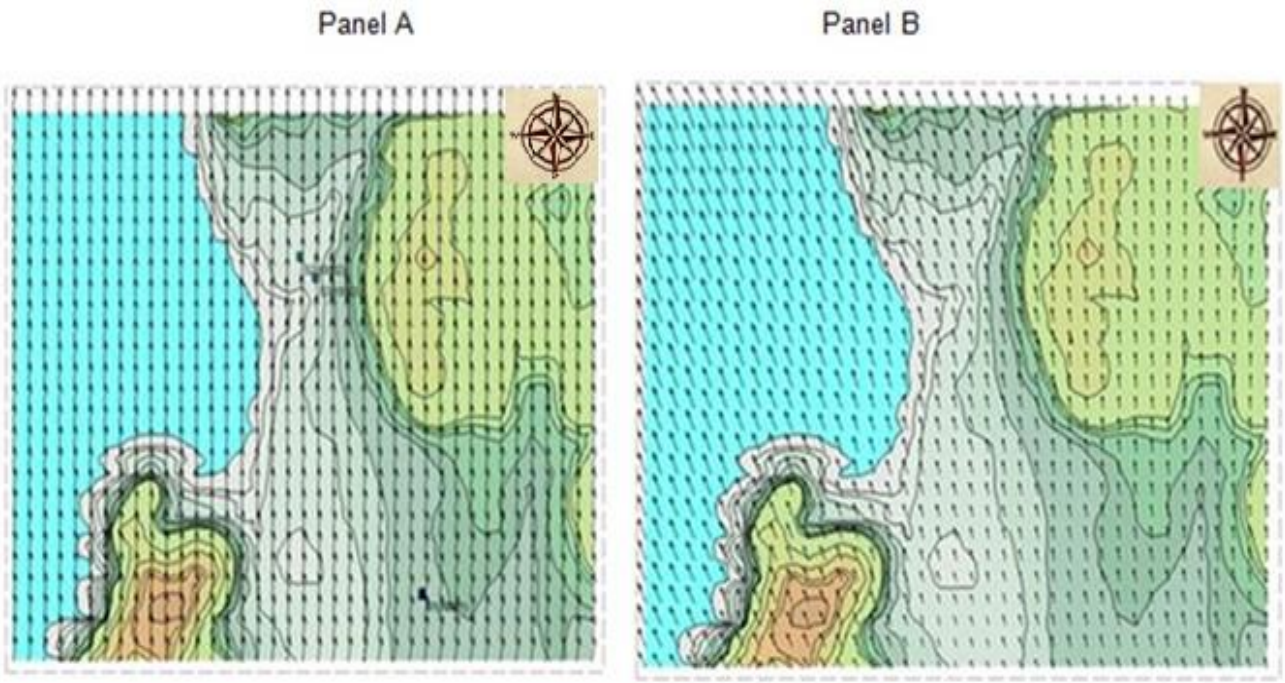


Figure 16: 2010 Annual CALMET (MM5) (Panel A) and measured wind data wind field for CTIA (Panel B).

Figure 15 & 16 show that although the most frequently occurring wind direction is southerly the comparison between Annual wind roses for CTIA MM5 and surface data are poorly correlated.

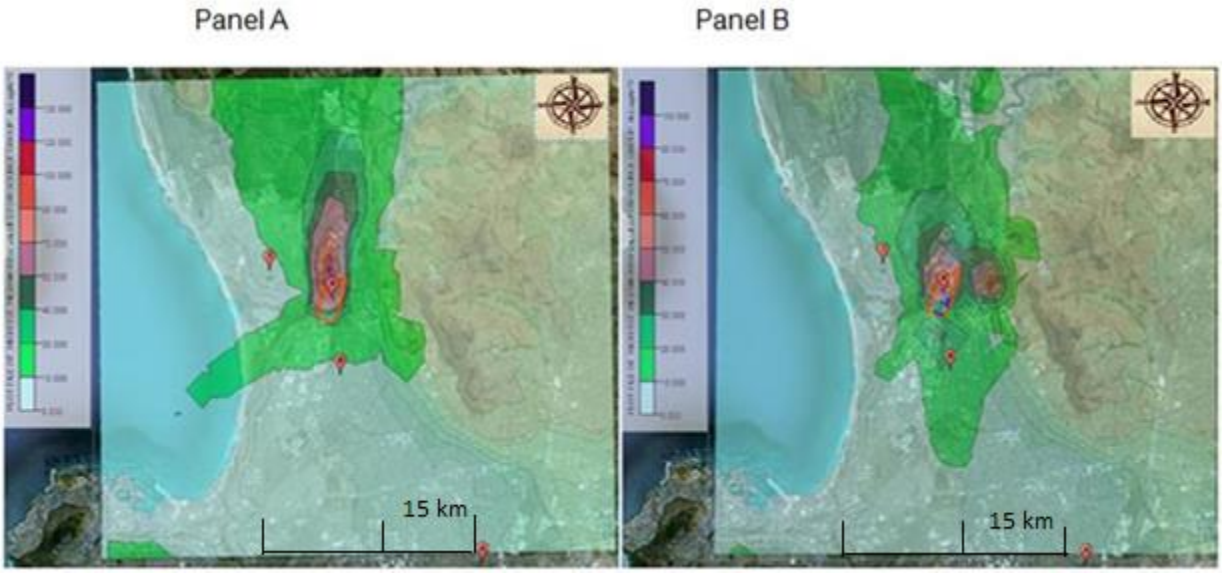


Figure 17: AERMOD modelled isopleths for March 2010, average SO_2 concentrations, Table View (Panel A) and CTIA (Panel B) meteorological data.

There are significant differences between the isopleths (Figures 17) based on Table View and CTIA meteorological data respectively. This also shows that modelling accuracy may be significantly compromised if representative local meteorological data are not used.

5.3.2 Upper Air data, mixing heights

In the Cape Peninsula, upper air soundings are only measured at the CTIA. Figure 18 present a comparison between mixing heights estimated by AERMET and CALMET using actual upper air data from CTIA.

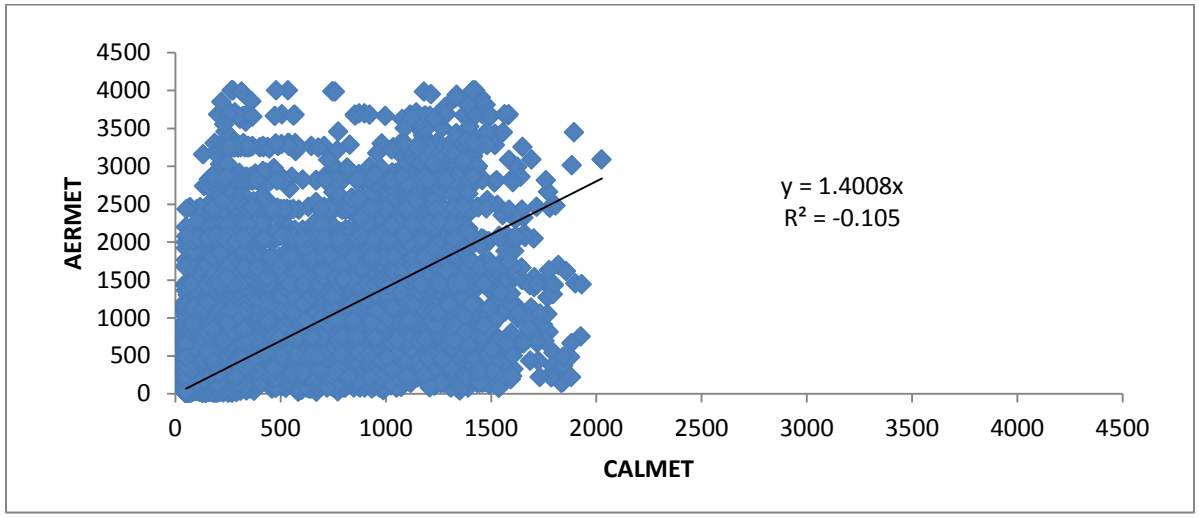


Figure 18: Comparison of mixing heights at CTIA, between AERMET and CALMET using upper air soundings, 2010.

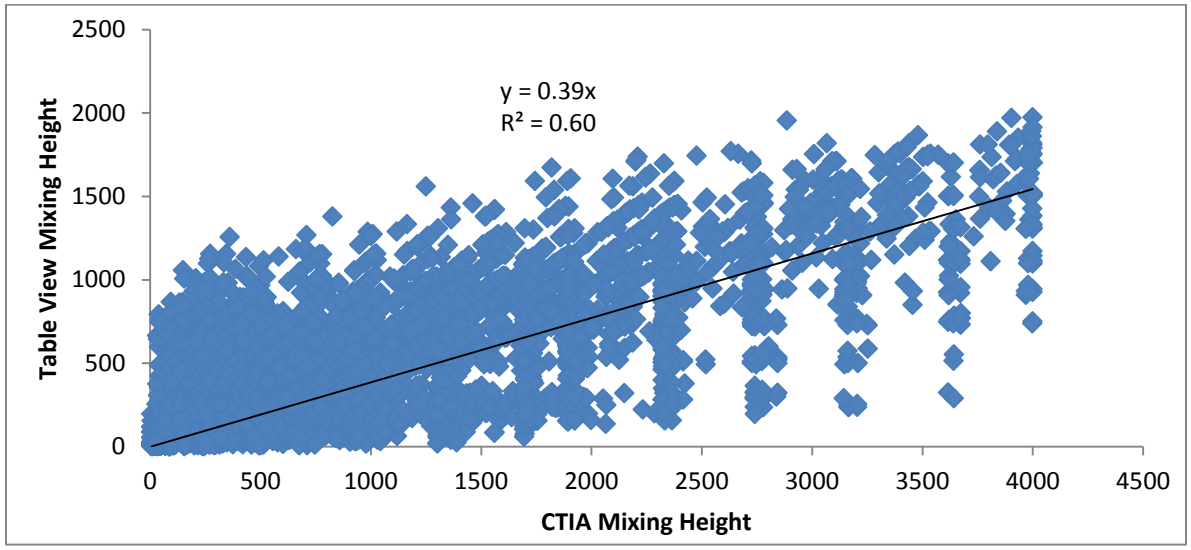


Figure 19: Comparison of mixing heights, using AERMET View™ Upper Air Estimator, between CTIA and Table View, 2010.

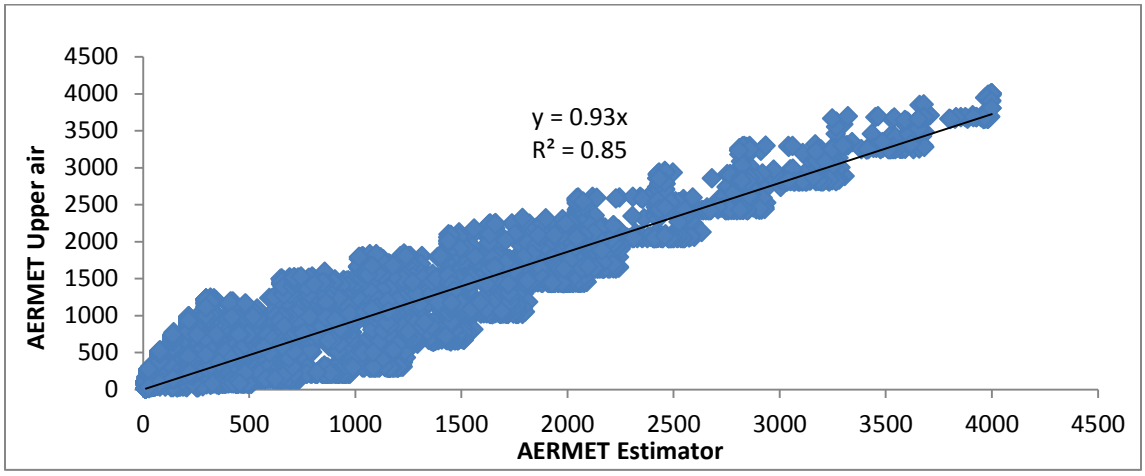


Figure 20: Comparison of mixing heights at CTIA, between AERMET estimator and AERMET using upper air data, 2010.

Figure 18 shows that for the year 2010 meteorological data, the AERMET and CALMET mixing heights (based on the CTIA upper air soundings) are poorly correlated (R^2=-0.105) (slope =1.401). AERMET View™ includes an Upper Air Estimator to estimate mixing heights based on surface data (with wind speed and direction from Table View, and humidity, cloud cover, surface temperature, and pressure from CTIA) as input variables. Figure 19 presents a comparison of mixing heights, using AERMET View™ Upper Air Estimator, between CTIA and Table View. For the year 2010 meteorological data, AERMET View™ Upper Air Estimator, between CTIA and Table View mixing heights are correlated (R^2= 0.60) but the Table View mixing heights are significantly lower than those for CTIA (slope =0.39).

Figure 20 shows that the mixing heights for the year 2010 meteorological data predicted by AERMET using actual upper air data and the AERMET estimator using surface data are in good agreement (R^2=0.853) (slope = 0.932). The AERMET Upper Air Estimator was used for further analysis. It was noted that when using upper air estimator in AERMET instead of upper air data (soundings), there were no significant changes on wind vectors at the CTIA, but when replacing upper air data with MM5 data in CALMET there was a significant change in wind direction (refer to figure 15&16). Table View and Bothasig local wind speed and direction data were therefore used combined with CTIA humidity, cloud cover, surface temperature, and pressure data for the AERMET modelling.

5.4 Geophysical terrain

5.4.1 Terrain Set Up.

Gridded terrain elevations for the modelling domain were derived from 3 arc-second DEM produced by the Department of Land Affairs, Cape Town. It is important to ensure that all model objects (sources, buildings, receptors) are defined in the same horizontal datum, WGS84 (South African datum). Elevations are in meters relative to mean sea level. The spacing of the elevations along each profile is 3 arc-seconds, which corresponds to a spacing of approximately 90 meters. The CALPUFF and AERMOD computational domains encompass areas of 39 km x 27 km and 21 km x 21 km respectively (Figure 21). A vertical and horizontal grid spacing of 0.5 km was selected to adequately represent the important terrain features. The raw terrain data were processed into each gridded field. These terrain fields effectively resolve major land features in the model domain. Below (Figure 21) are terrain isopleths for AERMOD and CALPUFF.

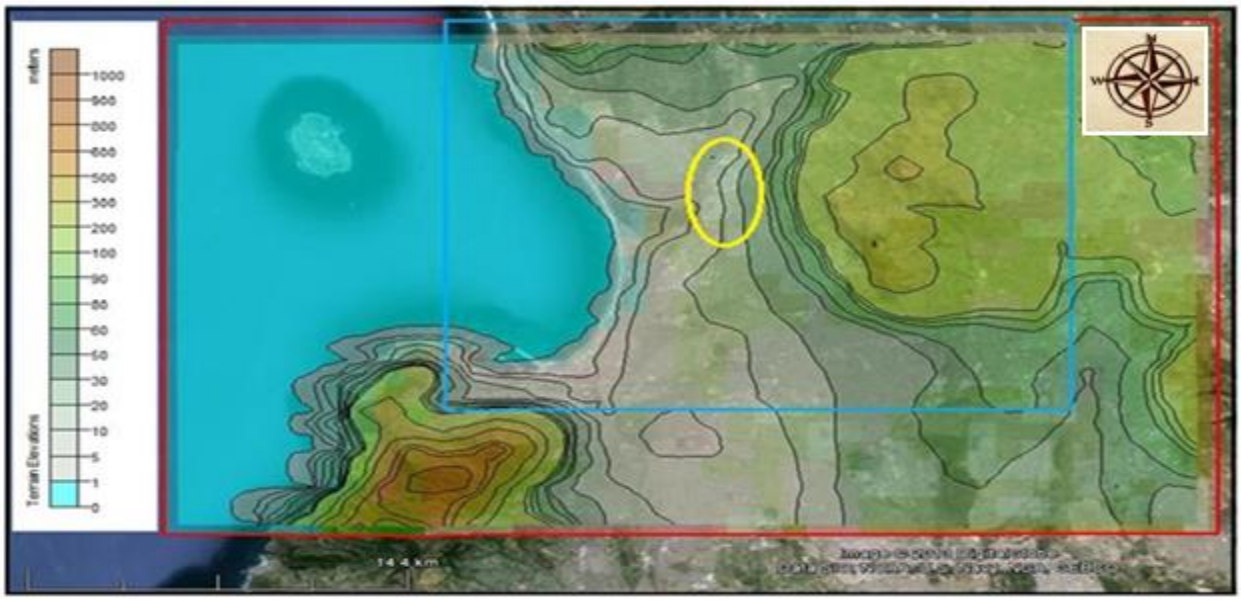


Figure 21: CALPUFF (red boundary), AERMOD (blue boundary) and Chevron Refinery (yellow circle) Terrain.

5.4.2 Land Use and Land Cover Set Up.

CALPUFF Land use and land cover (LULC) data were downloaded from the USGS at the 1:250,000-scale with file names corresponding to the 1:250,000-scale map names. Land use data were processed to produce a 1-km resolution gridded field of fractional land use categories and land use weighted values of surface and vegetation properties for each CALMET grid cell. AERSURFACE, designed to aid in obtaining realistic and reproducible surface characteristic values for the AERMOD modelling system requires input of land cover data from the USGS National Land Cover Data 1992 archives (NLCD92), at a spatial resolution of 30 meters, these resolutions include the modelled domain in the study. Below (Figure 22) is the land cover land use isopleths for AERMOD and CALPUFF.

Figure 22: CALPUFF (red boundary), AERMOD (blue boundary) and Chevron Refinery (yellow circle) Land use and Land Cover.

Figure 23 show sectors and surface parameters used in AERMET for the study. The three selected sectors were cultivated land, urban and water (fresh and sea). Table 4 show surface parameter values used.

Table 4: AERMET surface parameters.

	Albedo	***Bowen Ratio***	***Surface Roughness***
Cultivated land	*0.2800*	*0.750*	*0.0725*
Urban	*0.2075*	*1.625*	*1.0000*
Water	*0.1400*	*0.450*	*0.0010*

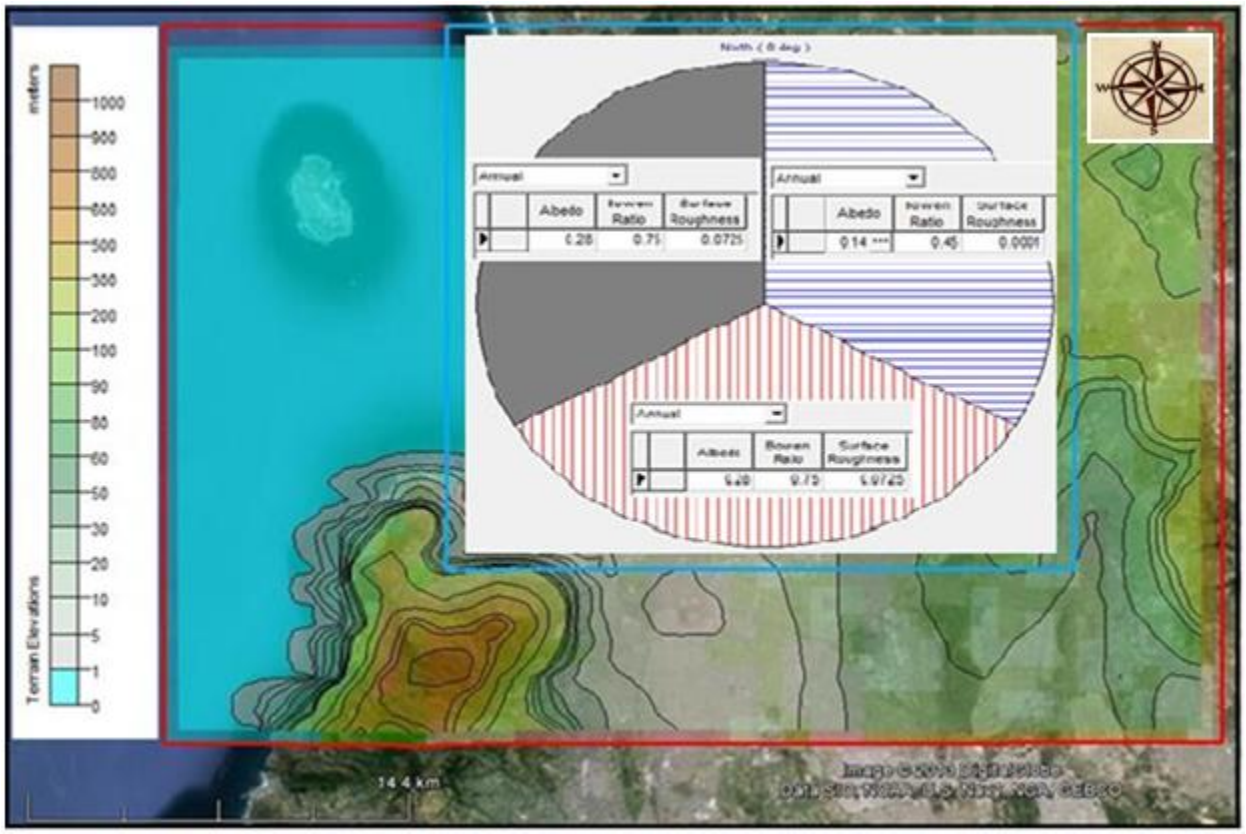


Figure 23: Sectors and Surface Parameters used in AERMET run.

5.5 Background Concentrations

Background data is used to represent the concentrations of pollutants in the air being blown into the modelled area. Usually that takes the form of hourly measurements from rural monitoring sites upwind of the modelling area. For Cape Town, rural monitoring data were not available and so a background dataset was derived from the available monitoring data: For NO_x, NO_2, PM_{10} and SO_2 for each hour, the lowest measured concentration ware taken for all Air Quality Monitoring Sites and for 0_3, the maximum concentration was taken. Below is a summary of the background data used in $\mu g/m^3$.

Table 5: City of Cape Town average measured background concentrations ($\mu g/m^3$) (City of Cape Town, 2007).

	NO_x	***NO_2***	***PM_{10}***	***SO_2***	***O_2***
Annual average	*28.0*	*10.5*	*18.3*	*3.9*	*40.2*
Maximum Hourly average	*561.0*	*74.0*	*169.0*	*36.0*	*221.0*

The City of Cape Town does not have background data for specific areas as the emission rates for all sources (traffic, point, area and volume) in the city have not been accurately calculated. Modelled concentrations do not include sources of SO_2 emissions other than the refinery, a comparison with monitored concentrations should include the contribution of background SO_2 sources at the monitoring stations but data for these sources, including vehicle emissions, were not available. We estimated the background contribution from monitored values during a refinery shutdown from 16 April to 4 May 2010. Table 6 below summarises the average concentrations at the two monitoring stations during this period, providing an estimate of the contribution of background sources at the monitoring stations during this period

Table 6: Average measured SO_2 concentrations during refinery shutdown: 16 April - 04 May 20

Station	***SO_2 concentration [µg/m^3]***		
	19-day average	***Maximum Daily value***	***Minimum Daily value***
Bothasig	*3.10*	*9.30*	*0.00*
Table View	*5.90*	*9.45*	*2.96*

5.6 Ambient Air Quality Standards for SO_2 Concentrations.

The National Ambient Air Quality Standards, promulgated 24 December 2009 (Government Gazette 2009), included the standard for SO_2, reflected in Table 7. The Standard reflects both maximum concentrations as well as maximum 'allowable exceedences at the different averaging periods.

Table 7: Ambient Air Quality Standard for SO_2

Averaging period	***Concentration [µg/m^3]***	***Allowable exceedences***
1 hour	*350*	*88*
24 hours	*125*	*4*
1 year	*50*	*0*

5.7 AERMOD and CALPUF Modelled Ambient Concentrations

The performance of AERMOD and CALPUFF modelling systems in predicting SO_2 concentrations when excluding background SO_2 concentration and deposition were analysed. Table 8 below depicts the model output SO_2 concentration (in µg/m^3)

Table 8: AERMOD and CALPUFF Modelled Ambient SO_2 Concentrations.

Average Period	***Receptor Grid***	***Concentration Matrix***	***Concentration from AERMOD [µg/m³]***	***Concentration from CALPUF [µg/m³]***	***%(AERMOD-CALPUFF) AERMOD***
1 hour	*Coarse*	*1st High*	*6245*	*1553*	*75*
24 hour	*Coarse*	*1st High*	*352*	*172*	*51*
Annual	*Coarse*	*1st High*	*72*	*12*	*83*

As seen in Table 8, the maximum 1-hour average SO_2 concentration from CALPUFF was about 75% less than that predicted by AERMOD. The maximum 24-hour average SO_2 concentration from CALPUFF was about 51% less than that predicted by AERMOD. The annual average SO_2 concentration from CALPUFF was about 83% less than that predicted by AERMOD. The annual average SO_2 concentration for AERMOD and CALPUFF are mostly concentrated around the source (Figure 24 and 25), with AERMOD predicting a maximum concentration of 72 µg/m^3 and CALPUFF predicting a maximum of 12 µg/m^3 for the period . The AAQS for annual average SO_2 concentration is 50 µg/^{m3}. The 24-hour average SO_2 concentration for AERMOD is highly concentrated around the source, Table View, Dunoon and Bothasig, with AERMOD predicting a maximum concentration 352 µg/m^3 (Figure 26). CALPUFF predicted a maximum concentration of 172 µg/m^3 for 24-hour average SO_2 concentration (Figure 27). The AAQS for The 24-hour average SO_2 concentration is 125 µg/^{m3}. The first highest concentration predicted by AERMOD for 1-hour average SO_2 concentration was 6245 µg/m^3, with most of the modelled area above the 350 µg/m^3 AAQS (Figure 28). The first highest concentration predicted by CALPUFF for 1-hour average SO_2 concentration was 1553 µg/m^3, with some of the modelled area above the 350 µg/m^3 AAQS around the cultivated land (wine farms) (Figure 29).

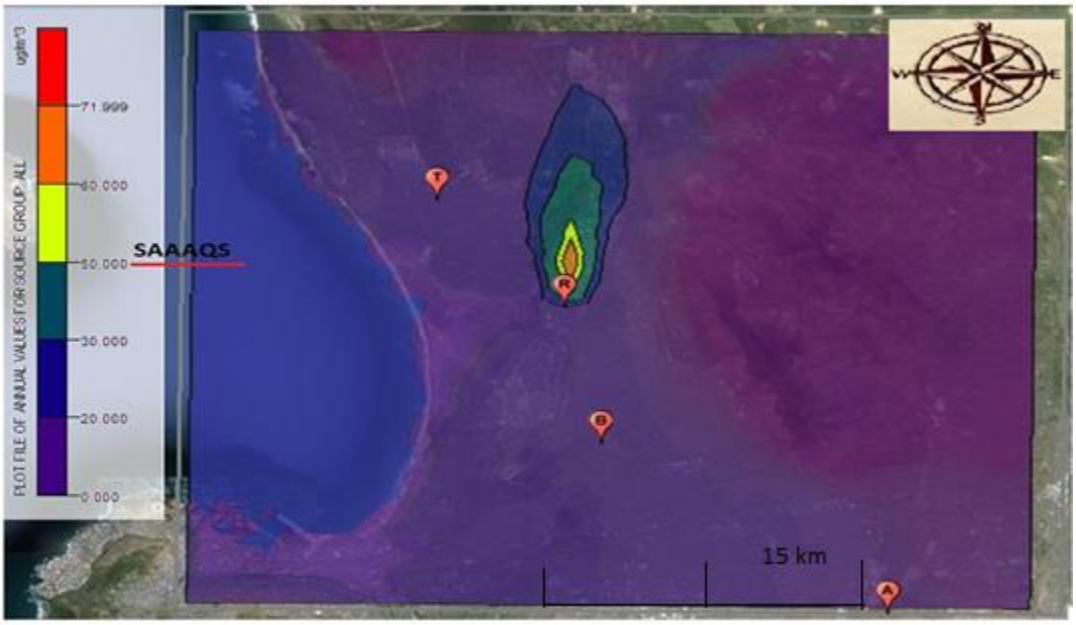


Figure 24: AERMOD modelled isopleths of annual average SO_2 concentrations, 2010.

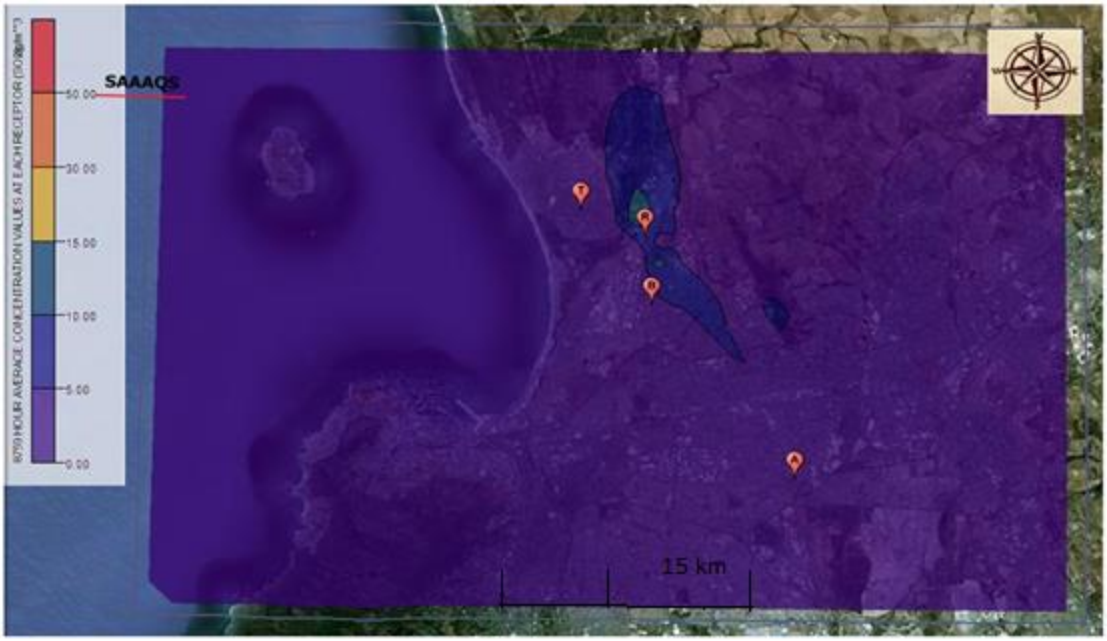


Figure 25: CALPUFF modelled isopleths of annual average SO_2 concentrations, 2010.

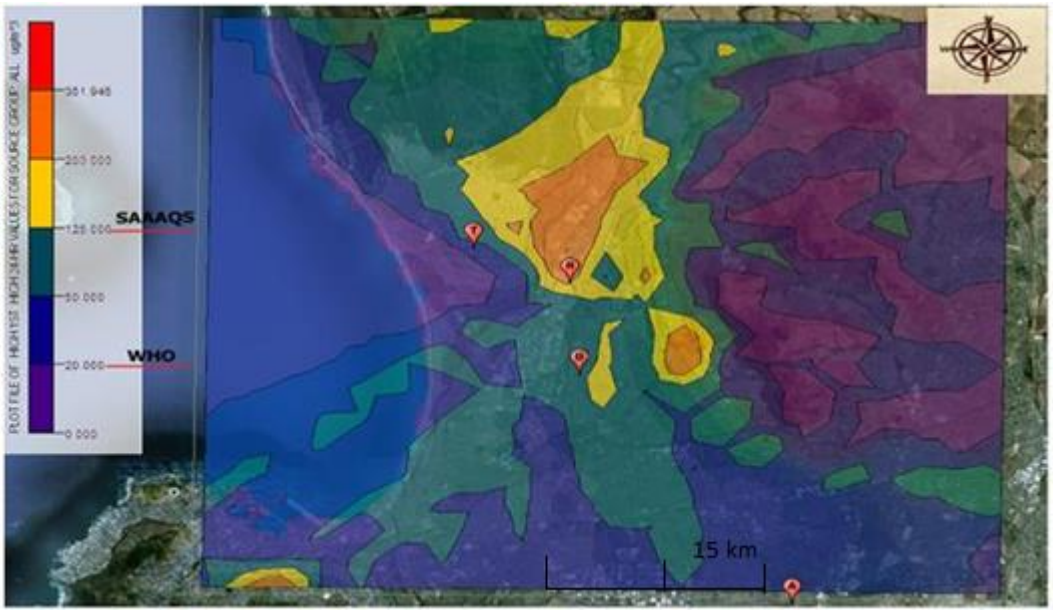


Figure 26: AERMOD modelled isopleths of 24hr average SO_2 concentrations, 2010.

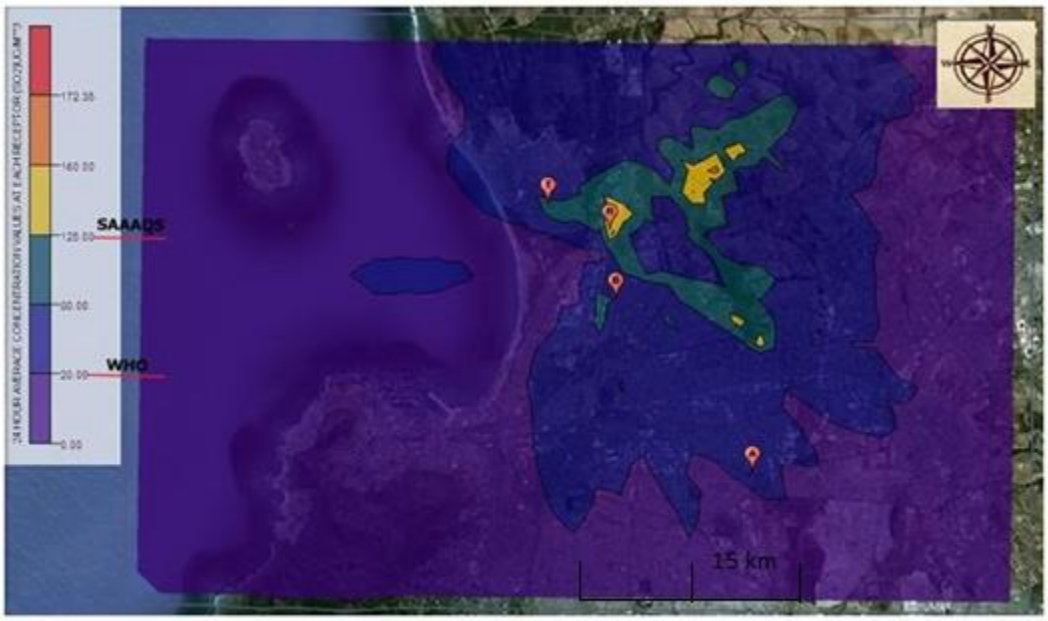


Figure 27: CALPUFF modelled isopleths of 24hr average SO_2 concentrations, 2010.

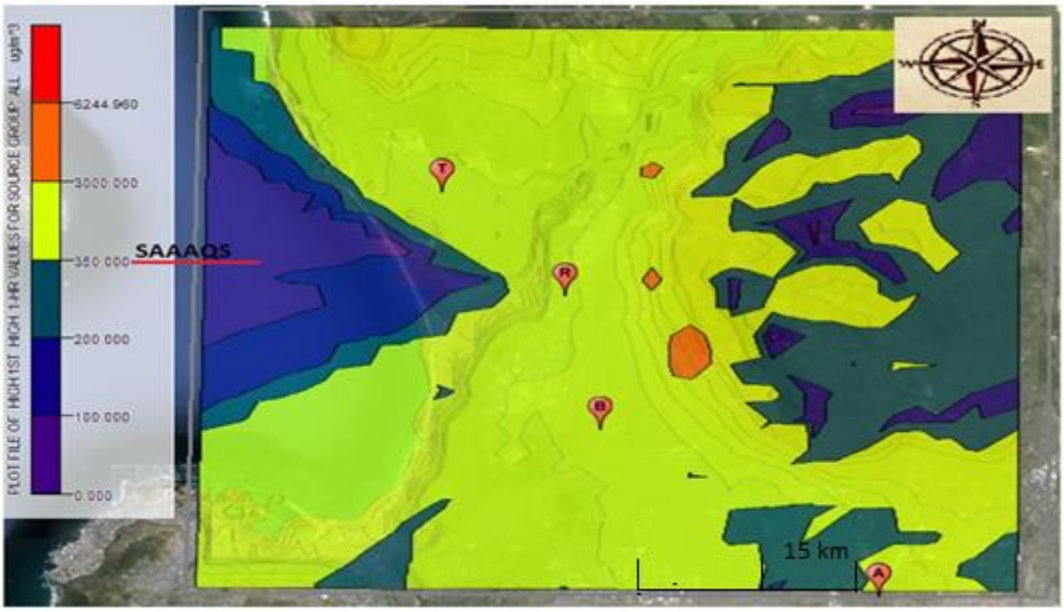


Figure 28: AERMOD modelled isopleths of 1hr average SO_2 concentrations, 2010.

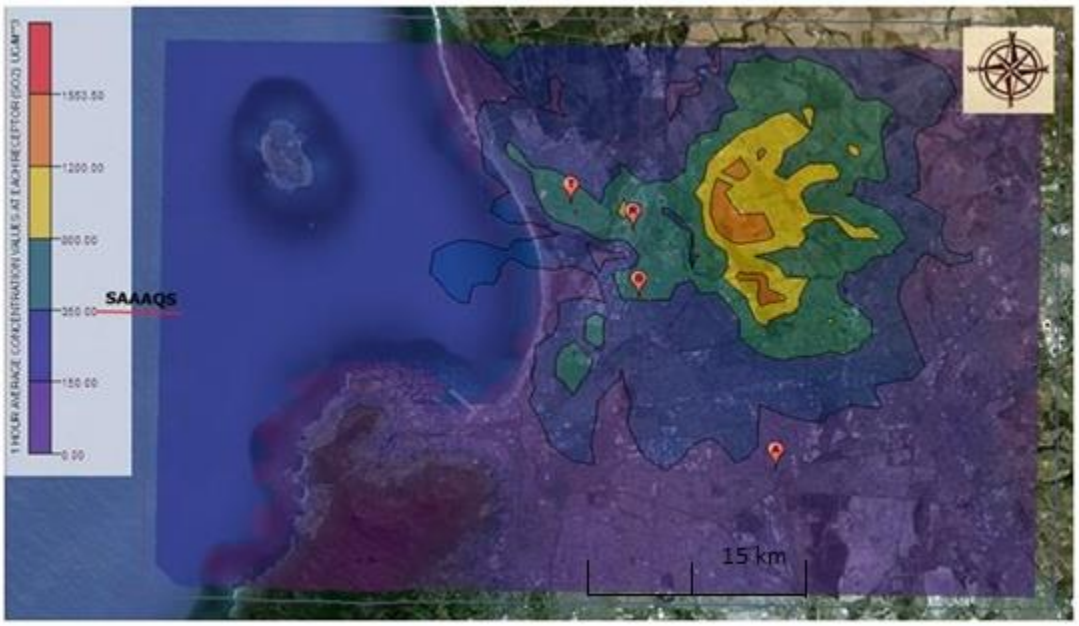


Figure 29: CALPUFF modelled isopleths of 1hr average SO_2 concentrations, 2010.

5.8 Comparison of Modelled Ambient Concentrations with Monitored Values

Evaluation of the performance of dispersion models is carried out by comparing modelled with measured concentrations. In this study model verification was conducted by comparing the measured daily average concentration values of the Bothasig and Table View monitoring stations with the model predicted values of AERMOD and CALPUFF at the same receptor points. Since Bothasig and Table View monitoring stations only monitor cumulative SO_2, the evaluation/comparison with modelled data was restricted to the daily average values. The results of the comparison are provided in Table 9 for the annual and 24-hr average values. The results showed AERMOD-modelled annual average values for 2010, based on refinery emissions only, are in good agreement with monitored values at the Table View and Bothasig sites, predicting the monitored values by -11% and +17% respectively. The 24-hr average AERMOD modelled values similarly are in good agreement with monitored values, on average over-predicting by 9% at Table View, although the day-to-day correlation is comparatively poor (r^2=0.32) Table View and (r^2=0.089) Bothasig (figure 30 & 31). CALPUFF-modelled average values for 2010, based on refinery emissions only, are in poor agreement with monitored values at the Table View site, under-predicting the monitored values by -61%; at the Bothasig site agreement is better (-20%) but in both cases the day-to-day correlations are comparatively poor (r^2=0.12) at Table View and (r^2=0.11) at Bothasig (Figures 30 and 31).

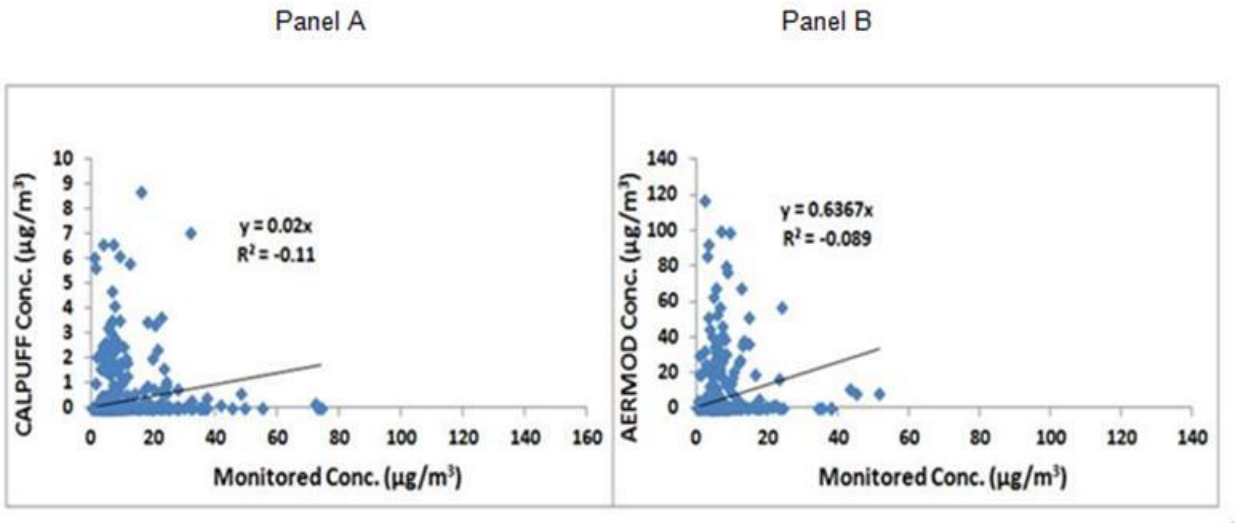
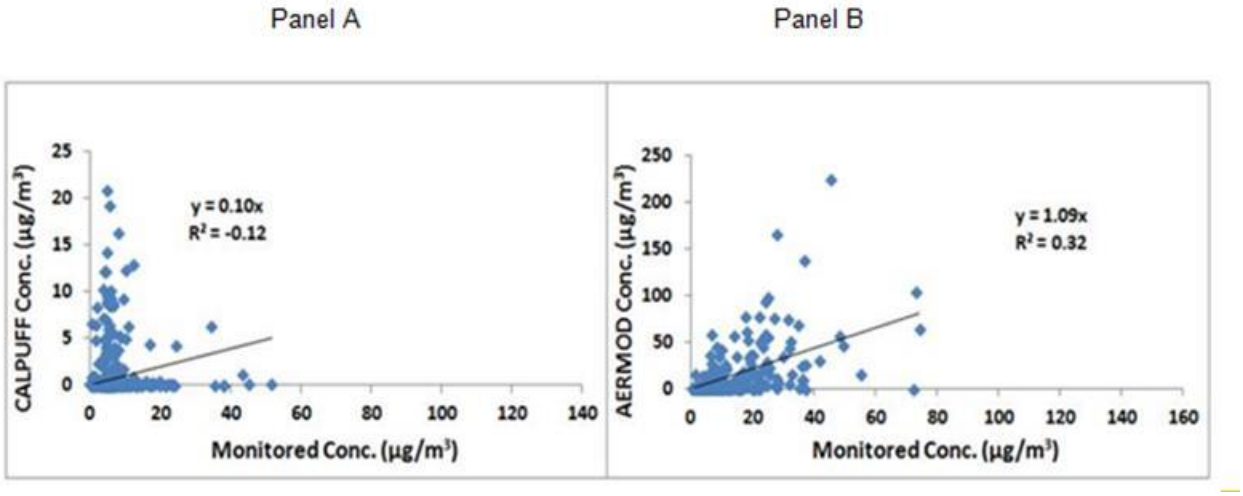


Figure 30: CALPUFF (Panel A) Vs AERMOD (Panel B), Monitored 24hr average SO_2 concentration at Bothasig.



Graph 31: CALPUFF (Panel A) , AERMOD (Panel B) vs Monitored 24hr average SO_2 concentration at Table View.

Table 9: 2010 Annual average SO_2 concentrations, modelled and monitored values.

Station	***2010 Average SO_2 concentration [µg/m³]***			***%(Modelled-Monitored) / Monitored***	
	Modelled AERMOD	*Modelled CALPUFF*	*Monitored*	*AERMOD*	*CALPUFF*
Bothasig*	*8.8*	*6.02*	*7.5*	*17%*	*-20%*
Table View	*9.3*	*4.07*	*10.5*	*-11%*	*-61%*

*One month's monitored data missing and modelled values exclude background concentration.

The AERMOD-modelled results values for 2010, based on refinery emissions only, were in good agreement with monitored values at the Table View and Bothasig sites compared to CALPUFF. To assess the coherence between the sulphur dioxide (SO_2) emission standard for the Petroleum Industry AERMOD model, with 2010 meteorology, was used. AERMOD modelled SO_2 concentrations were in good agreement with monitored ambient SO_2 concentrations (Table 9). We there used AERMOD for the rest of the modelling objectives. The differences between AERMOD and CALPUFF modelled concentrations are confirmed by direct comparison between the modelled concentrations, Figure 32.

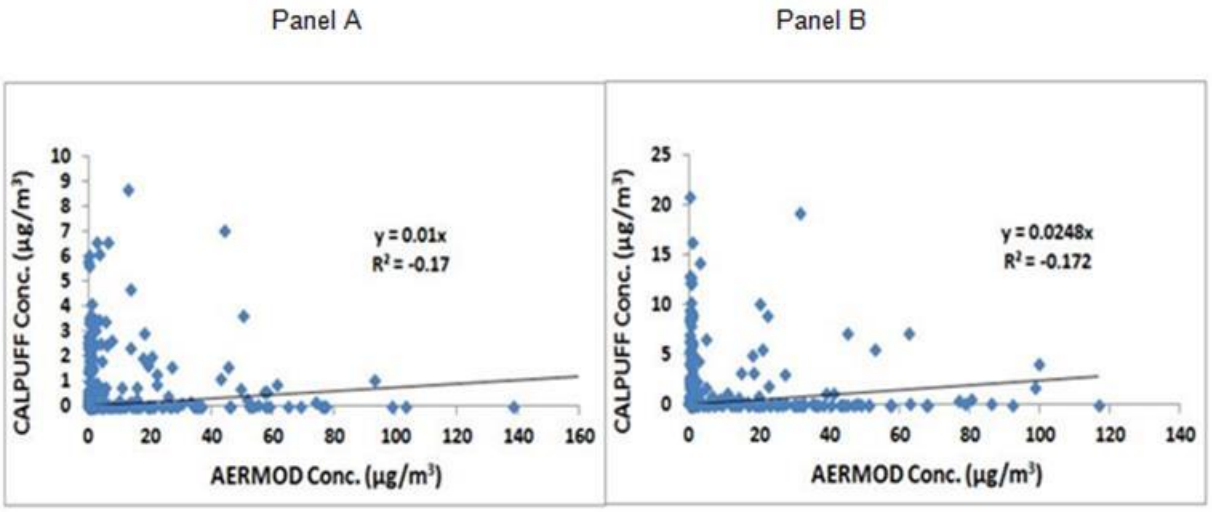


Figure 32: AERMOD Vs CALPUFF 24hr average SO_2 concentration at Table View (Panel A) and Bothasig (Panel B).

5.9 Comparison of AERMOD modelled concentrations with Ambient Air Quality Standards.

Table 10: AERMOD Modelled Ambient Concentrations exceedences.

AERMOD Number of exceedences	***AAQS Threshold***	***Table View***	***Bothasig***	***CTIA***
1-hour	*88*	*32*	*15*	*1*
24-hour	*4*	*3*	*1*	*0*
Annual	*0*	*0*	*0*	*0*

*One month's monitored data missing at Bothasig.

The threshold and number of exceedances recorded at three receptor (monitoring stations) within the study domain are reported for 1-hour, 24-hour and annual standard over the1-year period (2010) in Table 10. The total number of exceedances predicted by AERMOD in the modelling domain, for the 1hr averaging period, was 350. At the Table View station AERMOD predicted 32 exceedences of the 1h average (Figure 35). The total number of exceedances predicted by AERMOD for the 1hr averaging period at Bothasig was 15 (Figure 35). For the 24hr averaging period AERMOD recorded 3 at Table View(Figure 33), 1 at Bothasig number of

exceedences. AERMOD recorded no exceedances for the annual average period within the study domain. The Table View and Bothasig monitoring stations did not record any ambient exceedences for 2010.

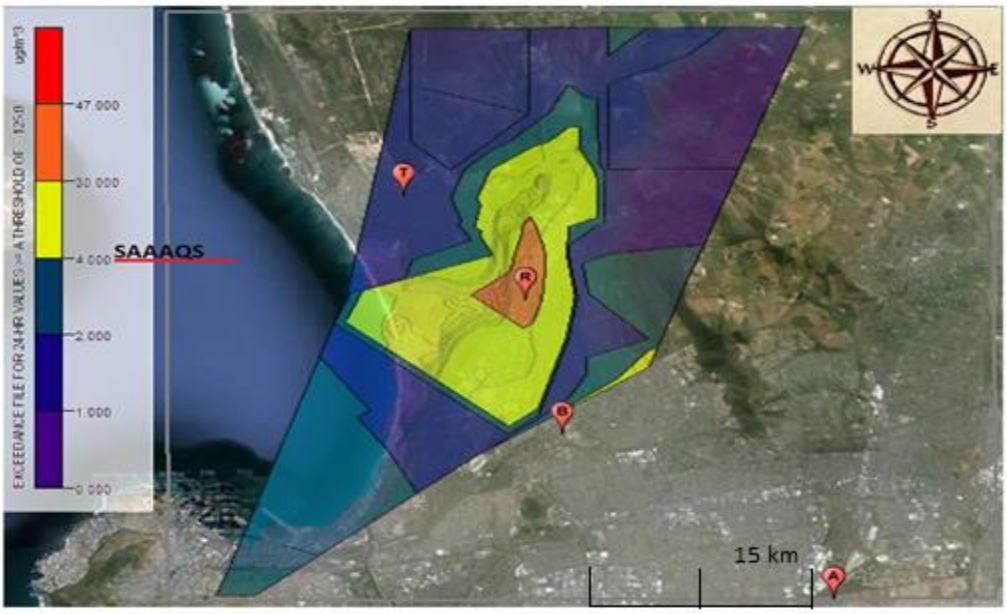


Figure 33: AERMOD modelled isopleths 24hr exceedences average SO_2 concentrations, 2010

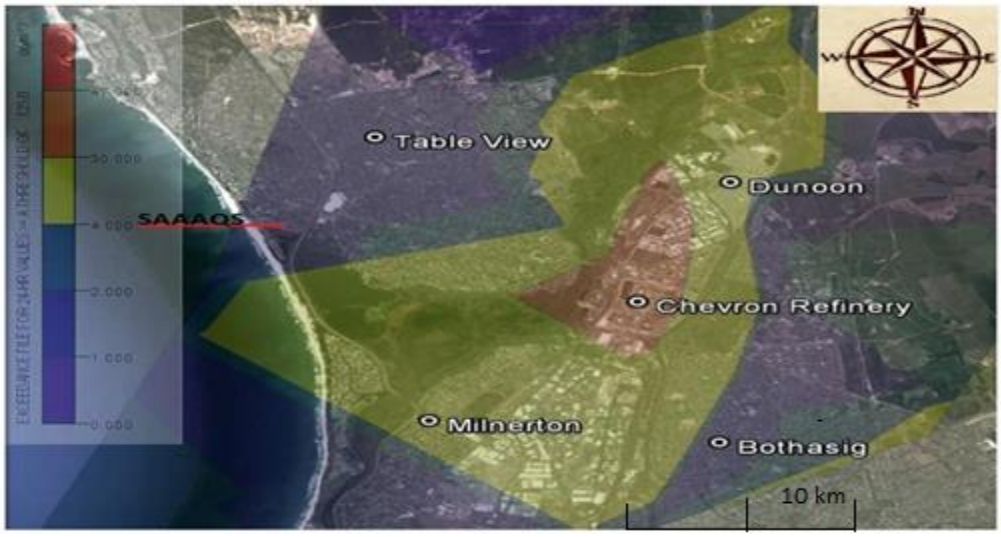


Figure 34: AERMOD modelled isopleths 24hr exceedences average SO_2 concentrations zoomed in overlay, 2010

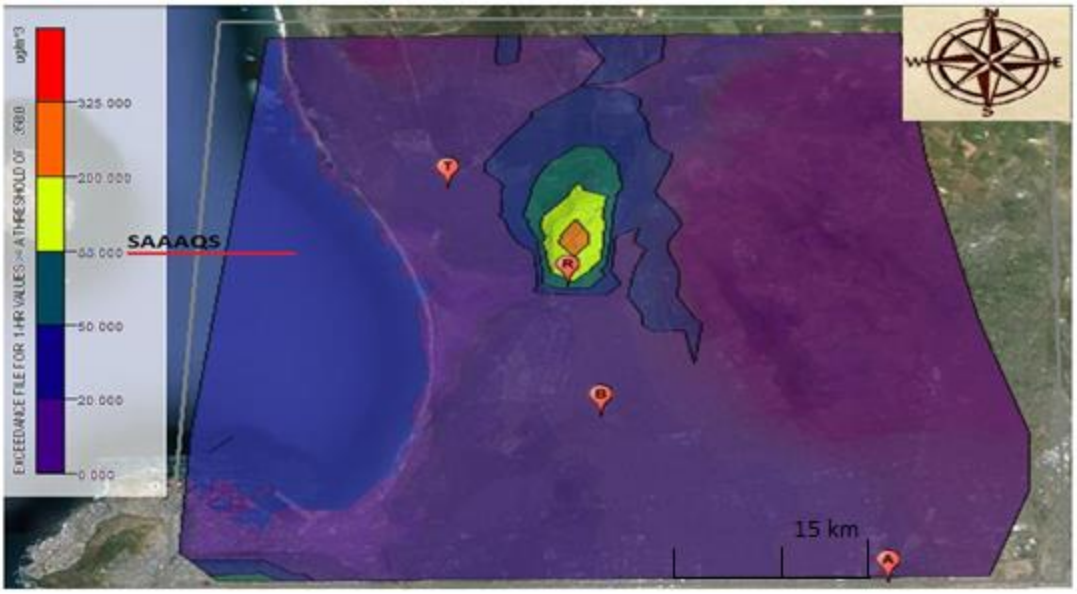


Figure 35: AERMOD modelled isopleths of 1hr exceedences average SO_2 concentrations, 2010

5.10 Modelling at refinery Emission Limits.

The SO_2 emission limit for an existing Category 2 (Petroleum Industry) Listed Activity is 0.8kg/day/t of crude throughput (Government Gazette 2010, Category 2, sub-category 2.1). Chevron Refinery has a regulated throughput of 100 000bbls/day approximately 13 500t/day crude, at a crude oil density of 850kg/m^3. Although the average 2010 emission rate was 143g/s SO_2, there was a large day to day variability, with standard deviation of 49.6 g/s. Therefore 16% (58 days per year) of the daily values were above Average +1SD, that is above 193g/s SO_2 (17tSO_2/day) and 2.3% (8 days per year) would be above 242g/s SO_2 (21tSO_2/day).

The emission limit for the Chevron Refinery would (when compliance comes into effect in 1 April 2015) be 125g/s, compared with the 2010 actual emissions case (average 143g/s, SD: 49.6g/s). To assess whether the AAQS would be met if the refinery reduced its total SO_2 emissions to the emission limit of 125g/s, emission rates from the stacks with the highest emission rates were reduced to the values in Table 11 and all other stacks emission rates were kept constant at their average values, to give a total of 125 gSO_2/s For every hour all stacks were kept constant at 125 g/s and the AERMOD model was re-run with 2010 meteorology. Figures 28 and 30

represent AERMOD modelled isopleths based on 2010 meteorology but with constant total SO_2 emissions of 125 g/s, the future emission limit.

Table 11: Stack annual average emission.

Annual Average SO_2 g/s	**Stack 1**	**Stack 2**	**Stack 3**	**Stack 4**	**Stack 5**	**Stack 6**	**Stack 7**	**Stack 8**	**Flare 1**
143	*7.61*	*4.22*	*23.26*	*4.39*	*0.01*	*0.04*	*23.48*	*77.56*	*2.30*
125	*7.61*	*4.22*	*20.26*	*4.39*	*0.01*	*0.04*	*18.48*	*67.56*	*2.30*

After the 15% reduction on the permitted value (125 g/s case), there was a significant change of concentration compared to the 2010 actual emissions case (average 143g/s, SD: 49.6g/s) (Table 12 and Figure 36 to 38). A maximum 1-hour average concentration of 432 µg/m^3 was predicted by the 125 g/s run case, compared to the 6245 µg/m^3 previously predicted by the 143 g/s run case (Figure 38). For the 24-hour average SO_2 concentration, the 125 g/s case predicted maximum SO_2 concentration of 48 µg/m^3 compared to the 352 µg/m^3 previously predicted by the 2010 actual emissions case (average 143 g/s, SD: 49.6g/s) (Figure 37). The maximum annual average concentration predicted by 143 g/s run case was 71 µg/m^3 in comparison with 11 µg/m^3 predicted in the 125 g/s run case (Figure 36).

Table 12: AERMOD Modelled Ambient SO_2 Concentrations for 2010 Actual Daily Emissions Case (143 g/s average, SD: 49.6 g/s) and the 125 g/s constant emissions case

Average Period	***Receptor Grid***	***Concentration Matrix***	**AERMOD predicted concentrations *(at* 2010 Actual Daily Emissions 143g/s run*)* *[µg/m^3]***	**AERMOD predicted concentrations *(at* 2010 Actual constant *125g/s run)* *[µg/m^3]***
1 hour	*Coarse*	*1st High*	*6245*	*432*
24 hour	*Coarse*	*1st High*	*352*	*48*
Annual	*Coarse*	*1st High*	*72*	*11*

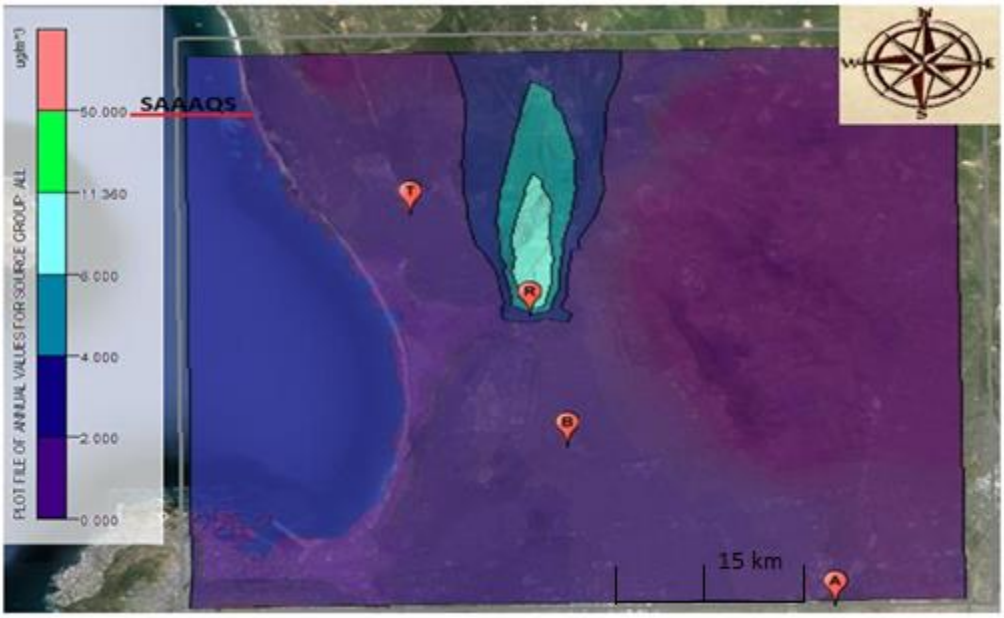


Figure 36: AERMOD modelled isopleths: 125g/s case for annual average SO_2 concentrations, 2010 meteorology.

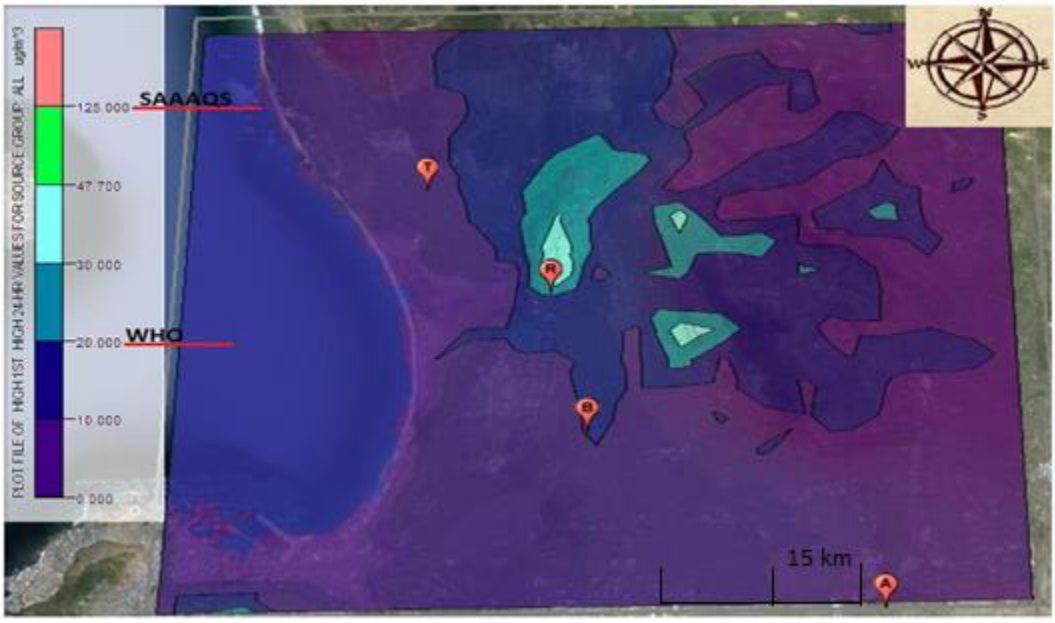


Figure 37: AERMOD modelled isopleths: 125g/s case for 24hr average SO_2 concentrations, 2010 meteorology.

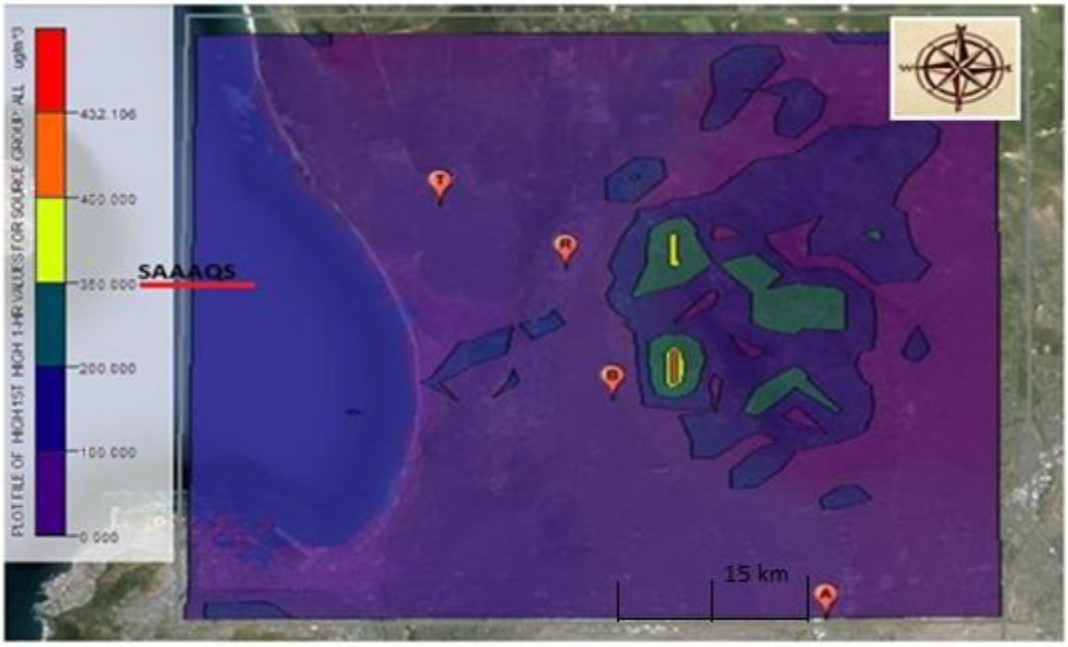


Figure 38: AERMOD modelled isopleths:125g/s case for 1hr average SO_2 concentrations, 2010 meteorology.

5.11 Comparison of AERMOD (125 g/s case) modelled concentrations with Ambient Air Quality Standards

The1hr average SO_2 concentrations predicted 7 exceedences fewer than the NAAQS allowable 88 exceedences for the 125 g/s run case with no allowable exceedences exceeded for the 24hr and annual average SO_2 concentrations (Table 13). The 15% of the daily values were above Average +1SD, 143+1SD, compared with the constant 125 g/s case.

Table 13: AERMOD Modelled Ambient SO_2 Concentrations 125 g/s case.

Number of exceedences	***AAQS Threshold***	***Modelled Table View***	***Monitored Table View***	***Modelled Bothasig***	***Monitored Bothasig***
1-hour	*88*	*0*	*0*	*0*	*0*
24-hour	*4*	*0*	*0*	*0*	*0*
Annual	*0*	*0*	*0*	*0*	*0*

Chapter 6: Conclusions and Recommendations.

6.1 Conclusions

The AERMOD modelled isopleths show that the 2010 annual average SO_2 concentrations exceeded the South African Standard of 50 µg/m^3 in a small area in the immediate vicinity of the refinery. The hourly and 24-hourly average standards for SO_2 of 350µg/m^3 and 125µg/m^3 respectively were exceeded in significantly larger area. The allowable number of exceedences for hourly and 24-hourly averages were also exceeded. This shows that emissions from the refinery resulted in the exceedance of the SO_2 AAQS during 2010.

If the 2010 emission rates were adjusted downwards to match the emission standards (to be complied with from 1 April 2015), AERMOD modelling indicates that the annual and 24-hr Ambient Air Quality Standards would not be exceeded. AERMOD modelling prediction show that the 1-hr Ambient Air Quality Standards would be exceeded in two small areas, but the allowable number of exceedences for the 1-hr averages would not be exceeded. Based on this case study, it was concluded that the Emission Standards are therefore coherent with the Ambient Air Quality Standards. There is no reduction of the refinery SO_2 emissions required to ensure that AAQS are complied with from 1 April 2015 but reduction of refinery SO_2 emissions are required to be reduced to ensure that 24hr average concentrations set by WHO are complied with. Meteorological conditions, terrain and other factors that affect modelled ambient concentration may be different for the other crude oil refineries, and a different conclusion may be reached if a comparable exercise was done in these cases.

Background concentration was estimated from monitored values during a refinery shutdown from 16 April to 4 May 2010. The average 19 days average SO_2 background concentration values ware 5,90 µg/m^3at Table View and 3.10µg/m^3 at Bothasig with highest recorded concentration value of 9.45 µg/$m^3$and 9.30 µg/m^3 respectively. Measured annual (year 2007) SO_2 background concentrations values far afield from the City of Cape Town were 3.90 µg/m^3 with a highest recorded concentration value of 36.0 µg/m^3. These estimates of background concentrations cannot simply be added to the modelled values, but they do provide an estimate of the possible incremental contribution of the background to modelled ambient values, and confirm that the refinery is the largest source of SO_2 emissions in the modelling domain.

A comprehensive set of meteorological data is available for the Cape Town International Airport (SynopNo 68816) but this station is 14km from the refinery. To assess the validity of using airport data for modelling dispersion from the Table View, we compared the wind vectors for the two locations during one month (March 2010). For the month of March 2010, daily wind direction at the Table View station is poorly correlated (r^2=0.53) with CTIA data, although there is negligible bias between the two stations (slope = 1.03). Wind speed is better correlated (r^2=0.63) but CTIA wind speeds are about 50% higher on average at the airport site (slope=1.54). There are significantly more low wind speed days at the Table View site compared with the airport site. These results demonstrate that meteorological conditions may differ significantly even over relatively short distances. The significant differences between the isopleths (Figures 17) based on Table View meteorological and CTIA meteorological respectively also show, as expected, that modelling accuracy may be significantly compromised if representative local meteorological data are not used (Figure 14).

The AERMOD-modelled results for annual average values for 2010, based on refinery emissions only, were in good agreement with monitored values at the Table View and Bothasig sites, predicting the monitored values by -11% and +17% respectively. The 24-hr average values similarly are in good agreement with monitored values, on average over-predicting by 9% at Table View, although the day-to-day correlation is comparatively poor (r^2=0.32 for Table View and r^2=0.089 Bothasig) between modelled and ambient monitored concentrations. These results are consistent with Gaussian dispersion modelling in that averaged results are expected to be better correlated than paired results. The CALPUFF-modelled results for annual average values for 2010, based on refinery emissions only, were in poor agreement with monitored values at the Table View and Bothasig sites, under-predicting the monitored values by -61% and -20% respectively with the day-to-day correlation comparatively poor (r^2=0.12) Table View and (r^2=0.11) Bothasig. AERMOD gave better results (in good agreement with ambient monitored values) in this situation, and therefore used AERMOD.

CALPUFF modelled values differed significantly compared with AERMOD modelled values and monitored values – daily /annual average values. The use of CTIA meteorological (wind speed and direction) data and local Table View meteorological (wind speed and direction) data also produced different results (100 and 130 µg/m^3) for the AERMOD modelled SO_2 concentrations.

These results emphasise the importance of validating modelled outputs against ambient measurements if the modelled results are to be used in a regulatory context. This conclusion is reinforced by a recent US EPA publication (Grosh T.G et al, 1998) which demonstrated that modelled outputs are sensitive to estimates of input parameters such as albedo, Bowen ratio, and surface roughness.

6.2 Recommendations.

Monitored data do not show exceedences – modelling shows that areas of high exceedences are not located at the points of highest concentrations. AAQS should be framed to use modelling in addition to monitoring to determine compliance.

Petroleum refineries are complex systems of multiple linked operations that convert the refinery crude and other intake into useful products. The specific operations used at a refinery depend on the type of crude refined and the range of refinery products. For this reason, no two refineries are exactly alike. Depending on the refinery age, location, size, variability of crude and product slates and complexity of operations, a facility can have different operating configurations and significantly different air emission sources. This will result in relative differences in the quantities of air pollutants emitted and the selection of appropriate emission management approaches. For the 125 g/s case predicted ambient concentrations are below the AAQS yet they exceed the WHO 24h average Guidelines. Both AAQS and Emission Limits are subject to periodic (5 year) review and may be revised downwards in the future to achieve a continuous improvement in ambient air quality.

Air dispersion modelling is an important regulatory tool for modelling the spatial distribution of priority pollutants from various sources; however the ability to accurately model source contributions to pollutant concentrations is strongly dependent upon the model input data, in particular, the emission rates from point, volume and area sources and meteorological data. Formats of these data files should be available in all formats for models recommended in the 2012 air dispersion draft regulation.

The emissions inventory and modelling methodologies are used to estimate concentrations of air pollution attributes for air pollutants; however, outdoor concentrations should include background concentrations accurately to estimate total ambient concentrations of air toxics, it is necessary to account for these background concentrations that are not represented by atmospheric modelling emissions. It is therefore recommended that the City of Cape Town to annually measure background concentration and make it available to public for air dispersion modelling use and provide a comprehensive emission inventory so that all emission sources can be accounted for in modelling studies.

When performing dispersion modelling for a project, the selection of meteorological data can play a major role in the outcome of the modelling results. The Guideline on Air Quality Models (U.S. EPA, 2005), states in Section 8.3.1.1 that the user should acquire sufficient meteorological data "to ensure that worst-case conditions are adequately represented in the model results." Based on the U.S. EPA use of local meteorological data to ensure modelling validation and accuracy is highly recommended.

Regulatory air dispersion modelling practices in South Africa are being standardised for regulatory purposes and to ensure that dispersion modelling practices are undertaken in a compatible form to ensure that results from one dispersion model study can be compared directly to those from another. This can only be ensured if the 2012 draft regulation for validation of dispersion modelling is compulsory not optional as per draft regulation.

Air quality monitoring networks in South Africa is currently operated by National, Provincial and Local Government Departments across the country in order to provide air quality data to the South African Air Quality Information System. Based on this research finding a monitoring station is recommended in areas of high SO_2 concentrations outside the source.

6.3 Further research issues

Emission Limits for different listed activities sources need be evaluated against Ambient Air Quality Standards (Government Gazette, 2010) because meteorological conditions, terrain and other factors that affect modelled ambient concentration may be different for other sources, and a different conclusion may be reached if a comparable exercise was done in other cases.

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Appendices

Source Emission data.

Table 1: Daily SO_2 data in tons/day.

	02F-201 Stack	2F-1 Combined	4F-1 Combined	YIP Stack	No 1 FCCU Stack	56F-201 Stack	Major Combined	71F-1	Flare Stack
1/1/2010	0.48	0.70	0.24	4.72	2.26	0.00	4.24	0.00	0.02
1/2/2010	0.48	0.75	0.24	4.88	2.25	0.00	4.27	0.00	0.02
1/3/2010	0.46	0.81	0.24	3.62	2.33	0.00	4.18	0.00	0.00
1/4/2010	0.44	0.84	0.24	4.75	2.31	0.00	4.18	0.00	0.01
1/5/2010	0.46	0.82	0.24	5.85	2.13	0.00	4.20	0.00	0.00
1/6/2010	0.48	0.80	0.24	4.95	2.30	0.00	4.36	0.00	0.00
1/7/2010	0.48	0.73	0.24	5.19	2.14	0.00	4.05	0.00	0.05
1/8/2010	0.48	0.73	0.24	5.04	2.13	0.00	4.10	0.00	0.05
1/9/2010	0.48	0.76	0.24	5.15	2.13	0.00	4.12	0.00	0.06
1/10/2010	0.46	0.79	0.24	4.97	2.18	0.00	4.12	0.00	0.05
1/11/2010	0.46	0.74	0.24	4.83	2.15	0.00	4.23	0.00	0.02
1/12/2010	0.46	0.72	0.24	4.67	2.13	0.00	4.25	0.00	0.06
1/13/2010	0.46	0.79	0.24	5.47	2.18	0.00	4.31	0.00	0.00
1/14/2010	0.46	0.74	0.24	6.82	2.24	0.00	5.65	0.00	0.05
1/15/2010	0.46	0.71	0.25	6.08	2.16	0.00	5.38	0.00	0.06
1/16/2010	0.46	0.73	0.24	5.84	2.17	0.00	5.16	0.00	0.06
1/17/2010	0.46	0.72	0.25	6.07	2.09	0.00	4.60	0.00	0.06
1/18/2010	0.46	0.74	0.24	6.36	2.18	0.00	4.66	0.00	0.00
1/19/2010	0.46	0.74	0.24	6.41	2.20	0.00	5.23	0.00	0.00
1/20/2010	0.42	0.60	0.24	6.23	2.16	0.00	4.99	0.00	0.00
1/21/2010	0.41	0.51	0.24	5.49	2.13	0.00	5.42	0.00	0.12
1/22/2010	0.48	0.70	0.00	6.44	2.21	0.00	5.11	0.00	0.00
1/23/2010	0.48	0.69	0.00	1.68	2.30	0.00	8.21	0.00	0.00
1/24/2010	0.48	0.67	0.00	1.66	2.30	0.00	9.33	0.00	0.00
1/25/2010	0.48	0.66	0.00	3.72	2.29	0.00	9.15	0.00	0.00
1/26/2010	0.48	0.66	0.00	3.69	2.27	0.00	9.72	0.00	0.00
1/27/2010	0.47	0.63	0.00	3.83	2.14	0.00	8.26	0.00	0.00
1/28/2010	0.44	0.60	0.27	1.90	1.65	0.00	8.08	0.00	0.00
1/29/2010	0.50	0.66	0.25	3.04	1.65	0.00	9.55	0.00	0.00
1/30/2010	0.58	0.64	0.25	3.00	1.61	0.00	11.06	0.00	0.00
1/31/2010	0.63	0.66	0.25	2.91	1.58	0.00	11.69	0.00	0.00

Table 2: AERMOD Emission file.

```
SO HOUREMIS 10 1 1 1 STCK1 7.61107271179889 583.9 8.39
        10 1 1 1 STCK2 4.21783609251095 649.9 0
        10 1 1 1 STCK3 20.262893485175 499.5 2.33
        10 1 1 1 STCK4 4.39327770453564 756.6 0.03
        10 1 1 1 STCK5 0.0065449203668445 2 518.2 0
        10 1 1 1 STCK6 0.039621398530577 589.4 0.01
        10 1 1 1 STCK7 18.4837978121834 525.1 19.71
        10 1 1 1 STCK8 67.5563318814791 544.6 48.99
        10 1 1 1 FLARE1 2.29632685956587 1273 0.05
        10 1 1 2 STCK1 7.61107271179889 593.1 8.39
        10 1 1 2 STCK2 4.21783609251095 651.2 0
        10 1 1 2 STCK3 20.262893485175 493 2.33
        10 1 1 2 STCK4 4.39327770453564 750.5 0.03
        10 1 1 2 STCK5 0.0065449203668445 2 519.6 0
        10 1 1 2 STCK6 0.039621398530577 589.2 0.01
        10 1 1 2 STCK7 18.4837978121834 527.4 19.71
        10 1 1 2 STCK8 67.5563318814791 547 48.99
        10 1 1 2 FLARE1 2.29632685956587 1273 0.05
        10 1 1 3 STCK1 7.61107271179889 591.1 8.39
        10 1 1 3 STCK2 4.21783609251095 651.4 0
        10 1 1 3 STCK3 20.262893485175 490.4 2.33
        10 1 1 3 STCK4 4.39327770453564 753.6 0.03
        10 1 1 3 STCK5 0.0065449203668445 2 519.8 0
        10 1 1 3 STCK6 0.039621398530577 586.6 0.01
        10 1 1 3 STCK7 18.4837978121834 528.1 19.71
        10 1 1 3 STCK8 67.5563318814791 543 48.99
        10 1 1 3 FLARE1 2.29632685956587 1273 0.05
        10 1 1 4 STCK1 7.61107271179889 583.6 8.39
        10 1 1 4 STCK2 4.21783609251095 652.5 0
        10 1 1 4 STCK3 20.262893485175 495 2.33
        10 1 1 4 STCK4 4.39327770453564 751.6 0.03
        10 1 1 4 STCK5 0.0065449203668445 2 519.5 0
        10 1 1 4 STCK6 0.039621398530577 585.5 0.01
        10 1 1 4 STCK7 18.4837978121834 527.6 19.71
        10 1 1 4 STCK8 67.5563318814791 543.2 48.99
        10 1 1 4 FLARE1 2.29632685956587 1273 0.05
        10 1 1 5 STCK1 7.61107271179889 576.5 8.39
        10 1 1 5 STCK2 4.21783609251095 654.7 0
        10 1 1 5 STCK3 20.262893485175 500.6 2.33
        10 1 1 5 STCK4 4.39327770453564 747.2 0.03
        10 1 1 5 STCK5 0.0065449203668445 2 516.4 0
        10 1 1 5 STCK6 0.039621398530577 587.3 0.01
```

Table 3: CALPUFF Emission file.

PTEMARB'	9	1	34	2010001	0	2010365	23	5
SO2'								
64								
STCK1	271328.8	6252297	60.96	2.68	1616.58	0	0	
STCK2	271329.7	6252305	60.96	1.68	16.6	0	0	
STCK3	271375.9	6252471	91.44	2.53	16.98	0	0	
STCK4	271382	6252277	59.13	3.35	16.86	0	0	
STCK5	271451.1	6252240	53.35	0.91	16.64	0	0	
STCK6	271457.2	6252341	53	0.9	17.07	0	0	
STCK7	271452.9	6252400	59.5	1.2	17.32	0	0	
STCK8	271559.6	6252608	91.44	3.05	19.04	0	0	
FLARE1	271451.5	6253017	53.34	0.92	21.35	0	0	
2010001	0	2010001	0					
STCK1	583.9	5.55	8.39					
STCK2	649.9	8.1	0					
STCK3	499.5	2.77	2.33					
STCK4	756.6	54.62	0.03					
STCK5	518.2	26.15	0					
STCK6	589.4	0	0.01					
STCK7	525.1	49.07	19.71					
STCK8	544.6	0	48.99					
FLARE1	1273	0.23	0.05					
2010001	1	2010001	1					
STCK1	593.1	5.55	8.39					
STCK2	651.2	8.1	0					
STCK3	493	2.77	2.33					
STCK4	750.5	54.62	0.03					
STCK5	519.6	26.15	0					
STCK6	589.2	0	0.01					
STCK7	527.4	49.07	19.71					
STCK8	547	0	48.99					
FLARE1	1273	0.23	0.05					
2010001	2	2010001	2					
STCK1	591.1	5.55	8.39					
STCK2	651.4	8.1	0					
STCK3	490.4	2.77	2.33					
STCK4	753.6	54.62	0.03					
STCK5	519.8	26.15	0					
STCK6	586.6	0	0.01					
STCK7	528.1	49.07	19.71					
STCK8	543	0	48.99					
FLARE1	1273	0.23	0.05					

Meteorological Data

Table 4: Daily monitored ambient SO_2 data.

DATE Limit	DAILY AVERAGE 125 µg/m³	DAILY MAXIMUM 10 MINUTE AVERAGE 500 µg/m³	DAILY MAXIMUM 15 MINUTE AVERAGE 266 µg/m³	DAILY MAXIMUM HOURLY AVERAGE 350 µg/m³
1-Jan-09	44.32	62.20	60.87	55.02
2-Jan-09	41.94	62.20	60.87	54.37
3-Jan-09	40.35	51.08	50.60	49.05
4-Jan-09	41.29	56.10	55.60	49.89
5-Jan-09	41.74	56.10	55.60	50.36
6-Jan-09	39.68	63.00	61.33	53.93
7-Jan-09	36.53	83.60	75.40	61.59
8-Jan-09	35.19	89.80	82.73	76.66
9-Jan-09	33.89	89.80	82.73	74.46
10-Jan-09	32.60	39.90	37.87	35.34
11-Jan-09	33.08	43.30	41.60	37.12
12-Jan-09	33.96	52.80	51.73	45.59
13-Jan-09	24.77	52.80	51.73	46.20
14-Jan-09	11.69	36.60	35.13	34.12
15-Jan-09	9.41	16.20	15.00	12.76
16-Jan-09	10.28	16.20	15.20	12.86
17-Jan-09	10.94	18.20	16.40	13.63
18-Jan-09	12.99	18.90	16.60	15.80
19-Jan-09	17.31	30.10	27.73	24.54
20-Jan-09	23.20	42.70	39.73	32.80
21-Jan-09	23.52	58.40	53.33	40.10
22-Jan-09	18.70	34.40	31.18	29.70
23-Jan-09	18.08	29.80	27.60	25.58
24-Jan-09	21.20	63.90	58.00	45.51
25-Jan-09	22.64	84.30	82.67	56.81
26-Jan-09	21.92	84.30	82.66	63.71
27-Jan-09	21.38	49.90	43.53	35.98
28-Jan-09	24.46	103.20	90.00	76.14
29-Jan-09	24.79	103.20	90.00	76.78
30-Jan-09	21.01	28.30	26.80	25.00
31-Jan-09	22.00	29.30	27.13	25.20
1-Feb-09	25.73	56.60	48.33	42.86
2-Feb-09	19.35	56.60	48.33	42.88
3-Feb-09	4.96	31.00	29.33	26.45
5-Feb-09	0.32	1.90	1.60	1.15
6-Feb-09	0.48	1.90	1.60	1.05
7-Feb-09	0.51	2.00	1.87	1.31
8-Feb-09	0.40	2.00	2.00	1.41
9-Feb-09	0.20	2.00	2.00	1.20

Table 5: Daily monitored Surface data

Date	Month	day	hr	Rain	Temp	Speed	Dir	Hum	Press	Tcld
2010	1	1	1	0.0	20.7	4.4	184	84	1009	1
2010	1	1	2	0.0	20.3	3.9	184	88	1009	2
2010	1	1	3	0.0	20.9	4.4	188	82	1009	2
2010	1	1	4	0.0	20.3	4.7	187	86	1008	2
2010	1	1	5	0.0	19.7	5.3	187	92	1008	2
2010	1	1	6	0.0	19.7	5	186	92	1008	1
2010	1	1	7	0.0	20.6	5.1	190	84	1008	1
2010	1	1	8	0.0	21.0	4.7	181	82	1009	3
2010	1	1	9	0.0	22.5	4.9	182	76	1010	2
2010	1	1	10	0.0	24.0	5.8	185	67	1010	2
2010	1	1	11	0.0	25.6	5.7	191	61	1009	2
2010	1	1	12	0.0	26.7	6.4	197	60	1009	2
2010	1	1	13	0.0	27.5	6.1	191	58	1009	1
2010	1	1	14	0.0	26.8	6.6	191	60	1008	1
2010	1	1	15	0.0	26.5	7.3	190	62	1008	1
2010	1	1	16	0.0	26.1	7.2	188	63	1007	1
2010	1	1	17	0.0	24.9	7.8	192	66	1007	1
2010	1	1	18	0.0	24.3	7.7	189	68	1006	1
2010	1	1	19	0.0	23.4	7.5	192	70	1006	1
2010	1	1	20	0.0	21.8	7.5	187	76	1006	1
2010	1	1	21	0.0	21.8	5.5	183	76	1006	1
2010	1	1	22	0.0	22.1	5.1	182	74	1006	1
2010	1	1	23	0.0	21.9	5.2	186	75	1007	1
2010	1	1	24	0.0	21.5	5.2	186	77	1006	1
2010	1	2	1	0.0	21.4	4.5	187	78	1006	1
2010	1	2	2	0.0	21.5	4.4	184	77	1005	1
2010	1	2	3	0.0	21.2	3.6	181	78	1005	1
2010	1	2	4	0.0	20.8	3.1	178	80	1004	0
2010	1	2	5	0.0	20.5	3	176	84	1004	0
2010	1	2	6	0.0	19.9	2.7	174	88	1004	0
2010	1	2	7	0.0	20.4	2.9	166	86	1004	0
2010	1	2	8	0.0	21.8	3	174	82	1004	0
2010	1	2	9	0.0	24.3	3	194	69	1004	0
2010	1	2	10	0.0	26.3	2.8	241	62	1004	0

Table 6: Daily monitored Upper air data

SynopNo	Date	Time	DeltaT	Pressure	Temp	Hum	Dewpt	GPM	Winddir	Windsp
68,816	CAPE TOWN WO		Lat:	-33.97	Long:	18.60	Height: 42 m			
68816	2010/07/05	23:22	0	1009.7	13.8	88	11.8	42.0	310	4.5
68816	2010/07/05	23:22	60	967.9	11.5	84	8.9	398.0	300	10.3
68816	2010/07/05	23:22	120	929.8	9.4	84	6.8	732.0	289	7.9
68816	2010/07/05	23:22	180	891.5	6.7	89	4.9	1080.0	279	5.3
68816	2010/07/05	23:22	240	859.9	6.0	69	0.7	1375.0	301	9.0
68816	2010/07/05	23:22	300	826.0	6.8	39	-6.2	1707.0	314	16.0
68816	2010/07/05	23:22	360	792.8	3.9	57	-4.0	2041.0	319	18.7
68816	2010/07/05	23:22	420	760.6	2.4	79	-0.9	2377.0	322	22.5
68816	2010/07/05	23:22	480	730.4	2.7	64	-3.4	2704.0	318	29.4
68816	2010/07/05	23:22	540	700.1	1.2	54	-7.1	3047.0	323	33.5
68816	2010/07/05	23:22	600	669.4	-1.9	63	-8.0	3405.0	324	34.7
68816	2010/07/05	23:22	660	638.9	-5.1	69	-10.0	3775.0	324	39.3
68816	2010/07/05	23:22	720	609.7	-7.6	29	-22.5	4140.0	317	39.4
68816	2010/07/05	23:22	780	582.9	-9.3	6	-39.9	4489.0	315	38.4
68816	2010/07/05	23:22	840	558.8	-9.9	3	-48.0	4815.0	310	37.5
68816	2010/07/05	23:22	900	534.2	-11.9	4	-45.1	5160.0	306	37.8
68816	2010/07/05	23:22	960	511.1	-14.3	15	-35.7	5496.0	303	38.9
68816	2010/07/05	23:22	1020	488.3	-16.2	7	-44.5	5841.0	302	40.8
68816	2010/07/05	23:22	1080	465.9	-18.5	5	-48.6	6191.0	300	39.7
68816	2010/07/05	23:22	1140	444.4	-21.4	6	-49.7	6541.0	298	43.5
68816	2010/07/05	23:22	1200	424.9	-24.1	6	-51.0	6871.0	294	43.2
68816	2010/07/05	23:22	1260	408.9	-25.7	7	-51.2	7150.0	295	44.2
68816	2010/07/05	23:22	1320	394.2	-27.2	7	-52.3	7415.0	293	45.3
68816	2010/07/05	23:22	1380	379.9	-28.3	5	-56.7	7679.0	292	38.5
68816	2010/07/05	23:22	1440	363.0	-30.9	5	-57.8	8003.0	291	36.3
68816	2010/07/05	23:22	1500	342.3	-34.4	7	-58.8	8417.0	292	34.5
68816	2010/07/05	23:22	1560	321.7	-37.8	5	-63.6	8849.0	291	37.8
68816	2010/07/05	23:22	1620	303.0	-40.7	4	-67.5	9257.0	295	38.0
68816	2010/07/05	23:22	1680	287.7	-43.4	6	-66.7	9608.0	292	37.8
68816	2010/07/05	23:22	1740	276.3	-45.9	8	-66.4	9878.0	290	39.2
68816	2010/07/05	23:22	1800	268.3	-44.6	7	-66.7	10073.0	286	44.3
68816	2010/07/05	23:22	1860	261.1	-42.8	5	-68.1	10257.0	290	44.3
68816	2010/07/05	23:22	1920	249.0	-40.7	2	-73.7	10580.0	294	46.0
68816	2010/07/05	23:22	1980	231.7	-38.4	0	-75.3	11072.0	299	44.4
68816	2010/07/05	23:22	2040	215.1	-41.9	0	-77.7	11580.0	295	43.1
68816	2010/07/05	23:22	2100	200.6	-45.4	0	-80.0	12048.0	292	46.0
68816	2010/07/05	23:22	2160	191.9	-47.1	0	-81.2	12343.0	289	44.7
68816	2010/07/05	23:22	2220	185.5	-47.8	0	-81.7	12568.0	291	42.6
68816	2010/07/05	23:22	2280	178.3	-49.6	0	-82.9	12826.0	292	41.5
68816	2010/07/05	23:22	2340	168.7	-52.1	0	-84.6	13186.0	294	40.2
68816	2010/07/05	23:22	2400	157.7	-54.8	0	-86.5	13621.0	294	41.9
68816	2010/07/05	23:22	2460	146.8	-56.6	0	-87.8	14076.0	297	41.0
68816	2010/07/05	23:22	2520	138.0	-59.4	0	-89.7	14466.0	302	41.8
68816	2010/07/05	23:22	2580	131.5	-61.6	0	-91.2	14767.0	303	45.9
SynopNo	Date	Time	DeltaT	Pressure	Temp	Hum	Dewpt	GPM	Winddir	Windsp
68816	2010/07/05	23:22	2640	127.1	-60.8	0	-90.7	14978.0	294	44.5
68816	2010/07/05	23:22	2700	121.2	-60.7	0	-90.6	15272.0	294	39.4
68816	2010/07/05	23:22	2760	112.8	-60.8	0	-90.7	15721.0	301	33.8
68816	2010/07/05	23:22	2820	102.8	-62.5	0	-91.9	16292.0	291	29.3
68816	2010/07/05	23:22	2880	95.5	-65.2	0	-93.8	16746.0	297	29.5
68816	2010/07/05	23:22	2940	89.8	-64.5	0	-93.3	17116.0	296	33.4
68816	2010/07/05	23:22	3000	86.0	-62.8	0	-92.1	17382.0	296	31.2

Geophysical Data.

Table 7: Land Use Land Cover

GEO.DAT 2 Header structure with coordinate parameters
by MAKEGEO
Produced V rersion : 2.29 Level: 70327
by Version -
Generated CALPUFF View - 5.0.2 0.523809524 /201 2

UTM

34S

WGS-84 0 2/21/2003

5
125 87 226.38 6218.354 0 700 0.7

KM M

- (1=new)
1 #NAME? EDATA categories

14 51 55 - NLU, IWAT1, IWAT2
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10 20 -20 30 40 51 61 62 70 80 90

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