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Verification of the ADMS 4 Air Quality Model in determining the SO_2 dispersion during the 2006 and 2007 winter over Elandsfontein, South Africa.

by

Marthinus Dewald Retief Ras

A mini-dissertation submitted in partial fulfilment of the requirements for the degree of

MASTER OF SCIENCE

in the

Department of Environmental Studies
Faculty of Natural and Agricultural Sciences

UNIVERSITY OF PRETORIA
February 2010

DECLARATION

I hereby declare that the mini-dissertation that I hereby submit for the degree M.Sc. (Air Quality Management) at the University of Pretoria is my own work and that it has not been previously submitted by me for degree purposes at any other university. I also declare that all the sources I have quoted have been indicated and acknowledged by complete references.

Signature

Date

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Verification of the ADMS 4 Air Quality Model in determining the SO_2 dispersion during the 2006 and 2007 winter over Elandsfontein, South Africa.

Marthinus Dewald Retief Ras

Promoter:	Prof. C. J. DeW. Rautenbach
Department:	Environmental Studies
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Degree:	Master of Science (Air Quality Management)

Summary

ADMS 4 is a relatively new generation air quality dispersion model program written by Cambridge Environmental Research Consultants in the UK and used to verify datasets in the USA on several types of plants, in various settings across the country. Typical results indicate an approximate 20% under prediction. It was decided to use this model to verify SO_2 emissions typical of the Eastern Highveld, which has several varying industries emitting SO_2 gases in the region. Two datasets were identified with complete data recorded, supplied by ESKOM as measured at their Elandsfontein site for the winter periods mid 2006 and 2007. The meteorological data recorded at Elandsfontein was used for the model and the SO_2 predicted emissions by ADMS 4 then compared to the actual measured SO_2 emissions at the monitoring site, to determine the efficiency level of ADMS 4. Efficiency levels of 42% for the 2006 dataset and 58% for the 2007 dataset were achieved. The high level of under prediction is ascribed to the influence of the local petrochemical refinery (SASOL) as well as the local steelworks plants also emitting SO_2 gas, but was not entered into the model database for evaluation in conjunction with the power stations' emissions data.

ACKNOWLEDGEMENTS

The author wishes to express his appreciation to the following persons and organizations for their assistance and contribution in making this dissertation a success:

1) Dr. Kristy Ross of Eskom Research and Innovation Department, Eskom, Johannesburg for her assistance and permission in accessing the necessary data recorded at their Elandsfontein monitoring station for the two study periods, as well as her suggested guidelines for the study in general.

2) Ms. Renee Thomas of Airshed Planning Professionals (Pty) Ltd for her help and assistance in running the data through the ADMS 4 software program.

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TABLE OF CONTENTS

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LIST OF TABLES & FIGURES

TABLES:

FIGURES:

LIST OF SYMBOLS & ABBREVIATIONS

SYMBOLS:

µ	:	Micro

ABBREVIATIONS:

ADMS 4	:	Atmospheric Dispersion Modelling System 4
ESKOM	:	Electricity Supply Commission
SASOL	:	South African Coal and Oil Ltd.
GPS	:	Global Positioning System
SO_2	:	Sulphur Dioxide gas
ppb	:	Parts per billion
$\mu g/m^3$	:	Micro grams per cubic meter
C	:	Celsius
m/s	:	Meters per second
km	:	Kilometre
CFES	:	Centre for Environmental Studies

CHAPTER 1

INTRODUCTION

1.1 BACKGROUND

The interest in the Eastern Highveld of South Africa for air quality studies is immediately apparent when one understands the easy availability of coal as a natural resource and cheap energy source. In most places, the coal seams lie very close to ground surface, greatly simplifying coal extraction, cost effective and therefore highly attractive to mine. This has attracted several types of high consuming coal industries, which impacts area air quality due to coal combustion. Several years of effective pollution control has been successfully implemented by the local electricity supplier, ESKOM, as there has been a steady increase of sulphur dioxide as primary pollutant, which is as a result of increased power demand over the years due to increased economic growth of the country (Rorich, *et al.,* 2000).

In general, air quality models use mathematical methods to attempt to copy or simulate the physical processes that impact air pollutants when they are released, dispersed and then react in our atmosphere. Initial work on employing mesoscale numerical models (Jury, *et al.,* 1992*)* was suggested as a methodology to use as an input into dispersion predictive models, but today's advanced air quality models automatically incorporate the mathematical workup. The data that these models require to run effectively are datasets obtained from meteorological data measured at weather monitoring sites and physical data like rates of emissions from smoke stacks and the height of those smoke stacks. Plotted wind roses employing wind frequency data or converted pollution data readings (Guastella, *et al.,* 2005) are successfully used as precursors to final model applications. During ADMS dispersion model evaluations in urban and industrial sites in the UK, the sensitive nature of wind speeds, especially wind directions, were revealed for the comparisons of predicted and measured concentrations at monitoring sites. Nonetheless, good correlations were found between predicted and measured values of the SO_2 pollutant (Carruthers and Lester, *et al.,* 2000). The models can then describe the primary pollutants entering the atmosphere as well as predicting or determining secondary pollutants that are formed due to complex chemical reactions that occur in the atmosphere under favourable conditions.

Air Quality models are furthermore used to control air pollution by identifying source contributions, thereby assisting in the design of effective counteracting strategies. The models are used to verify and permit new source processes if the ambient air quality standards are not exceeded; or if necessary, to assist with the employment of additional pollution control requirements. Alternatively, models are used in the prediction of future pollution actions from several sources in close proximity after the implementation of a regulatory program, so that through the program harmful exposure to pollutants to humans can be estimated.[a] Models originating from the US EPA, like the Industrial Source Complex Dispersion (ISCD) model has been successfully employed to estimate ground level concentrations of sulphur dioxide originating from cement kiln stacks, proving their use as a successful point source tool during waste conversion to energy in the cement industry (Gaylard, 1996).

Several articles have already been published by the originators of the software on datasets taken from field observations or readings supplied from the United Kingdom as well as from the USA, where prediction efficiencies have been determined by using the ADMS 4 model (Hanna, *et al.*, 1999*)*. The first and second datasets concerned non-buoyant tracer releases within an oil refinery complex and from area and volume sources in an open field respectively. The last three data bases dealt with buoyant plumes taken from tall stacks in power plants. In the case of each dataset, the difference lay in the settings where these plants were situated. One plant was surrounded by low lying flat farmland, the other plant was situated in an urban environment and the third surrounded by complex terrain, where the monitors were situated at elevations higher than the stacks. From these studies that compared ADMS 4 to AERMOD and the ISC3 air quality models, it was found that ADMS 4 under predicted by 20% with a scatter of about a factor of two. Furthermore, the ADMS 4 model had about 53% of its predictions within a factor of two compared to the observations actually taken. If one had to consider only the highest predicted and observed concentrations, ADMS 4 under predicted on average by about 20%.

The ADMS 4 program is a new generation dispersion model which is practical in its application to simulate a wide range of short-ranged buoyant and passive releases into the atmosphere, either in combination or individually. The program was developed in the United

Kingdom by a governmental and industrial combined consortium under guidance of Cambridge Environmental Research Consultants (CERC). It is capable of simulating continuous plumes and short duration puff releases. The model can provide useful information up to distances of 100 km downwind from the emitting source. The model uses two parameters for its calculations: the Monin-Obukhov length (L_{MO}) as well as the boundary layer height (h) in its skewed Gaussian concentration distribution to calculate dispersion of the pollutants under convection conditions.

Other features include long-term outputs in terms of averages, percentiles or number of emissions exceeding limits and objectives for direct comparison. The nature of the pollution sources, whether they be point or line sources, can time vary periodically, seasonally or on an hourly basis. The model can calculate concentration and deposition fluxes from a line, area, volume, continuous point or directional release (jet) point of view (CERC, 2007).

Some of the advantages that ADMS 4 has as a modelling program include the requirement of only one level of near ground observations to be input. It can include surface conditions such as soil moisture, surface albedo and surface roughness length. Surface roughness characteristics impact dispersion rates as well as vertical profiles of wind and temperature in the surface layer and therefore it becomes an important variable in determining the dispersion in the vicinity of refineries, as in the case of SASOL Secunda, coal fired power stations and steel industries as found in the Eastern Highveld region.

The algorithms used in the ADMS 4 software quantify the partial penetration of an elevated plume. The resultant pollutants that are left to diffuse back to the earth's surface depend on the stability of the inversion and the buoyancy of the plume. This constraint is important for extreme or average buoyant plumes combining with reasonably low level inversions. This characteristic is conducive to the types of temperature inversions that are typically experienced in the winter period nights over the study domain. A study carried out in 1985 by GERC using the "Indianapolis" dataset and an SF_6 tracer in conjunction with the ADMS 4 model, indicated over-predictions of source concentrations during the daytime convective conditions close to the source and an under-prediction of distances up to 3 km from source. During night-time, a consistent under-prediction was experienced and put down to air turbulence (Carruthers and Dyster, *et al.*, 2000).

Studies comparing the ADMS model to the UK, R-91 as well as the US, ISC-ST Gaussian dispersion models in conjunction with archived LIDAR data showed higher levels of predictability in maximum ground-level pollutant concentrations, in convective conditions for elevated sources. Errors were smoothly distributed about the zero errors and errors of maximum concentrations were unlikely to being more than a factor or two around the averages. The absolute sense of performance compared to the other models were good for expected stack heights greater than 30m and less than 80% of the boundary layer height in neutral or convective conditions (Carruthers, *et al.*, 1997).

ADMS 4's main applications include stack-height determinations, environmental impact assessments, odour modelling and safety planning by Air Quality regulators, government departments and consultancies as well as industrially based manufacturing companies to monitor the emissions of their operations. Other applications include Integrated Pollution Prevention and Control authorisations. The reason for the choice of using this model for this study was the new developments that had been created in version 4, compared to earlier versions of the ADMS model system. It is not the purpose of this thesis to compare various models presently available in the market, as this has already been done in a previous study by the developers of ADMS 4 (Hanna, *et al.*, 1999).

[a] http://www.epa.gov/ttn/scram/aqmindex.htm

1.2 AIM AND OBJECTIVE OF THIS STUDY

The overall aim of the study is to assess the ADMS 4 dispersion model by seeing what the efficiencies of the model have to offer and by determining the measure of over- or under prediction capability; the viability can be determined whether this model could be used as a tool to accurately measure source pollution in the future. This will be achieved by the following objective:

<u>OBJECTIVE</u>

To demonstrate or verify the use of ADMS 4 as an effective air quality predictive modelling tool, by simulating air emissions releases in the Eastern Transvaal Highveld (ETH) region of study and to see whether via emissions measurements performed at the measuring station, it can be estimated which source was the originator of the emission.

1.3 ORGANISATION OF THE REPORT

CHAPTER 2 discusses the “study domain” and describes the area in South Africa, the Eastern Highveld weather characteristics typical of the study period chosen, namely the regions’ winter period and the farming and industrial activities present in the area.

CHAPTER 3 discusses the methodology of baseline data collection activities taken from the chosen weather station, namely Elandsfontein and illustrates the equipment used and identifies the data sets chosen for the two periods under study.

In CHAPTER 4, the Elandsfontein data is manipulated by using wind directions, pollution concentrations of SO_2 which is input into WARPLOT wind rose generating software, as well as the ADSM 4 wind rose software to determine general direction and extent of the pollution patterns, as an initial estimate before physical emissions data are entered into ADMS 4 for calculated predictions at the receptor site.

In CHAPTER 5, the power stations emissions data and meteorological data (from the monitoring station) are then entered into the model to determine maximum emissions experienced over the identified grid area of the time dataset chosen. The ADMS 4 results and graphic comparisons are compared and discussed.

In CHAPTER 6 conclusions are drawn from the predictions and final efficiencies of the model are determined, as well as recommendations made to improve the practical use of the model and methodology for future potential determinations.

In CHAPTER 7, the references are highlighted of researched articles and readings performed to substantiate the research report.

CHAPTER 2

CHARACTERISTICS OF THE EASTERN HIGHVELD ("STUDY DOMAIN")

The Eastern Highveld study area is situated mainly in the western side of the Mpumalanga province, overlapping the eastern and south-eastern border of Gauteng province. The study area is defined by the following map coordinates: 25.8234S 28.8224E, 25.8638S 30.2406E, 27.1541S 30.1846E and 27.1263S 28.8271E. Prominent towns in the area are Witbank, Ermelo, Bethal, Secunda, Kinross, Evander, Leandra and Trichardt, each supporting local farming communities and within themselves delivering negligible industrial manufactured goods or services. Mixed farming is practised in the region, mainly with cattle (beef and dairy), sunflower seed, grain sorghum and maize production. (See Figure 1 indicating a map of the Eastern Highveld region reflecting towns and main arterials through the area.)

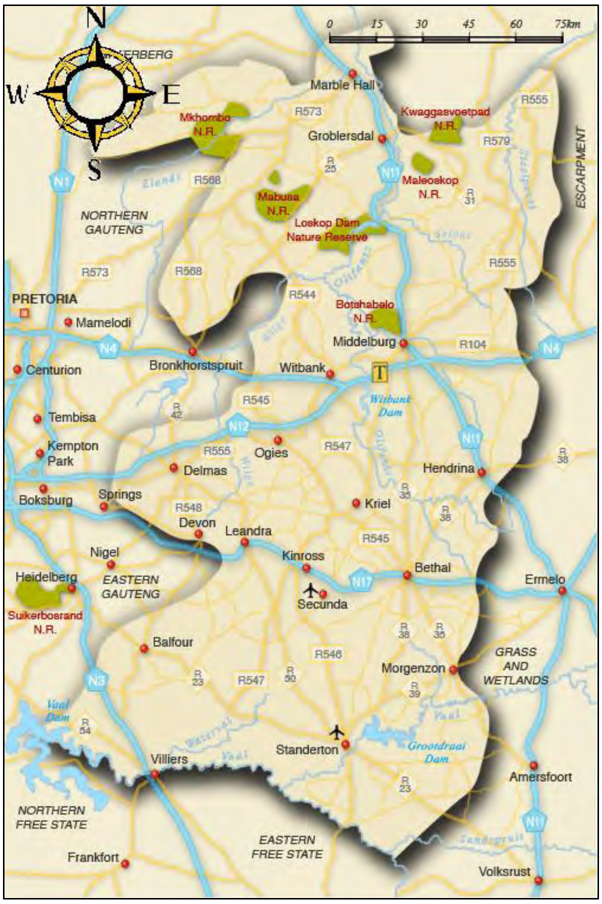

Figure 1: Map of the region described as the Eastern Highveld [b]

[b] http://www.roomsforafrica.com/dest/south-africa/mpumalanga/regions/highveld-and-cosmos.

The most significant industry found in this region is coal mining, to support via coal production, the countries' most concentrated cluster of ten electricity generating power stations, producing power for the sub-Sahara African region.

A second pertinent industry is synthetic fuel manufacture from coal, as described by the Fischer-Tropsch method and produced by SASOL II and III at Secunda, covering a total area of some 13 km^2. By gasification of 40.5 million tons of low grade coal per annum from the surrounding coal mines, SASOL produces hydrocarbon fuels like diesel, petrol, LPG (Liquid Petroleum Gas) and several chemical by-products such as alpha olefins used in the plastics and fertilizer industries (Okonkwo, 2007). An aerial view of these refinery plants can be seen in Figure 2.

Figure 2: An aerial view of the Sasol II & III Plants at Secunda (with permission of Google Earth).[c]

[c] Google Earth (26.5572S, 29.1581E)

The close confines of these two refinery plants in conjunction with the number of power generating plants and coal mining operations, together probably create the sum total volume of South Africa's contribution of global warming emissions, defined as the primary pollutants which are Sulphur and Nitrogen oxides (NO_X and SO_X), Carbon Monoxide (CO), particulate matter (PM) and volatile organic compounds (VOC) which impact the regions' air quality levels extensively (Fuggle, *et al*., 2000).

Other influencers to air quality emissions in the area are the steel plants on the outskirts of the Witbank, namely Columbus Steel (to the east of Witbank), Highveld Steel & Vanadium Corporation (to the west of Witbank) as well as the extensive coal mining operations in and around the region that emit sulphurous compounds. Of these are the spontaneous combustion of coal discard and other carbonaceous materials on coal discard dumps that emit sulphur oxide compounds, as well as rogue emissions from the underground coal mine fires which leach large amounts of sulphur oxide compounds through the ground and shafts, impacting low level air quality characteristics (Fuggle, *et al*., 2000).

Situated in and around these in mines, power stations and other polluting related industries are local informal settlements of permanently employed, as well as unemployed migrant labour and their families that burn biomass as well as the locally mined coal for heating and cooking purposes. The change in volumes of these emissions are also seen to be seasonally influenced, as these volumes increase over the late autumn, winter and early spring periods of the year. This further aggravates the air quality levels of the boundary layer of the atmosphere in conjunction with stable temperature inversions that develop during this period.

Lastly, the eastern highveld region is characterised by an undulating low lying landscape at a high altitude, in the region of 1650 meters above sea level, mainly of Themeda Veld of temporary cultivated grassland (30%) and unimproved grassland (60%). Soil characteristics are primarily clay in nature. The winter period in this region is prone to veldt fires which are started for a variety of reasons and therefore also contributes to the pollution of the boundary atmospheric layer, as can be seen in Figure 3.

Figure 3: The flat cultivated and unimproved grassland that is typical of the region, as well as the frequent veldt fires that occur during the winter periods.

The area experiences mainly summer rainfall patterns which varies between 600 and 750 mm per annum. Moderate summer day temperatures are experienced with an average range of 22 ^{0}C and 24 ^{0}C during the summer months and an average day temperature range of between 12 ^{0}C and 14 ^{0}C during the winter months. Winter months are also characterised by low lying early morning fog which generally starts dissipating by mid morning. Night temperatures tend to average between 0 ^{0}C and 5 ^{0}C during the winter months, as can be seen in Figure 4 (Mbeki, 2005).

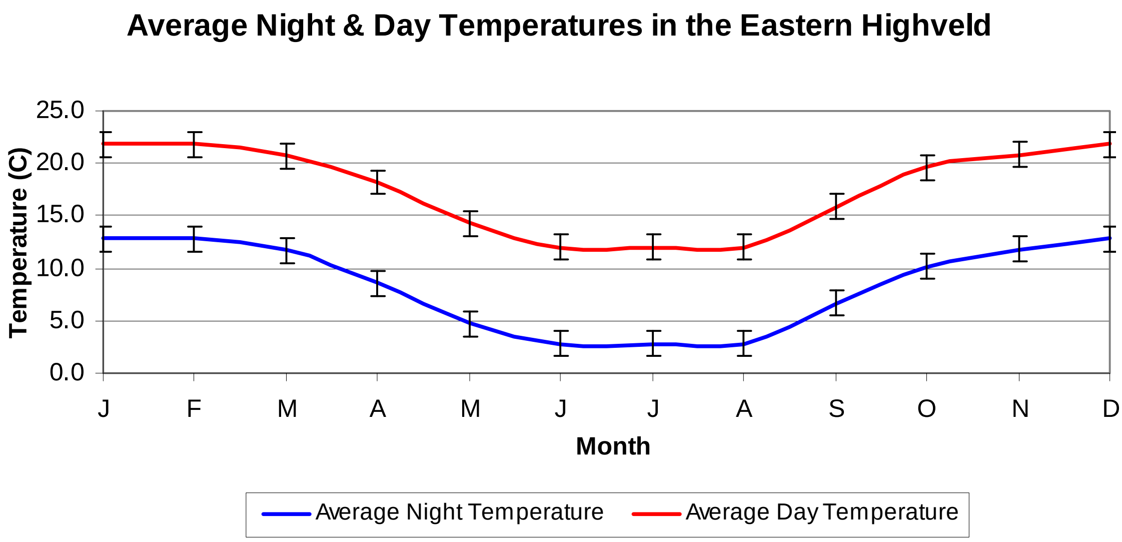

Figure 4: The average day & night temperatures of the region clearly indicate the stable temperature inversions common for the May to August period of the year. (data from Mbeki, with permission).[d]

[d] (Mbeki, 2005)

CHAPTER 3

METHODOLOGY

3.1 TIME INTERVALS AND DATA COLLECTION SITES

It was decided to concentrate on a centrally situated air quality monitoring site to all the power stations, as well as the oil refinery in the area of study. The site, known as Elandsfontein, is an ESKOM owned and managed air quality monitoring site and is situated on a slight rise in comparison to the neighbouring countryside, with an elevation of 1768m above sea level (altitude accuracy approximately 17.5m) and GPS coordinates of longitude: 29.4174E and latitude: 26.2453S (with a GPS position accuracy of approximately 10.86m).

Figure 5: An aerial view of the Elandsfontein site taken from the turnoff at the R544 Bethal road (with permission of Google Earth).[e]

[e] Google Earth (26.2453S, 29.4173E)

The testing equipment and their parameters are listed in Table 1 that were used to generate the data over the test period. The ozone testing equipment was replaced in 2007, where the TECO 49 unit was replaced by a Monitor Labs 9841B unit. As this parameter was not one of the variables inputted into the ADMS 4 model, it did not impact the subsequent model predictions made of SO_2 content in the air over the two given periods.

Figure 6: A zoomed photograph indicating the Elandsfontein site on the hill in the distance, situated at the base of the radio tower.

Table 1: The list of air quality station equipment at the Elandsfontein monitoring station.

Test Parameter	Equipment Make and Model
Wind Direction, Speed and **Velocity**	RM Young combined head
Temperature	RM Young thermistor probe
Rain Gauge	Automatic tippler measuring 0.2 mm
NO_1, NO_2, NO_X	TECO 17C
SO_2	TECO 43C
Ozone	TECO 49 (2006), Monitor Labs 9841B (2007)
H_2S	TECO 43A SO_2 with a TECO H_2S convertor
Sigma Theta	By calculation
SO_4 & NO_3	Rupprecht & Patashnick 8400S and 8400N pulse generators with R & P pulse.
Beta Gauge	Eberline FH 621-R

Figure 7: The Elandsfontein physical testing & monitoring facility.

Data available from this site were supplied by ESKOM's Research and Technology Centre in Rosherville, Johannesburg and carefully studied for practical use in such a study. Two sets of data were identified for their relevance and practicality as: (1) each set had complete and continued readings recorded for an approximate period of ten to fourteen days, (2) both sets were recorded over the July, August periods which coincide well with stable, boundary layer inversions that form over the study area during the southern hemisphere winter period. The inversions help concentrate the levels of air quality gas pollutants for ease of detection and measurement.

The meteorological data necessary for input into the model, namely: temperature, wind direction and wind speed were recorded every hour, on the hour and therefore 24 readings taken for every day. The first set of data readings identified for use was for the period: 14th to 27th July 2006, 14 days with a sum total of 336 data readings. The second identified period: 25th July to 4th August 2007, 11 days with a sum total of 264 data readings.

The methodology for this specific study was to use the meteorological data recorded at Elandsfontein in conjunction with the power stations' combustion figures, stack heights and other physical characteristics and use it as the input information for the air quality model. The SO_2 pollutant predictions calculated from the model for the receptor site, namely Elandsfontein, would then be compared to the true values of SO_2 measured and recorded at the Elandsfontein station and efficiencies of the model compared.

CHAPTER 4

RESULTS

4.1 DATA MEASUREMENT AT THE POWER STATIONS AND ELANDSFONTEIN

From the two identified ESKOM Elandsfontein datasets chosen to be studied, it was decided to plot wind roses as well as SO_2 pollution roses to determine which specific power stations were responsible for the SO_2 emissions at the time. General outlines of the pollution roses were then superimposed on the Eastern Highveld map (see Figure 8) to estimate the origin of the emission. The corresponding SO_2 quantities (in parts per billion, ppb) were then entered into the wind rose generating software in place of the wind speeds and the wind direction then used as the other variable for the rose plot. The positions of the power stations and SASOL with their corresponding distances in relation to the Elandsfontein test facility can be seen in Table 2.

Table 2: The GPS positions as well as the relative distances from the power stations as well as SASOL in relation to Elandsfontein.

	Latitude	Longitude	Distance from Elandsfontein (km)
Arnot Power Station	25.9439S	29.7912E	50.12
Duvha Power Station	25.9610S	29.3383E	32.56
Hendrina Power Station	26.0266S	29.6028E	30.54
Kendall Power Station	26.0881S	28.9689E	48.02
Kriel Power Station	26.2535S	29.1791E	23.77
Lethabo Power Station	26.7403S	27.9750E	153.63
Matla Power Station	26.2831S	29.1393E	28.03
Majuba Power Station	27.0999S	29.7698E	101.20
Tutuka Power Station	26.7757S	29.3521E	59.29
SASOL Refinery	26.5572S	29.1581E	43.21
Elandsfontein Test Site	26.2453S	29.4174E	N/A

Although Grootvlei and Komati power stations are shown on the maps, these two power stations were mothballed over the dataset periods and therefore did not generate power with resultant SO_2 emissions.

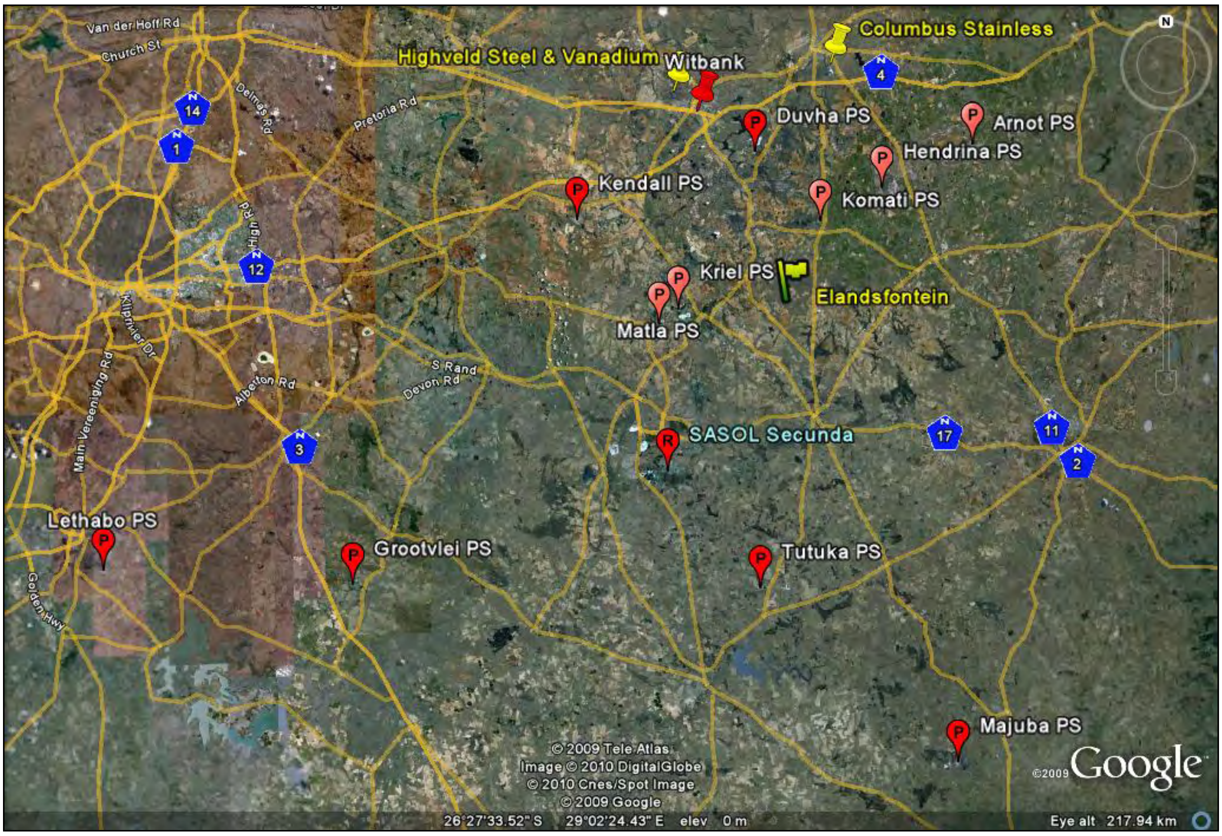

Figure 8: The Eastern Highveld region depicting the high emissions industries and clearly indicating the position of the Elandsfontein test site in relation (with permission of Google Earth).[f]

[f] Google Earth (26.2453S, 29.4173E)

4.1.1 THE 14th TO 27th JULY 2006 DATASET

The wind speed and direction data was plotted in wind rose plotting software to determine the wind rose for the period. (See Figure 9). Hereafter the corresponding SO_2 values measured at Elandsfontein were plotted in the same wind rose software using the wind direction data to determine an SO_2 pollution rose. (See Figure 10).

The SO_2 pollution wind rose was then superimposed on the Eastern Highveld area map (see Figure 11) to estimate the industries or power stations that could have been responsible for the SO_2 emissions measured at the monitoring site.

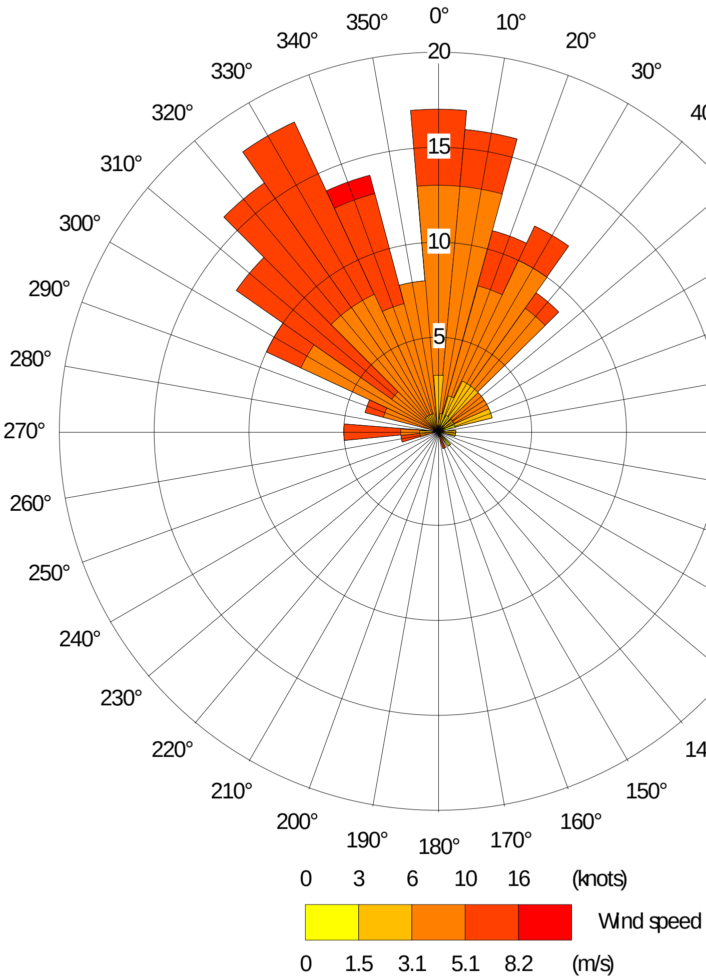

Figure 9: The wind rose for the July 2006 period dataset. The two bands of significance are the 0 – 30 degree band as well as the 300 – 340 degree band.

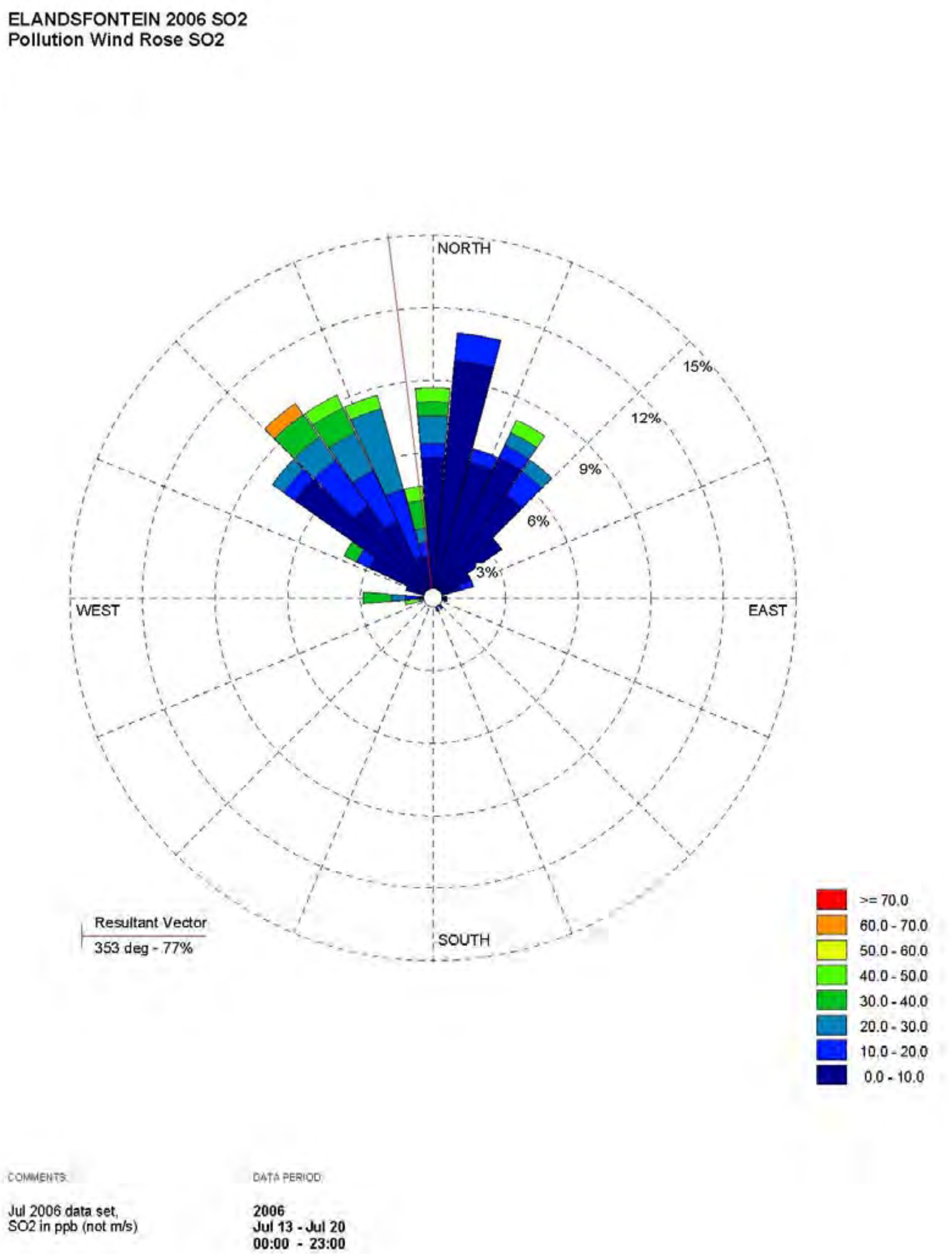

Figure 10: The SO_2 pollution rose using the wind direction and SO_2 data from the July 2006 dataset.

From Figure 11, it would seem that Arnot, Hendrina and Duvha power stations could be responsible for the 0 to 30 degree directional band of emissions measured at the monitoring station, in combination with the largest directional band (300 to 340 degrees) emissions possibly influenced by Kendal power station to the west.

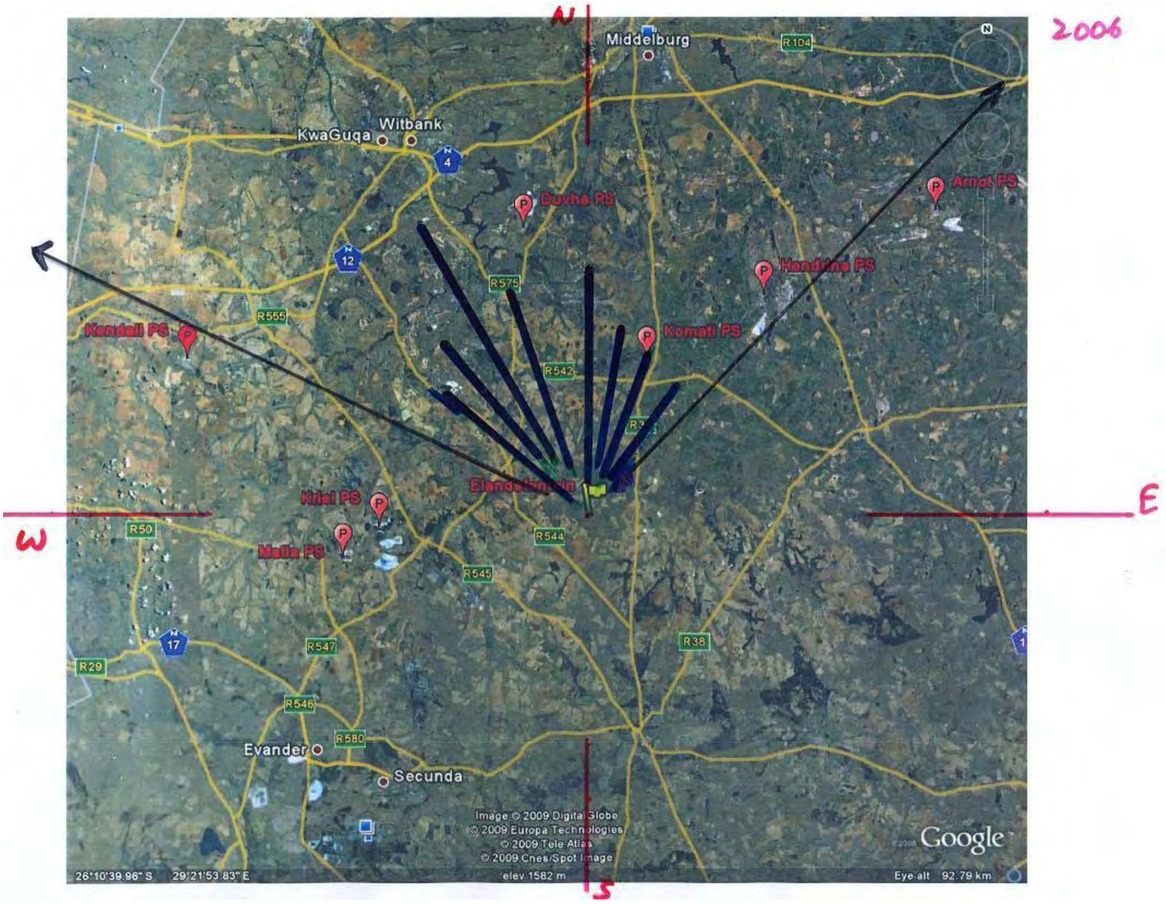

Figure 11: The area of SO_2 emission is seen drawn within the arrowed upwards pointing wedge on the Eastern Highveld map (with permission of Google Earth).[g]

[g] Google Earth (26.2453S, 29.4173E)

4.1.2 THE 25th JULY TO 4th AUGUST 2007 DATASET

Similarly to the July 2006 dataset, the wind speed and direction data for 2007 was plotted in wind rose plotting software to determine the wind rose for the period. (See Figure 12). Hereafter, the corresponding measured SO_2 values were plotted using the wind direction data to determine the SO_2 pollution rose. (See Figure 13). The SO_2 pollution wind rose was then also superimposed on the Eastern Highveld area map (see Figure 14) to estimate the industries or power stations responsible for the SO_2 emissions measured at Elandsfontein.

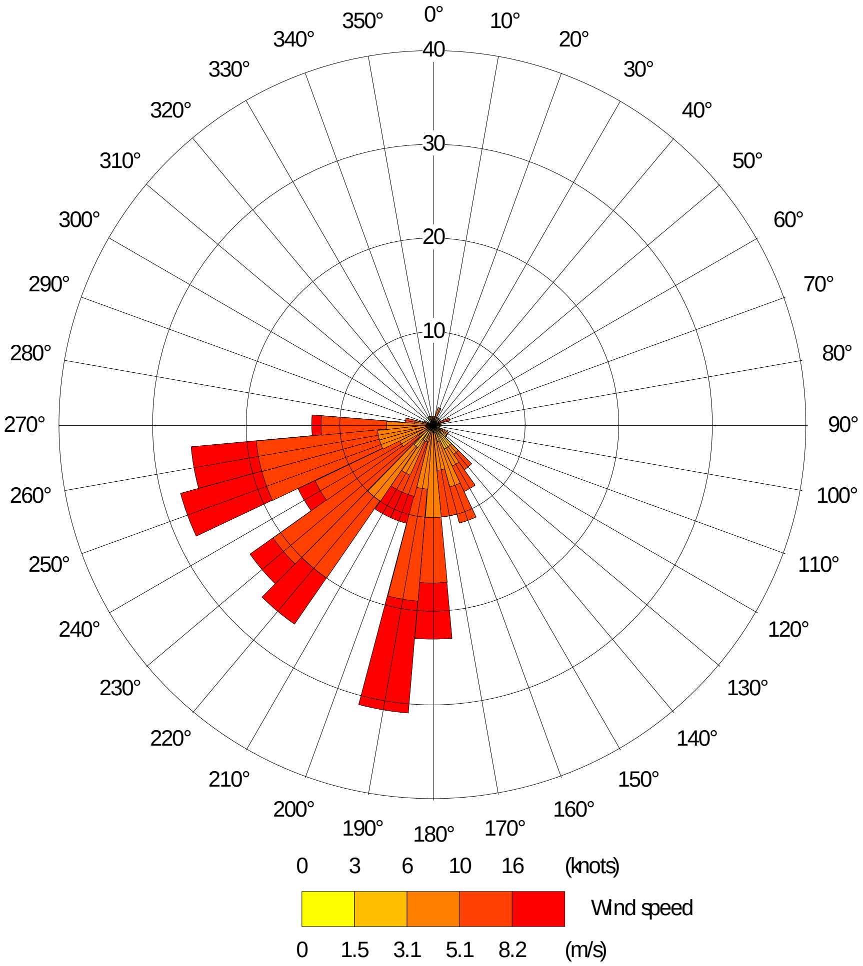

Figure 12: The wind rose for the July - August 2007 period dataset. The two bands of significance are the 220 - 260 degree band as well as the 180 - 190 degree band.

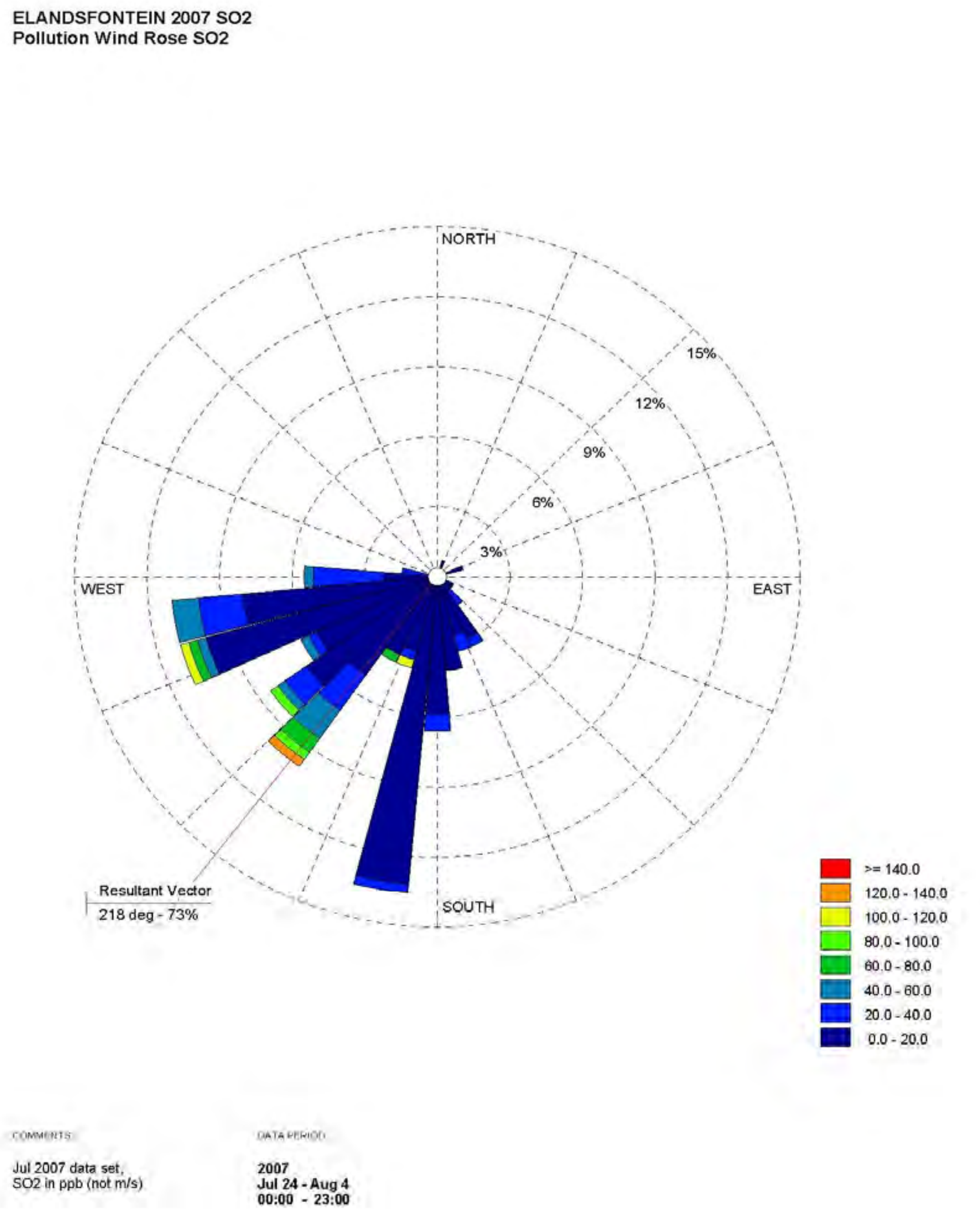

Figure 13: The SO_2 pollution rose using the wind direction and SO_2 data from the July to August 2007 dataset.

From Figure 14, the contributory emissions measured at Elandsfontein would seem to originate from the Majuba and Tutuka power stations as seen by the 180 to 190 degree directional emissions bands. However, the biggest emissions influence would seem to originate from Lethabo power station (the 260 degree band) and with further emissions originating from Kriel and Matla power stations.

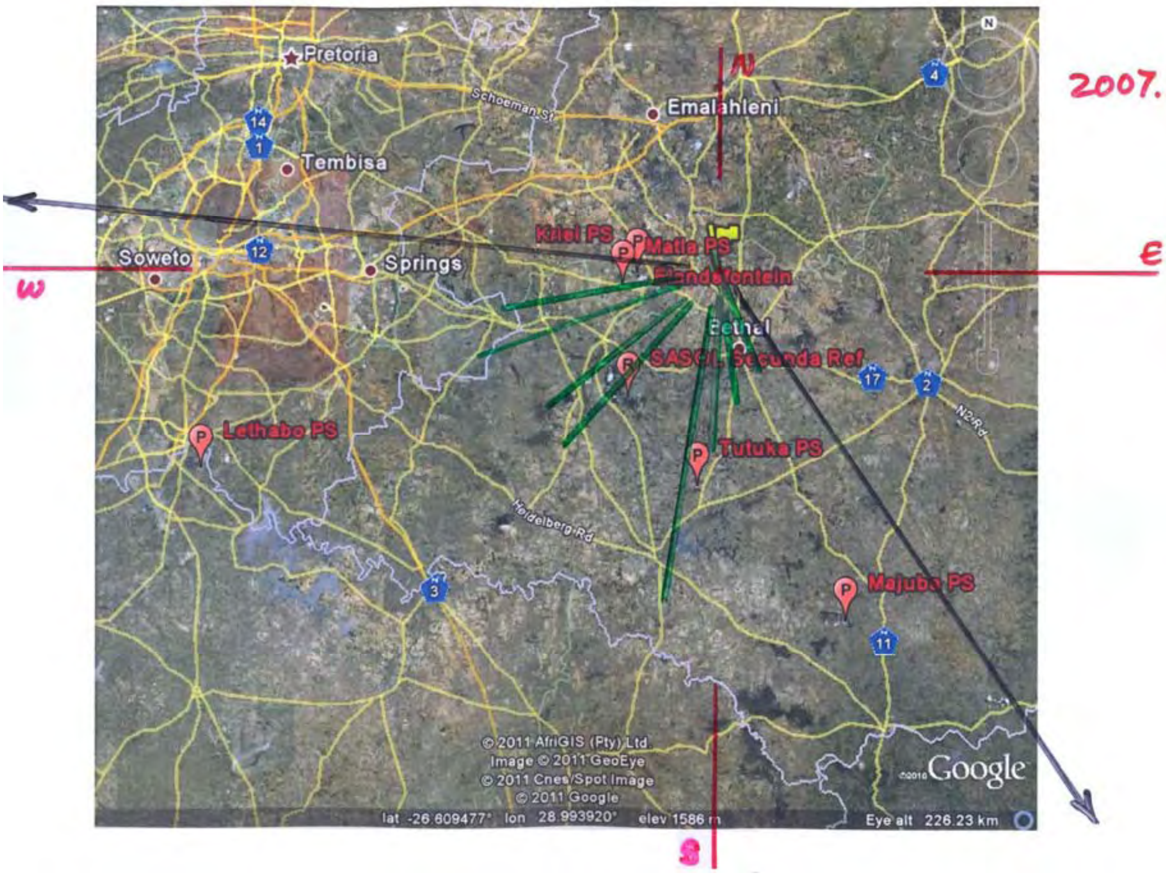

Figure 14: The area of SO_2 emission is seen drawn within the downwards pointing arrowed wedge on the Eastern Highveld map (with permission of Google Earth).[h]

[h] Google Earth (26.2453S, 29.4173E)

The pollution rose for each dataset, superimposed on regional maps, gives reasonably clarity as to which emitting industry's parameters and coal combustion data, or quantified annual SO_2 generation emissions can be sourced for input into the data for the model for evaluation or verification against actual measured quantities.

4.2 DATA MANIPULATION AND IMPORT INTO ADMS 4 RE-ANALYSIS DATA

The emissions data for each power station, supplied by ESKOM, needed to be manipulated in a favourable format for input into the program. The information for the 2006 dataset and the 2007 dataset are listed below in Tables 3 and 4 respectively. (Different datasets had to be used for 2006 and 2007, as these were the only complete sets of data that were monitored on-site at Elandsfontein due to equipment downtime and loss of data for various reasons.) The annualised reported SO_2 production had to be corrected to a monthly figure and then converted into a grams per second rate for ease of model calculation when hourly meteorological data was used. This rate was lastly divided by the number of stacks per power station site, as the estimated position of the stacks on the station site, as well as in relation to each other, had to be calculated using GPS grid data. The grid positions of the stations are used (not reflected in the following tables, but previously reported in Table 2 earlier in this report) by the model to set up an area grid of emission points, to be able to plot the highest emission points in its output graphics.

4.2.1 THE 14th TO 27th JULY 2006 POWER STATION EMISSIONS DATA

Table 3: ESKOM Power Station physical and emissions data for the July 2006 dataset.

Stack	**Height**	**Velocity**	**Diameter**	**Temp**	**SO_2 Emissions**		**No.**	**Emissions Rate**
	(m)	**(m/sec)**	**(m)**	**(^{0}C)**	**(Tons/m)**	**(g/sec)**		**(g/sec/stack)**
Hendrina	155.5	19.4	11.1	129.4	8484	3273.2	2	1636.6
Arnot	195	20.3	11.1	137.8	6089	2349.2	2	1174.6
Duvha	300	25.5	12.5	130	22368	8629.6	2	4314.8
Kendal	275	24.1	13.5	125.5	25245	9739.6	2	4869.8
Kriel	213	16.6	14.3	130	8239	3178.6	2	1589.3
Matla 1-3	213	19.4	14.3	124	11622.5	4484.0	1	4484.0
Matla 4-6	275	25.5	12.5	124	11622.5	4484.0	1	4484.0

From Table 3 above, one will notice a significant difference (not just in the physical dimensions of stack heights, temperatures or stack diameters of each power station) but the difference in emissions that each stack delivers once the final rates are determined. In this table it is clear that Duvha, Kendal and Matla generated significant higher levels of SO_2 per second per stack for this time period. (As identified from the pollution rose, Figure 10 and the mapped pollution directions, Figure 11 being the main contributory emitters for that time period.)

4.2.2 THE 25th JULY TO 4th AUGUST 2007 POWER STATION EMISSIONS DATA

From Table 4, the higher generators of SO_2 were Tutuka, Kriel and Matla power stations. However, there now reflects a downturn in SO_2 production from Matla power station with a significant increase in SO_2 production from Kriel during the time period, nearly a year later. This could be ascribed to possible turbine generating downtime experienced by Matla for this period and where Kriel power station has had to compensate for generating capacity.

Table 4: ESKOM Power Station physical and emissions data for the July to August 2007 dataset.

Stack	Height	Velocity	Diameter	Temp	SO_2 Emissions		No.	Emissions Rate
	(m)	(m/sec)	(m)	(^{0}C)	(Tons/m)	(g/sec)		(g/sec/stack)
Majuba	250	29.8	12.3	130	15558	6002.3	2	3001.2
Tutuka	275	24.9	12.3	130	13543.5	5225.1	2	2612.6
Lethabo	275	25.3	12.0	126	17163	6621.5	2	3310.8
Kriel	213	16.6	14.3	130	11404.5	4399.9	2	2199.9
Matla 1-3	213	19.4	14.5	124	9436.5	3640.6	1	3640.6
Matla 4-6	275	25.5	12.5	124	9436.5	3640.6	1	3640.6

The above data with the grid information of Table 2 as well as the Elandsfontein meteorological data was then entered into the program to generate, on a grid system, the predicted highest SO_2 levels expected at the receptor site, namely the Elandsfontein monitoring station. (As identified from the pollution rose, Figure 13 and the mapped pollution directions, Figure 14 being the main contributory emitters for that time period.)

4.3 VERIFICATION WITH ELANDSFONTEIN DATA

Figures 15 & 16 reflect the actual measurements of the meteorological data used to input into ADMS 4 as well as the actual levels of SO_2 (measured in ppb) for the two time periods under study. The wind speeds (meters per second), SO_2 and temperature (^{0}C) are plotted against time. The wind speeds and wind directions are reflected in the wind roses for the time periods, seen in Figures 9 & 12.

4.3.1 THE 14th TO 27th JULY 2006 DATASET

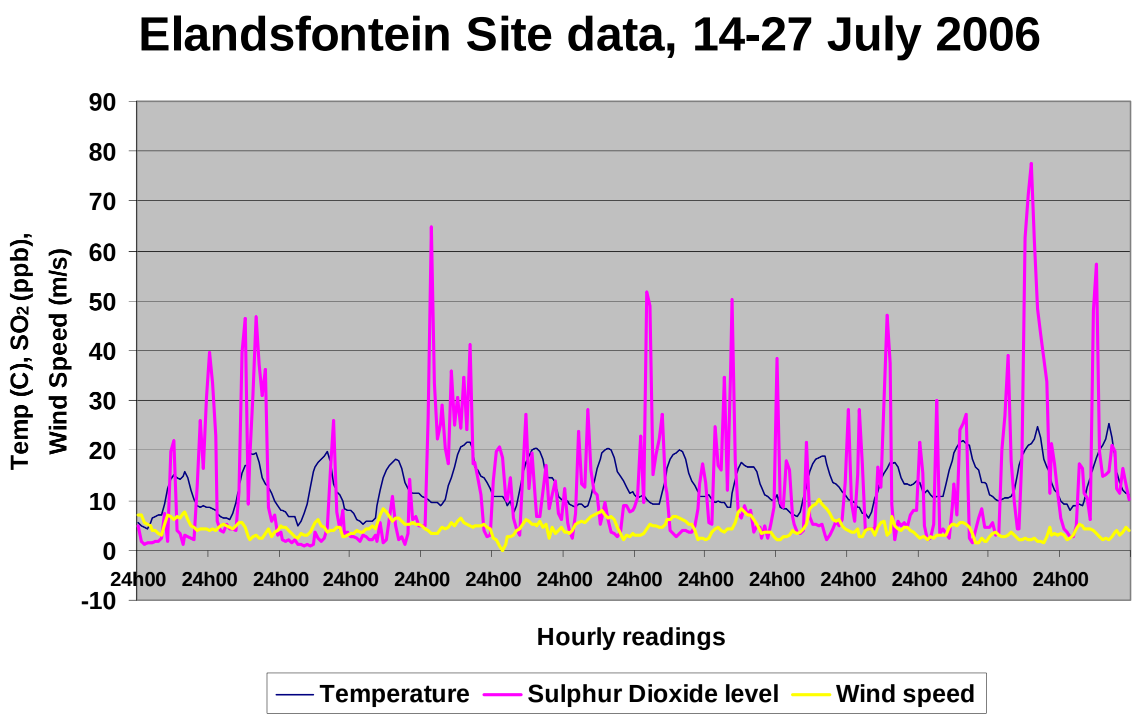

Figure 15: Physical hourly readings taken at Elandsfontein monitoring site of the Temperature, SO_2 levels and Wind Speed measurements, July 2006 dataset.

From the graphs the temperatures clearly show a steady frequency as they fluctuate between the day temperatures, all averaging in the region of just under 20 ^{0}C for the day temperature and averaging between 5 ^{0}C to just under 10 ^{0}C for the low night time temperatures. Wind speeds do not fluctuate significantly and seem to fluctuate between approximately 2 meters/second and 8 meters/second.

The SO_2 emission spikes or maximums do not seem to follow similar consistent trends. They seem to vary between day and night puff emissions, not specifically adhering to night time only maximums measured, as one would expect with the probability of winter night boundary inversions developing.

4.3.2 THE 25th JULY TO 4th AUGUST 2007 DATASET

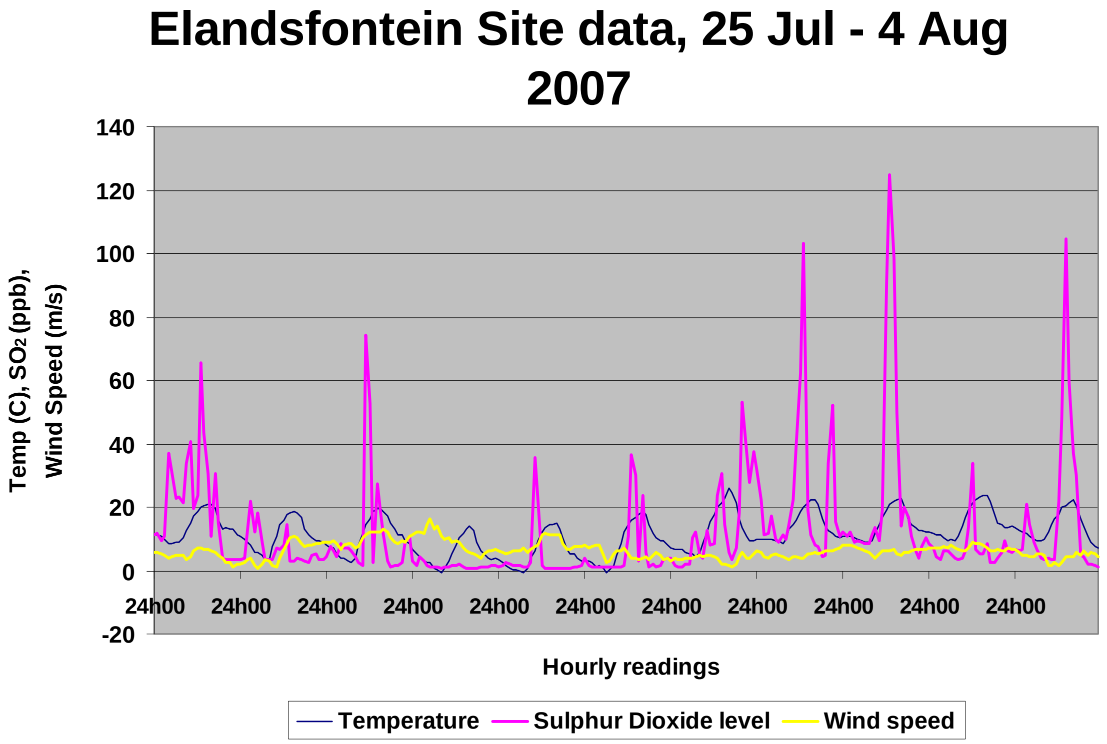

Figure 16: Physical hourly readings taken at Elandsfontein monitoring site of the Temperature, SO_2 levels and Wind Speed measurements, July to August 2007 dataset.

Just as seen in Figure 15 of the Elandsfontein measured data for 2006, the 2007 data reflect very similar temperature fluctuations between day and night, but with a slight increase for some of the day temperatures exceeding 20 ^{0}C, as the period approaches the warmer Spring season. Wind speeds initially well exceed the 10 meters/second mark, but then calm down to similar speeds experienced in 2006, namely in the region of approximately 2 meters/second and 8 meters/second. The SO_2 puff emission maximums start showing steadier patterns with maximum values being recorded during daytime temperatures, especially toward the latter part of the study period.

CHAPTER 5

DISCUSSION

5.1 ADMS 4 GRAPHIC OUTCOMES

Two sets of graphical outcomes (highest hourly as well as second highest hourly) were generated for comparison purposes to reflect the regional emission patterns and to compare the effect each source had on the region for the study period. Reflecting on the two results, the highest hourly gave the best reflection for the short time frame chosen for the two datasets. The second highest hourly would have given a better reflection had a one year time frame set of meteorological data been used. The second highest would then smooth out the possibility of fluctuations and missing data that might have occurred in the measured meteorological data throughout the year.

5.1.1 THE 14th TO 27th JULY 2006 DATASET

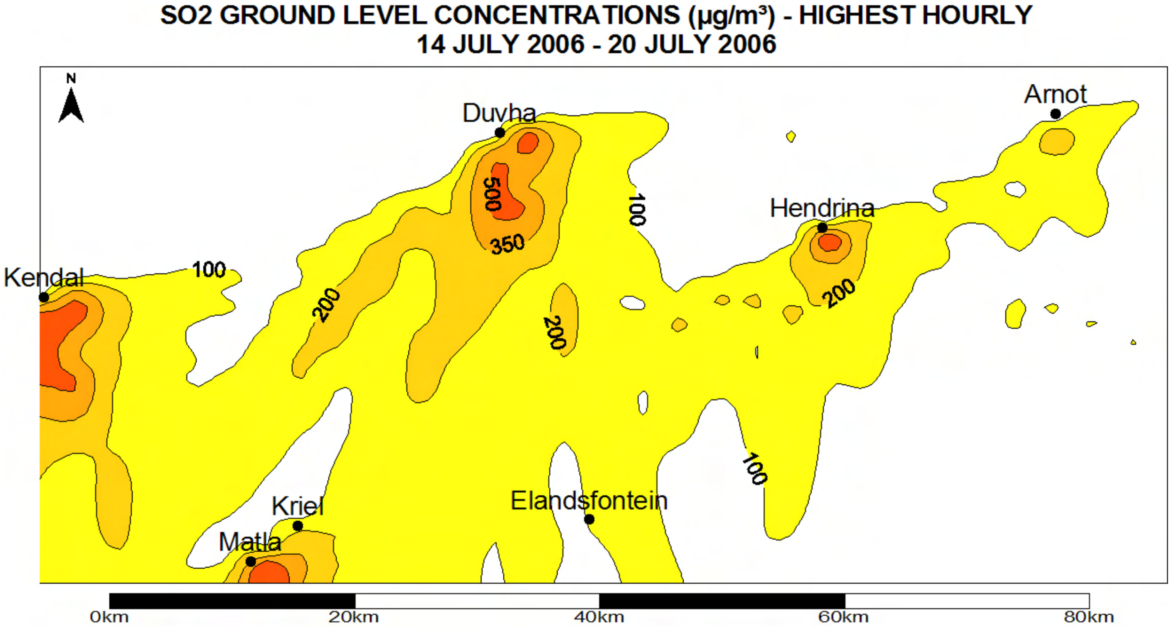

Figure 17: ADMS 4 graphic grid display of the ground level SO_2 concentration of the highest hourly readings for the July 2006 dataset.

The Elandsfontein monitoring station (seen in Figure 17 above, lying centre below) on the edge of the 100 µg/m^3 (38 ppb) band of SO_2 emissions spread, with the major contributors estimated by ADMS 4 being Hendrina, Duvha, Kriel, Matla and Kendal power stations. This ties in moderately well with the wind rose (Figure 9) as well as with the pollution rose (Figure 10) earlier on in the report. However, there remains a band of SO_2 emissions, between 310 degrees and 340 degrees, the area between Duvha and Kendal power stations that is unaccounted for.

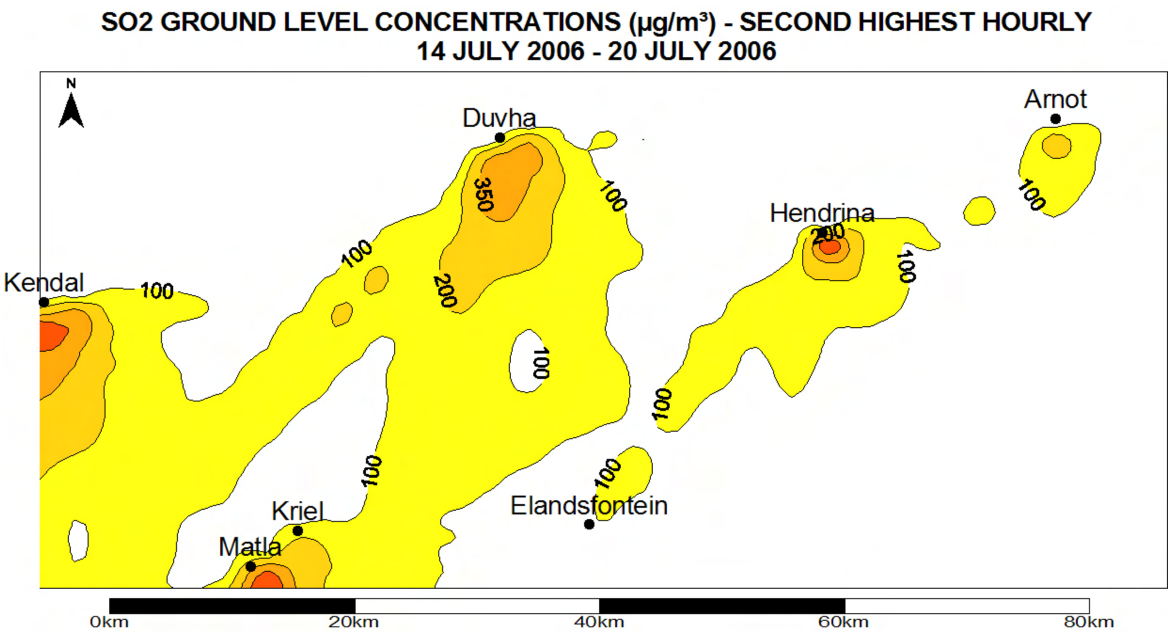

Figure 18: ADMS 4 graphic grid display of the ground level SO_2 concentration of the second highest hourly readings for the July 2006 dataset.

Figure 18 above depicts the second highest hourly emission for the region, a lesser degree of dispersion graphically displayed, but yet still confirming the five power stations' influence for the SO_2 emissions measured for the time period.

5.1.2 THE 25th JULY TO 4th AUGUST 2007 DATASET

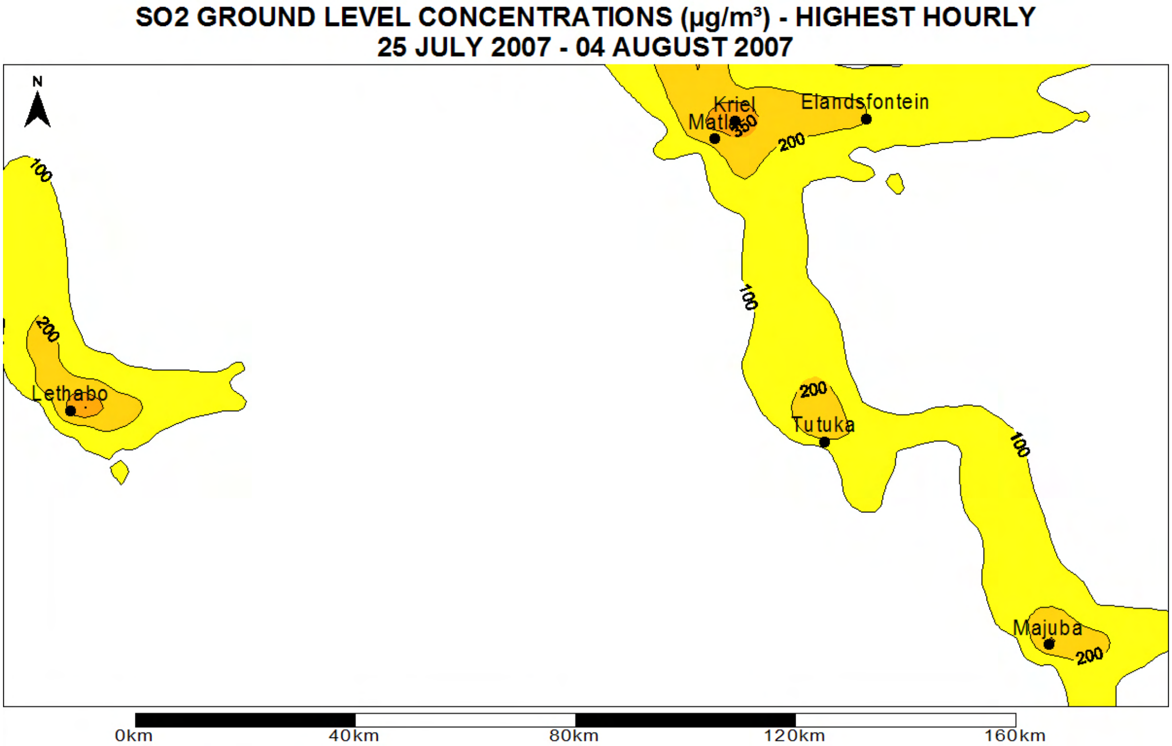

Figure 19: ADMS 4 graphic grid display of the ground level SO_2 concentration of the highest hourly readings for the July to August 2007 dataset.

The model determines the grid area of SO_2 dispersion influences for the 2007 dataset and places Elandsfontein in the upper right-handed area of the grid, on the edge of the 100 and 200 µg/m^3 (38 ppb and 76 ppb respectively) bands of SO_2 dispersion, to the right of Kriel and Matla power stations. Other role players of the SO_2 source dispersion are Majuba (101 km away), Tutuka (59.3 km away) and Lethabo (153.6 km away) power stations dotted to the south and east south-east from Elandsfontein.

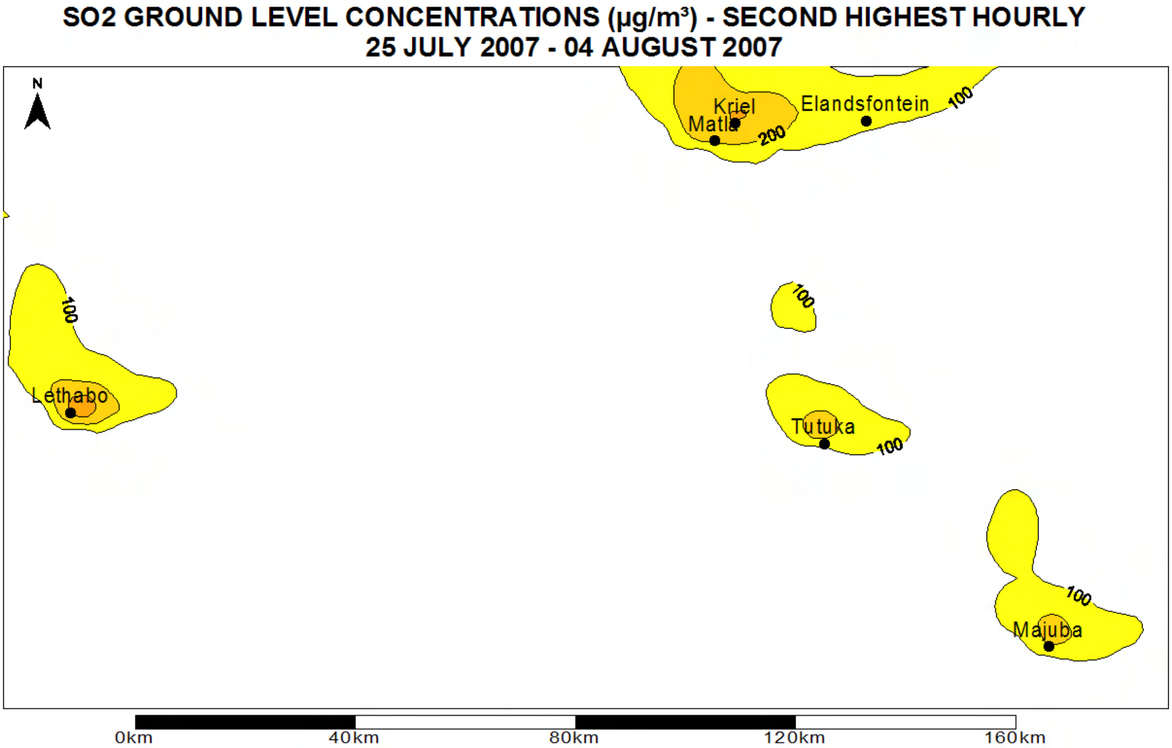

Figure 20: ADMS 4 graphic grid display of the ground level SO_2 concentration of the second highest hourly readings for the July to August 2007 dataset.

Figure 20 above depicts the second highest hourly emission for the region, a lesser degree of dispersion graphically displayed, but yet still confirming the five power stations' influence for the SO_2 dispersion measured for the time period. In this case Elandsfontein is situated on the edge of the 100 µg/m^3 (38 ppb) band of the SO_2 dispersion, east of Kriel and Matla power stations.

5.2 COMPARISON WITH THE ELANDSFONTEIN MEASURED DATA

The data generated from the model for the two study periods was produced in grid (and not time and date) format, identifying the highest and second highest predicted values. With further manipulation of the data of individual power stations' emissions contribution is determined. The highest and second highest maxima of the grid were identified and each station's effect to that maximum graphically displayed.

5.2.1 THE 14th TO 27th JULY 2006 DATASET

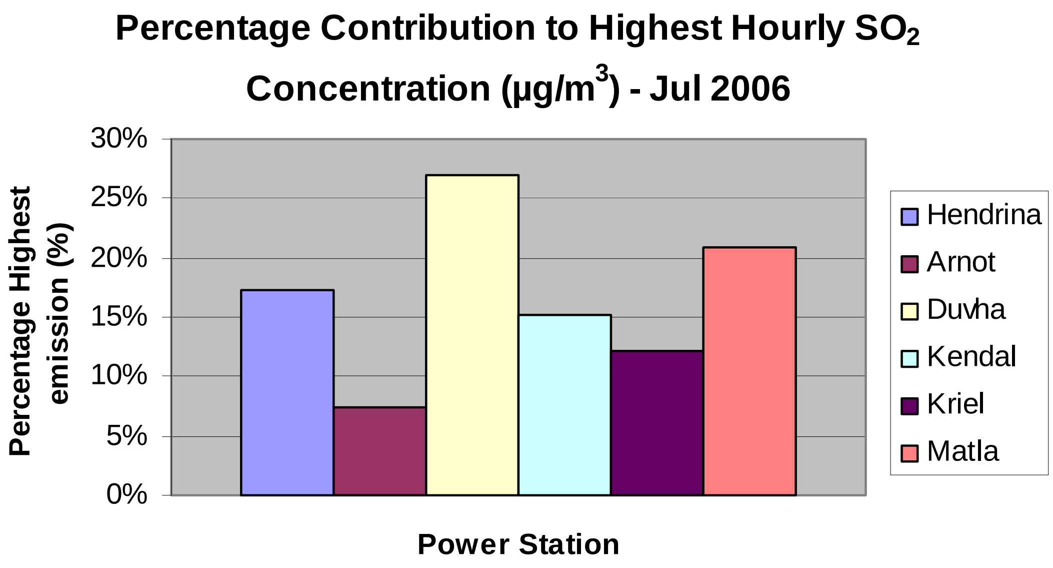

Figure 21: Percentage contribution by power station of the highest hourly SO_2 concentration during the July 2006 study dataset.

The model prediction for the receptor site (Elandsfontein) is summarised in Figure 21 above with the percentage contribution of each SO_2 emitting source. These results partly tie in with the results from the wind and pollution rose images as seen in Figures 9 & 10. However, the greatest direction of pollutant contribution is seen originating from the 320 degree to the 340 degree directional bands. No power station lies within this band as can be seen in the map of Figure 11. The model therefore could not identify the SO_2 emitting source, as data was not entered into the model for assessment of any other SO_2 emitting industry other than power stations. The band seems to clearly indicate the probability of a maximum emissions and a dispersion in that time period of the SO_2 gases emanating from a steelworks industry west of Witbank, specifically Highveld Steel and Vanadium.

From Figure 22 below, the prediction of the power station emissions contribution taken from the second highest hourly data from the model indicates the lesser level of accuracy if one had to study the map in Figure 11, where Matla and Kriel power stations are way off the dispersion area for the SO_2 pollution band reflected by the pollution rose, as indicated in Figure 10.

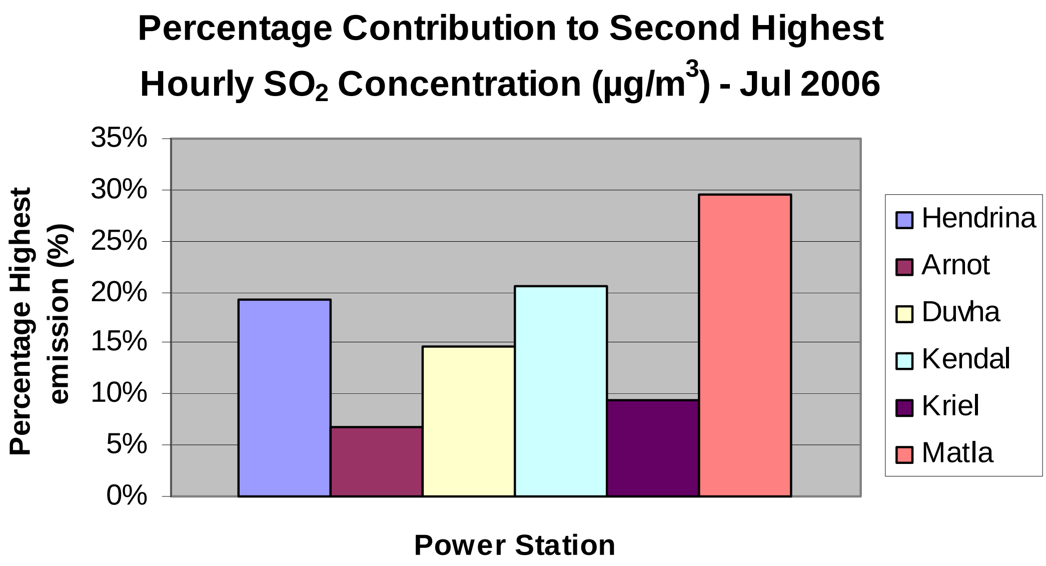

Figure 22: Percentage contribution by power station of the second highest hourly SO_2 concentration during the July 2006 study dataset.

5.2.2 THE 25th JULY TO 4th AUGUST 2007 DATASET

The model prediction data at the receptor site (Elandsfontein) for this time period indicates a majority percentage highest concentration of SO_2 emissions contribution from Matla and Kriel power stations, with minimal contribution by Tutuka, Majuba as well as Lethabo power stations, as seen in Figure 23 below. As the last three power stations are situated very far from the receptor site (59 km, 101 km and 153 km respectively, compared to the initial two), it would be acceptable to say that their contribution would be negligible as the SO_2 gases would have been dispersed far to thinly through the region before being detected at Elandsfontein.

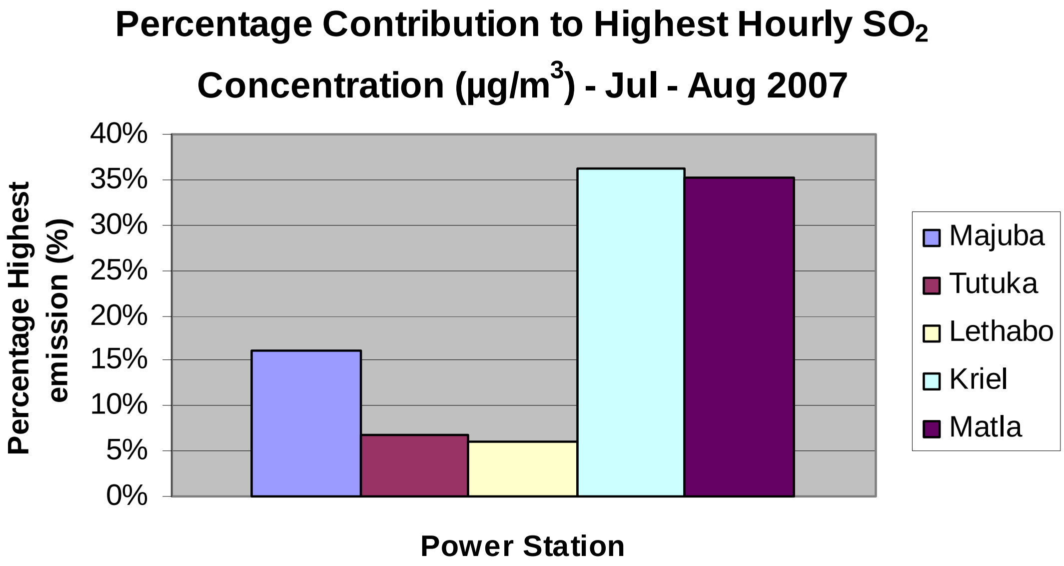

Figure 23: Percentage contribution by power station of the highest hourly SO_2 concentration during the July to August 2007 study dataset.

Whilst Kriel and Matla stations are practically due west from Elandsfontein and would justify the 250 degree to 270 degree directional band of emissions, the 220 degree to 250 degree directional band is unaccounted for. Although Lethabo power station falls within this band, Lethabo is situated too far off to have any real direct impact. However, the source not accounted for and data not entered into the air quality model is the emissions data for the SASOL Refinery, which is situated right in the middle of this band, as well as being situated 43 km away from Elandsfontein. SASOL is known for its substantial annual SO_2 emissions (approximately 210,000 tonnes SO_2 in 2005, 230,000 tonnes SO_2 in 2006 and 230,000 tonnes SO_2 in 2007)[i] and it would be reasonable to assume that this would account for the pollution roses' specific shape, as indicated by Figure 13.

From Figure 24 below, the prediction of the power station emissions contribution taken from the second highest hourly data from the model indicates the lesser level of accuracy if one had to study the map in Figure 14, where Matla power station now plays the major role and Kriel power station plays the lesser role in the dispersion area or SO_2 pollution band, as reflected by the pollution rose and indicated in Figure 13.

[i]http://www.sasol.com/sasol_internet/downloads/annual_review2007_1193997146684.pdf (p. 74)

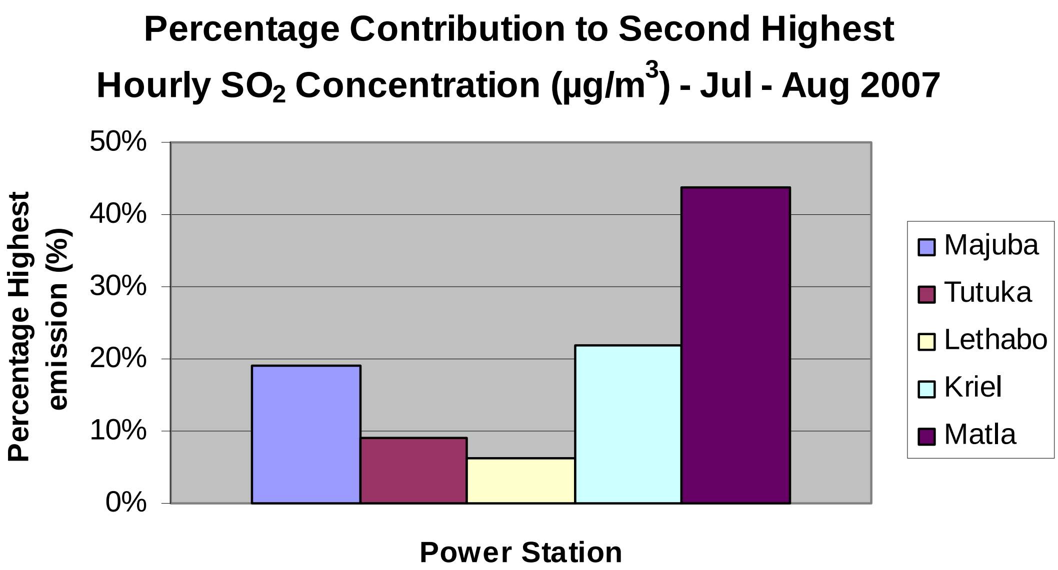

Figure 24: Percentage contribution by power station of the second highest hourly SO_2 concentration during the July to August 2007 study dataset.

The efficiencies of the ADMS 4 model predictions were determined by taking the maximum estimated emission of SO_2 by the model as predicted at the Elandsfontein receptor site and comparing it to the actual maximum measured SO_2 emission at the monitoring site for the two study periods.

The July 2006 dataset indicates a 42% efficiency for the highest hourly readings and a 40% efficiency for the second highest hourly readings. In comparison to this, the July to August 2007 dataset indicates a 58% efficiency for the highest hourly readings and a 38% efficiency for the second highest hourly readings. Table 5 summarises the efficiencies.

Table 5: ADMS 4 predicted values compared to the actual measurements taken at Elandsfontein monitoring site, reflecting the model's efficiency.

Study Period	**Highest Hourly**		**ADMS 4**	**Second Highest Hourly**		**ADMS 4**
	Measured (ppb)	**Predicted (ADMS 4) (ppb)**	**Under Predicted (%)**	**Measured (ppb)**	**Predicted (ADMS 4) (ppb)**	**Under Predicted (%)**
14 – 20 July 2006	77.5	32.5	**42**	77.5	31.2	**40**
25 July – 4 August 2007	124.9	72.1	**58**	124.9	46.9	**38**

CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

6.1 CONCLUSIONS

The findings of the results from both datasets for July 2006 and July to August 2007 suggest that the predictions made by the ADMS 4 air quality modelling program grossly under predict the measured values and therefore create doubt on its effectiveness of use in industry. This compared to the literature findings where datasets used in the USA to evaluate and compare ADMS 4 to other models, found an under prediction of approximately 20%. It would seem the biggest contributory factor to the high level of under prediction is the unaccounted for presence of other industrial operations in close proximity of the test region, that also produce SO_2 emissions. The fact that their emission data was not entered into the overall model database made the final results inaccurate, compared to the true dispersion that was actually present over the region at the time.

Here specific reference is made to the abundant coal mining operations present, of which the most are open cast mining operations, due to the fact that the coal seams lie close to the ground surface. Several of these operations have large coal dumps situated on site where spontaneous combustion of the coal occurs, or present underground coal mine fires exist, emitting SO_2 at low levels within the boundary layer atmosphere. Other larger SO_2 emitters that have without a doubt skewed the results of the study are the petrochemical refineries, as well as the two steel plants east and west of Witbank. These plants' emissions data are not readily available to the public due to the sensitive nature of the pollution and potential legal implications that might follow if made public.

A third source of fugitive emissions are the informal settlements burning coal for heating and cooking purposes and where low level SO_2 emissions are released into the boundary layer of the atmosphere. Had these source emissions data been available and been entered into the model, a more representative prediction would most probably have been achieved and a more accurate simulation to the pollution roses been found.

6.2 RECOMMENDATIONS

For this model to find practical use or implementation, it is suggested that each manufacturing industry in the Eastern Highveld region that emits any one of the primary air quality pollutants from its process, by law test, monitor and submit their annual emissions to a central, regional air quality database.

With government agency monitored data from strategically placed stations in the area, monitoring the region's informal housing establishments as well as veldt fires that occur from time to time, would produce a more accurate footprint of the region's annual pollutant volumes and patterns. This would facilitate the effective implementation and use of air quality models, like the ADMS 4 model, to further predict the expected effects of rogue emissions, or unplanned releases that might occur by industry in the future.

Furthermore, as the regions' industries evolve or develop, the presence of an existing network of monitoring stations and regular model usage would create effective control and policing of the regions' air quality levels. This would have dual benefit to industry by utilising air quality model technology to develop programs that will assist them to put control measures in place, or further develop their processes to counteract their emissions.

CHAPTER 7

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