APPENDIX Q –

ATMOSPHERIC DISPERSION SIMULATION METHODOLOGY

Dispersion Model Selection

Dispersion models compute ambient concentrations as a function of source configurations, emission strengths and meteorological characteristics, thus providing a useful tool to ascertain the spatial and temporal patterns in the ground level concentrations arising from the emissions of various sources. Increasing reliance has been placed on ground level air pollution concentration estimates from models as the primary basis for environmental and health impact assessments, risk assessments and determining emission control requirements. Care was therefore taken in the selection of a suitable dispersion model for the task at hand. For the current study, it was decided to use the US Environmental Protection Agency's CALMET meteorological model and the CALPUFF dispersion model in combination.

Most regulatory dispersion models, such as the widely used Industrial Source Complex (ISC) model and the relatively new AERMOD model, are based on the steady-state plume assumption, with meteorological inputs for these models assuming a horizontally uniform flow field. Usually the winds are derived from a single point measurement, which is often made at a nearby non-complex terrain site. The meteorological processors for the regulatory models do not adjust the winds to reflect terrain effects. The steady-state flow fields either do not or only partially reproduce the terrain-induced spatial variability in the wind field. In addition to which, the straight-line trajectory assumption of the plume models cannot easily handle curved trajectories associated with terrain-induced deflection or channelling. These limitations of plume models can significantly affect the models ability to correctly represent the spatial area of impact from sources in complex terrain, in addition to the magnitude of the peak values in certain instances.

CALPUFF is a regional Lagrangian Puff model suitable for application in modelling domains of 50 km to 200 km. Due to its puff-based formulation the CALPUFF model is able to account for various effects, including spatial variability of meteorological conditions, dry deposition and dispersion over a variety of spatially varying land surfaces. The simulation of plume fumigation and low wind speed dispersion are also facilitated.

CALPUFF requires as a minimum the input of hourly average surface meteorological data. In order to take full advantage of the model's ability to simulate spatially varying meteorological conditions and dispersion within the convective boundary layer it is, however, necessary to generate a three-dimensional wind field for input to the CALPUFF model. The CALMET model may be used to generate such a three-dimensional wind field for input to the CALPUFF model.

The CALMET meteorological model contains a diagnostic wind field module that includes parameterized treatments of terrain effects, including slope flows, terrain channelling and kinematic effects, which are responsible for highly variable wind patterns. CALMET uses a two-step procedure for computing wind fields. An initial guess wind field is adjusted for terrain effects to produce a Step 1 wind field. The user specifies the vertical layers through which the domain wind is averaged and computed, and the upper air and surface meteorological stations to be included in the interpolation to produce the spatially varying guess field. The Step 1 (initial guess) field and wind observational data are then weighted through an objective analysis procedure to produce the final (Step 2) wind field. Weighting is undertaken through assigning a radius of influence to stations, both within the surface layer and layers aloft. Observational data are excluded from the interpolation if the distance between the station and a particular grid point exceeds the maximum radius of influence specified (EPA, 1995b; Scire and Robe, 1997; Robe and Scire, 1998).

By using CALMET and CALPUFF in combination it is possible to treat many important complex terrain effects, including spatial variability of the meteorological fields, curved plume trajectories, and plume-terrain interaction effects. Maximum hourly average, maximum daily average and annual average concentrations will be simulated through the application of CALPUFF, using as input the relevant emissions data and the three-dimensional CALMET data set.

Chemical Transformation Modelling

CALPUFF allows for first order chemical transformation modelling to determine gas phase reactions for SO_x and NO_x. Chemical transformation rates were computed internally by the model using the RIVAD/ARM3 Scheme. This scheme allows for the separate modelling of NO_2 and NO, whereas the default MESOPUFF II Scheme only makes provision for the combined modelling of NO_x. The RIVAD/ARM3 scheme treats the NO and NO_2 conversion process in addition to the NO_2 and total NO_3 and SO_2 to SO_4 conversions, with equilibrium between gaseous HNO_3 and ammonium nitrate aerosol. The scheme uses user-input ozone data (together with modelled radiation intensity) as surrogates for the OH concentration during the daytime when gas phase free radical chemistry is active.

Dispersion Model Data Requirements

Receptor Locations and Modelling Domain

The meteorology was modelled and the dispersion of pollutants simulated for an area covering ~50 km (east-west) by 50 km (north-south), with ambient ground-level concentrations and deposition levels being simulated for over 2500 receptor points. The regular Cartesian receptor grid selected has a resolution of 1000 m by 1000 m. Discrete receptor points were specified for each of the off-site monitoring locations to facilitate the simulation of concentrations and deposition at these locations for application in the validation and calibration of the model.

Meteorological Data Inputs

CALMET was used to simulate the wind field within the study area. Upper air data required by CALMET includes pressure, geopotential height, temperature, wind direction and wind speed for various levels. No upper air readings exist for the region with the nearest station located in Pietersburg. Use was therefore made of ETA model data obtained from the SAWS. Twice daily data are available for five sounding levels. The closest ETA data point to the Matimba Power Station is ~20 km northwest. The initial guess field in CALMET was therefore determined as a combined weighing of surface winds at three surface weather stations, vertically extrapolated using Similarity Theory (Stull, 1997) and the upper air winds. Surface data from the Ellisras Weather Service Station was included together with the data from two, Eskom monitoring stations (i.e. Zwartwater and Grootstryd).

The CALMET meteorological model requires hourly average surface data as input, including wind speed, wind direction, mixing depth, cloud cover, temperature, relative humidity, pressure and precipitation. The mixing depth is not readily measured and needed to be calculated based on readily available data, viz. temperature and predicted solar radiation. The daytime mixing heights were calculated with the prognostic equations of Batchvarova and Gryning (1990), while night-time boundary layer heights were calculated from various diagnostic approaches for stable and neutral conditions.

The data availability for the surface and upper are data used in the current study is given in Table B-1.

Table B.1 Data availability for surface and upper air data for the period 2001 to 2003.

Data	Station	Period		
		2001	2002	2003
Surface data	Ellisras	100%	100 %	100 %
	Zwartwater(1)	64%	90 %	69%
	Grootstryd(2)	0 %	0 %	100 %
Upper air data	ETA	100 %	42 %	76%

Notes:
The Zwartwater monitoring station was decommissioned in October 2003.
The Grootstryd monitoring station was started in October 2003.

A three dimensional meteorological data set for the region was output by the CALMET model for application in the CALPUFF model. This data set parameterised the spatial (horizontal and vertical) and temporal variations of parameters required to model the dispersion and removal of pollutants, including: vertical wind speed, wind direction, temperature, mixing depths, atmospheric stability, (etc.). Meteorological parameters were projected at various heights above the ground, viz.: 20m, 200m, 500m, 1500m, and 3000m. In projecting vertical changes in the windfield, temperature (etc.) it was possible to accurately parameterize the atmospheric conditions characteristic of within valley layers, transitional layers and atmospheric layers located above the terrain. The three-dimensional data set was generated for the base-case years selected (2001 to 2003) and comprised hourly averages for each parameter thus providing information for each time interval required by the non-steady state CALPUFF dispersion model.

Source and Emissions Data Inputs

Source parameter requirements for input into the CALPUFF model include stack height, diameter, exit temperature, exit velocity, elevation of stack base above sea level and co-ordinates. Emissions per sources are also required as input to the model (see Section 4 for input source data for the current study).

Model Accuracy and Verification

Comparisons between CALPUFF results, and results generated by the Industrial Source Complex Model Short Term version 3 (ISCST3) model, have shown that CALPUFF is generally more conservative (Strimatis et al., 1998). The ISC model typically produces predictions within a factor of 2 to 10 within complex topography with a high incidence of calm wind conditions. When applied in flat or gently rolling terrain, the USA-EPA (EPA 1986) considers the range of uncertainty of the ISC to be -50% to 200%. CALPUFF predictions have been found to have a greater correlation with observations, with more predictions within a factor of 2 of the observations when compared to the ISC model (Strimatis et al., 1998). It has generally been found that the accuracy of off-the-shelf dispersion models improve with increased averaging periods. The accurate prediction of instantaneous peaks are the most difficult and are normally performed with more complicated dispersion models specifically fine-tuned and validated for the location. The duration of these short-term, peak concentrations are often only for a few minutes and on-site meteorological data are then essential for accurate predictions.

In order to assess whether the dispersion model selected and populated is predicting in the correct order of magnitude, dispersion model results are compared to air pollutant concentrations measured at air quality monitoring stations.

Validation of Dispersion Model Results

In order to validate the dispersion model results predicted sulphur dioxide concentrations were compared to measured concentrations from the various monitoring stations (Tables B.2 and B.3). Predicted concentrations and frequencies of exceedance were found to significantly exceed measured concentrations at all monitoring stations indicating that the dispersion model was overpredicting.

The margin of accuracy of the CALPUFF model is typically in the range of –50% to +200% (i.e. ranging from underpredicting by 50% to overpredicting by 200%). Predicted concentrations as a fraction of measured concentrations would therefore be anticipated to be in the range of 0.5 to 2.0. From Table B.3 it is evident that the model significantly overpredicted concentrations at most monitoring sites, particularly sites located in the near field. The model overpredicted both the magnitude of concentrations and the frequency of air quality limit exceedances. The reasons for the model overpredicting could not be ascertained despite an extended investigation. There are three main reasons why predictions would significantly deviate from measured results: (i) source and emissions data were not adequately characterised, (ii) ambient measurements are questionable, (iii) the model is not accurately parameterising the prevailing atmospheric dispersion. Steps taken to check, and if necessary improve, model accuracy are described below.

Accuracy of source and emissions data – The stack parameters for existing Matimba Power Station operations were confirmed. Stack monitoring data were obtained from a one year stack monitoring campaign conducted by Wits University personnel on one of the six flues. Emission concentrations from all flues were given as being similar. Comparisons between the emissions data generated on the basis of coal qualities and quantities and the measured emissions served to confirm that the measured sulphur dioxide emission rates were higher than those estimated. The estimated emissions were therefore not an overestimate of actual releases. Measured diurnal variations in stack emissions were also used in subsequent dispersion modelling in an attempt to improve the correlation between predictions and measurements.

Accuracy of ambient air quality monitoring data - Initially reference was only made to the Zwartwater and Grootstryd monitoring data sets. During the investigation additional ambient air quality monitoring data were obtained to check the model accuracy including the M1 – M5 monitoring campaign data, the RON1 – RON10 passive diffusive monitoring station data, the University of Witwatersrand caravan data (only 1 month available) and the Waterberg monitoring campaign data. All the ambient air quality monitoring data served to indicate that the dispersion model was overpredicting.

Table B.1 Predicted and measured sulphur dioxide concentrations during baseline operations

PREDICTED Sulphur Dioxide Concentrations	Station	Highest hourly (µg/m³)	Highest Daily (µg/m³)	Annual Average (µg/m³)	Frequency of Exceedance (%) of Hourly Limit of 350 µg/m³	Frequency of Exceedance (%) of Daily Limit of 125 µg/m³
	Grootstryd	1385	217	37	4.38	6.3
	Zwartwater	1006	167	27	2.90	2.5
	Waterberg	525	98	9	0.17	0.0
	M1	249	35	2	0.01	0.0
	M2	1775	180	33	3.13	5.8
	M3	2071	219	23	2.15	5.2
	M4	713	103	19	0.74	0.3
	RON1	1431	233	37	4.45	6.3
	RON3	404	70	10	0.05	0.0
	RON4	595	72	5	0.15	0.0
	RON5	945	199	16	0.74	1.1
	RON6	952	120	21	1.06	1.1
	RON7	740	120	11	0.32	0.3
	RON8	949	104	4	0.24	0.3
	RON9	461	58	4	0.24	0.0
	RON10	401	38	2	0.05	0.0
	CARAVAN	1821	183	19	1.04	3.0
MEASURED Sulphur Dioxide Concentrations	**Station**	**Highest hourly (µg/m³)**	**Highest Daily (µg/m³)**	**Annual Average (µg/m³)**	**Frequency of Exceedance (%) of Hourly Limit of 350 µg/m³**	**Frequency of Exceedance (%) of Daily Limit of 125 µg/m³**
77% avail. over 1.5 years	Grootstryd	620	103	14.0	0.08	
55% over 2.5 yrs	Zwartwater	825	98	14.1	0.07	
69% over 5 yrs	Waterberg	565	99	16.1	0.03	0.0
Aug 1991 to Jan 1992	M1	398	72	10.6	0.03	
Aug 1991 to Jan 1992	M2	560	69	14.8	0.02	
Aug 1991 to Jan 1992	M3	806	176	19.0	0.23	2.19
Aug 1991 to Jan 1992	M4	487	87	13.4	0.03	
Dec 2004 – Oct 2005	RON1			6.5		
Dec 2004 – Oct 2005	RON3			10.5		
Dec 2004 – Oct 2005	RON4			2.2		
Dec 2004 – Oct 2005	RON5			6.9		
Dec 2004 – Oct 2005	RON6			11.3		
Dec 2004 – Oct 2005	RON7			6.1		
Dec 2004 – Oct 2005	RON8			5.6		
Dec 2004 – Oct 2005	RON9			5.6		
Dec 2004 – Oct 2005	RON10			2.6		
16 June - 10 July 2006	CARAVAN	172	33			

Table B.3 Predicted sulphur dioxide concentrations during baseline operations given as a fraction of the measured sulphur dioxide concentrations (significant overpredictions indicated in bold print)

PREDICTED as a fraction of the MEASURED	Station	Highest hourly (fraction)	Highest Daily (fraction)	Annual Average (fraction)	Frequency of Exceedance of Hourly Limit (fraction)	Frequency of Exceedance of Daily Limit (fraction)
	Grootstryd	**2.2**	**2.1**	**2.6**	55.5	
	Zwartwater	1.2	1.7	1.9	39.5	
	Waterberg	0.9	1.0	0.6	6.4	
	M1	0.6	0.5	0.2	0.4	
	M2	**3.2**	**2.6**	**2.3**	128.6	
	M3	**2.6**	1.2	1.2	9.4	2.4
	M4	1.5	1.2	1.4	23.9	
	RON1			**5.7**		
	RON3			0.9		
	RON4			**2.5**		
	RON5			**2.3**		
	RON6			1.9		
	RON7			1.8		
	RON8			0.8		
	RON9			0.8		
	RON10			0.9		

Improvement of meteorological input data to dispersion model – Due to the region being located a significant distance from the nearest upper air station, the decision was taken to purchase ETA model data from the South African Weather Services to improve the model's characterisation of airflow, temperature (etc.) variations with height.

Given the accuracy of the source and emissions data used as input to the model, and the relative consistency of the measured concentrations it was concluded that the model was not accurately parameterising the atmospheric dispersion potential of the region despite the improved meteorological input dataset. The decision was therefore taken to apply a correction factor of 0.5 to the dispersion model results. Predicted sulphur dioxide concentrations, given the implementation of a correction factor of 0.5, are compared to measured concentrations from the various monitoring stations in Tables B.4 and B.5.

Table B.4 Predicted and measured sulphur dioxide concentrations during baseline operations (given correction factor of 0.5 for model predictions)

PREDICTED Sulphur Dioxide Concentrations	Station	Highest hourly (µg/m³)	Highest Daily (µg/m³)	Annual Average (µg/m³)	Frequency of Exceedance (%) of Hourly Limit of 350 µg/m³	Frequency of Exceedance (%) of Daily Limit of 125 µg/m³
	Grootstryd	693	109	18	0.95	0.0
	Zwartwater	503	84	13	0.50	0.0
	Waterberg	262	49	5	0.00	0.0
	M1	125	17	1	0.00	0.0
	M2	888	90	17	0.88	0.5
	M3	1036	110	12	0.48	0.3
	M4	356	52	9	0.06	0.0
	RON1	715	117	19	0.90	0.0
	RON3	202	35	5	0.00	0.0
	RON4	298	36	3	0.01	0.0
	RON5	473	99	8	0.15	0.0
	RON6	476	60	11	0.09	0.0
	RON7	370	60	5	0.05	0.0
	RON8	475	52	2	0.06	0.0
	RON9	230	29	2	0.00	0.0
	RON10	201	19	1	0.00	0.0
	CARAVAN	911	91	9	0.23	0.3
MEASURED Sulphur Dioxide Concentrations	**Station**	**Highest hourly (µg/m³)**	**Highest Daily (µg/m³)**	**Annual Average (µg/m³)**	**Frequency of Exceedance (%) of Hourly Limit of 350 µg/m³**	**Frequency of Exceedance (%) of Daily Limit of 125 µg/m³**
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Dec 2004 – Oct 2005	RON5			6.9		
Dec 2004 – Oct 2005	RON6			11.3		
Dec 2004 – Oct 2005	RON7			6.1		
Dec 2004 – Oct 2005	RON8			5.6		
Dec 2004 – Oct 2005	RON9			5.6		
Dec 2004 – Oct 2005	RON10			2.6		
16 June - 10 July 2006	CARAVAN	172	33			

Table B.5 Predicted sulphur dioxide concentrations during baseline operations given as a fraction of the measured sulphur dioxide concentrations (given correction factor of 0.5 for model predictions) (significant over or under predictions indicated in bold print)

PREDICTED as a fraction of the MEASURED	Station	Highest hourly (fraction)	Highest Daily (fraction)	Annual Average (fraction)	Frequency of Exceedance of Hourly Limit (fraction)	Frequency of Exceedance of Daily Limit (fraction)
	Grootstryd	1.1	1.1	1.3	**12.0**	
	Zwartwater	0.6	0.9	1.0	**6.8**	
	Waterberg	0.5	0.5	**0.3**	0.0	
	M1	**0.3**	**0.2**	**0.1**	0.0	
	M2	1.6	1.3	1.1	**36.2**	
	M3	1.3	0.6	0.6	**2.1**	**0.1**
	M4	0.7	0.6	0.7	1.8	
	RON1			**2.9**		
	RON3			0.5		
	RON4			1.2		
	RON5			1.1		
	RON6			0.9		
	RON7			0.9		
	RON8			**0.4**		
	RON9			**0.4**		
	RON10			**0.4**		