The application of photochemical modelling for the City of Johannesburg AQMP

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Municipalities are required to develop an Air Quality Management Plan (AQMP) in order to work towards mitigating the negative impacts of air quality on human health and the environment. The 2016 AQMP for the City of Johannesburg (CoJ) incorporated photochemical modelling to assist in air quality “hotspot” and scenario analyses. The complex emission source profile of CoJ (like many urban areas) necessitated the use of a one-atmosphere chemistry model. The Comprehensive Air Quality Model with Extensions (CAMx) photochemical model was used to accomplish this. A regional and CoJ specific emissions inventory was developed for both management and modelling purposes; which fed into the model hotspot analysis (also as a baseline) and the basis of the scenarios. This paper will present the various methodologies employed to effectively apply CAMx in CoJ, results and strengths and limitations encountered in the process.

Keywords: Air quality management, modelling, emissions, Johannesburg

1. Introduction

As specified by the Air Quality Act (Section 15(2)) municipalities are required to develop an Air Quality Management Plan (AQMP) in order to work towards mitigating the negative impacts of air quality on human health and the environment. Prior to any regulatory requirement the City of Johannesburg (CoJ) developed an AQMP in 2003; which laid the general foundation for accomplishing many air quality related tasks to ensure improved air quality. The 2003 AQMP did not however include air quality modelling.

The 2016 AQMP for CoJ incorporated photochemical modelling to assist in air quality “hotspot” analysis. The complex emission source profile of CoJ (like many urban areas) necessitated the use of a “one-atmosphere” chemistry model to account for accurate transformation and interactions of the various pollutants within a single simulation (hence the term “one-atmosphere” as opposed to dispersion model simulations which are often separated by source categories). A similar study was done by Lourens et al., (2015) which applied a photochemical box model (MECCA-MCM; Butler 2009); in which while a comprehensive near explicit chemical mechanism was utilized, much of the meteorology and emissions remained static. Therefor chemistry in the model is handled well while emissions characterization and transport was not. The MECCA-MCM simulated NOx and ozone to a reasonable degree however input and thus output was spatially (and temporally to a large extent) aggregated. The spatial aspect was required for the 2016 AQMP for CoJ and the Comprehensive Air Quality Model with Extensions (CAMx) photochemical model was used to accomplish this (www.camx.com; Ramboll-Environ, 2016). A regional and CoJ specific emissions inventory was developed for both management and modelling purposes with a base year of 2014, which fed into the hotspot analysis. This paper discusses the various methodologies employed to effectively apply CAMx in CoJ, results and strengths and limitations encountered in the process.

2. Methods

CAMx requires gridded and temporally representative emissions, meteorology, boundary conditions and photolysis rates. This input must be prepared for all modelling domains; ideally at the domain native resolutions (coarse domain input can be interpolated finer however this is not ideal). Figure 1 shows the model domains used for the CoJ AQMP.

The 3 km resolution domain captures regional transport of pollutants to ensure inter-municipality impacts are represented; while a finer 1 km resolution nest resolves detailed urban scale features of dispersion and chemistry. CAMx incorporates two-way nesting such that mass is conserved within the parent domain (important for nesting in air quality models).

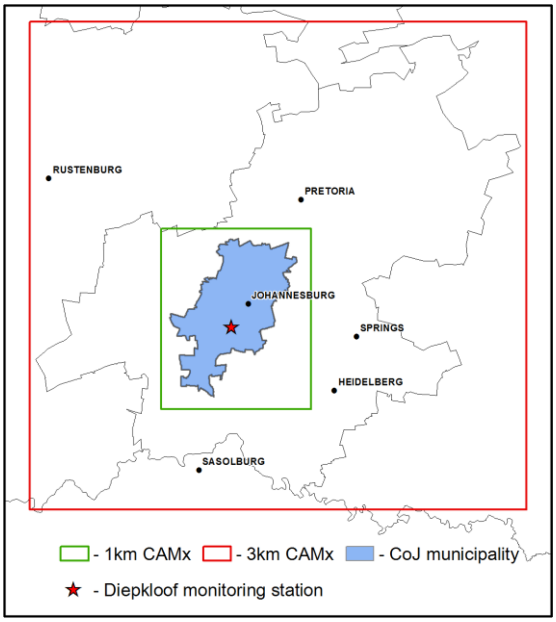

Figure 1: CAMx model domains and location of monitoring station used for validation

2.1 Meteorology

The Weather Research and Forecasting model (WRF-ARW 3.8.1; Skamarock et al., 2008) was used to simulate meteorological data for use in air quality modelling, but also feeding into dust and biogenic VOC emissions modelling. WRF was configured to run over three domains at 9km, 3km and 1km resolutions with 30 vertical layers. The 3 km and 1 km resolution nests were positioned over each of the corresponding CAMx domains (though larger in extent) while the synoptic scale 9km resolution parent domain extended over South Africa. WRF initialization and boundary conditions are specified by the National Centers for Environmental Prediction (NCEP) Climate Forecast System (CFS) version 2 (Saha et al., 2011). Data assimilation was not used for this WRF run. WRF simulations were compared to observations at five stations around Gauteng (OR Tambo airport, Lanseria airport, Rand airport, Wonderboom airport and Johannesburg Botanical Gardens). On average, across all sites, WRF over-estimates hourly temperature (by 2.17 ^{o}C) and wind (U by 1.68 m/s; V by 2.15 m/s). WRF also over-estimates rainfall at the two sites where rainfall data was available (OR Tambo and Johannesburg Botanical Gardens).

2.2 Emissions

A comprehensive emissions inventory was developed for the base year 2014; with the following sources included for modelling:

- Biogenic VOC
- Biomass burning
- Airports aircraft LTO (landing and take-off)
- Household fuel combustion
- Wind-blown dust from tailings facilities
- Industrial sources
- On-road vehicles.

2.2.1 Biogenic VOC

BVOC were modelled using the Model of Emissions of Gases and Aerosols from Nature (MEGAN; Guenther et al., 2006). Input comprised of plant functional types (using MODIS MCD12Q1), leaf area index (using MODIS MCD15A2H) and meteorological parameters (such as rainfall and temperature) from the WRF simulations. Output includes speciated hourly BVOC emission rates for both model domains.

2.2.2 Biomass burning

Emissions from fires were derived from the Fire Inventory from NCAR (FINN) (Wiedinmyer et al., 2011). The FINN inventory is a dataset of daily emissions from biomass burning with a global coverage at 1 km resolution. The location and timing of fires are provided by the MODIS instrument aboard the NASA Terra and Aqua polar orbiting satellites. The MODIS also provides information on the vegetation burnt allowing for the classification of vegetation type and matching them to the available global fuel loadings and emissions factors. Emissions factors used are taken from Andreae and Merlet (2001) and Akagi et al. (2013). Emissions of CO, PM, NOx, NH_3, SO_2, CH_4, CO_2, Hg, HCN as well as VOC speciated for commonly used air quality modelling chemical mechanisms are included in the datasets. The 1 km resolution means that smaller fires are not captured and thus this sector may be under-estimated.

2.2.3 Airports aircraft LTO

Due to the presence of large airports in the region this is a potentially high intensity source of NOx, VOC and PM. Emissions only from aircraft LTO are considered. At minimum level of aircraft activity is required to estimate emissions. To date LTO information from Lanseria airport (a private airport) is unavailable. Detailed LTO activity was available for OR Tambo through communications with airports operations personnel. This included LTO for international, domestic and regional flights; and included aircraft models/types. Emission factors for these aircraft were derived from International Civil Aviation Organization publications (ICAO, 2011). The lack of data from Lanseria airport means NOx emissions for the CoJ will be under-estimated. However NOx emissions estimated for OR Tambo are significant at 3984.32 tons per annum and will impact Ekurhuleni.

2.2.4 *Household fuel combustion*

Emissions due to household use of paraffin, LPG, coal and wood were estimated using a top-down approach. An estimate for fuel consumption was based on the annual published DOE energy balance data (DOE, 2012; available online). Census 2011 energy household energy preference information is then used to proportionally disaggregate the national consumption down to Small Area Levels (SAL). Fuel consumption at SAL was then further spatially disaggregated using Spot Building Count (SBC) spatial database developed by Eskom and CSIR; which is based on SPOT 5 satellite 2.5 m national coverage (Mudau, 2010). In terms of emission factors, a mix of those from Makonese et al. (2015) and the US EPA AP-42 database were used. The use of national energy balance derived fuel consumption and Census 2011 information introduces uncertainty. A bottom-up approach may yield better results but this requires targeted surveying of communities within the CoJ.

2.2.5 *Wind-blown dust*

This emissions sector was made up of 12 tailing storage facilities (TSFs) around Gauteng; identified as particularly problematic. Emission rates of wind-blown dust from these TSFs were estimated using the ADDAS model (Burger et al., 1997; Burger, 2010 and Liebenberg-Enslin, 2014). This model is based on the dust emission scheme of Marticorena and Bergametti (1995) and Shao et al. (2011). The model inputs include material particle density, moisture content, particle size distribution and site specific surface characteristics such as whether the source is active or undisturbed. Soil sampling and particle size distribution analysis were done for 10 TSFs and the results were used to further constrain the model. WRF meteorological output provided the model with wind speed, wind direction and temperature. Thus ADDAS was forced with hourly meteorological fields; which meant that wind gusts are unaccounted for. This means it is likely that wind-blown dust emissions from the TSFs are under-estimated.

2.2.6 *Industrial sources*

The focus of this sector was on industrial emitters within CoJ but also those in neighbouring municipalities (particularly those close to the borders). For listed activity sources within CoJ, emission estimates were derived from emission reports (sourced from CoJ officials and GDARD) or if those were not available the Minimum Emissions Standards (MES) from the respective Atmospheric Emissions Licenses (AEL) were used. It was possible to estimate emissions for 37 listed activity sources. In terms of controlled emitters (small boilers in this case) emissions for only 8 of the identified 52 could be estimated. For listed activity sources outside CoJ 33 of the 140 facilities identified were estimated (using any publicly available information such as EIAs). While it is likely that an under-estimation of emissions from industrial sources is possible due to not all sources being quantified, the use of an MES as a representative industrial emission rate will be an over-estimate. These uncertainties non-withstanding it is unsurprising that the bulk of industrial emissions are due to Kelvin power-station with 76% NOx and 88% SO_2 contributed to the industrial sector.

2.2.7 *On-road vehicles*

Emissions were estimated for private passenger, commercial passenger, public transport and freight vehicles operating on Gauteng roads. The Gauteng Strategic Travel Demand Model (GSTDM) was used to derive Vehicle Kilometres Travelled (VKT) and vehicle speed on road classes 1-3, i.e. secondary roads were not included. The TDM is able to spatially capture VKT in an appropriate manner in terms of allocation to the different roads. Hot running (i.e. thermally stabilized engine and exhaust treatment) emission factors are derived from the COPERT 4 (version 11.3) model. Secondary roads are not included as the GSTDM is a macroscale model designed to evaluate travel demand and movement on a provincial scale. As a result, emissions are under-estimated.

Figure 2 shows the relative contribution of each source sector to total NOx, SO_2, NMVOC and PM_{10} within the boundaries of CoJ. As such LTO emissions from OR Tambo are not included in the figure.

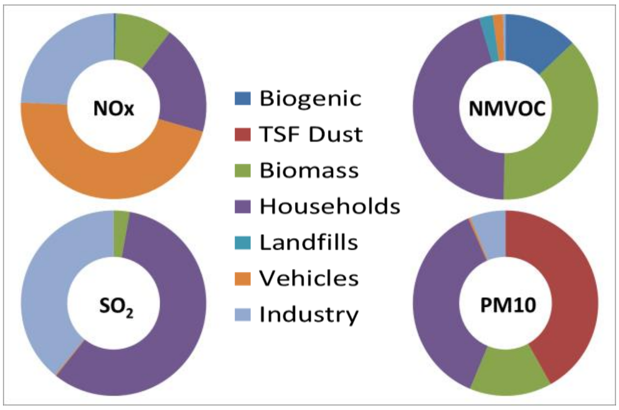

Figure 2: Relative source contribution to criteria pollutants within the emissions inventory

2.3 Initial and boundary conditions

CAMx was run for each month in parallel, i.e. all 12 months are run at once. A spin-up period of 3 days was used prior to the start of each month. Thus, initial conditions are required at the start of the 3-day spin-up. Similarly, boundary conditions are required for the 3 km resolution domain since CAMx is a limited area model and pollutants entering the domain need to be specified on an hourly basis. For the CAMx runs both initial and boundary conditions on the Model for Ozone and Related Chemical Tracers (MOZART-4; Emmons et al., 2010) output provided to the WRF-Chem community via the NCAR Atmospheric Chemistry, Observations and Modelling (ACOM) MOZART download page (http://www.acom.ucar.edu/wrf-chem/mozart.shtml).

2.4 Photolysis rates

Photolysis rates are estimated using the NCAR TUV radiative transfer model with lookup tables for the photochemical reactions to be considered for CAMx (in this case those specified by Carbon Bond 2005). Absorption due to total column ozone is considered in TUV and is derived from Ozone Monitoring Instrument (OMI) data. CAMx then also modifies absorption (and then photolysis rates) due to simulated aerosols.

3. Results

3.1 Model validation

Model output was compared to the only station within CoJ with good data coverage for 2014, i.e. the Diepkloof station (see Figure 1) run by DEA as part of the Vaal Triangle Airshed Priority Area network. The station is heavily impacted by vehicle emissions and domestic fuel burning and has the potential to be impacted by the Mooifontein TSF if threshold wind speeds and direction towards the station has occurred.

Table 1. Statistics for NO_2, PM_{10}, SO_2 and ozone at Diepkloof.

Pollutant	NO_2	O_3	PM_{10}	SO_2
% data	81	83	81	71
Ave Obs (model units)	22	33	40	5.2
Ave CAMx (model units)	5.8	37	24	3.8
FAC2[1] (Fraction)	0.11	0.71	0.37	0.42
NMB[2] (%)	-75	14	-42	-26
NMGE[3] (%)	77	46	72	86
r	0.46	0.45	0.07	0.07

[1] Fraction of the predictions within a factor of two of the observed values (1.0 = perfect)

[2] Mean bias between predictions and observations and then normalized by observations

[3] Absolute mean bias between prediction and observation and then normalized by observations

NO_2 is heavily under-estimated at Diepkloof. This is primarily due to the lack of secondary roads within the TDM. In terms of absolute differences, the NMGE shows that differences between model and observed are small for ozone with a slight over-estimation. In terms of timing of simulated concentrations, NO_2 and ozone are simulated reasonably well, as these are governed primarily by photochemistry (i.e. sunlight), while more fine scale sources such as those impacting ambient SO_2 and PM10 are not timed well at Diepkloof. The model simulates a later evening PM_{10} peak than observed and does not simulated a midday SO_2 peak (graphs not shown here). Both PM_{10} and SO_2 are also under-estimated with SO_2 performing better.

Figure 3 shows the temporal characteristics of ozone measurements at Diepkloof compared to those simulated by CAMx. While the diurnal timing of peak ozone is captured, the model simulates higher night-time ozone. In terms of monthly variation, the model simulates a higher average in general (contributed by the night-time over estimation) though particularly so for the first half of the year.

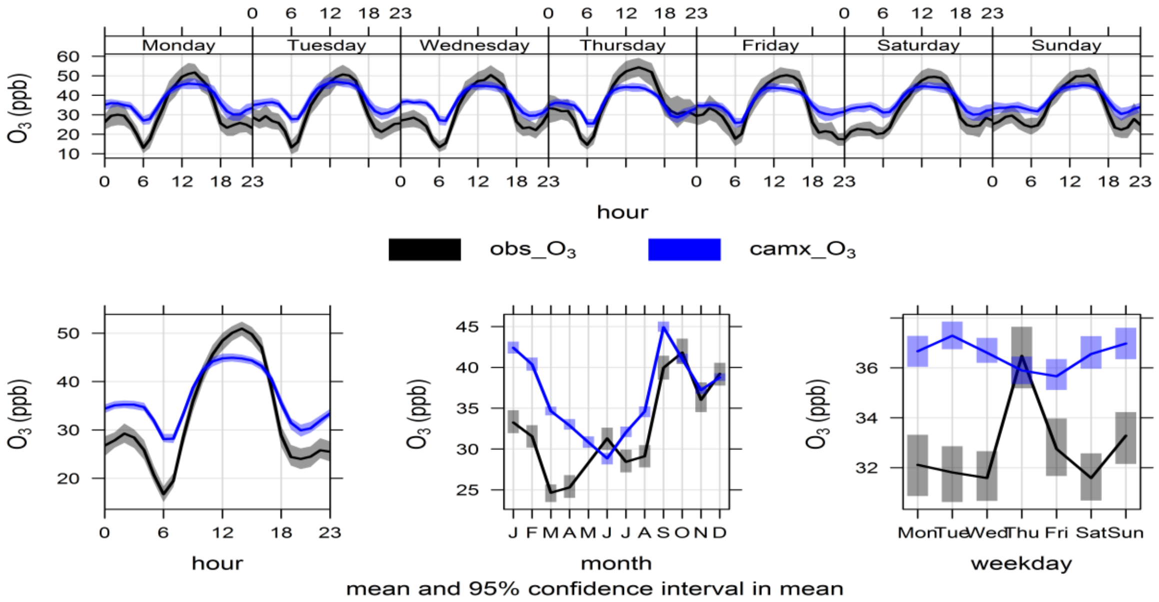

Figure 3: Time variation plot of ozone comparing modelled vs observed at Diepkloof

3.1 Pollution “hot-spots”

Spatial plots of averaged model concentrations show various pollutant “hot-spots” around the CoJ. Presented here are plots of NO_2, ozone, PM10 and SO_2 at averaging periods relevant to national ambient guidelines.

Figure 4 shows the 99th percentile of hourly concentrations for a year for NO_2. Concentrations are highest around heavier traffic zones but also around Kempton Park. This is due to OR Tambo airport and Kelvin power station emissions. This area is simulated to exceed the national guideline of 106 ppb. While it is also very likely that the guideline is exceeded within CoJ, the under-estimation of NOx emissions due to TDM estimation do not allow to model to show this. However, the relative spatial distribution is clear.

Figure 5 shows modelled 99th percentile of 8-hour ozone. Ozone titration is clearly seen along major traffic routes (as well as the Kempton Park region) with ozone concentrations being higher between these routes. Due to higher NOx sources (particularly Kelvin power station) within the inventory around the east rand (Ekurhuleni), higher concentrations of ozone are modelled along the West Rand.

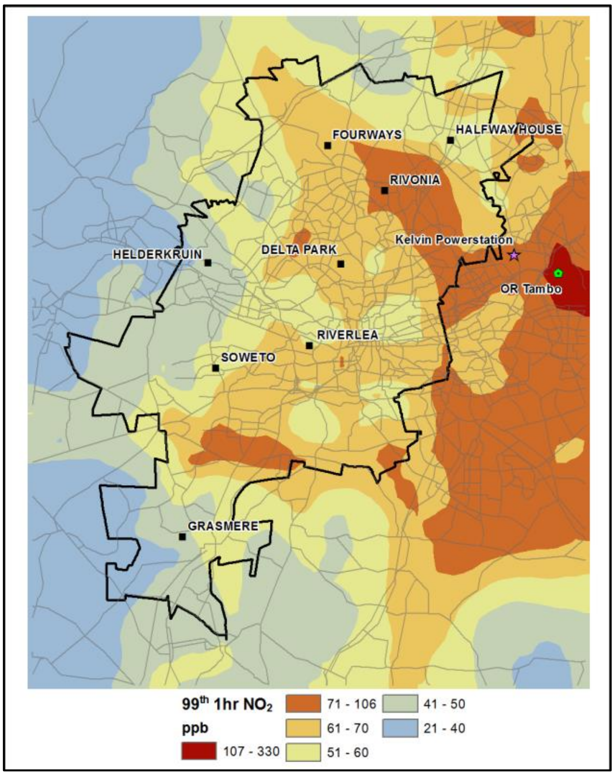

Figure 4: Modelled 99th percentile of hourly NO_2

Figure 6 shows modelled 99th of 24-hour averaged PM_{10}. A majority of the hotspots are around TSFs included in the emissions inventory. Others are found to be around heavier domestic fuel usage (according to Census 2011) of wood or coal (e.g. Tembisa, Thembalihle and Protea South).

A high concentration is modelled north of Tembisa due to the inclusion of a clamp kiln facility.

Figure 7 shows modelled 99th percentile of 24-hour average SO_2. A large region of high concentrations is centred on the Kempton Park region; and this is primarily due to the Kelvin power station. The hotspots simulated to the south of Johannesburg are due to domestic coal use (around Protea South and Thembalihle), a large brick kiln facility (south of Thembalihle) and traffic along the N12 (high density of diesel vehicles simulated by the TDM west of Protea South).

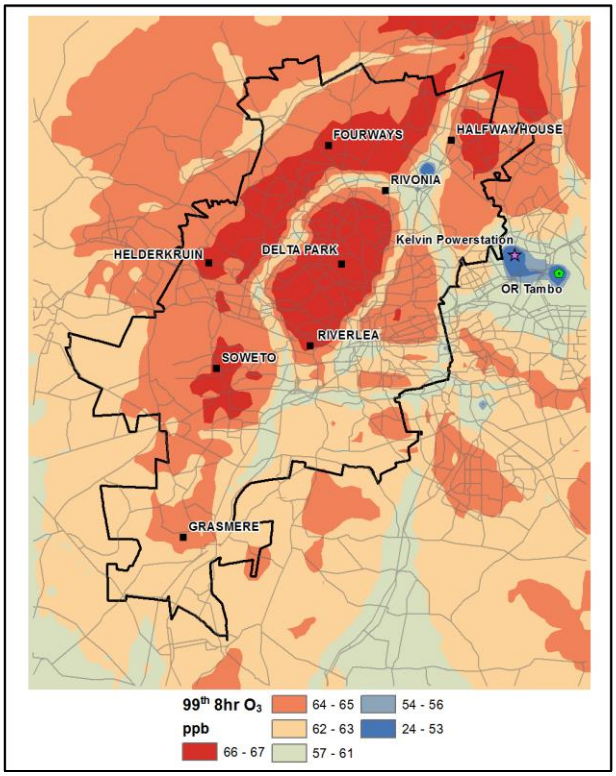

Figure 5: Modelled 99th percentile of 8-hourly ozone

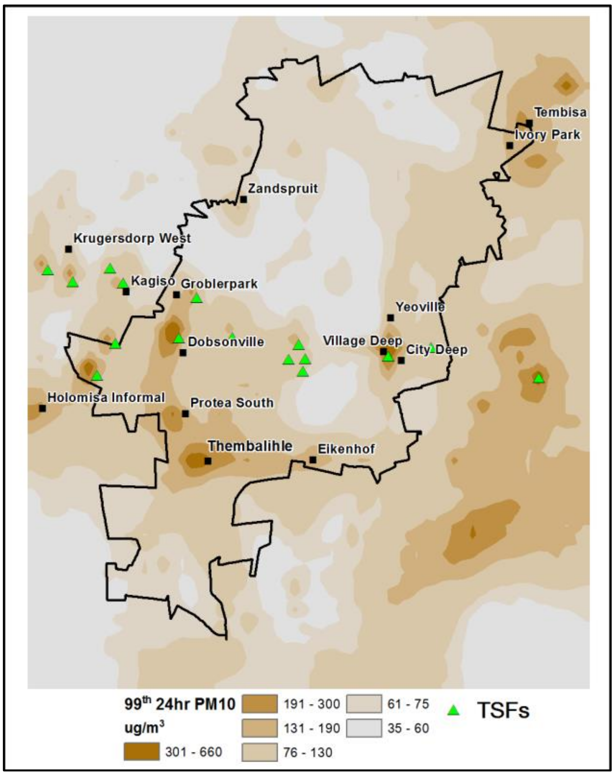

Figure 6: Modelled 99th percentile of 24-hour PM10 (TSFs shown as green triangles)

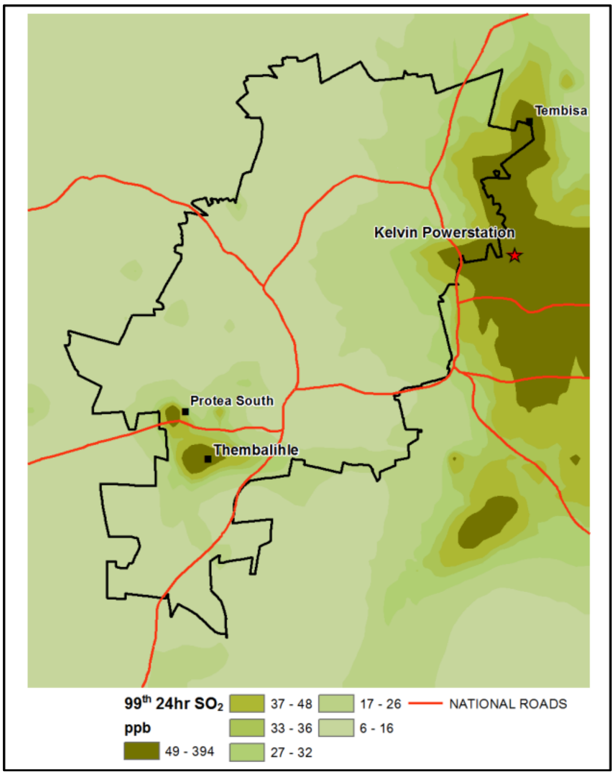

Figure 7: Modelled 99th percentile of 24-hour SO_2

4. Conclusions

The application of a photochemical air quality model to the development of an AQMP is useful in that a variety of sources are modelled as a "one-atmosphere" simulation. Chemical interactions and transformations are described within the model resolution and as such provide information regarding the area wide distribution of ambient air quality; which is what an AQMP is meant to address. In order to make use of such a tool, a comprehensive emissions inventory (spatially and temporally disaggregated) was required. This also resulted in the municipality wide emissions inventory being as comprehensive and descriptive as possible.

Much of the model uncertainty within the CoJ AQMP was due to under-estimating NOx emissions from traffic. This was domain wide; while a potential lack of industrial emissions also contributed to localized uncertainty (seen at Diepkloof for SO_2). Indeed, missing stationary sources would account for much localized under-estimations and a prime example would be the omission of Lanseria Airport LTO. These have great potential to contribute to NOx emissions in the area. These uncertainties notwithstanding, a spatial distribution of air quality due to domain wide sources was possible to simulate.

The role of traffic is clear even with the under-estimated NOx emissions. Busy routes are regions of higher NOx concentrations while these regions are also simulated to show lower ozone concentrations. Further away from these busy routes, ozone concentrations are simulated to be higher. Ozone thus has a potential to have limited areas of elevated concentrations due to the complex road network and possible interaction with biogenic VOC emissions from within the City. The region around Kelvin power station is also important for NOx as the station is a very high emitter with an elevated stack; while OR Tambo is also estimated to be a contributor to NOx in the area. The significance in an urban setting is high as these are extremely high NOx emitters in very close proximity to residential areas. This will impact human health; as well as chemistry of the area by promoting ozone formation further afield (i.e. away from these sources). This applies to SO_2 as well with local impacts due to SO_2 and potential PM impacts due to sulfate formation further away.

While the emissions inventory in the 2016 AQMP laid a solid foundation; individual emission sectors (particularly on-road vehicles and domestic fuel combustion) require further work to refine to a more representative point. This is an on-going effort and the City has an implementable plan to achieve this as laid out in the AQMP. An immediate benefit of using a photochemical model such as CAMx (as opposed to dispersion modelling) is that secondary pollutants are simulated in a consistent way; i.e. the model accounts for chemistry in a more realistic manner than simplistic parameterizations used in dispersion models. For example VOC oxidation impacts ozone formation and also results in secondary VOC which go further on to react. Atmospheric chemistry is important for arguably all criteria pollutants and thus to simulate ambient air quality these reactions need to be accounted for. The impact for example of Kelvin power station on both near field NOx concentrations and area wide ozone formation is simulated by CAMx. A similar consideration is necessary in accounting for both impacts on air quality in the immediate vicinity of high traffic zones as well as their regional effect on ozone. As progress is made in the emissions inventory work subsequent model studies utilizing photochemical air quality models will paint an even clearer picture.

5. Acknowledgments

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