The comparability of modelled concentrations using alternative meteorological datasets: A case study of SO_2 dispersion from a large stationary source

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The Department of Environment Affairs (DEA) recently (December 2012) published, for public comment, guidelines for regulatory air quality modelling, including guidance on modelling input requirements, and protocols and procedures to be followed to ensure comparability of results. Due to the relative scarcity of site- representative meteorology, the proposed Regulations propose mainly qualitative criteria for the acceptable use of alternative meteorology, that is meteorology representative of the site but not local to it. Modellers are also not required to validate their modelling but are required to use ambient air quality measurements to evaluate modelling results *but only if these measurements are available*. We explore the comparability in modelled concentrations when using different sets of surface and upper air data, using a case study of SO_2 emissions from a large stationary source (an oil refinery), and compare AERMOD modelled concentrations against monitored values. Cape Town International Airport (CTIA) surface data, 14km from the refinery, differed significantly from that of local meteorological stations. AERMOD modelled SO_2 concentrations based on CTIA surface and upper air data differed significantly from those based on local (Table View) data. Good agreement with monitored ambient concentrations and is achieved using the combination of local (Table View) surface meteorology and Lakes Environment's Upper Air Estimator using both Table View and CTIA surface data to estimate mixing heights.

Keywords: AERMOD, air pollution meteorology, sulphur dioxide, refinery emissions, representative meteorology.

1. Introduction

Air quality models such as AERMOD (American Meteorological Society/Environmental Protection Agency Air Regulatory Model) require surface meteorological data, including the wind speed and direction, and upper air soundings, that are representative of the modelling domain (US EPA 2004). However the representativety of available meteorological data is not easily established, even if measurement sites are relatively close to emission sources (US EPA, 2009). The proposed South African regulations for air dispersion modelling, whilst recognising the relative scarcity of site-representative meteorology, propose mainly qualitative criteria for the acceptable use of alternative meteorology (DEA, 2012). Yet the choice of surface and upper air datasets may have a significant influence on predicted ambient concentrations, demonstrated through this case study.

Our case study comprises of the modelling of SO_2 emissions from the Chevron Refinery, located in Milnerton, Cape Town and the dominant SO_2 point source in the modelling domain, including the evaluation of the representivity of different meteorological datasets. Surface meteorological data are available at Table View and Bothasig ambient air quality monitoring stations, located within 5km of the refinery, but upper air soundings, done twice daily, are only available at the Cape Town International Airport (CTIA), 14 to 17km from the refinery.

Lakes Environment's AERMOD View™ (Jesse L 2009) was used with local meteorology (Cape Town International Airport and meteorological stations local to the refinery), reported daily SO_2 emissions and local terrain data as inputs to model the dispersion of SO_2 emitted by the Chevron Refinery (Milnerton). We report on the comparability of CTIA wind speed and direction data with corresponding Table View and Bothasig data, and mixing heights estimated using CTIA upper air data compared with mixing heights estimated using AERMOD View™'s Upper Air Estimator. Model-predicted ambient concentrations are compared with monitored data.

2. Methodology

2.1 The modelling domain

The modelling domain, on a 1kmx1km grid, shown is in Figure 1. The approximate Universal Transverse Mercator (UTM) coordinates of the facility are 261 to 284 km East and 6242 to 6263 km North.

relatively flat terrain between the two sites. The wind roses (Figure 4) are significantly different and CTIA wind speeds are about 50% higher than Table View wind speeds although wind directions are reasonably well correlated particularly if much of the scatter in the regions 300° to 60° is noted as an artefact.

AERMOD requires upper air data, only available at the CTIA, to estimate mixing heights. However Lakes Environment's AERMOD View™ suite includes a mixing height estimator that uses surface data as inputs. To evaluate the utility of the mixing height estimator, we compared CTIA mixing heights estimated using upper air soundings vs mixing heights calculated using the estimator, Figure 5.

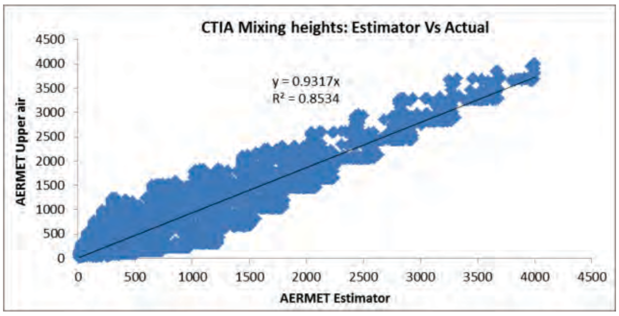

Figure 5: Comparison of AERMET estimates of mixing heights: based on upper air soundings and Estimator based on surface data

There is good agreement between AERMET estimates of mixing heights based on CTIA upper air soundings and estimated using surface data (slope = 0.93, R^2=0.85).

The estimate of mixing height has a major influence on modelled concentrations. Figure 6 compares mixing heights estimated using Table View surface wind vectors, and mixing heights estimated using CTIA upper air soundings.

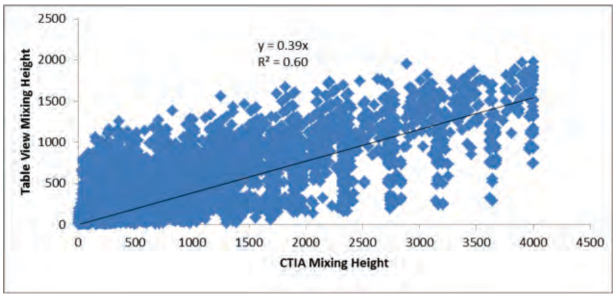

Figure 6: Comparison of mixing heights, using AERMET View™ Upper Air Estimator on Table View data, and CTIA Upper Air data, 2010.

The mixing heights are moderately well correlated (R^2=0.6), but Table View mixing heights are significantly lower (y=0.39) than CTIA mixing heights.

3.3 SO_2 concentration isopleths: CTIA meteorology vs Table View meteorology

As may be expected from the differences in mixning height estimates using Table View (close to the emissions source) meteorological data and CTIA meteorological data, estimates on ambient concentrations differ significantly (Figure 7).

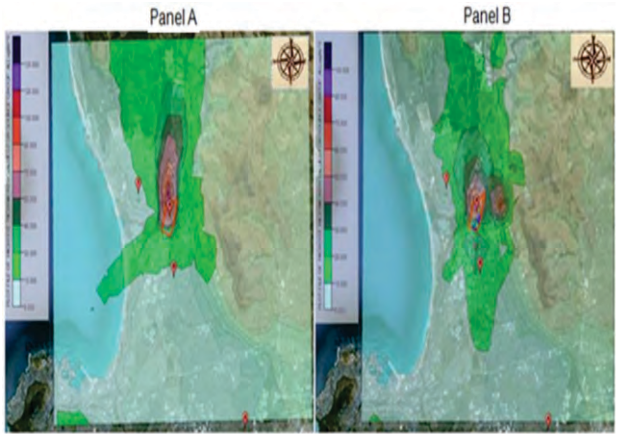

Figure 7: AERMOD modelled isopleths for March 2010, annual average SO_2 concentrations: Table View (Panel A) and CTIA (Panel B) meteorological data.

3.4 SO_2 concentration isopleths: validation

Modelling of dispersion from the refinery was based on Table View wind vectors and mixing heights estimated using the AERMET estimator with Table View and CTIA surface data as inputs. To validate the modelling, predicted concentrations are compared with monitoring data, Table 1.

Table 1: 2010 Annual average SO_2 concentrations, modelled and monitored values.

Station	2010 Average SO2 concentration [µg/m³] AERMOD Modelled	Monitored	%(Modelled-Monitored)/ Monitored
Bothasig*	8.8	7.5	17%
Table View	9.3	10.5	-11%

4. Discussion and Conclusions

The wind vectors at the Table View, about 4km from the modelled emission source, differ significantly (50 from those at the CTIA, about 14km from the source, both in respect of hourly wind speed and wind direction. The average wind directions are similar, but the hour to hour correlation is poor. Table View wind speeds are on average about 50% lower than CTIA wind speeds, and moderately correlated (R^2=0.63). Annual wind roses also differ significantly.

Figure 1: Modelling domain (R: Refinery; T: Table View and B: Bothasig monitoring stations; A: CTIA)

2.2 Meteorological data

Cape Town International Airport (CTIA) surface data and upper air soundings were supplied by the South African Weather Service (SAWS); surface data (wind speed and direction) at Table View and Bothasig were supplied by the City of Cape Town.

2.3 Land use and terrain data

AERSURFACE, using the land cover data from the USGS National Land Cover Data 1992 archives (NLCD92) provided the required values for the AERMOD modelling system.

2.4 Emissions data

The refinery emissions data for the year 2010 are based on the daily emissions values reported to the City of Cape Town Licensing Authority.

3. Results

3.1 Comparison of wind speed and direction, CTIA vs Table View station

To assess the validity of using CTIA meteorological surface data for modelling dispersion from the refinery we compared the wind vectors for the two locations, Figures 2 and 3, during one month (March 2010). For the month of March 2010, daily wind direction at the Table View station (4km from the refinery) is comparatively poorly correlated (R^2=-0.53) with CTIA (14km from the refinery) data, although there is negligible bias between the two stations (slope = 1.03). Wind speed is better correlated (R^2=0.63) but CTIA wind speeds are about 50% higher on average (slope=1.54) and there are significantly more low wind speed days at the Table View site compared with the airport site.

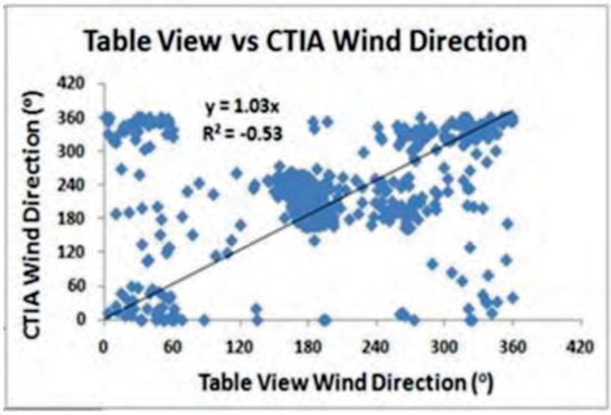

Figure 2: Comparison of hourly wind direction, CTIA vs Table View monitoring stations

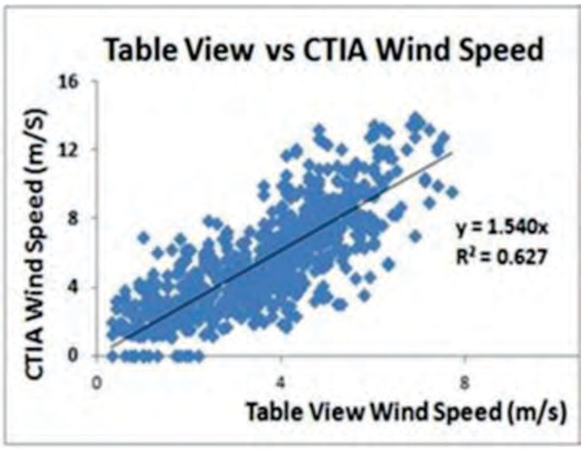

Figure 3: Comparison of hourly wind speeds, CTIA vs Table View monitoring stations

A comparison of the wind roses (Figure 4, Panels A and B) for the two monitoring stations reflects the differences in wind vectors.

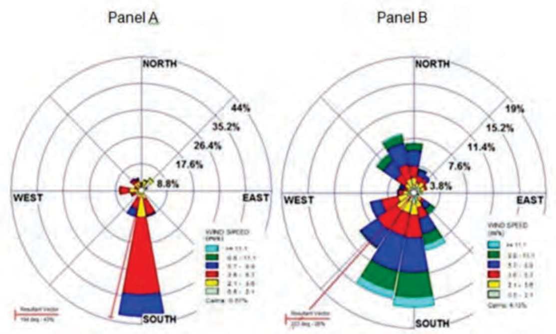

Figure 4: Wind rose CTIA (Panel A) and Table View (Panel B) monitoring stations

3.2 Upper air data, mixing heights

Comparison of the CTIA and Table View wind vectors (Figures 2, 3 and 4) showed that CTIA wind vectors are not representative of the site conditions even though the CTIA is only 14km from the refinery, with

Mixing heights estimated using the AERMOD View™ Upper Air Estimator are well-correlated with those using CTIA upper air soundings (y=0.93; R^2=0.85). Estimator mixing heights based on Table View surface data differ significantly from those based on CTIA data (y=0.39, R^2=0.60). Corresponding concentration isopleths also differ significantly.

Concentration isopleths modelled using Table View surface data and the the mixing height estimator, using both Table View and CTIA surface data, are in good agreement with monitored values at two monitoring stations (+17%, -11%) located within 5km of the emission source.

5. Acknowledgments

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