APPLICATION OF THREE AIR QUALITY MODELS TO THE PILBARA REGION

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Summary

This paper discusses findings from the evaluation of three air quality models in the Pilbara region. TAPM is a complex model that predicts the local meteorology as well as ground-level concentrations (glcs) of primary and secondary pollutants. DISPMOD and AUSPLUME are simpler Gaussian-plume based models for passive pollutants and require meteorological observations as input. Over a 12-month period, TAPM is shown to reproduce the meteorology well, and both TAPM and DISPMOD satisfactorily predict glcs of nitrogen oxides (NO_x) at Dampier, 9 km from the main emitter. However, the lack of a fumigation module in AUSPLUME causes it to consistently underestimate the higher concentrations. DISPMOD and AUSPLUME are also run using TAPM-predicted 'observations' as input and there is very little difference in the results from those obtained when actual observations are used. The performance of all three models at the King Bay monitor, 4 km from the main emitter, is less satisfactory, and possible reasons are discussed. TAPM's predictions for the secondary pollutants nitrogen dioxide (NO_2) and ozone (O_3) compare well with the observations at Dampier.

Keywords: Pilbara, sea breeze, air quality modelling, TAPM, DISPMOD, AUSPLUME, Burrup Peninsula, fumigation

1. Introduction

The Pilbara region of Western Australia occupies a large part of the sparsely-populated northwest of the state. The coastal towns of Dampier and Karratha, 1500 km north of Perth, service local industry (established on the Burrup Peninsula as a result of offshore natural gas) and the ore-loading facilities set up to ship ore transported by rail from inland mining areas. Figure 1 shows a map of the area with monitoring sites and significant emitters. In a study of regional meteorological data (Physick, 2001; Physick et al. 2000), it was established that low-level coastal winds in the Burrup Peninsula region were predominantly north-easterly to south-easterly from April to August, and north-westerly to south-westerly from September to March. However in those transition months between summer and winter, there were many days when the wind direction in the lowest 800 m rotated through 360° over a 24-hour period, often for several consecutive days. It was surmised that the wind behaviour on such days may lead to recirculation of coastal emissions back to the source region, and this was supported by some preliminary simulations with the air quality model TAPM. Coastal fumigation was also identified as an important process for the dispersion of plumes from elevated sources.

In this paper, results are presented from application of three models, TAPM, DISPMOD and AUSPLUME, to the dispersion of emissions in the region. Meteorological results from TAPM and ground-level concentrations from year-long simulations (1999) with all three models are compared with NO_x observations at the Department of Environmental Protection of Western Australia (DEPWA) monitoring station at Dampier and the Woodside Offshore Petroleum monitor at King Bay (Figure 1). TAPM predictions of O_3 and NO_2 are also compared to data from the Dampier station.

2. Data

2.1. Surface data

Meteorological and air quality data were taken in the Pilbara region from early 1998 until the end of 2001. Monitoring stations for meteorology, including surface wind, temperature (at 2 and 10 m), relative humidity, shortwave and net radiation, pressure and rainfall were installed at Karratha and Dampier (see Figure 1) in the Burrup Peninsula area by DEPWA in early 1998. The Dampier station also measured O_3, NO, NO_2, CO and PM_{10}. At King Bay, a monitor operated by Woodside measured hourly averages of O_3, NO, NO_2, and SO_2 between 1 January and 31 October 1999. Meteorological data were also taken at Bureau of Meteorology (BoM) stations at Legendre Island and Karratha airport, and at Maitland Estate by Woodward-Clyde. Beyond the Peninsula region, DEPWA surface data were collected at Wickham, 50 km east along the coast from Karratha, and at Radio Hill, 28 km south of Karratha. At all stations, meteorological and air quality data were measured as 10-minute averages. Upper-air data, not used in this paper, were regularly taken at Karratha (sounder) and Port Hedland (radiosondes), and at both locations for special observing periods (Physick et al. 2000).

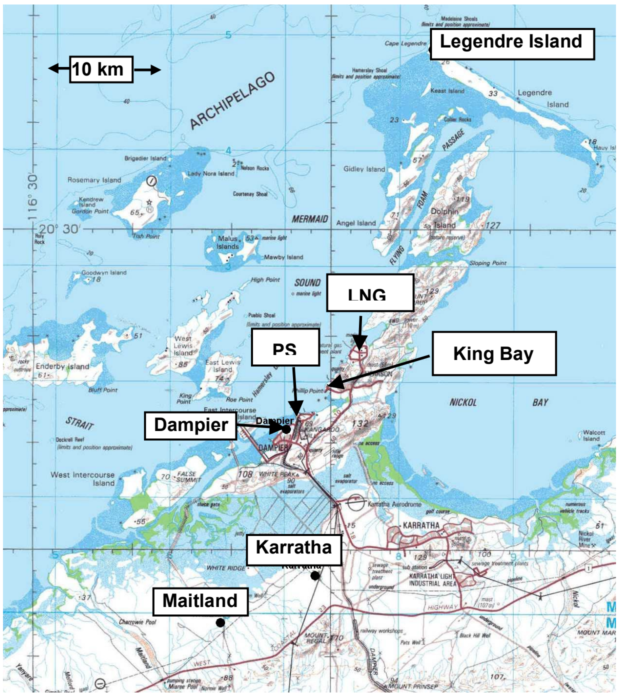

Figure 1. The Burrup Peninsula region, including the data sites Legendre Island, King Bay, Dampier, Karratha and Maitland, and the emission point sources Dampier power station (PS) and the liquefied natural gas (LNG) plant.

2.2. Emissions data

Over the modelled year, *Woodside liquefied natural gas plant (LNG)* emissions were specified to vary quarterly, rather than hourly or daily. A total of 32 point sources were specified on the site, with NO_x and VOCs being the dominant emissions. The sum of NO_x emissions, expressed as NO_2 mass equivalent and assuming a NO/NO_x ratio of 0.9, varied from 176 g s^{-1} to 194 g s^{-1} over the four quarters. Over the same period, VOC emissions remained constant at 1958 g s^{-1}. Knowing the individual emissions and reactivities of the dominant VOC constituents (parafin, toluene, xylene and benzene), a weighted reactivity of .0012 was calculated and used to obtain the emission rate of R_{smog} (reactivity multiplied by VOC emission rate) for input to TAPM.

Dampier power station emissions for 1999 were specified each hour for every day of the year. NO_x emissions, expressed as NO_2 mass equivalent and assuming a NO/NO_x ratio of 0.9, were typically 12 g s^{-1}, varying between 20 g s^{-1} and 6 g s^{-1}. VOC emissions were typically 0.11 g s^{-1}. A reactivity of .0012 was used to obtain R_{smog}. A buoyancy enhancement factor of 1.27 was calculated, to take account of the 70 m spacing of the two stacks.

Area sources included Dampier and Karratha townships, several main roads, ship-loading facilities, the two main shipping lanes, and storage depots. Emissions from these sources remained constant for all hours of the year, and were small compared to LNG emissions. For example for the ship-loading facilities, typical values of NO_x, expressed as NO_2 and assuming a NO/NO_x ratio of 0.9, were 14 g s^{-1} on a 1-km square grid. Largest VOCs were emitted at a rate of 2.8 g s^{-1} from the towns. A reactivity value of .0067 was used to convert to R_{smog}.

Emissions from *biogenic sources* on the inner emissions grid (see section 3.4.2) varied with time of day, but not with day of the year, so that vegetation emitted at the same rate on both hot days and cool days. Maximum emissions each day of NO_x from soil, expressed as NO_2 and assuming a NO/NO_x ratio of 1.0, were .082 g s^{-1} while VOCs were 0.28 g s^{-1}. A reactivity value of .0067 was used to convert to R_{smog}.

On the outer *biogenic emissions* grid, specified VOC emissions were assumed to be at 30ºC and a photosynthetic active radiation level (PAR) of 1000 μmol m^{-2} s^{-1}. When the emissions are input in this way, TAPM is able to calculate hourly VOC emissions which are a function of temperature and PAR. VOC emissions were given a value of 0.28 g s^{-1}. The specified value for NO_x emissions (0.048 g s^{-1}) is a mean of the inner grid value over 24 hours.

A single value of background O_3 (25 ppb) was used for all months of the year. It is also necessary to assign a background value for Rsmog, partly to account for a general background concentration of VOCs but also to compensate for the omission of some inorganic radical-producing reactions in the GRS photochemical mechanism. After some preliminary simulations, a value of 0.1 was chosen.

A factor to be taken into consideration when comparing model concentrations with observations is that levels of pollutants (especially O_3) are enhanced in smoky air transported to the Burrup Peninsula from fire areas inland. Eighteen such days, identified by high PM10 levels and Bureau of Meteorology visibility reports from Port Hedland, were discarded from the NO_x and O_3 model comparisons. Analysis of the Dampier monitoring data suggests that peak O_3 values are increased by up to 20 ppb in smoky air. Further discussion can be found in Physick and Blockley (2001).

3. Models and Grid Configurations

3.1. TAPM

TAPM (Hurley, 1999) was developed at CSIRO Atmospheric Research and consists of prognostic meteorological and air pollution modules that can be run for multiple-nested domains. The meteorological module is an incompressible, non-hydrostatic, primitive equation model for three-dimensional simulations. It predicts the three components of the wind, temperature, humidity, cloud and rainwater, turbulent kinetic energy and eddy dissipation rate, and includes a vegetation/soil scheme at the surface and radiation effects. The model is driven by the Bureau of Meteorology's LAPS (Limited Area Prediction System) analysis fields (on a 75 km-spacing grid) of winds, temperature and specific humidity, which account for the larger-scale synoptic variability. TAPM is run for much finer grid spacings and predicts the meteorology at smaller scales.

The air pollution module solves prognostic equations for pollutant concentration using predicted wind and turbulence fields from the meteorological module. It includes gas- and aqueous-phase chemical reactions based on an extended version of the Generic Reaction Set (GRS) developed at CSIRO Energy Technology, a plume-rise module, and wet and dry deposition effects.

3.2. DISPMOD

DISPMOD is a Gaussian-plume based air quality model for coastal regions, and was designed to simulate the downward fumigation of an elevated plume as it intersects a growing thermal internal boundary layer (TIBL) within onshore flow (Rayner and Blockley, 2001). It was developed as an aid in setting emission limits for industry in the Kwinana industrial complex, situated on the coast south of Perth. As input, it needs surface winds at hourly or shorter intervals, stability parameters and a thermal stability profile when winds are onshore. For offshore winds, it uses the more traditional Gaussian-plume algorithms and needs PBL heights at intervals of one hour or less as input. The meteorological inputs required by DISPMOD are collected at a single point and then applied over the entire model domain.

3.3. AUSPLUME

AUSPLUME is a standard Gaussian-plume based air quality dispersion model. It was developed by the Victorian EPA and is widely accepted and used for regulatory purposes within Australia (Lorimer, 1986). Its input requirements are hourly wind speed, wind direction, temperature, PBL height, and stability parameters. AUSPLUME does not have any explicit algorithms for simulating fumigation of elevated plumes.

3.4. Grids

3.4.1 TAPM

The simulations were carried out on three nested grids (each 21 x 21 x20 gridpoints) with grid spacings of 10, 3 and 1 km for the meteorology. The grid spacings for the corresponding air quality simulations over the same domains were 5, 1.5 and 0.5 km. All grids were centred at (20º39', 116º43') – near Dampier and (470400, 7716500) in Australian Map Grid coordinates. Terrain elevation was obtained from AUSLIG data (250 m resolution). For the 1-km grid, land-use classification in the data set accompanying the TAPM modelling package was changed from a land category to water for gridpoints corresponding to the Dampier Salt Farm at the lower end of the Burrup Peninsula. A roughness length of 0.9 m was assigned to Burrup Peninsula gridpoints by changing the land-use category in that region to low dense forest, which simulates the rough rocky landscape.

3.4.2 Dampier emissions grid

The DEPWA area emissions (anthropogenic plus biogenic) consist of values at 1-km intervals on a 31 x 33 grid centred at AMG coordinates (475500, 7714500), about 5 km east of Dampier. In order to cover all three TAPM grids, another (outer) emissions grid was created to account for biogenic emissions outside the inner grid. This grid consisted of 71 x 71 gridpoints, centred at (470400, 7716500) – the centre of the TAPM grids - with a 3-km spacing.

3.4.3 AUSPLUME and DISPMOD grids

Simulations carried out using DISPMOD and AUSPLUME used a single 1-km spaced grid centred near Dampier (AMG coordinates 470400, 7716500, same as for TAPM), with a domain size of 21x21 gridpoints.

4. Modelling results

4.1 Meteorology

Table 4.2 shows various model evaluation statistics for DEP's Dampier (coastal) and Karratha (12 km inland) sites for surface wind speed, u- (east-west) and v- (north-south) wind components, temperature and relative humidity from the 1-km grid spacing simulations. The results are very similar for the 3-km spaced grid. At both sites, statistics are very encouraging as RMSEs are well below the standard deviation in the observations, the indexes of agreement (IOA) are especially high, and at Dampier the variance in observations and model are very similar. The modelled temperature at Karratha shows more variability than is observed, mainly due to cooler temperatures at night on many occasions. *IOA* values from other studies reported in the literature lie between 0.5 and 0.7 for wind speed, while the few temperature values reported are less than 0.6. The model's performance varies from month to month, but the statistics are acceptable throughout the year. In an initial simulation, the modelled wind speeds at Dampier were higher than observed by about 20% in the annual statistics. This discrepancy was less in those months in which westerly winds (off the sea) predominate and greater when easterly winds are most common, suggesting that the model is unable to resolve small-scale terrain or other objects which contribute to a blocking or sheltering effect at this site. In an attempt to parameterise such small-scale variations in the terrain on the Burrup Peninsula, roughness length in this area was set to 0.9 m.

Table 4.2: Annual statistics at Dampier and Karratha for TAPM simulation of 1999 for the following surface variables (10 m above the ground): wind speed (WS10), the east-west component of the wind (U10), the north-south component of the wind (V10), temperature (TEMP), and relative humidity (REL. H).

VARIABLE	MEAN_OBS	MEAN_MOD	RMSE	IOA	SKILL_V	SKILL_R
DAMPIER						
WS10	3.8	4.0	1.72	0.68	0.89	0.99
U10	0.3	-0.3	2.09	0.90	1.04	0.63
V10	0.0	0.2	1.87	0.85	1.00	0.74
TEMP	25.8	25.6	1.88	0.94	1.12	0.49
REL. H	60.9	60.6	12.99	0.86	1.00	0.71
KARRATHA						
WS10	4.4	4.4	1.78	0.79	0.76	0.77
U10	0.2	-0.4	2.17	0.92	0.86	0.53
V10	-0.3	0.2	2.11	0.86	1.10	0.74
TEMP	25.6	25.2	3.89	0.90	1.50	0.78
REL. H	60.3	56.6	16.46	0.87	1.14	0.75

KEY: OBS = Observations, MOD = Model Predictions, MEAN = Arithmetic mean, STD = Standard Deviation, RMSE = Root Mean Square Error, IOA = Index of Agreement (0=no agreement, 1=perfect agreement), SKILL_V = (STD_MOD)/(STD_OBS) (near to 1 shows skill), SKILL_R = (RMSE)/(STD_OBS) (<1 shows skill).

4.2 NO_x

Results are presented in terms of mean and maximum concentration, percentile concentrations, and robust highest concentration (RHC). The RHC approach (Cox and Tikvart, 1990) recognises that peak (maximum) concentrations are highly variable, in models and observations, and uses information contained in the upper end of the concentration distribution to calculate a robust statistic (RHC) for model comparison purposes. In this study, we have used the 11^{th} highest concentration, and the mean of the top-ten concentrations, to project to the RHC.

The Dampier monitoring station is on the coast, 9 km from the LNG plant and 1-km from the Dampier power station. The NO_x statistics for Dampier from the TAPM simulation on the 0.5-km spaced grid are shown in Figure 2. Although the highest concentration for the year is under-estimated only by about 15%, there is a greater discrepancy between model and observations for the RHC and 99.9^{th} percentile concentration. Also shown in Figure 2 are statistics from DISPMOD and AUSPLUME simulations, using either an observed meteorology file from Dampier or a file consisting of TAPM-predicted meteorology at the LNG gridpoint. For all simulations, DISPMOD also used TAPM-predicted stability profiles during onshore flow. DISPMOD results, for both observed and predicted meteorology input, are very similar to the TAPM results, while the AUSPLUME concentrations are less than 50% of the observed values for all statistics. AUSPLUME and DISPMOD under-predict for percentiles lower than the 99^{th} because their input files did not include area emissions.

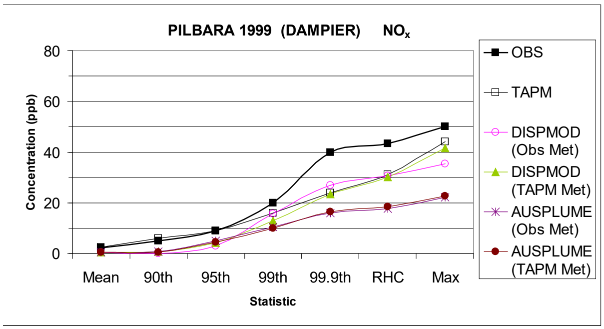

Figure 2. Annual mean, maximum, robust highest concentration (RHC) and percentile statistics for modelled (0.5-km grid) and observed NO_x at Dampier for 1999. The curves represent different models with alternative input, as detailed in the text.

The King Bay monitoring station is 4 km along the coast from the LNG plant, and statistics from the three models are shown in Figure 3. Although TAPM and DISPMOD predict the maximum concentration well, TAPM over-predicts at all other concentrations and DISPMOD predicts too high for statistics above the 95^{th} percentile. AUSPLUME does best of the three models for all concentrations except the maximum.

Although it is probably too time-consuming to run a 12-month TAPM simulation for NO_x at a resolution of 0.25 km grid spacing (at least on a single computer), it is of interest to see the effect of this finer resolution on NO_x concentrations at Dampier. A simulation was done at this spacing for the months of July and August, when the highest concentrations are observed. The results, and those for a 0.5 km spacing, are shown for various percentiles in Figure 4. Finer resolution does improve the higher concentrations, but RHC is still underestimated, by almost 25%.

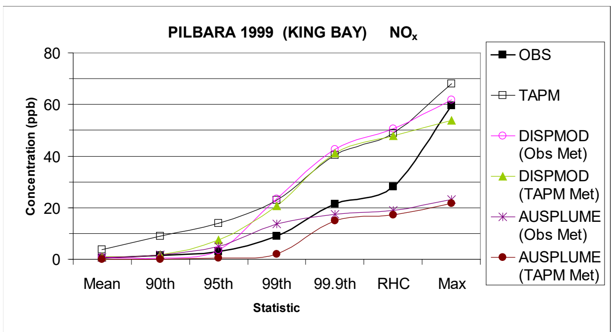

Figure 3. Annual mean, maximum, robust highest concentration (RHC) and percentile statistics for modelled (0.5-km grid) and observed NO_x at King Bay for 1999. The curves represent different models with alternative input, as detailed in the text.

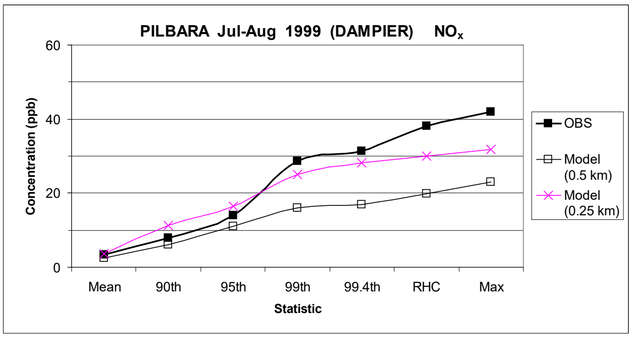

Figure 4. Mean, maximum, robust highest concentration (RHC) and percentile statistics for modelled (0.5-km and 0.25-km grids) and observed NO_x at Dampier for July-August 1999.

4.3 NO_2 and O_3

For the secondary pollutants NO_2 and O_3, model results are compared with data at the Dampier station. The modelled NO_2 results (from the 0.5-km spaced grid) in Figure 5 are in good agreement with the observations, although the maximum concentration is about 40% higher than observed. This case, in which the peak concentration is considerably higher than other concentrations, illustrates the value of the robust highest concentration (RHC), a statistic that mitigates the undesirable influence of unusual events.

Simulations for O_3 with various grid spacings showed that it is not necessary to use smaller spacings than 3 km, for either comparison with Dampier observations or when predicting a regional maximum. Figure 6 shows the modelled and observed annual statistics for O_3, for the 3-km and 0.5-km spaced grids, and it can be seen that the higher concentrations are simulated well. The middle-range of concentrations between 25 and 35 ppb is underestimated by the model, and this is reflected in the model's variance, which is only half that of the observations. Time series show that the diurnal amplitude of the O_3 signal is often underestimated, including many occasions when the winds are steady from the south or east, suggesting that biogenic VOC emissions may not be large enough. However, this characteristic may also arise from assumptions in the GRS photochemical mechanism in TAPM, which lead to an under-production of radicals (M. Cope, personal communication).

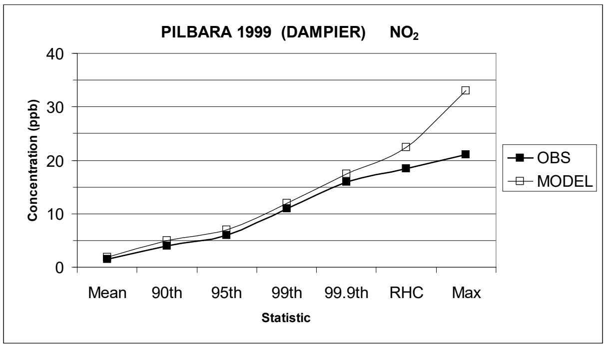

Figure 5. Annual mean, maximum, robust highest concentration (RHC) and percentile statistics for modelled (0.5-km grid) and observed nitrogen dioxide at Dampier for 1999.

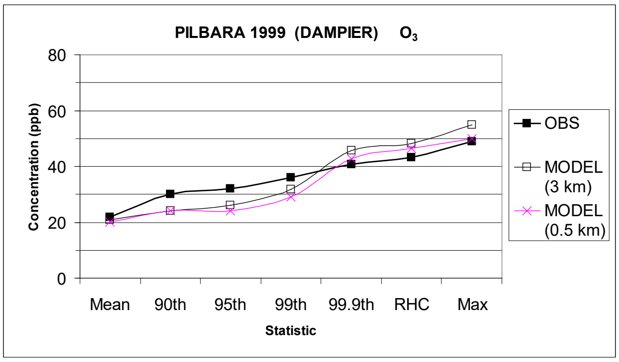

Figure 6. Annual mean, maximum, robust highest concentration (RHC) and percentile statistics for modelled (3-km grid) and observed O_3 at Dampier for 1999.

5. Discussion and Summary

Although TAPM and DISPMOD have been shown to perform satisfactorily when used for NO_x in the Burrup Peninsula region, an under-estimate of concentrations at Dampier and an over-estimate at King Bay suggest that the modelled LNG plumes are being brought to the ground too close to the plant. It is possible that the TAPM temperature/stability profiles are not being predicted correctly at all times and further work is being carried out along these lines. However, the variability in atmospheric stability as the plumes travel along the irregular coastline from source to monitors is an especially difficult aspect for the models to simulate.

The higher concentrations observed at Dampier and King Bay are due to fumigation of elevated plumes, a process that AUSPLUME is unable to simulate. Consequently, it predicts lower concentrations than the other two models.

As well as runs using observed meteorology files, DISPMOD and AUSPLUME simulations were also done using meteorology files generated by TAPM. It was encouraging to see that there was very little difference between the results using either observed or predicted input for both models.

TAPM was also run in a chemistry mode with the results compared to hourly-averaged NO_2 and O_3 data at Dampier. Agreement was good for NO_2 and for the lower and upper ranges of O_3 concentrations, with under-prediction in the middle ranges. Satisfactory results were obtained using a 1.5-km grid spacing for NO_2 and 3 km for O_3, with negligible improvement when the grid spacings were decreased further.

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