Final Report

Meteorological and Dispersion Modelling Using TAPM for Wagerup

Phase 2: Dispersion

Prepared for
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Contents

Executive Summary

The Wagerup alumina refinery of Alcoa World Alumina Australia is located about 130 km south of Perth in Western Australia. The work presented in this report is part of a study entitled "Meteorological and Dispersion Modelling Using TAPM for Wagerup", consisting of three closely defined objectives. This report addresses the second objective (Phase 2: Dispersion), which was to:

- evaluate CSIRO's The Air Pollution Model (TAPM) for air quality predictions at Wagerup using a database of emissions from the Wagerup Refinery to model hourly-averaged ambient air concentrations of pollutants for appropriate periods and compare them with observations, and

- identify dominant pathways for the transport of the refinery emissions to the ground level in the surrounding district.

Results from Phase 1 (Meteorology), Phase 3A (TAPM modelling for Health Risk Assessment – Current Emission Scenarios) and Phase 3B (TAPM modelling for Health Risk Assessment – Expanded Refinery Scenario) are reported in the CSIRO (2004a), CSIRO (2004b) and CSIRO (2004c) reports, respectively.

TAPM is a prognostic meteorological and air pollution dispersion model developed by CSIRO Atmospheric Research (see http://www.dar.csiro.au/tapm). The meteorological component of TAPM predicts the local-scale flow, such as sea breezes and terrain-induced circulations, given the larger-scale synoptic meteorology. The air pollution component uses the model-predicted meteorology to estimate the pollutant concentrations in the region surrounding the emission source.

The specific components of the Phase 2 objective included:

- An analysis of the oxides of nitrogen (NO_x) data from Alcoa's Upper Dam and Boundary Road monitoring stations measured during a one-year period (1 April 2003–31 March 2004[1]), and an analysis of ANSTO perfluorocarbon tracer data obtained on 13 and 14 August 2002.

- Running TAPM for NO_x and ANSTO tracer data simulations, analysis of the model results, and comparison of the hourly-averaged model results with the data.

- For some periods, running of TAPM with building effects and local wind data assimilation.

- Calculation of a standard set of performance statistics for the model runs so that the performance of TAPM in estimating concentrations of air pollutants from given emissions can easily be compared with other models.

[1] The NO_x data at Upper Dam were available only till 12 December 2003.

- An analysis of the total suspended particulate (TSP) data measured at the Residue Disposal Area (RDA) obtained for one year, and comparison of the model winds with the observed RDA winds when high TSP concentrations are observed.

- Identification of dominant meteorological and dispersion mechanisms governing the relative frequency of model events in the Yarloop area.

Information on the Refinery NO_x sources and their emission rates (constant with time), and tracer source characteristics was supplied by Alcoa. Alcoa also supplied the observed ambient concentrations of NO_x, total suspended particles, and ANSTO tracers.

In order to evaluate TAPM (version 2.6), it was run with four nested grid domains, with the innermost grid resolution of 0.5 km for meteorology and 0.25 km for dispersion. For pollutant dispersion, the innermost domain was about 7 km × 7 km, whereas the outermost domain was about 300 km × 300 km. Model inputs included the Wagerup-specific land-use database and a Refinery-generated heat flux of 150 W m^{-2}, both derived as part of the Phase 1 work.

The model evaluation focused on the ability of the model to describe the high concentration occurrences that are observed occasionally during the year and which are of most interest in impact assessments. For air pollution model evaluation, specific statistics are commonly used, including quantile-quantile (q-q) plots, and statistical measures, such as the robust highest concentration (RHC), and these were used in this study. The evaluation procedure involved comparison of modelled and observed concentrations that were unpaired in time and/or space.

The results of the Phase 2 are in summary:

- There is evidence that almost all of the Boundary Road NO_x data are heavily influenced by unquantified non-Refinery emissions, which are not included in the modelling, whereas the NO_x data from Upper Dam are the most extensive data set of measurements available that show a strong Refinery signature. Consequently, the emphasis was placed on the model comparison with the Upper Dam data for assessing the TAPM performance.

- The TAPM modelling performs well at Upper Dam. Considering all the statistical measures for high-end concentration (i.e. the maximum 1-hour average to the 99^{th} percentile), the ratio of the modelled concentration to the observed concentration lies within 0.9–1.3. The model-observation comparison agrees to within the uncertainties in the model physics, inputs and concentration data.

- Inclusion of building wake effects in the model does not make a significant difference to the predictions. However, it is physically realistic to include them.

- Slight improvement in the TAPM predictions is achieved with the inclusion of the Refinery-generated heat flux.

- Wind data assimilation has mixed impact on pollution predictions. The results for NO_x at Upper Dam show that the assimilation of local wind data in TAPM makes the modelled concentrations somewhat higher, and slightly improves the prediction of the top few concentrations. The ANSTO tracer-modelling results show that for

Calciner 4 and Boiler 1, the wind data assimilation worsens the predictions, and for the 100-m Multiflue it improves the predictions.

- Meteorological data currently available for wind data assimilation do not cover the whole model year, and at the Residual Disposal Area have quality problems. More meteorological and pollution observations would be necessary to examine the impact of wind data assimilation on predictions within the larger, topographically complex domain of interest.

- TAPM is able to describe the observed high wind speeds corresponding to high dust events at RDA moderately well, with a correlation coefficient (*r*) between 0.6–0.7.

- Comparison of evaluation results reported in the present study with other modelling studies suggests that TAPM's overall performance at Wagerup is on par with its performance elsewhere for annual data measured at sparse monitoring networks.

- Using odour as a tracer, TAPM was run for the one-year period to identify meteorological and dispersion factors governing model events in Yarloop. A model event was defined using a somewhat arbitrary threshold value. The diurnal variation of the relative number (or the relative frequency) of model events qualitatively agrees with that of the relative number of complaints in the area.

- The maximum number (13%) of model events occur in the later morning, which closely matches the maximum number of complaints (15%) that occur at about the same time. Model events are most intense in the late morning when the airflow is such that Yarloop is frequently downwind of the Refinery.

- The modelling shows that the dominant meteorological and dispersion pathways that cause events at Yarloop due to the Refinery emissions are: morning inversion break-up fumigation and subsequent shallow convection, and strong winds and/or cloudy conditions (77% of events); nighttime drainage flows from the escarpment with westerly flows aloft (15% of events); and low/calm wind conditions (8% of events).

- In terms of the meteorological variables that are used in routine modelling applications, the highest frequencies of model events are encountered when Yarloop is directly downwind of the Refinery; surface wind speed is moderately strong; atmospheric stability is neutral, slightly unstable or moderately unstable; and the boundary-layer height is less than about half a kilometre.

Additional conclusions from Appendix A

The NO_x emissions initially supplied by Alcoa were constant throughout the annual model simulation period. Subsequent to the completion of the NO_x modelling, Alcoa supplied sufficient data to enable daily NO_x emission rates to be calculated. The Appendix A of this report presents the revised modelled ground-level concentrations based on these daily emission rates. The new results show that the approach of combining the buoyancies of the plumes from the Calciners 1–3 flues and those from the Boilers 1–3 flues, and treating them as effective single sources, produces better model performance at Upper Dam than when these flues are treated separately in the

model (as was done in the report). For all the high-end concentration measures (i.e. the maximum 1-hour average to the 99th percentile) at this site, the ratio of the modelled concentration to the observed concentration ranged between 0.8–1.0. It is concluded that the observations support the use of plume buoyancy enhancement for modelling the emissions from the two Multiflue stacks of the Wagerup Refinery.

Glossary

Simple definitions of various technical terms are given here to assist the reader. If required, the reader should look to other sources for more formal and technical definitions.

ABL	Atmospheric Boundary Layer. The ABL is the lowest 100 to 3000 m of the atmosphere modified by the earth's surface. The ABL responds to surface forcings (i.e. heating, cooling, and roughness) with a time scale of about an hour or less, and its extent is deeper in the daytime and shallower in the nighttime. It is often turbulent and is capped by a temperature inversion (see definition below).
Aerosol	A suspension of fine solid, liquid or mixed-phase particles in air.
AGL	Height Above Ground Level
ANSTO	Australian Nuclear Science and Technology Organisation (http://www.ansto.gov.au/)
AUSPLUME	A simple, steady-state, Gaussian plume dispersion model used for predicting ground-level concentrations of pollutants from a variety of sources. It is a regulatory model developed and approved by EPA Victoria and other regulatory agencies. AUSPLUME requires input, which typically contains hourly values of temperature, wind speed, wind direction, stability, and mixing height.
Buoyancy enhancement	An increase in the effective buoyancy of a plume as a result of merging with another buoyant plume. This leads to greater plume rise of the combined plume than of the individual plumes.
CALMET	Computer code providing the meteorological input for the dispersion model CALPUFF. It is driven by observed or large-scale model meteorology and is capable of calculating temporally and spatially varying wind fields.
CALPUFF	An air pollution dispersion model developed by Earth Tech Inc. (USA). It simulates the transport and diffusion of a plume via the puff approach in which a plume is described as consisting of a series of puffs. CALPUFF typically uses meteorological data generated by the processor CALMET. (http://www.src.com/calpuff/calpuff1.htm)
CAR	CSIRO Atmospheric Research (http://www.dar.csiro.au)
Combined source	The representation of two or more closely-spaced emission sources which have similar emission characteristics by a single source.

Convective mixed layer	Also called convective boundary layer, mixed layer or mixing layer. A type of atmospheric boundary layer (ABL) characterised by vigorous turbulence, generated by the solar heating of the ground, tending to stir and mix pollutants particularly in the vertical.
CSIRO	Commonwealth Scientific and Industrial Research Organisation (http://www.csiro.au)
Diffusion	In air pollution meteorology the words dispersion and diffusion are often used interchangeably. This is also the case in this report. However, strictly speaking the two words mean different things. Diffusion refers to dilution of pollutants by turbulent eddies in the atmosphere whose dimensions are smaller than that of a pollutant plume or a puff (see also Dispersion).
Dispersion	Dispersion refers to the movement or transport of pollutants horizontally or vertically by the wind field and their dilution by atmospheric turbulence. Dispersion includes both transport and diffusion of pollutants (see also Diffusion).
Emission rate	Specifies the rate at which gas or particles are emitted from a source. The quantity is usually expressed in units of grams per second.
Ensemble average	The value of a meteorological variable found by averaging over many independent descriptions or realizations of that variable. Also, an average taken over many different flow realizations that have the same initial and boundary conditions.
EPAV	Environment Protection Authority of Victoria (Australia) (http://www.epa.vic.gov.au)
Eulerian approach	An approach to describing atmospheric diffusion in which the behaviour of species is described relative to a fixed coordinate system.
Exit temperature	The temperature of the gas released from a source.
Exit velocity	The velocity at which gases are emitted from source. For a stack, the volume flow rate from the stack is obtained by multiplying the exit velocity by the internal cross-sectional area of the top of the stack.
GASP	Global AnalySis and Prediction. A meteorological modelling system currently used by the Australian Bureau of Meteorology that can provide the large-scale (synoptic) meteorological input needed in the models TAPM and CALMET.
Inversion	An atmospheric layer in which temperature increases with

	altitude (e.g. the layer above the atmospheric boundary layer). These layers are stable and resistant to vertical mixing and hence may restrict the dispersion of pollutants. Properly described as a temperature inversion.
Lagrangian approach	An approach to describing atmospheric diffusion in which concentration changes are described relative to the moving fluid.
LAPS	Limited Area Prediction System. A meteorological modelling system previously used by the Australian Bureau of Meteorology that can provide the large-scale (synoptic) meteorological input needed in the model TAPM.
mg	Milligram (1 mg = 10^{-3} gram = 0.001 gram). One thousandth of a gram
mg m^{-3}	Milligram per cubic metre. 1 mg m^{-3} = 1000 μg m^{-3}
NBL	Neutral Boundary Layer. A type of atmospheric boundary layer (ABL) that forms when winds are strong and/or when there is negligible heating or cooling of the ground (e.g. overcast conditions). The turbulence responsible for mixing under these conditions is generated by wind shear.
NO	Nitric oxide
NO_x	Oxides of nitrogen (commonly NO_x = NO + NO_2)
NO_2	Nitrogen dioxide
OU	Odour Unit. The odour units are dimensionless and are effectively "dilutions to odour threshold." An odour present at a concentration of 1 OU will be discerned as odourless by approximately half the population. 10 OU represents a mixture, which if diluted by 10 will then have an odour detected by 50% of the respondents and so forth.
Percentile	The p^{th} percentile is a value so that roughly *p*% of the data are smaller and (100-*p*)% of the data are larger than this value; the 50^{th} percentile is called the median. Quantile is a more general definition than percentile.
pg	Picogram (1 pg = 10^{-12} gram = 0.000000000001 gram). One trillionth of a gram
pg m^{-3}	Picogram per cubic metre. 1 pg m^{-3} = 0.000001 μg m^{-3}
Pollutant	Used in this report in the non-legal sense to refer to a chemical species being modelled by air pollution dispersion models, such as TAPM.

ppb	Parts per billion (by volume): 1 ppb = 1/1000 ppm.
ppm	Parts per million (by volume): a unit for the concentration of a gas in the atmosphere based on the mixing ratio approach. A concentration of 1 ppm is equivalent to a volume of 1 cubic metre of pure undiluted gas in 1 million cubic metres of air. The expression ppm (or ppb) is without dimensions. The ppm (or ppb) unit is useful because its value is unaffected by changes in temperature and pressure, and also because many sampling techniques are based on volume concentrations. Concentrations of gaseous compounds can be converted from mixing ratio units, e.g. ppm units (volumetric), to density units, e.g. mg m^{-3} (mass/volume), using the following formula: $$C(\text{mg m}^{-3}) = \frac{273.15 \times M_w \times C}{22.4136 \times (273.15 + T)},$$ where C is the concentration (ppm), M_w is the molecular weight of the gas, and T is the ambient temperature in degrees Celsius. At a temperature of 0 degrees Celsius, the conversion factor from 1 ppm to mg m^{-3} for nitrogen dioxide (NO_2) is 2.050.
Prognostic equation	Any equation governing a system that contains change with time of a quantity, and therefore can be used to determine the value of that quantity at a later time when the other terms in the equation are known.
Quantile	The fraction (or percent) of points below the given value. That is, the 0.3 (or 30%) quantile is the point at which 30% percent of the data fall below and 70% fall above that value. Certain quantiles have special names. The 0.25-, 0.50-, and 0.75-quantiles are called the first, second and third quartiles. The 0.01-, 0.02-, 0.03-, ... , 0.98-, 0.99-quantiles are called the first, second, third, ... , ninety-eighth, and ninety-ninth percentiles.
Q-q plot	A graphical data analysis technique for comparing the distributions of two data sets. The plot consists of the following: vertical axis = estimated quantiles from data set 1; horizontal axis = estimated quantiles from data set 2. However, it is common to directly plot the one data set against the other. That is, the actual quantile level is not plotted. Hence, in an air pollution model evaluation application, the q-q plot is essentially a plot of the sorted observed concentrations against the sorted predicted concentrations.

RDA	Residue Disposal Area
RHC	Robust Highest Concentration. A robust test statistic calculated using information contained in the upper end of the distribution of concentrations.
SBL	Stable Boundary Layer. A type of atmospheric boundary layer (ABL) that develops during the night when the ground is substantially cooler than the air above it, thus forming a stable temperature gradient with height in the air that opposes vertical motions of air and resulting in little ambient turbulence.
SKM	Sinclair Knight Merz (an environmental consulting company)
Stochastic	Stochastic is synonymous with "random". It is used to indicate that a particular subject is seen from point of view of randomness. Stochastic is often used as counterpart of the word "deterministic", which means that random phenomena are not involved.
TAPM	The Air Pollution Model. A prognostic meteorological and air pollution dispersion model developed by CSIRO Atmospheric Research (http://www.dar.csiro.au/tapm). The meteorological component of TAPM predicts the local-scale flow, such as sea breezes and terrain-induced circulations, given the larger-scale synoptic meteorology. The air pollution component uses the model-predicted three-dimensional meteorology and turbulence, and consists of a set of species conservation equations and an optional particle trajectory module.
Temperature inversion	see Inversion
TSP	Total Suspended Particulates– all particles below about 50 µm in diameter suspended in the atmosphere.
US EPA	United States Environmental Protection Agency (http://www.epa.gov)
WA	Western Australia
W m^{-2}	Watts per square metre
Wind data assimilation	A technique in which at one or more locations in a meteorological model, the wind speed and wind direction in the model are adjusted to those observed in the atmosphere. The model adjusts its airflow at this and surrounding locations to ensure that the model wind speed and direction at the location closely follow that observed.

µg	Microgram (1 µg = 10^{-6} gram = 0.000001 gram). One millionth of a gram
µg m^{-3}	Microgram per cubic metre: a unit for the concentration of a gas or particulate matter in the atmosphere based on the density approach (mass per unit volume of air). Concentrations of gaseous compounds can be converted from density units, e.g. mg m^{-3} (mass/volume), to mixing ratio units, e.g. ppm units (volumetric), using the following formula: $$C(\text{ppm}) = \frac{22.4136 \times (273.15 + T) \times C}{273.15 \times M_w},$$ where C is the concentration (mg m^{-3}), M_w is the molecular weight of the gas, and T is the ambient temperature in degrees Celsius. At a temperature of 0 degrees Celsius, the conversion factor from 1 mg m^{-3} to ppm for nitrogen dioxide (NO_2) is 0.488.

1. Introduction

The Wagerup alumina refinery of Alcoa World Alumina Australia is located about 130 km south of Perth in Western Australia, 25 km inland from the coast and in the western foothills of the north-south Darling escarpment. The local communities in the proximity of the Refinery include Yarloop, about 3 km south of the Refinery; and Hamel and Waroona, approximately 5 km and 8 km north of the Refinery (see Figure 1).

The work presented in this report was carried out as Phase 2 of the CSIRO proposal entitled "Meteorological and Dispersion Modelling Using TAPM for Wagerup" to Alcoa World Alumina Australia (referred to as Alcoa hereafter). The overall project currently consists of the following components:

- evaluation of the capability of CSIRO's The Air Pollution Model (TAPM) to acceptably produce meteorological predictions matching available field observations at Wagerup (*Phase 1: Meteorology*);

- evaluation of TAPM for air quality predictions at Wagerup using a database of emissions and observed ambient air concentrations (*Phase 2: Dispersion*); and

- use of TAPM modelling as input for the Health Risk Assessment (HRA) and the Public Environmental Review Document concerning the Wagerup Refinery expansion plans (*Phase 3: HRA concentration modelling*).

Results from Phase 1 (Meteorology), Phase 3A (TAPM modelling for Health Risk Assessment – Current Emission Scenarios) and Phase 3B (TAPM modelling for Health Risk Assessment – Expanded Refinery Scenario) are reported in the CSIRO (2004a), CSIRO (2004b) and CSIRO (2004c) reports, respectively.

This report addresses the objectives of Phase 2 as set out in the original proposal and the subsequent variations. Overall, the objective of Phase 2 is:

"Based on acceptable performance of the model compared to observed meteorology (in Phase 1), to then use TAPM (version 2.6) and a database of emissions from the Wagerup Refinery to model hourly-averaged ambient air concentrations of pollutants for appropriate periods and compare them with observations. Identify dominant pathways for the transport of the refinery emissions to the ground level in the surrounding district."

The following summarises the components of this report:

Section 2 briefly describes TAPM. The model settings that are common to the runs reported here are presented in Section 3.

Section 4 describes the evaluation method used and the TAPM evaluation results. In Section 4.2, using the Refinery NO_x emissions data provided by Alcoa, TAPM is applied to an annual database (1 April 2003–31 March 2004) of hourly-averaged oxides of nitrogen (NO_x) data from Alcoa's Boundary Road and Upper Dam monitoring

stations near the Refinery. The period selected is the same as that for meteorological predictions in Phase 1 (CSIRO, 2004a). The NO_x simulations are performed with three separate model options: a base run, the base run with building effects, and the base run with building effects and wind data assimilation. Additionally, a 4-month winter run is performed without the Refinery-generated heat flux to establish the extent of influence this heat flux exerts on the NO_x concentrations. The modelled concentrations are compared with the measured levels.

TAPM simulations of the ambient concentrations that resulted from the ANSTO tracer releases from three Refinery stacks (Calciner 3, Calciner 4 and Powerhouse Boiler) on 13 and 14 August 2002, both with and without wind data assimilation, and comparison of the model results with the tracer data, are reported in Section 4.3.

In Section 4.5, the ability of TAPM to simulate the (high) wind speeds and the corresponding wind directions observed at the Residue Disposal Area (RDA) weather station, for the hours when there are occurrences of elevated concentrations of total suspended particulates (TSPs) observed around the RDA area, is investigated. TAPM does not have a dust rise module for estimating dust emissions, and the scope of this part of the report is limited to testing the model winds when elevated dust concentrations occur.

Section 5 compares the performance of TAPM at Wagerup with other TAPM studies and models involving industrial point sources.

In Section 6, TAPM modelling with two tracer releases, representing two major Refinery odour point sources, is carried out. The hourly-averaged model concentrations are used to estimate relative frequencies of model events in Yarloop, and the results are compared with the relative complaints frequencies. The definition of a model event uses a somewhat arbitrary threshold value; however, the actual threshold value is not critical since our model analysis is focused on the identification the possible meteorological and dispersion factors that lead to model events in the Yarloop area.

Section 7 gives conclusions derived from the work presented in this report.

Appendix A details additional NO_x analysis and modelling carried out following the provision of more detailed emission data by Alcoa, subsequent to the completion of the NO_x modelling presented in this report.

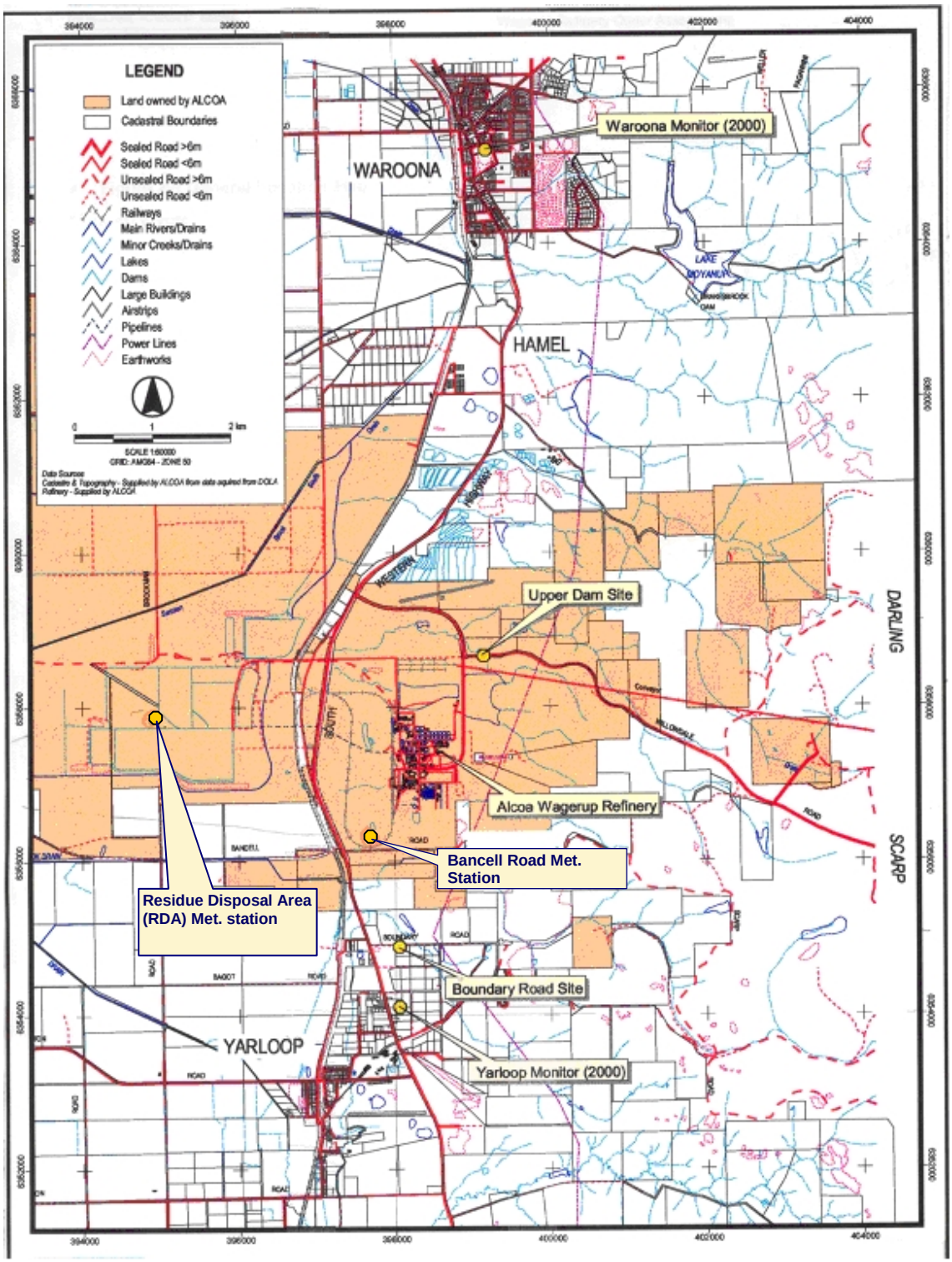

Figure 1: A map of the Wagerup area showing the Alcoa Wagerup Refinery, Bancell Road meteorological station, Residue Disposal Area (RDA) meteorological station, Boundary Road air quality monitoring station, and the Upper Dam monitoring site. The Yarloop monitoring site and the Waroona Monitor are non-operative. To the east of the Refinery is the north-south Darling escarpment (adapted from SKM, 2002).

2. TAPM

The Phase-1 (meteorology) report of the present project (CSIRO, 2004a) provided a brief introduction of the various classes of air pollution models, and discussed the advantages offered by the prognostic approach used by CSIRO's The Air Pollution Model (TAPM) over some of the other commonly-used air pollution models. Although a brief description of TAPM has been given in the CSIRO (2004a) report, we summarise TAPM here again for the sake of completeness.

TAPM is a three-dimensional, prognostic meteorological and air pollution model (see Hurley, 2002; http://www.dar.csiro.au/tapm/ for model details). The model uses a complete set of mathematical equations governing the behaviour of the atmosphere and the dispersion of pollutants. The global databases input to TAPM include terrain height (given at a resolution of about 300 m for Australia), land use, sea-surface temperature, and synoptic meteorological analyses. All input datasets, except emissions, accompany the TAPM software, and are easily transferred through a graphical user interface to nested grids for the region of interest.

The meteorological component of TAPM uses the large-scale weather information (synoptic analyses or, potentially, weather forecasts), typically obtained from the Bureau of Meteorology LAPS (Limited Area Prediction System) or GASP (Global Analysis and Prediction) analyses at a horizontal grid spacing of about 100 km at 6-hourly intervals as boundary conditions for the model outer grid. These synoptic data are for the horizontal wind components, temperature and moisture, and are obtained from the output of a Bureau of Meteorology meteorological model(s) that assimilates meteorological observations from a network of stations. The vertical levels of the synoptic analyses are in a scaled pressure coordinate system. For the present application, the lowest of these correspond typically to 0, 75, 200, 425, 650, 875, 1100, 1325 and 1800 m above mean-sea level. TAPM then 'zooms-in' from the 100-km data to model local scales at a finer resolution using a one-way nested approach to improve efficiency and resolution, predicting local-scale meteorology (typically down to a resolution of 1 km), such as sea breezes and terrain induced flows.

The model solves a set of momentum equations for the horizontal wind components, the incompressible continuity equation for the vertical velocity in a terrain-following coordinate system, and scalar equations for potential virtual temperature, specific humidity of water vapour, cloud water and rain water. Pressure is determined from the sum of hydrostatic and optional non-hydrostatic components. Explicit cloud microphysical processes are included. The turbulence closure terms in the mean equations use a gradient-diffusion approach, including a counter-gradient term for the heat flux, with eddy diffusivity determined using prognostic equations for turbulent kinetic energy and eddy dissipation rate. A weighted vegetative canopy, soil and urban land-use scheme is used to predict energy partitioning at the surface, while radiative fluxes, both at the surface and at upper levels, are also included. Boundary conditions for the turbulent fluxes are determined by Monin-Obukhov surface-layer scaling variables and parameterisations for stomatal resistance.

Atmospheric models are not perfect, and greater resolution cannot always ensure great gains in model skill. However, sometimes it is possible to improve model results by assimilating available meteorological data in a model. Wind data assimilation is where

at one or more locations in the model, the wind speed and wind direction in the model are adjusted to those observed in the atmosphere. The model adjusts its airflow at this and surrounding locations to ensure that the model wind speed and direction at the location closely follow that observed. There are several methods for assimilating data in a model. In TAPM, wind observations can optionally be assimilated into the momentum equations as nudging terms. In nudging, the model is pushed gently towards observed values. The nudging term is time dependent; it forces the model every time step – more when the observations are current and less at earlier and later times. Observations at any height can be included, and the observations can influence a user-specified number of model levels and horizontal radius for each site. The nudging term should be large enough to be noticed by the model, but not so large that it dominates over other terms in the equation. Model predictions with assimilation would be very close to the assimilated observations, but may not be exactly the same. Good quality and continuous records of meteorological data are essential for assimilation purposes.

The air pollution component of TAPM consists of an Eulerian (fixed location) grid-based set of conservation equations for species for determining a spatially explicit distribution of time varying ground-level pollutant concentrations, either using the Eulerian grid-based approach and/or a Lagrangian particle approach targeted at important point sources. In the Lagrangian mode (where the model coordinates essentially move with the air flow), mass is represented as a puff in the horizontal direction and as a particle in the vertical direction. The pollutants are transported and dispersed according to the air motions determined by the meteorological component.

Previous versions of TAPM have been used, for example, to model year-long meteorology and air pollution for the industrial area of Kwinana (Hurley et al., 2001); to model year-long urban meteorology, photochemical smog and particulate matter in Melbourne (Hurley et al., 2003); and to compare with international model validation data sets (Luhar and Hurley, 2003).

3. TAPM Settings

The same version 2.6 of TAPM that was used in Phase 1 was also used for all the simulations presented in this report. All simulations included one extra spin-up day at the start.

Four nested domains with horizontal grid resolutions of 20, 7, 2, and 0.5 km for meteorology, and 10, 3.5, 1, and 0.25 km for plume dispersion were used. The lowest ten of the 25 vertical levels were 10, 25, 50, 100, 150, 200, 250, 300, 400 and 500 m, with the highest model level at 8 km. The default databases of soil properties, topography, and the monthly sea-surface temperature and deep soil parameters were used. In all the runs reported in this document, the Lagrangian mode was used for the dispersion calculations. Unless stated otherwise, the Wagerup-specific land-use database and a refinery-generated surface heat flux value of 150 W m^{-2}, both derived as part of the Phase 1 work (CSIRO, 2004a), were used.

Some TAPM runs included building wake effects and/or assimilation of the local surface wind data. A total of 29 rectangular buildings were considered, ranging in height from 8 m to 42 m. The locations and the horizontal size of these buildings are

shown in Figure 2, together with some of the major Wagerup Refinery point sources (O. Pitts, personal communication, 20 August 2004).

Other model settings that varied from run to run are given below in relevant sections. Unless stated otherwise, all times in this report refer to end of sampling hours.

All model runs, except the ANSTO runs in Section 4.3, were performed on two computer clusters, one using the Intel Pentium IV processors and the other AMD Athlon processors. Both clusters run under the Linux operating system and used the TAPM code compiled using the Absoft Fortran 90/95 compiler (version 3.0). The ANSTO runs were performed on an IBM compatible personal computer with an Intel Pentium III processor and Lahey/Fujitsu Fortran 95 compiler (version 5.6).

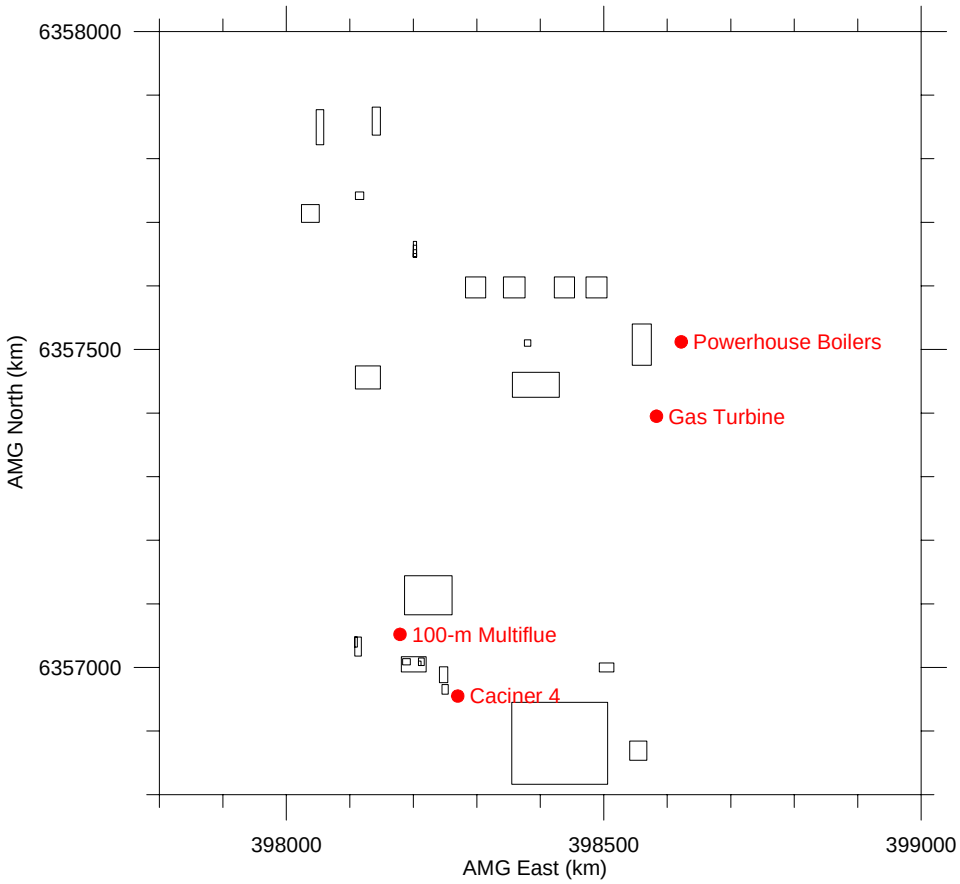

Figure 2: The locations and the horizontal size of the buildings used in selected TAPM runs with building effects. Some of the major Refinery point sources are shown by solid circles (data from O. Pitts, personal communication, 20 August 2004).

4. Evaluation of TAPM

The following sections present an evaluation of TAPM for air quality predictions at Wagerup using Refinery emissions data and observed ambient air concentrations.

4.1. Performance measures for evaluating air pollution models

Methods used for air pollution model evaluation are generally different from those used for meteorological model evaluation. In the case of meteorological model evaluation, a point-by-point comparison of the observed and predicted mean (e.g., hourly averaged) meteorological quantities (e.g., wind speed, wind direction and temperature) is normally made. Hence, the observed and predicted quantities that are paired in both time and space are used to determine model performance through the calculation of a series of statistical measures, such as the mean, the root mean square error, the correlation and the index of agreement. This was the method used in the Phase 1 work of the present project (CSIRO, 2004a).

Methodologies for the comparison of modelled air concentrations with observed field data are still evolving, and evaluation schemes used can be application specific (ASTM, 2000). The above point-by-point procedure for meteorological comparison is generally not followed for evaluation of an air pollution model via the use of observed and predicted ground-level concentrations, especially when limited data are available from sparse monitoring networks (as is the case with Wagerup). This is because the stochastic nature of atmospheric dispersion, governed by the instantaneous, random motions of the air (i.e. turbulence), can lead to large differences between model predictions and observations during a given hour. For example, small differences between the wind direction fields (both the mean and fluctuating part) used by the model and the actual fields can cause the location and magnitude of the predicted concentration at a point to be very different from the observed values at the same point at the same time. This uncertainty increases as the dimensionality (or the degree of freedom) of the diffusion process increases, that is from point-source plumes to line-source plumes and to areas-source plumes. Under these circumstances it is more meaningful to compare the observed and predicted concentration distributions formed using values that are unpaired in time and/or space.

Point-by-point comparison of the model and observed concentrations is not used even when large quantities of data are available from intensive field studies designed for model evaluation with a much denser receptor network than routinely-operated monitoring networks. For example, air pollution model evaluation using data from the well-known Kincaid and Indianapolis field experiments is generally performed using only the observed and predicted centreline concentrations on sampling arcs unpaired in space (hence, this way, the stochastic uncertainty associated with the influence of wind direction on concentration is eliminated) (see for example, Luhar and Hurley, 2003). For Wagerup, data are available from a very sparse receptor network: the NO_x data are available for one year or longer, but only at two locations, whereas tracer data are available at 11 receptors but only for a total of 13 hours. Hence, for the purpose of evaluating TAPM for Wagerup, we use the observed and predicted concentrations unpaired in time (and in space too for ANSTO tracer simulations).

The performance measures described below are used for model evaluation (e.g., Hurley et al., 2001, 2003; Venkatram et al., 2001, 2004).

Use of a quantile-quantile plot (also called a q-q plot) is common in model evaluation. This graphical technique is used for determining if two datasets with equal sample size (i.e. observed and predicted concentrations) come from populations with a common distribution. Normally, a q-q plot is a plot of the quantiles of the first data set against the quantiles of the second data set. A quantile here means the fraction (or percent) of points below the given value. That is, the 0.9 (or 90%) quantile is the point at which 90% percent of the data fall below and 10% fall above that value. However, it is common to directly plot the one data set against the other. That is, the actual quantile level is not plotted. For a given point on the q-q plot, we know that the quantile level is the same for both points, but not what that quantile level actually is (see http://www.itl.nist.gov/div898/handbook/eda/section3/qqplot.htm). Hence, in an air pollution model evaluation application, the q-q plot is essentially a plot of the sorted observed concentrations against the sorted predicted concentrations. A 1:1 reference line is also plotted. If the two sets come from a population with the same distribution, the points should fall approximately along this reference line. The greater the departure from this reference line, the greater the evidence for the conclusion that the two data sets have come from populations with different distributions.

With the use of a q-q plot, many distributional aspects can be simultaneously tested. For example, shifts in location, shifts in scale, changes in symmetry, and the presence of outliers can all be detected from this plot. If the two data sets come from populations whose distributions differ only by a shift in location, the points should lie along a straight line that is displaced either up or down from the 1:1 reference line.

The main test of an air pollution model from the point of view of pollution management and regulatory applications is whether it can correctly predict the extreme (or high) end of the concentration frequency distribution constructed using data collected over a reasonably long period (e.g. one year). It is possible to check whether the model is performing well in predicting extreme concentrations by a visual inspection of the q-q plot. However, there are performance measures that can be used for a more quantitative evaluation. The robust highest concentration (RHC) (Cox and Tikvart, 1990) is such a performance measure, and is defined as:

$$RHC = C(R) + \left(\overline{C} - C(R)\right)\ln\left(\frac{3R-1}{2}\right),$$

where $C(R)$ is the Rth highest concentration and $\overline{C}$ is the mean of the top $R-1$ concentrations. The RHC is based on an exponential fit to the highest $R-1$ values of the cumulative frequency distribution. A value of $R = 11$ is used in the present analysis so that $\overline{C}$ is the average of the top ten concentrations, which is an accepted statistic for evaluation of model performance (Hanna, 1988). The RHC is preferred to the maximum value because it mitigates the undesirable influence of unusual (stochastic) events, while still representing the magnitude of the maximum concentration (unlike percentiles).

Frequently, percentiles are also used to compare model results with observations and to compare concentrations with air quality standards (including odour). The p^{th} percentile is a value such that roughly p% of the data are smaller and (100 – p)% of the data are

larger than this value; the 50th percentile is called the median. We use some of the top percentiles, as well as the maximum, the 2nd highest, the average of the top ten concentrations, and the mean, for model evaluation.

4.2. Modelling of oxides of nitrogen (NO_x)

Measured NO_x data from Alcoa's Boundary Road and Upper Dam monitoring stations were used for TAPM evaluation. The Boundary Road data were available for the one-year simulation period 1 April 2003–31 March 2004, whereas the Upper Dam data were available only till 12 December 2003. The AMG (Australian Map Grid) locations of these stations are (399.120 km E, 6358.450 km N) and (398.031 km E, 6354.875 km N), respectively, and they are about 1.5 km north-east and 2.5 km south of the Refinery, respectively (see Figure 1). The details of model evaluation are given below.

4.2.1 Model setup

TAPM was run for the period 1 April 2003–31 March 2004 with four nested domains of 31 × 31 horizontal grid points for the meteorology, and 25 × 25 horizontal grid points for the dispersion, all centred on the location 115°54.5′ E, 32°55.5′ S, which is equivalent to 397.932 km east and 6356.486 km north in the Australian Map Grid (AMG) coordinate system. The centre point is almost halfway between the Refinery Multiflue and the Bancell Road meteorological station.

Figure 3a–d shows the four successive model domains for meteorology, corresponding to a grid resolution of 20, 7, 2 and 0.5 km, respectively. The smaller, finer domain embedded in a meteorological domain represents the area and resolution for the NO_x dispersion calculations, at a grid resolution of 10, 3.5, 1 and 0.25 km, respectively. The innermost domain covers an area of 15 km × 15 km for meteorology and 6 km × 6 km for dispersion. The green-grey shading represents the terrain height at the same resolution as that used for meteorology.

Information on the Refinery NO_x sources and emissions was supplied by Alcoa on 7 September 2004 (file "WGCombinedEmissionsRev5.xls"), and is given in Table 1. CSIRO had no role in the development or verification of these emissions. The modelled concentrations are directly dependent on these emissions. If the emissions are different, then the modelled concentrations will be different. No temporal variation of the NO_x emissions is available; it is assumed that the emission rates do not vary significantly with time (see Appendix A for an update on emissions), and that they represent the average emission conditions.

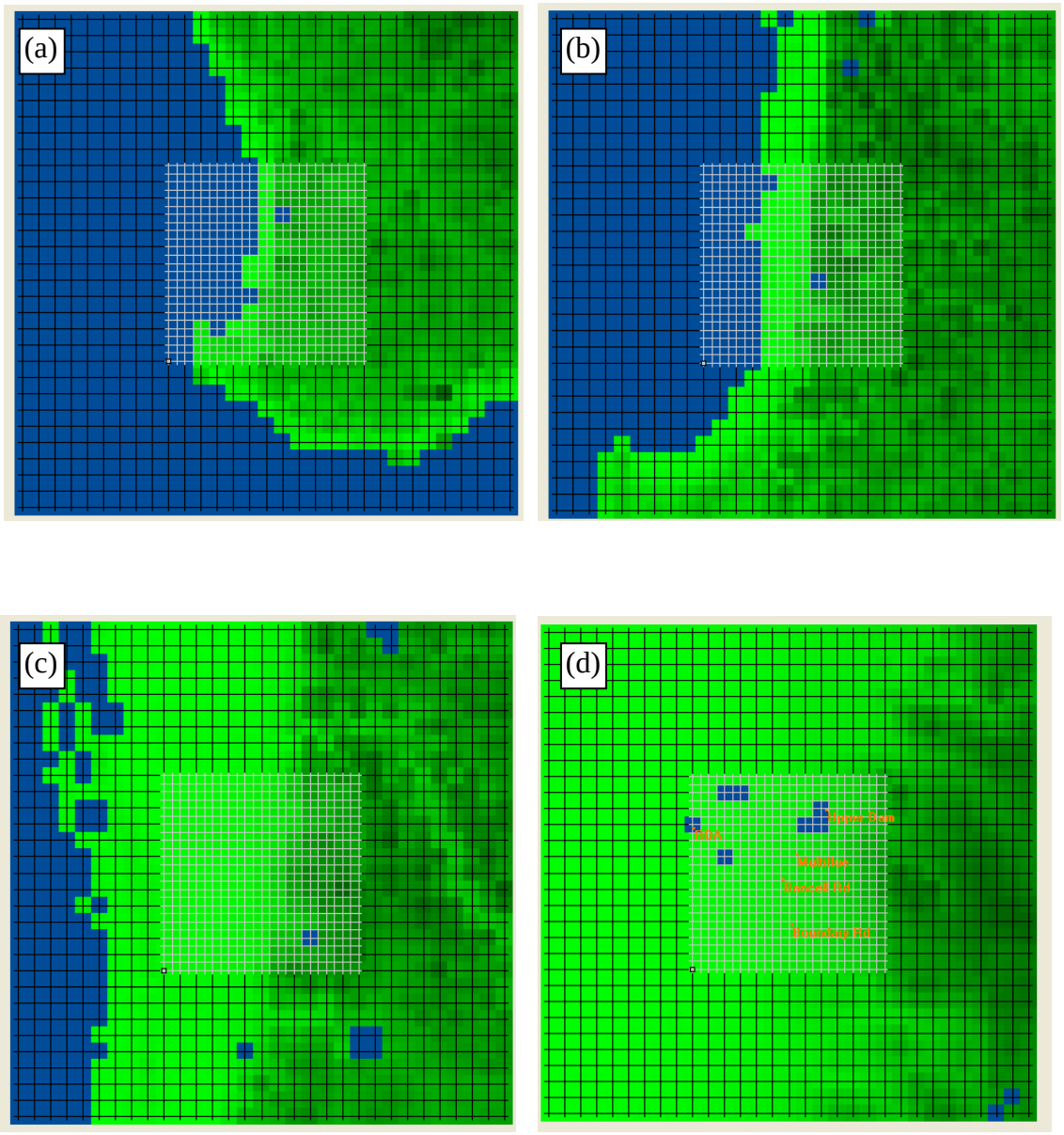

Figure 3: The horizontal grid domain used in TAPM for meteorology (31 × 31 grid points) and the smaller, finer horizontal grid domain for NO_x predictions (25 × 25 grid points). These domains are successively nested at a grid resolution of (a) 20, (b) 7, (c) 2 and (d) 0.5 km for meteorology, and (a) 10, (b) 3.5, (c) 1 and (d) 0.25 km for NO_x dispersion predictions.

Table 1: The NO_x sources and their characteristics used as input in TAPM (data supplied by Alcoa).

Source	AMG location		Source height (m)	Source radius (m)	Exit velocity (m s^{-1})	Exit temp. (°K)	NO_x emission rate* (g s^{-1})
	East (km)	North (km)					
Liquor Burner	398.179	6357.052	100	0.47	27.9	338	1.24
Calciner 1	398.179	6357.052	100	0.95	21.6	432	2.16
Calciner 2	398.179	6357.052	100	0.95	20.8	433	1.25
Calciner 3	398.179	6357.052	100	1.08	19.6	469	3.60
Calciner 4	398.270	6356.955	48.8	1.18	20.1	430	2.43
Boiler 1	398.622	6357.512	65	1.20	14.5	374	7.61
Boiler 2	398.622	6357.512	65	1.00	16.2	397	7.96
Boiler 3	398.622	6357.512	65	1.00	13.7	404	2.64
Gas Turbine	398.583	6357.395	40	1.52	22.4	371	3.00

* Expressed as NO_2.

TAPM was run in three configurations:

- *Run A*: TAPM with the Wagerup-specific land-use data base and refinery-generated surface heat flux,
- *Run B*: TAPM with the Wagerup-specific land-use data base, refinery-generated surface heat flux, and building effects,
- *Run C*: TAPM with the Wagerup-specific land-use data base, refinery-generated surface heat flux, building effects, and wind data assimilation.

In Run C, the hourly-averaged wind speed and wind direction measurements made at about 8 m AGL (above ground level) at the RDA and those at 30 m AGL at Bancell Road were used (the 30-m observations started from 18 July 2003). The RDA data for wind speeds less than 0.8 m s^{-1} were not used because of stalling issues associated with the cup anemometer at this site for low wind speeds (see CSIRO, 2004a). In the modelling, the horizontal radius of influence for the assimilated winds at both sites was taken as 5 km (which is the minimum for TAPM). In the vertical, the model options were selected such that the Bancell Road winds influenced the first four model levels, and the RDA winds the first two levels. This difference is due to the different heights of measurements at the two sites.

The hourly-averaged modelled NO_x concentrations on the innermost grid domain were extracted at the grid point nearest to each of the two monitoring sites (i.e. Boundary Road and Upper Dam) for comparison with the data. The modelled NO_x concentrations obtained in the units of $\mu g\ m^{-3}$ were converted to the units of parts per billion by volume (ppb) by multiplying them with a factor of 0.523. Note that when using mass and density units, both the ambient NO_x concentrations and the Refinery NO_x emissions are expressed in terms of NO_2 as is the practice in air pollution studies.

4.2.2 Data analysis

The 6-minute NO_x data taken at Alcoa's Upper Dam and Boundary Road monitoring stations were used to calculate hourly averages. Hourly periods for which there were more than 40% missing data were not included in the subsequent analysis. There were no NO_x data at Upper Dam for the period 13 December 2003 until the end of the model simulation period (i.e. 31 March 2004).

Figure 4 presents the variation of the measured NO_x concentration with the observed 30-m Bancell Road wind direction at (a) Upper Dam and (b) Boundary Road. (The 30-m wind observations started from 18 July 2003.) Figure 4a shows that a well defined peak at Upper Dam occurs when the winds are from the Refinery sector between 190°–240°, with the maximum value being about 35 ppb. There is a much smaller, but noticeable, peak, with a value of about 12 ppb, for northerly winds (between 330°–30°), which may suggest NO_x contributions from Hamel and/or Waroona.

Figure 4b shows that there is a reasonably well-defined peak for the (Refinery) wind direction sector 345°–30° at Boundary Road, with a maximum concentration of about 24 ppb. However, it is also apparent in Figure 4b that there is an even more pronounced concentration distribution for the wind direction sector between 150°–270°, which suggests that local sources in Yarloop and those in areas south-west of this monitoring station are contributing substantially. These sources may include the South Western Highway, which is only about 300 m west of the Boundary Road site, and the local traffic and other combustion sources in the Yarloop area.

The plots in Figure 4 do not include the NO_x data from 1 April 2003 to 17 July 2003 because the 30-m wind measurements at Bancell Road did not start until 18 July 2003 when the 10-m mast was replaced by a 30-m mast, measuring winds at both 10-m and 30-m levels. Even though there are 10-m wind data for the whole of the selected one-year period that can be used to plot the NO_x data against, there are measurement problems due to the sheltering of the 10-m wind sensor by the new mast when the flow is easterly (between about 45°–135°) (see CSIRO, 2004a). These problems are, therefore, applicable starting from 18 July 2003. However, the easterly wind sector is not critical in terms of contribution of NO_x sources when examining the variation of the NO_x concentration with wind direction at the two sites.

Figure 5 presents the variation of the observed NO_x concentration with the observed 10-m Bancell Road wind direction at (a) Upper Dam and (b) Boundary Road. The overall behaviour of NO_x versus 10-m winds in Figure 5 for both sites is qualitatively similar to that for NO_x versus 30-m winds in Figure 4. The two maxima in Figure 5b for Boundary Road occur under southerly and north-westerly flows, each with a value of about 55 ppb. These maxima are not present in Figure 4b because they occurred before the wind measurements at 30 m AGL started.

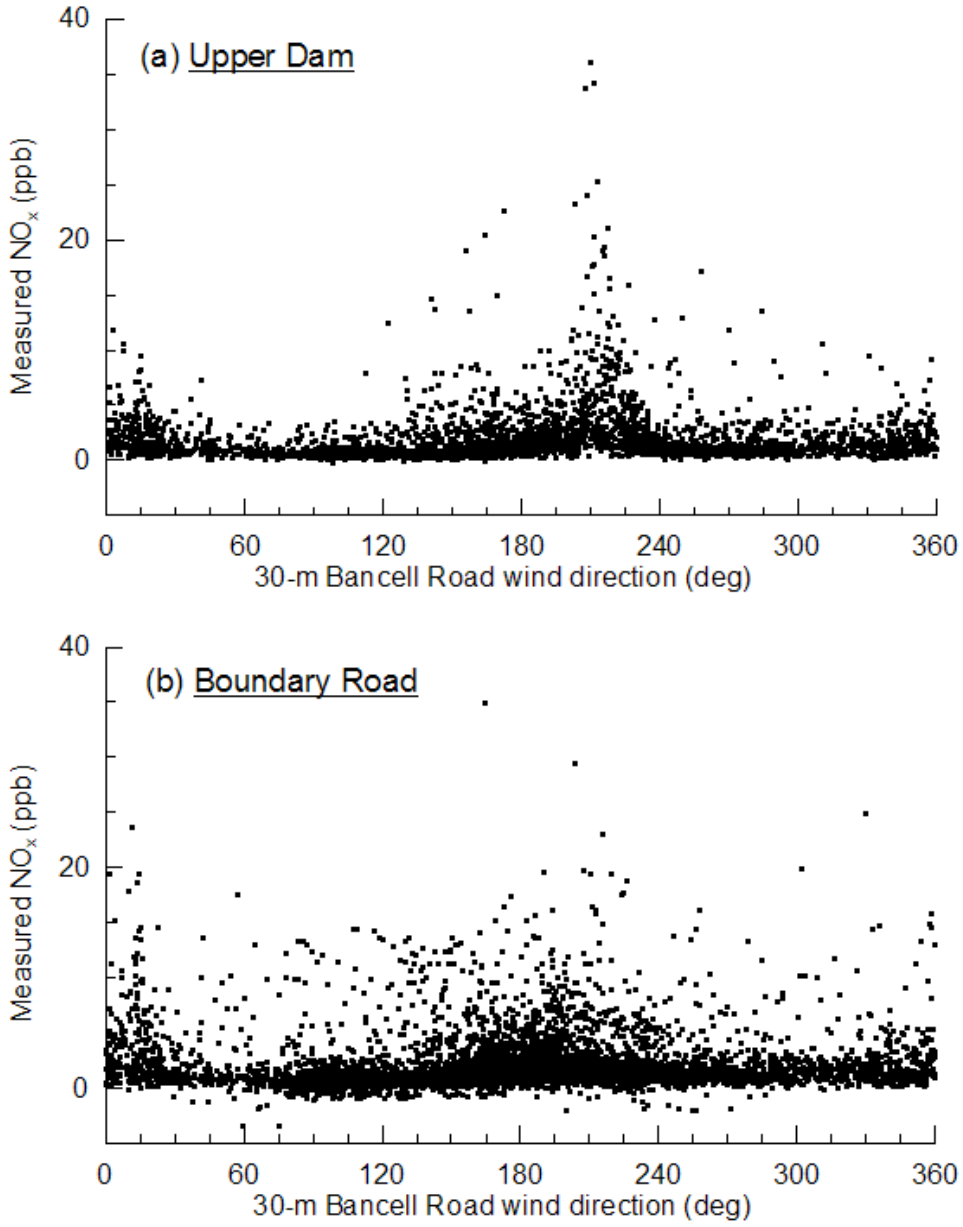

Figure 4: Variation of the observed NO_x concentration as a function of the observed 30-m Bancell Road wind direction at (a) Upper Dam and (b) Boundary Road.

The Upper Dam site is isolated from any interference from local NO_x sources to a greater extent than the Boundary Road site, and, therefore, the data from this site are more robust for the purpose of comparing them with the modelled NO_x concentrations due to the Refinery emissions. The above analysis suggests that this site is a good location for monitoring the footprint of the Refinery NO_x emissions.

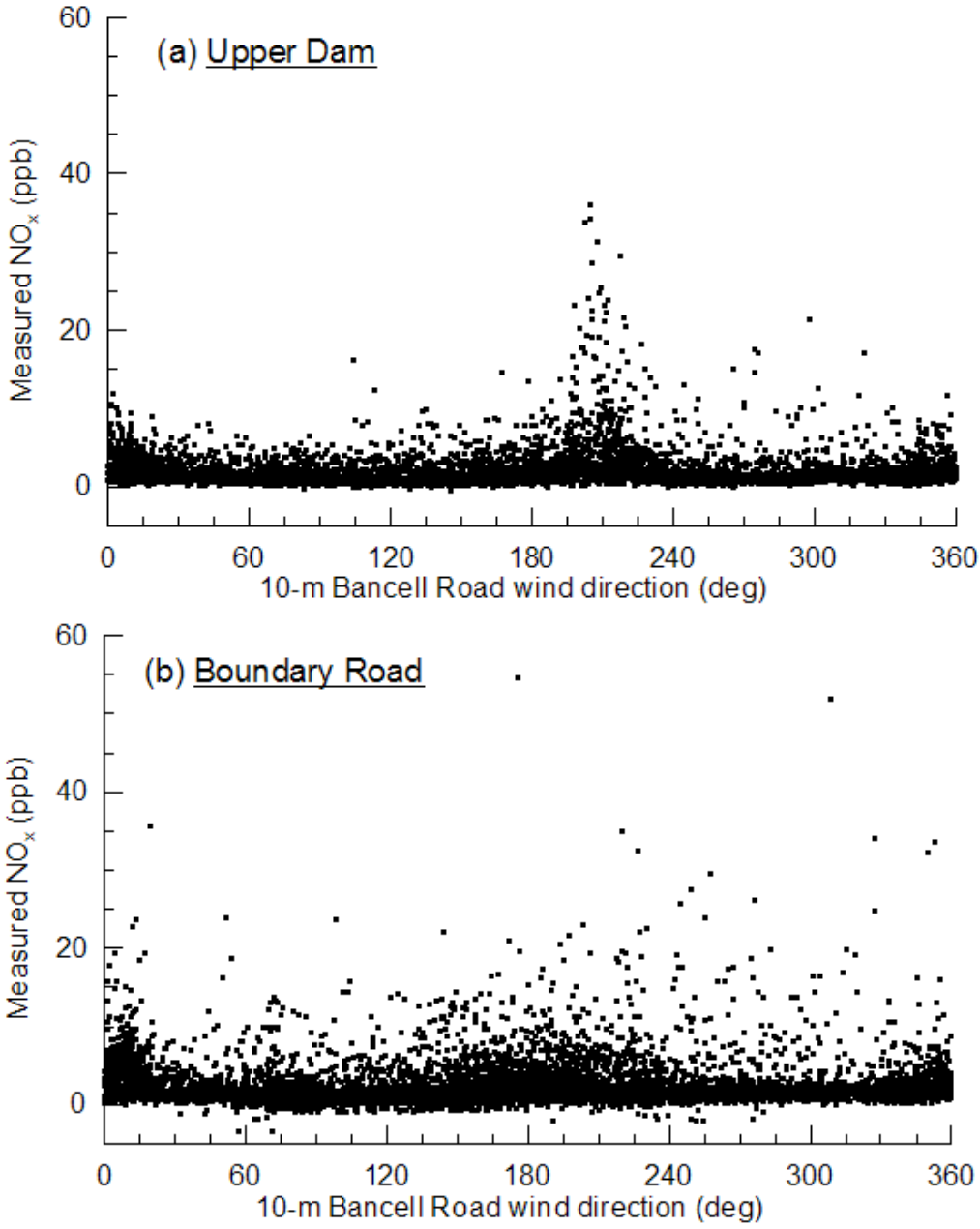

Figure 5: Variation of the observed NO_x concentration as a function of the observed 10-m Bancell Road wind direction at (a) Upper Dam and (b) Boundary Road.

The above NO_x features are also seen in previous analyses of Wagerup data. An analysis of 6-min NO_x data reported in CSIRO (2004d) for the measurement period March 2002–June 2003, indicates that dominant peaks at Upper Dam occur when the wind is from the refinery sector, and that all the dominant maxima at Boundary Road occur under westerly winds and not when the wind is from the plant. Most peaks were found to occur under low to moderate winds (< 4 m s^{-1}). An analysis by SKM (2002) of NO_x data at four sites (viz Upper Dam, RDA, Yarloop and Waroona) for the month of December 2000 also suggests that there were unambiguous peaks at Upper Dam when the winds were from the Refinery, but there were no dominant peaks at Yarloop (a site within Yarloop town, about 750 m south of Boundary Road) under such wind conditions.

4.2.3 Model evaluation

Figure 6 presents the variation of the modelled NO_x concentration with the modelled 25-m Bancell Road wind direction at (a) Upper Dam and (b) Boundary Road, obtained from Run B (without wind data assimilation). The modelled hours for which there are no observed NO_x data, are excluded from the plot. It is clear in Figure 6a and Figure 6b that high concentrations are predicted when the winds are from the Refinery sector. Comparison of Figure 6a with Figure 4a and Figure 5a indicates that the magnitude of the observed NO_x peak is predicted well by TAPM at Upper Dam. However, for many hours for which the observed concentrations are low (around 1–2 ppb), the model is predicting zero concentration. These low observed concentrations are presumably due to NO_x emissions from soil and other local/regional sources, which the present modelling does not take into account. Figure 6b indicates that at Boundary Road the model is predicting the magnitude of the observed high concentrations (as shown in Figure 4a and Figure 5a) well when the winds are from the Refinery wind sector.

Figure 6a and Figure 6b also show that occasionally even though the winds are not from the Refinery, the model predicts high concentrations. Meteorological factors such as turning of the wind with height, and also turning with distance travelled in the horizontal, means that the source of a pollutant peak may not necessarily be straight upwind of the sampling location. For example, the peaks at both sites when the wind direction is about 70°, which is due to low wind speeds close to the surface that become almost calm close to the stack release heights, thus resulting in a plume footprint that is more widespread than that under the conditions of moderate to high wind speeds.

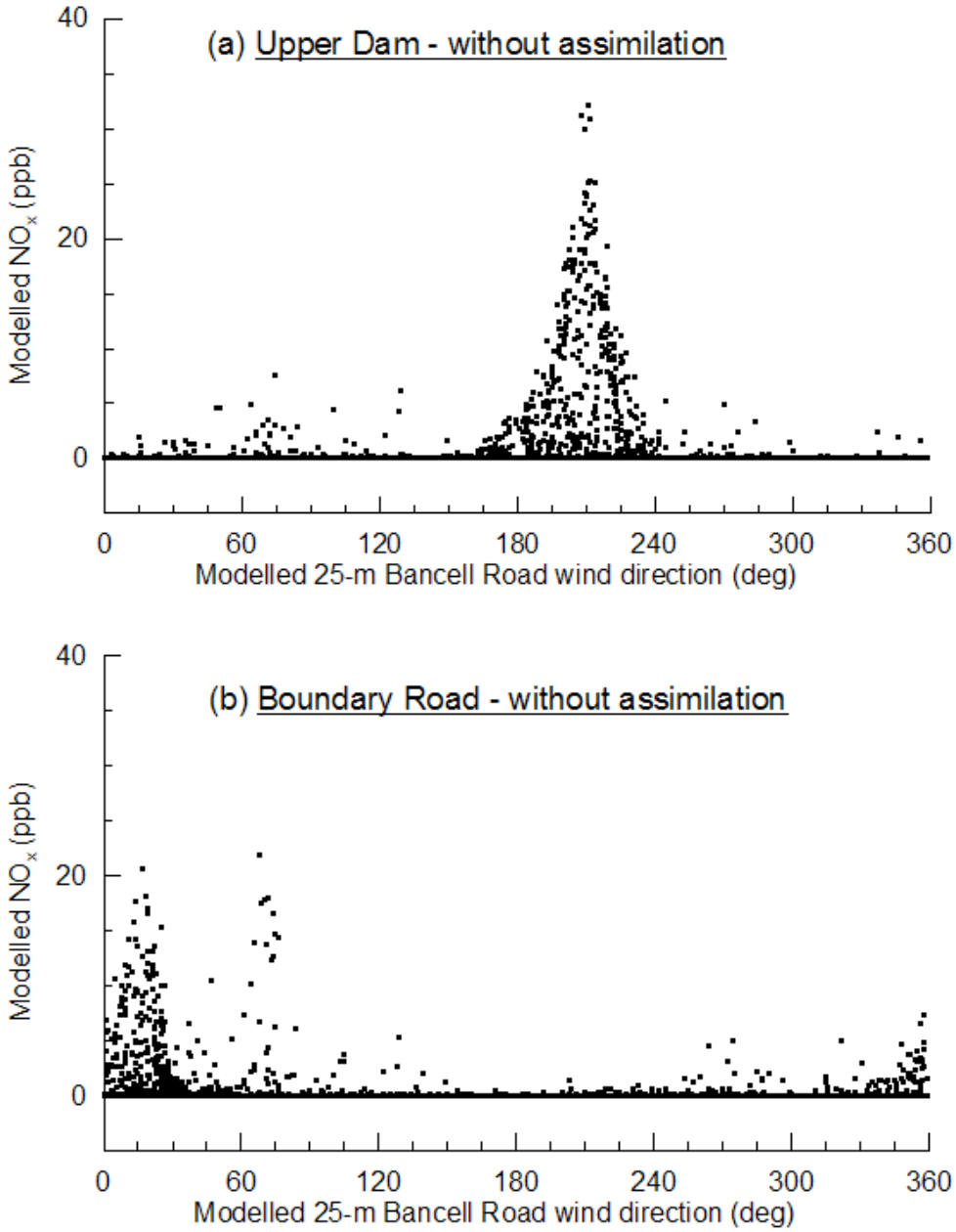

Figure 6: Variation of the modelled (Run B) NO_x concentration with the modelled 25-m Bancell Road wind direction at (a) Upper Dam and (b) Boundary Road.

Figure 7a and Figure 7b present the variation of the modelled NO_x concentration with the modelled 25-m Bancell Road wind direction at (a) Upper Dam and (b) Boundary Road, obtained from Run C (with wind data assimilation). As in the previous figure, the modelled hours for which the there are no observed NO_x data are excluded from the plot. Highest concentrations occur when the wind is directly from the Refinery direction. With wind data assimilation the peak value at Boundary Road (Figure 7b) is predicted to be larger and closer to the observed peak value than that without wind data assimilation. However, the peak value at Upper Dam remains almost the same with wind data assimilation as without wind data assimilation.

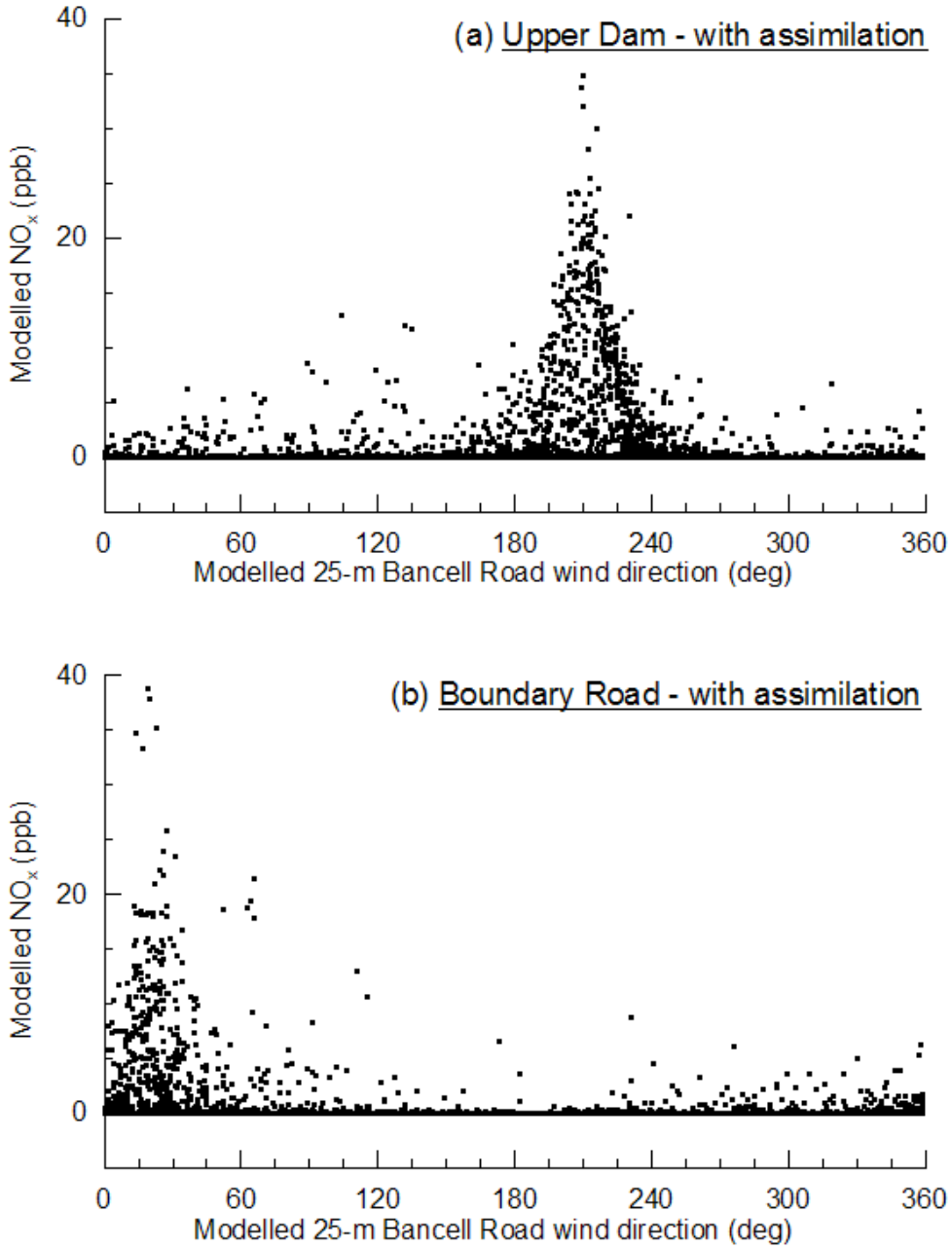

Figure 7: Variation of the modelled (Run C) NO_x concentration with the modelled 25-m Bancell Road wind direction at (a) Upper Dam and (b) Boundary Road.

To quantitatively evaluate the model for its capability of predicting ambient NO_x concentrations due to the Refinery sources, we only consider for Boundary Road the wind sector from the Refinery because of the possible interference, in other sectors, by sources other the Refinery that are not included in the modelling. Only those hourly periods for which the observed wind directions at Bancell Road were within 330°–80° were considered for comparison. This is a fairly wide range for the Refinery wind sector at Boundary Road, but it was selected (based on Figure 4 and Figure 5) to ensure that it covers dominant pathways by which the refinery plume reaches Boundary Road. For example, the model results in Figure 6 show that even when the mean wind direction is 70°, the Boundary Road site can experience relatively high concentrations under low wind speed conditions. The filtering was done using the observed wind directions at

10 m AGL for the period 1 April–18 July 2003 (up to 1200 h) and those at 30 m AGL for the remaining period up to 31 March 2004. The reason why the observed wind directions at 30-m, and not those at 10-m, were used for the latter period was because the 10-m wind sensor on the new 30-m mast, commissioned on 18 July 2003, is sheltered for the easterly flow by the mast. The wind direction range selected for filtering includes an easterly flow component, and, therefore the 30-m data, and not the 10-m data, were used.

Because the possible contribution from non-Refinery sources (i.e. sources other than the ones considered in the present model runs) to NO_x at Upper Dam is much less than that from Boundary Road, we consider all NO_x data at Upper Dam.

In the quantile-quantile (q-q) plot in Figure 8, the sorted predicted NO_x concentrations are plotted against the sorted observed NO_x values (i.e. independent of time) at Upper Dam for the three TAPM runs. Overall, all three runs perform well in simulating the observed concentration distribution. A comparison of the Run-A curve with the Run-B curve indicates that the inclusion of the building effects in the model does not make a significant difference in the predictions at Upper Dam. The assimilation of the wind data in TAPM (Run C) slightly improves the prediction of the top few concentrations, but leads to a slight overprediction of concentration distribution for the 8–20 ppb range compared to Run A and Run B. For observed concentrations between 4–8 ppb, Run C is closer to the observed distribution than the other two runs. The model predicts zero concentrations for the observed concentration distribution below about 4 ppb. This is presumably because of the absence of NO_x emissions from soil and other local/regional sources in the model.

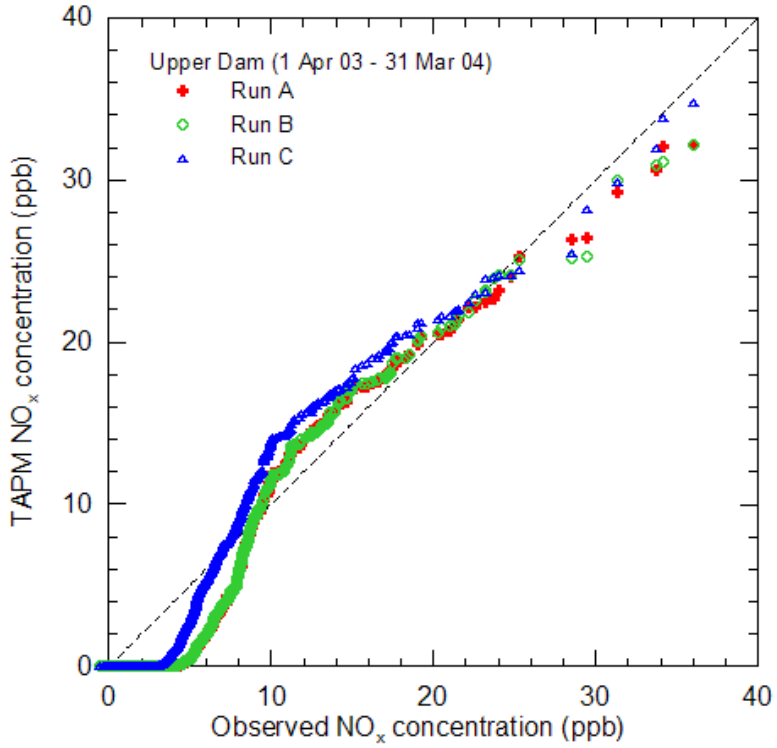

Figure 8: Quantile-quantile plots of the hourly-averaged modelled vs. observed NO_x concentrations for the three TAPM runs for Upper Dam.

Figure 9 presents plots of observed and modelled values of RHC and other performance values for the three TAPM runs at Upper Dam. These plots show that both Run A and Run B perform well in simulating the observed extreme statistics, with a slight underprediction (9%) of RHC. In both these Runs, the model underestimation is the largest for the 90^{th} percentile, which is dominated by the occurrences of low concentrations. For 90% of the time, the model predicts almost zero concentrations, while the observed values are below about 5 ppb. These results also show that the inclusion of buildings effects does not make any significant difference in concentration predictions (at this site). The NO_x sources considered include all the tall stacks within the Refinery, which are less likely to be influenced by the buildings than some of the smaller stacks and vents. Figure 9c for Run C demonstrates that the use of wind data assimilation in TAPM leads to a slight improvement in the model performance, especially in the prediction of the maximum concentration and the 95^{th} and 90^{th} percentiles, and is a superior fit than either Run A or Run B.

Modelled and observed values of the concentration statistics for Upper Dam are given in Table 2. It is clear that the model underestimates the observed mean value of 2.2 ppb. The mean value is dominated by the high frequency of low concentration events when the Refinery plume does not impact the monitoring site. These low concentrations are dominated by levels that are close to the background NO_x concentrations, which are not included in the model. There are unknowns about the background NO_x at Wagerup. Dabberdt and Dietz (1986) give a rural NO_x concentration of 3 ppb. Galbally et al. (1987) undertook measurements of the background NO_x concentration in the atmosphere at Griffith (NSW) and found that the concentration varied from 0.3 ppb to 3.6 ppb on a diurnal basis, with a nighttime maximum. They also found that the bulk of NO_x was NO_2. A background NO_x value of around 2 ppb added to the model predictions would be consistent with the observed mean value. Addition of this value to the modelled concentrations will simply lift all model values in Figure 9 by 2 ppb.

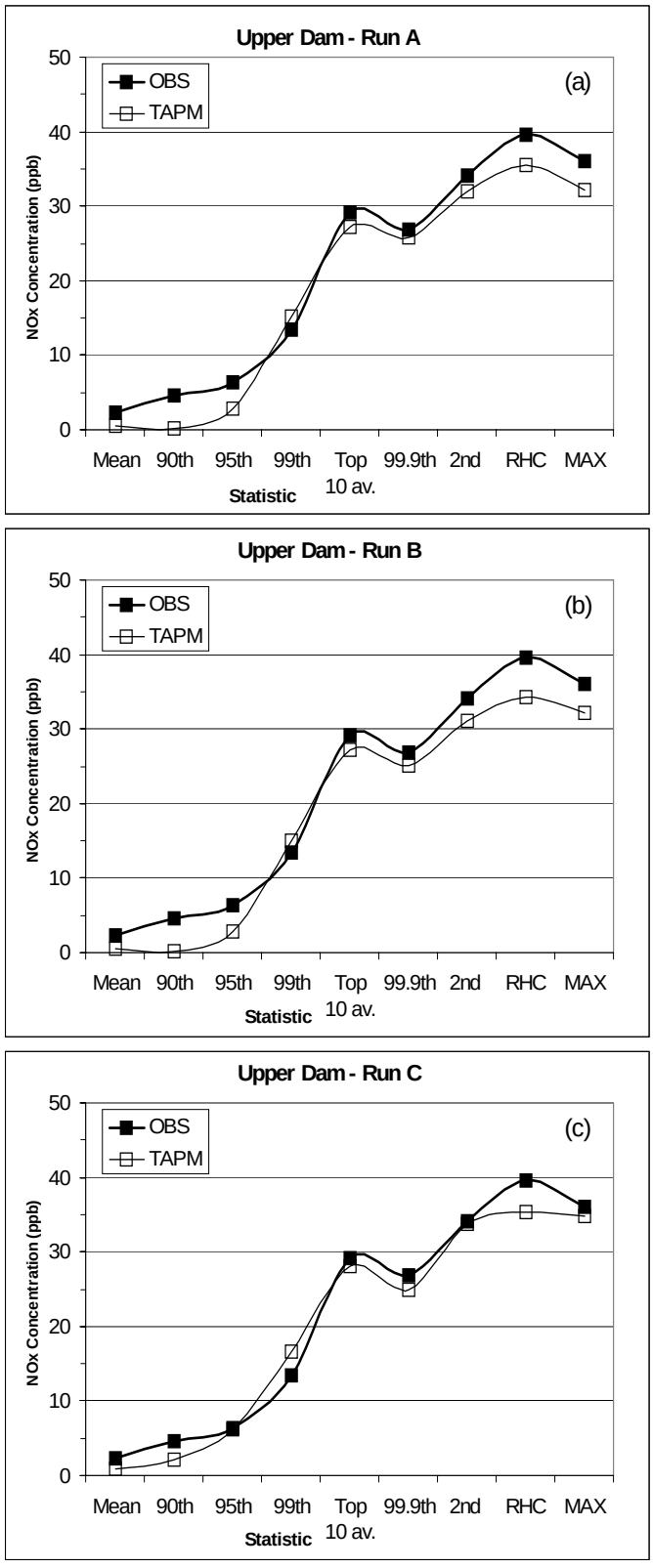

Figure 9: Observed and modelled annual maximum, robust highest concentration (RHC), 2nd highest concentration, average of the top ten concentrations, mean, and percentile statistics for NO_x concentrations at Upper Dam. The three plots correspond to the three model runs.

Figure 10 is a q-q plot for Boundary Road for the three TAPM runs. The Run A and Run B curves show that there is a tendency in the model to underestimate the observed concentration distribution. The inclusion of building effects (Run B) leads to a small decrease (of about 8%) in the top concentration levels at Boundary Road. It is apparent that for Boundary Road, the assimilation of the wind data in TAPM (Run C) improves the predictions compared with both Run A and Run B, although now there is some overestimation of the concentration distribution. This improvement with data assimilation is greater than that at Upper Dam. Note that, as discussed earlier, wind direction based data filtering has been used for Boundary Road data, giving a smaller sample size, and the amount of influence on the data due to non-Refinery sources even after filtering is not known.

From the model comparison perspective, the Boundary Road NO_x data are not as robust as the Upper Dam data. There is evidence, shown in Figure 4 and Figure 5, that the Boundary Road NO_x concentrations include contributions from non-Refinery sources (possibly from local traffic and Yarloop) that are as large as, or even larger than, the Refinery contributions. It is possible that non-Refinery sources (e.g. Waroona) contributed to Upper Dam NO_x also, but the wind sector analysis given earlier suggests that this contribution is much smaller than the Refinery contribution at Upper Dam.

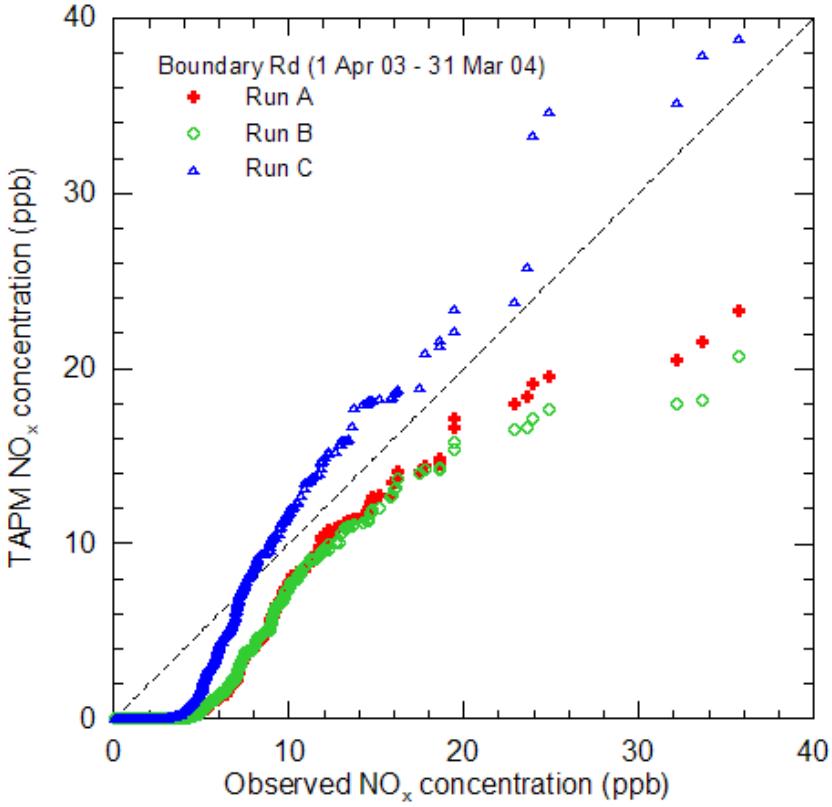

Figure 10: Quantile-quantile plots of the hourly-averaged modelled vs. observed NO_x concentrations for the three TAPM runs for Boundary Road.

Table 2: Modelled and observed annual statistics of NO_x concentrations at the Upper Dam (sample size = 5531) and Boundary Road (sample size = 1972) monitoring sites.

Statistic	Observed (ppb)	Run A* (ppb)	Run B* (ppb)	Run C* (ppb)
Upper Dam				
Mean	2.2	0.6	0.6	0.9
90th percentile	4.6	0.2	0.2	2.0
95th percentile	6.4	2.8	2.9	6.2
99th percentile	13.4	15.2	15.0	16.6
Average of top ten	29.1	27.2	27.2	28.1
99.9th percentile	26.8	25.8	25.1	24.9
2nd highest	34.1	32.1	31.2	33.8
RHC	39.5	35.5	34.3	35.4
Maximum	36.0	32.2	32.2	34.8
Boundary Road				
Mean	2.8	0.7	0.7	1.3
90th percentile	6.0	1.3	1.4	4.4
95th percentile	8.2	4.4	4.6	9.2
99th percentile	14.8	12.6	11.9	18.2
Average of top ten	25.4	18.9	17.0	29.7
99.9th percentile	32.2	20.5	18.0	35.3
2nd highest	33.6	21.6	18.2	37.9
RHC	37.6	26.6	21.9	44.4
Maximum	35.7	23.3	20.7	38.8

*An addition of a background NO_x concentration of 2 ppb in the modelled concentrations will increase values of all model statistics by 2 ppb.

Observed and modelled values of RHC and other performance measures for the three TAPM runs at Boundary Road are plotted in Figure 11. For Run A and Run B, the performance statistics are underestimated by the model. The RHC is underestimated by 30% for Run A, and by about 40% for Run B. For these runs, out of all statistics, the 99th percentile is closest to the observations. Again Run C provides a superior match to the observations than either Run A or Run B.

In Figure 11c, there is some overestimation of the model performance measures above the 95th percentile when the observed winds are assimilated in the model (Run C). In this case (Run C), the modelled RHC is 18% greater than the observed RHC, and there is reasonable agreement, with smaller differences of model and observed concentrations for all other high concentration statistics.

Table 2 gives the modelled and observed values of the concentration statistics for Boundary Road. As with Upper Dam, the model underestimates the observed mean value of 2.8 ppb, which is dominated by the high frequency of low concentration events which in turn are dominated by background concentrations. As for the pervious case, the addition of a background NO_x concentration of 2 ppb in the model concentrations would improve the prediction of the mean concentration, while having a proportionally much smaller effect on the high end of the concentration distribution.

As mentioned earlier, comparison of the model and observed concentrations paired in time is not adopted here. The performance measures calculated using observed and model values unpaired in time and/or space are used for model evaluation. However, such a method does not reveal whether the right results are obtained for the right reasons, i.e. whether the model performs well under a range of conditions during a given a year. Therefore, the performance test is carried out under four conditions: winter (1 April–30 September 2003), (b) summer (1 October 2003–31 March 2004), (c) daytime (0800–1900 h), and nighttime (2000–0700 h). We divide the modelled and observed NO_x concentrations into these four categories, and the q-q plots are then drawn. Figure 12 and Figure 13 present the q-q plots for Upper Dam and Boundary Road, respectively.

For Upper Dam, TAPM shows a bias towards underestimating the observed concentrations in winter (Figure 12a), whereas for summer the model overestimates (Figure 12b). (These two trends balance out in the full year's data to give the good agreement in Figure 8.) The model performance during the day is good (Figure 12c), but in the nighttime, TAPM underestimates the observed concentrations when the wind data assimilation is not used (Figure 12d). These figures also show that, at Upper Dam, wind data assimilation does not cause large differences in the predictions, except in the nighttime where it improves the predictions (by increasing the frequency of the southerly/south-westerly winds).

Wind data assimilation makes a bigger difference at Boundary Road than at Upper Dam. For Boundary Road, overall, the model concentrations computed with wind data assimilation are larger than those without (Figure 13). Generally, the high-end concentrations predicted by the model with wind data assimilation are in better agreement with the data and are higher than the observations (Figure 13a–d). The model without wind data assimilation underestimates the high-end concentrations under all four conditions.

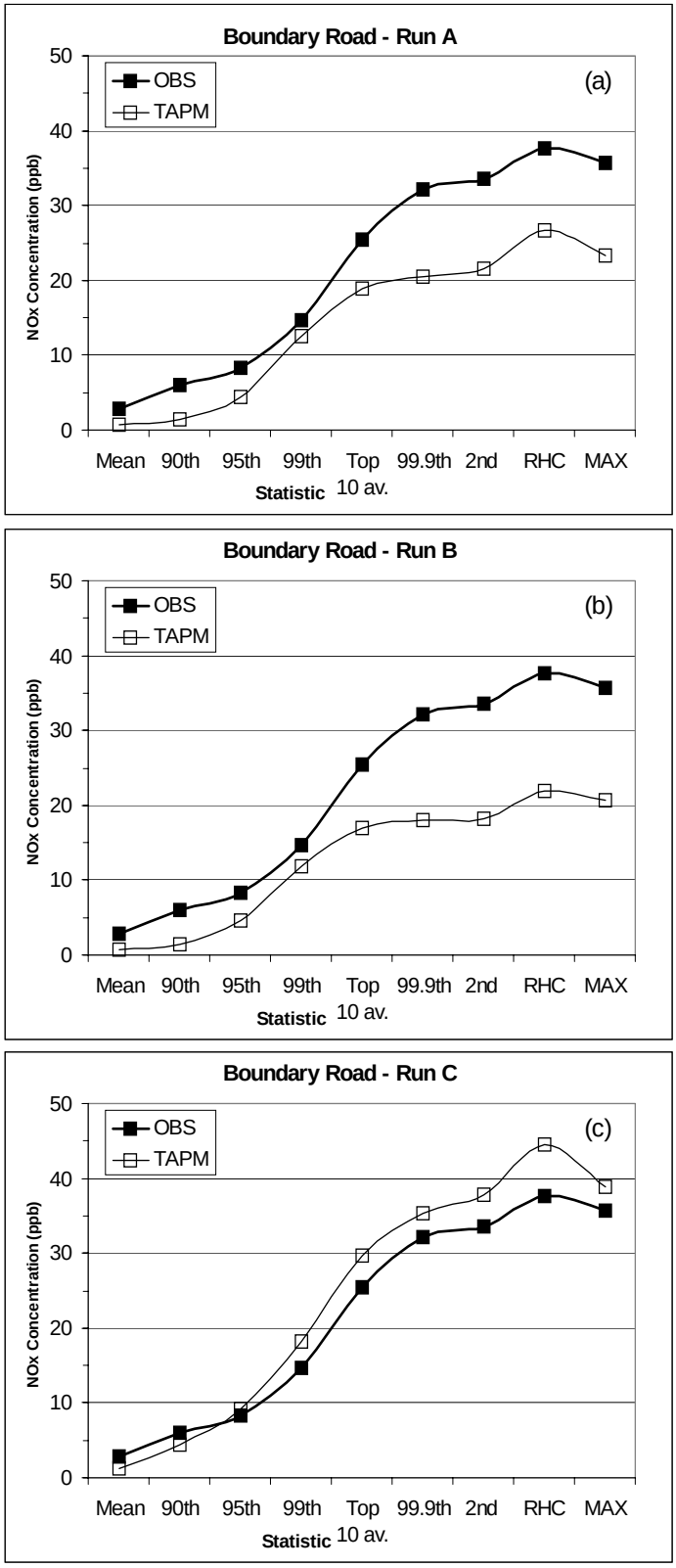

Figure 11: Observed and modelled annual maximum, robust highest concentration (RHC), 2nd highest concentration, average of the top ten concentrations, mean, and percentile statistics for NO_x concentrations at Boundary Road. The three plots correspond to the three model runs.

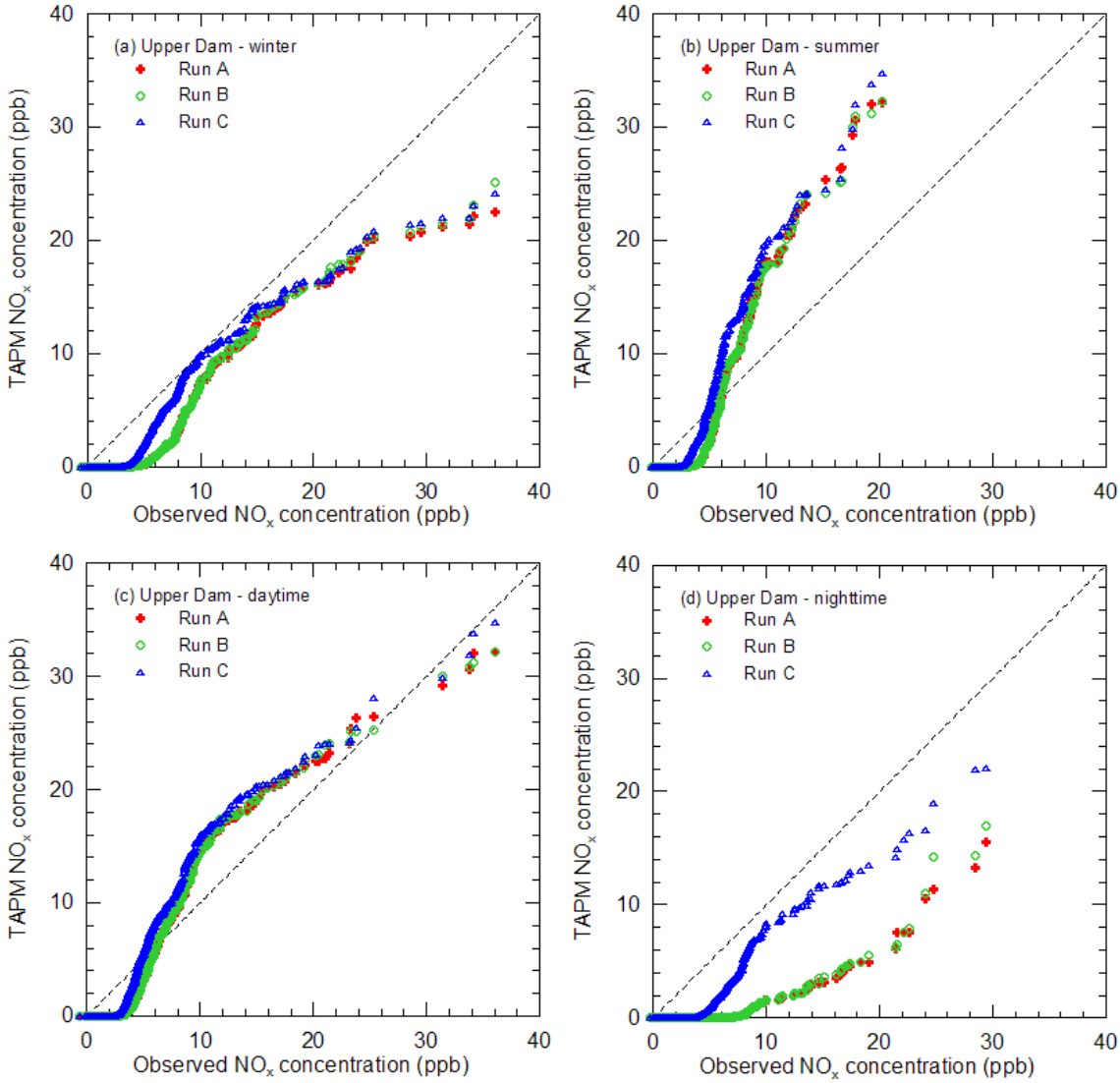

Figure 12: Quantile-quantile plots of the hourly-averaged modelled vs. observed NO_x concentrations for the three TAPM runs at Upper Dam for (a) winter (April–September 2003), (b) summer (October 2003–March 2004), (c) daytime (0800–1900 h), and nighttime (2000–0700 h). The number of data points for winter, summer, daytime and nighttime are 3874, 1657, 2801 and 2730, respectively.

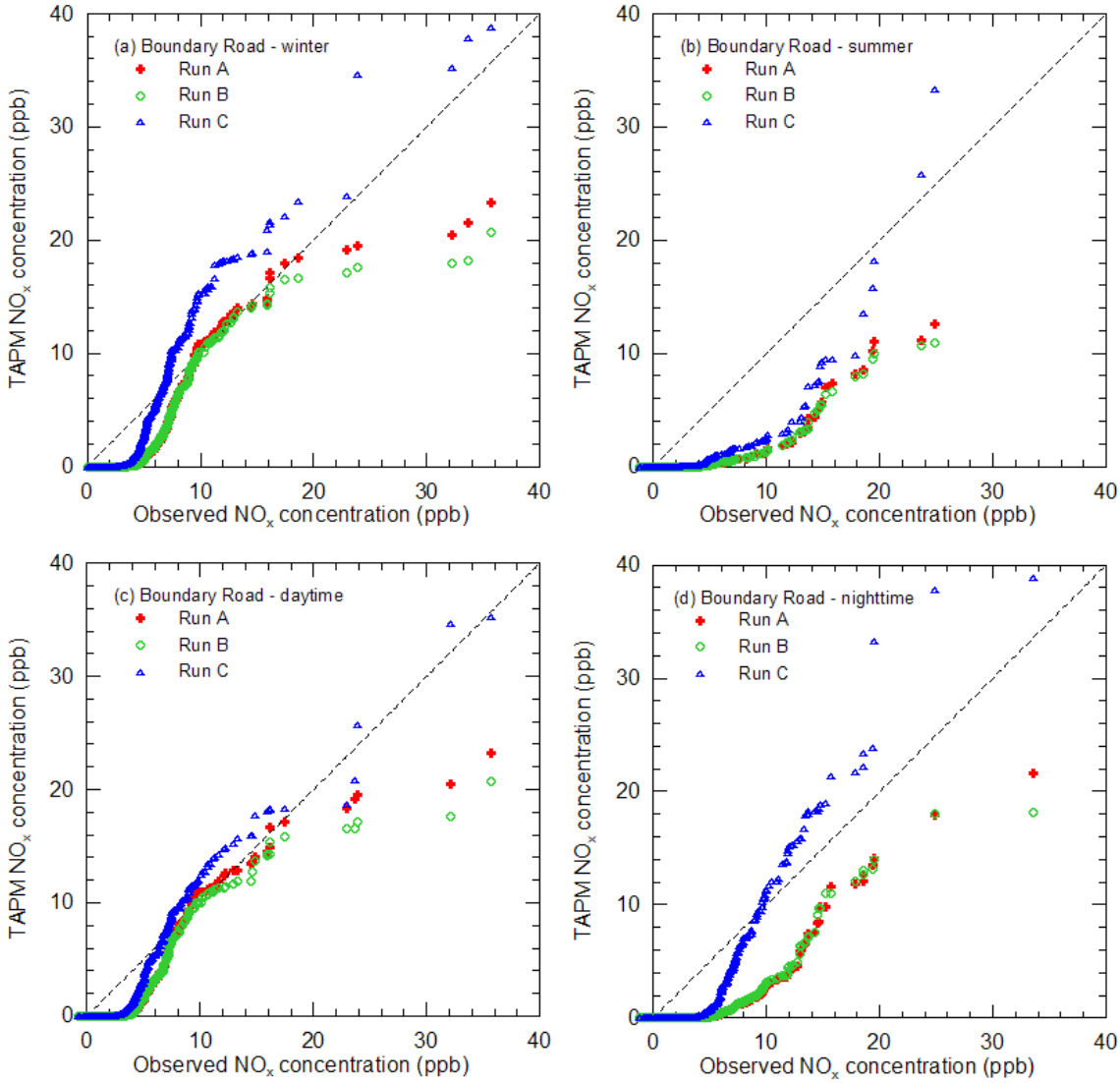

Figure 13: Quantile-quantile plots of the hourly-averaged modelled vs. observed NO_x concentrations for the three TAPM runs at Boundary Road for (a) winter (April–September 2003), (b) summer (October 2003–March 2004), (c) daytime (0800–1900 h), and nighttime (2000–0700 h). The number of data points for winter, summer, daytime and nighttime are 1599, 373, 890 and 1082, respectively.

Additional NO_x analysis presented in the Appendix A of this report suggest that almost all of the Boundary Road NO_x data are heavily influenced by unquantified non-Refinery emissions, which are not included in the modelling, whereas the NO_x data from Upper Dam are the most extensive data set available that show a strong Refinery signature. Consequently, the emphasis should be placed on the model comparison with the Upper Dam data for assessing the TAPM performance.

4.2.4 Influence of the Refinery-generated surface heat flux on dispersion

All the model runs discussed above include a refinery-generated heat flux of 150 W m^{-2} distributed over the Refinery surface area. This value was based on the heat-loss balance for Wagerup Refinery using known energy inputs, outputs and losses (see Phase 1 report by CSIRO (2004a)). In the CSIRO (2004a) report, it was found that the use of the refinery-generated heat flux together with the Wagerup-specific land-use pattern in TAPM slightly improved the surface temperature and relatively humidity predictions. In this section, we examine how much influence this additional heat flux in the model exerts on dispersion by performing an additional run for the (winter) period 1 May–31 August 2003, with the same setting as Run A above, but without the Refinery-generated heat flux.

Q-q plots of the observed and predicted NO_x concentrations with and without the refinery-generated heat flux at Upper Dam are given in Figure 14. The overall influence of the refinery-generated heat flux on the NO_x predictions is not large. The predictions are slightly improved for the mid-range concentrations between 15–24 ppb.

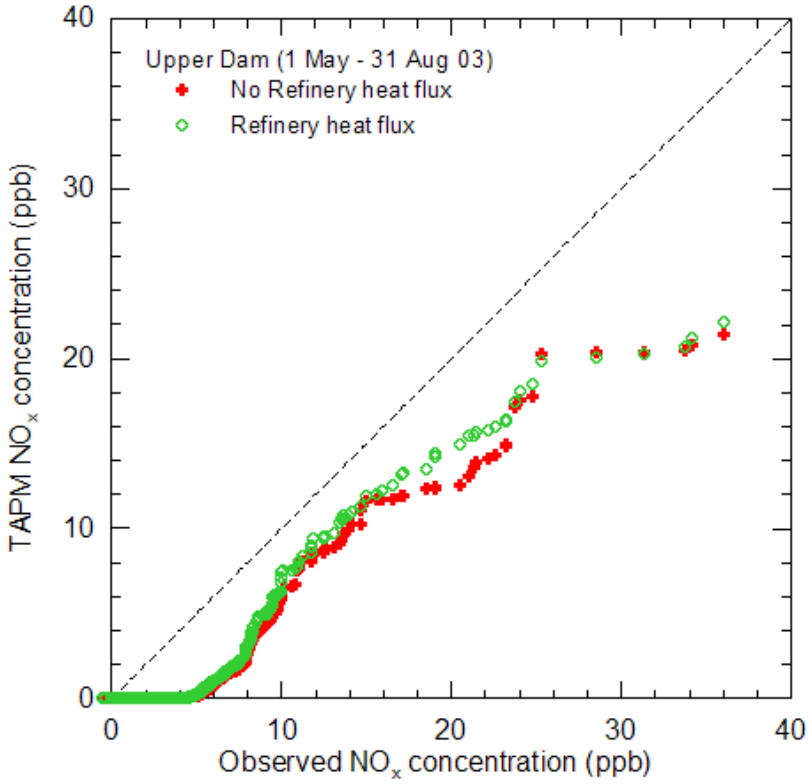

Figure 14: Quantile-quantile plots of the hourly-averaged modelled vs. observed NO_x concentrations at Upper Dam. The two curves correspond to results with and without the inclusion of Refinery-generated heat flux in the model.

Figure 15 is a q-q plot for Boundary Road. The differences between the two curves in this case are somewhat smaller than those in Figure 14 for Upper Dam, with the refinery-generated heat flux causing only a very slight increase in the predictions within the mid-range of concentration. The maximum concentration predicted with the refinery-generated heat flux is smaller than that obtained without this heat flux.

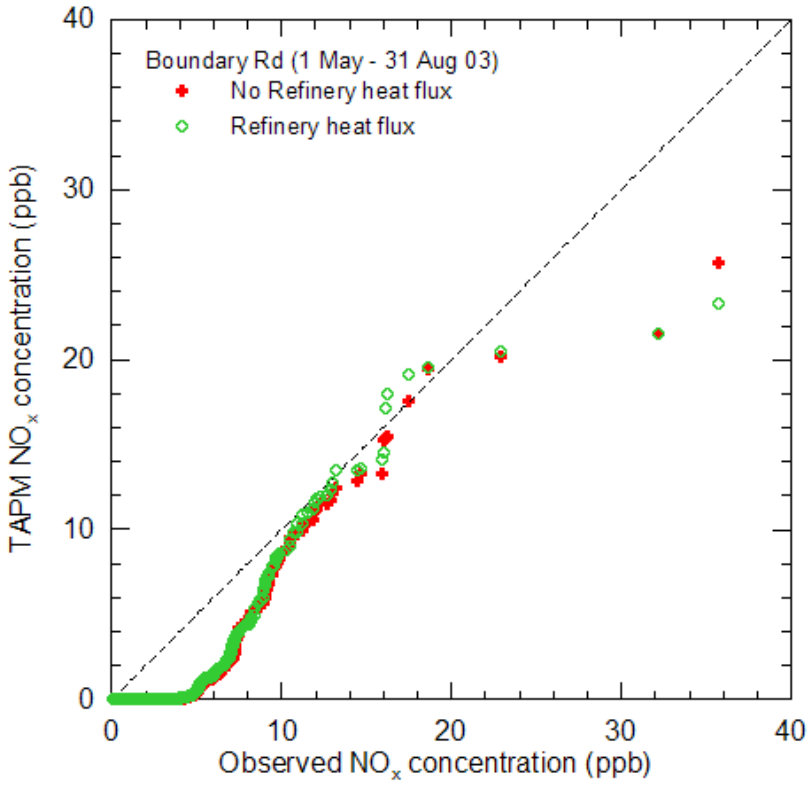

Figure 15: Quantile-quantile plots of the hourly-averaged modelled vs. observed NO_x concentrations at Boundary Road. The two curves correspond to results with and without the inclusion of Refinery-generated heat flux in the model.

The modelled and observed values of the concentration statistics obtained with and without the Refinery generated heat flux for Upper Dam and Boundary Road are summarised in Table 3. Overall, the inclusion of the Refinery generated heat flux slightly improves the model performance. This improvement is not significant for the high-end concentration statistics, but it is for the mid-range concentration values.

Table 3: Modelled and observed statistics of NO_x concentrations at the Upper Dam (sample size = 2469) and Boundary Road (sample size = 1197) monitoring sites with and without the inclusion of Refinery-generated heat flux in the model.

Statistic	Observed (ppb)	Model without Ref. heat flux* (ppb)	Model with Ref. heat flux* (ppb)
Upper Dam			
Mean	2.4	0.4	0.4
90th percentile	4.5	0.1	0.1
95th percentile	6.6	1.2	1.4
99th percentile	15.1	11.7	12.0
Average of top ten	28.5	19.1	19.5
99.9th percentile	32.6	20.5	20.5
2nd highest	34.1	20.8	21.2
RHC	37.8	26.8	25.2
Maximum	36.0	21.4	22.2
Boundary Road			
Mean	2.7	0.7	0.7
90th percentile	5.9	1.3	1.4
95th percentile	8.0	4.7	4.4
99th percentile	13.0	12.2	12.8
Average of top ten	20.6	17.7	18.1
99.9th percentile	30.4	21.3	21.3
2nd highest	32.2	21.5	21.6
RHC	31.4	26.3	26.4
Maximum	35.7	25.7	23.3

*An addition of a background NO_x concentration of 2 ppb in the modelled concentrations will increase values of all model statistics by 2 ppb.

4.3. Modelling of the ANSTO tracer data

The report SKM (2003a) gives details of the perfluorocarbon (PFC) tracer releases conducted by the Australian Nuclear Science and Technology Organisation (ANSTO) from a number of stacks of the Wagerup Refinery in the middle of 2002. The main objective of the tracer releases was to evaluate the effectiveness of the then newly-constructed 100-m Multiflue stack in the dispersal of Refinery effluents in the atmosphere. In the present modelling study, the emissions data given in the SKM (2003a) report were used. The data on the observed ambient atmospheric concentrations of the PFCs and the sampling locations were provided by Alcoa (P. Coffey, personal communication, 10 August 2004, files "Wag120802_final.xls", "Wag130802_final.xls", and "Wag140802_final.xls").

The ANSTO tracer releases were conducted over two field campaigns, before the construction of the 100-m Multiflue stack (15–17 June 2002) and after the construction (12–14 August 2002). In the present study, we only consider the data from the second campaign for the evaluation of TAPM because the sources considered for this campaign represent the present Refinery source characteristics. It is mentioned in the SKM

(2003a) report that the tracer data for 12 August 2002 were potentially contaminated due to tracer leakage when the tracer gases and ambient samples were stored overnight in the same room. Therefore, we exclude this day from modelling.

On 13 August 2002, the following tracers were released:

- PDCB (perfluorodimethylcyclobutane, C_6F_{12}) from the Calciner 3 flue of the 100-m Multiflue,
- PMCP (perfluoromethylcyclopentane, C_6F_{12}) from the 49-m Calciner 4 stack, and
- PMCH (perfluoromethylcyclohexane, C_7F_{14}) from the Boiler 1 flue of the 65-m Powerhouse Multiflue.

On 14 August 2002, the following tracers were released:

- PDCB from the Vacuum Pump flue of the 100-m Multiflue,
- PMCP from the 49-m Calciner 4 stack, and
- PMCH from the Boiler 1 flue of the 65-m Powerhouse Multiflue.

PDCB and PMCP are chemically distinct isomers. During 13–14 August 2002, a total of 17 locations (see Table 4) were selected for sampling the near-surface tracer concentrations downwind of the Refinery. During a given hour, 11 portable samplers were used for monitoring. The sampling locations were within almost a 60° sector south of the Refinery. Figure 16 shows the tracer sampling locations for the period 0900–1000 h on 13 August 2002 (from SKM, 2003a).

There were seven valid ambient sampling hours on 13 August (0800 h to 1400 h), and six on 14 August (0700 h to 1200 h). For each tracer, the total sample size was 77 on 13 August, and 66 on 14 August.

Table 4: Tracer sampling locations on 13–14 August 2002.

Sampler number	AMG East (km)	AMG North (km)
2	397.760	6356.151
3	398.010	6356.158
7	397.399	6354.963
9	397.664	6354.917
10	398.048	6354.875
12	398.481	6354.913
13	398.958	6354.934
17	398.374	6354.321
18	398.219	6353.728
19	398.567	6354.065
20	399.100	6354.255
22	397.391	6353.147
25	397.527	6354.304
51	396.594	6354.420
52	397.255	6354.411
56	397.036	6353.169
57	396.479	6353.159

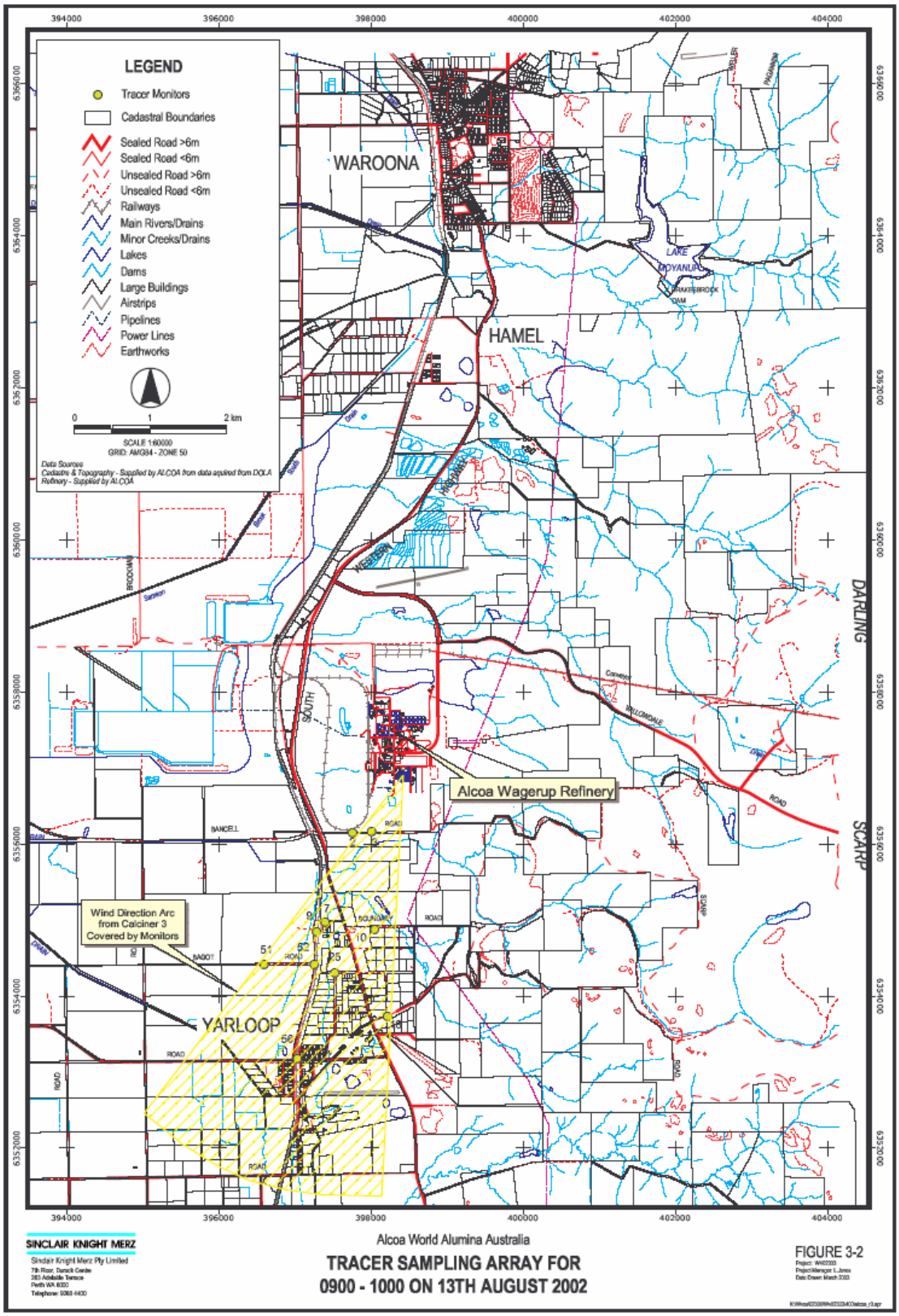

Figure 16: Tracer sampling network (yellow dots) for the period 0900–1000 h on 13 August 2002 (from SKM, 2003a).

4.3.1 Model setup for tracer simulations

To simulate the ANSTO tracer data, TAPM was run for the period 13–14 August 2002. Four nested domains of 31 × 31 horizontal grid points for the meteorology, and 33 × 33 horizontal grid points for the dispersion, all centred on the location 115°54.5′ E, 32°55.5′ S. The model runs included major buildings within the refinery. The emission parameters were taken from SKM (2003a), and are presented in Table 5. Values for the 100-m Multiflue exit temperature and velocity in Table 5 are based on the combined flow from the five individual flues with an equivalent diameter of 3.75 m. Similarly, these variables for Boiler 1 are based on an equivalent diameter for the three boiler flues of 3.71 m (SKM, 2003a).

Two sets of runs were performed:

- *Run A*: TAPM with Wagerup-specific land-use data base, refinery-generated surface heat flux, and building effects, and
- *Run B*: TAPM with Wagerup-specific land-use data base, refinery-generated surface heat flux, building effects, and wind data assimilation.

In the wind data assimilation run, the hourly-averaged wind speed and wind direction measurements at 10 m AGL at Bancell Road were used (the 30-m wind measurements at this site did not begin until mid July 2003), with the horizontal radius of influence taken as 8 km. In the vertical, model options were selected such that the Bancell Road winds influenced the first two model levels.

The hourly-averaged modelled tracer concentrations on the innermost grid domain were extracted at the grid point nearest to each of the tracer monitoring sites for comparison with the data.

Table 5: Emission parameters for the ANSTO tracer releases on 13–14 August 2002 (from SKM (2003a)).

Time	100-m Multiflue** (PDCB tracer)			Calciner 4 (PMCP tracer)			Boiler 1 (PMCH tracer)		
	Exit vel. ($m\ s^{-1}$)	Exit temp. (°C)	Emission rate ($mg\ s^{-1}$)	Exit vel. ($m\ s^{-1}$)	Exit temp. (°C)	Emission rate ($mg\ s^{-1}$)	Exit vel. ($m\ s^{-1}$)	Exit temp. (°C)	Emission rate ($mg\ s^{-1}$)
13 August									
0600–0700	19.1	181.6	12.8	19.3	173.4	-	13.7	118.6	14.4*
0700–0800	19.1	181.5	12.8	19.1	173.1	16.7	14.4	119.7	14.2
0800–0900	19.1	182.0	14.0	19.2	174.1	14.1	14.0	118.6	13.4
0900–1000	18.4	182.2	14.5	19.1	177.8	13.2	12.3	116.2	13.3
1000–1100	16.7	179.9	14.0	19.0	173.2	12.7	13.6	118.6	14.2
1100–1200	16.8	179.5	13.1	19.5	170.4	13.3	14.3	119.9	14.1
1200–1300	17.1	178.8	12.9	19.1	173.7	13.3	16.8	128.8	14.9
1300–1400	17.0	181.0	15.2	18.9	184.5	13.1	15.0	123.1	16.1
14 August									
0500–0600	13.1	167.2	13.0*	21.4	162.0	21.9*	15.4	121.7	14.5*
0600–0700	13.2	165.2	13.2	21.0	161.1	18.5	15.3	121.6	16.2
0700–0800	13.2	165.6	13.5	21.2	161.0	13.0	15.3	121.7	18.5
0800–0900	13.2	165.3	13.1	21.0	159.2	13.1	15.2	121.7	14.2
0900–1000	13.2	167.7	13.1	21.4	158.1	13.2	15.0	121.6	13.9
1000–1100	12.5	167.7	13.0	21.6	160.1	13.2	15.0	121.7	13.5
1100–1200	12.2	165.1	14.3	21.7	160.1	13.9	15.0	122.5	14.6

*The emission occurred only for part of the hour.
**On 13 August, the PDCB tracer was released from the Calciner 3 stack of the Multiflue, whereas on 14 August it was released from the Vacuum flue stack of the Multiflue.

4.3.2 Model results

Figure 17a and Figure 17b show the observed and TAPM-predicted variations of wind speed and wind direction, respectively, at 10-m AGL at the Bancell Road meteorological station for the period 13–14 August 2002. The data show that the peak wind speed increases from 5 $m\ s^{-1}$ on the first day to 8 $m\ s^{-1}$ on the second day, and that the wind direction is relatively steady. Overall, the model is performing very well in describing the data. In Figure 17a, the model is able to simulate the observed peak in wind speed at around 1200 h on 13 August and that at about 1400 h on 14 August. Similarly, the model is correctly predicting the dip in wind speed at 1900 h on 13 August. However, the TAPM wind speed after 1900 h on 14 August is much smaller than the observations. On both the days in late morning, the model predicts an early (anticlockwise) turning of the wind to the northerly direction compared to the data (Figure 17b). However, at about 2100 h on 14 August (hour 45 in the plot), the observed wind turns from northerly to southerly earlier than the model wind.

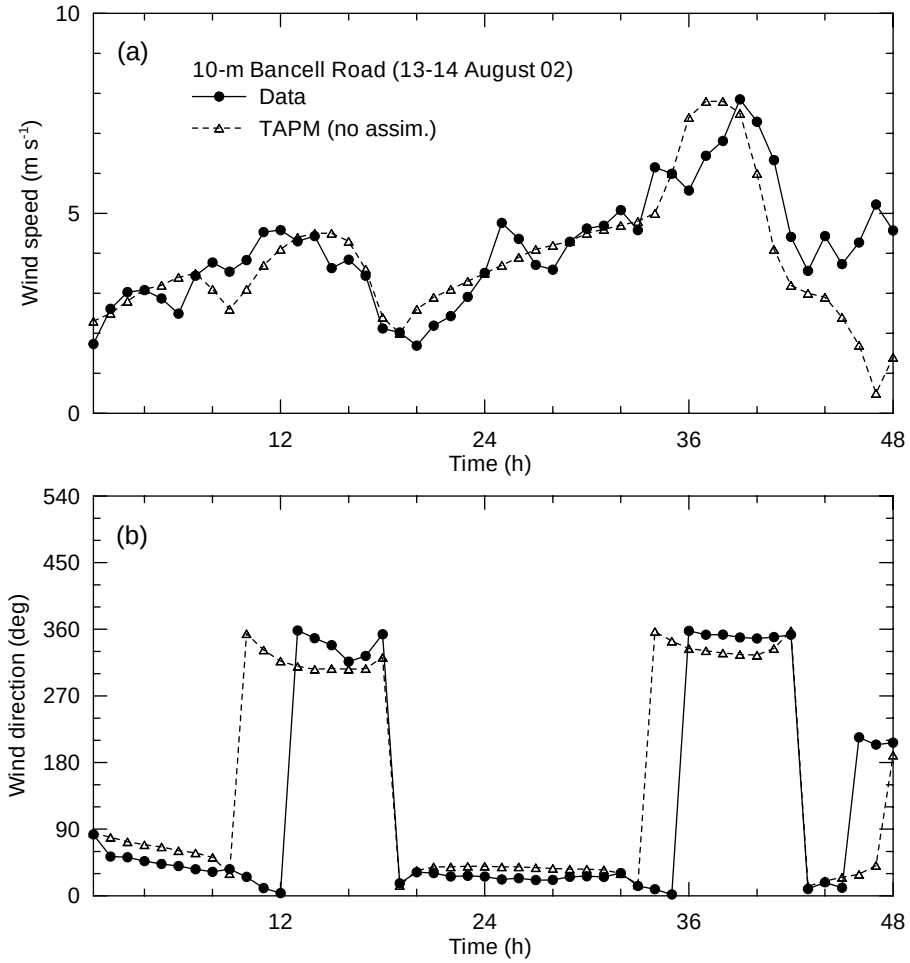

Figure 17: Time series of the hourly-averaged observed and modelled (a) wind speed, and (b) wind direction at 10-m AGL at the Bancell Road meteorological station for the period 13–14 August 2002.

The time series of the observed and modelled wind speed and wind direction at 10-m AGL at the Bancell Road meteorological station for the period 13–14 August 2002 when the observed 10-m winds at Bancell Road are assimilated in the model, are plotted in Figure 18a and Figure 18b. The correlation between the model predictions and the data is very high because the data have been assimilated in the model.

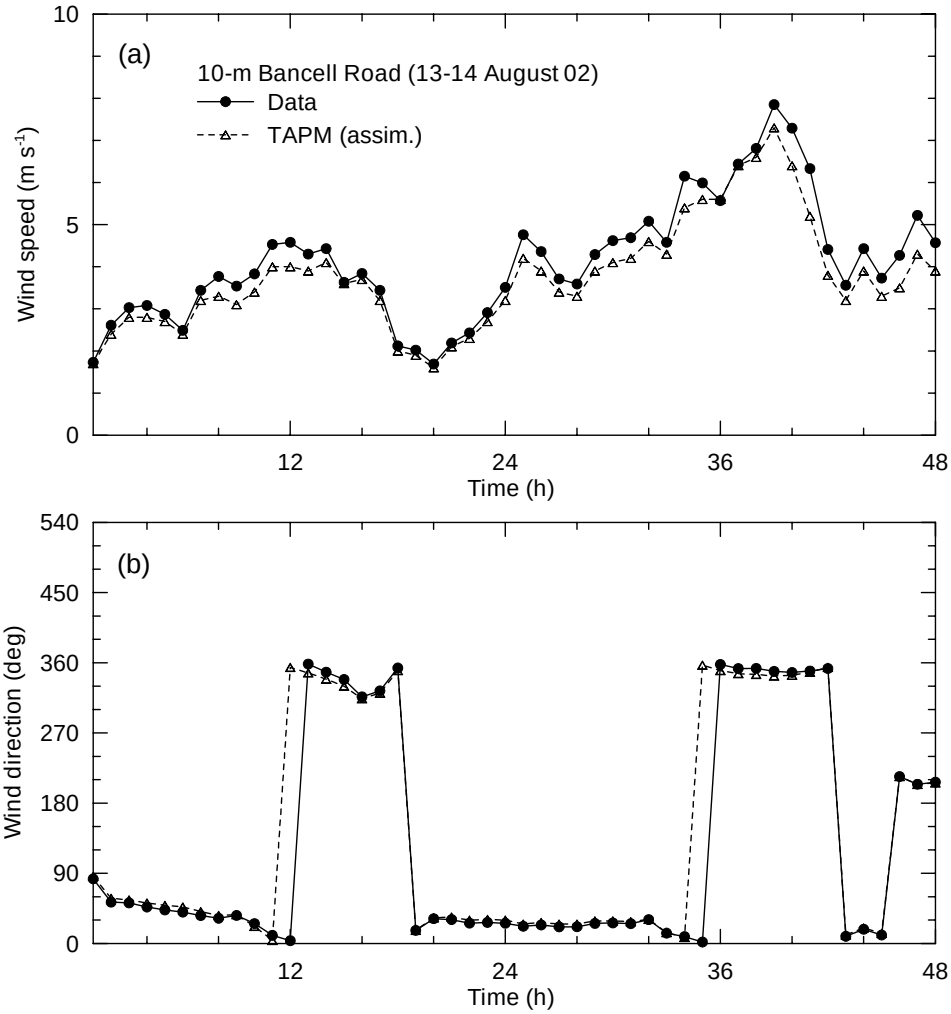

Figure 18: Time series of the hourly-averaged observed and modelled (a) wind speed, and (b) wind direction at 10-m AGL at the Bancell Road meteorological station for the period 13–14 August 2002 with wind data assimilation in the model.

The sample size of the ANSTO tracer study is very limited; there are only 13 observations for each of the 11 samplers located downwind of the Refinery. Hence, for each tracer, there are only 143 observations, with some samplers missing the plumes. This is in contrast to the much larger sample size of the hourly-averaged NO_x concentrations routinely monitored at Boundary Road and Upper Dam, for which the model performance could be evaluated for each site with the modelled and observed levels unpaired in time. One advantage of the tracer data is that the emission rates are accurately known, and plumes from individual sources can be monitored separately without any background influence. Because of the limited tracer sample size, we evaluate the model performance using the modelled and observed tracer concentrations that are unpaired in both space and time.

As in the case of NO_x comparison, the focus is on whether the highest observed and modelled tracer concentrations are similar. In the q-q plot in Figure 19, the sorted predicted tracer concentrations obtained from Run A are plotted against the sorted observed tracer values (i.e. independent of time and position) for each of the three tracer sources in order to examine any model bias over the concentration distribution. The plot indicates that there is a bias in the model to underpredict concentration distribution due to the 100-m Multiflue, and to overpredict the high-end concentration levels due to

Calciner 4 and Boiler 1, except for the maximum concentration due to Calciner 4 which is underpredicted by the model. Figure 20 presents a q-q plot for Multiflue and Boiler 1 with reduced axis limits to improve clarity. Figure 19 and Figure 20 are very similar to the TAPM comparison plots in Figure 5.8 given in the SKM (2003a) report on tracer modelling. However, some improvements with the present TAPM modelling are noticeable. For example, the top two concentrations due to Calciner 4 are better predicted. Also, the concentrations between 1000–3000 pg m^{-3} for Boiler 1, and the overall q-q curve for Multiflue above 3000 pg m^{-3} are reproduced better. This is probably due to the inclusion of the refinery-generated heat flux and/or the Wagerup specific land use in the model. For the 100-m Multiflue, there are a series of observed concentrations within the range 0–3000 pg m^{-3} that are modelled as zero concentrations.

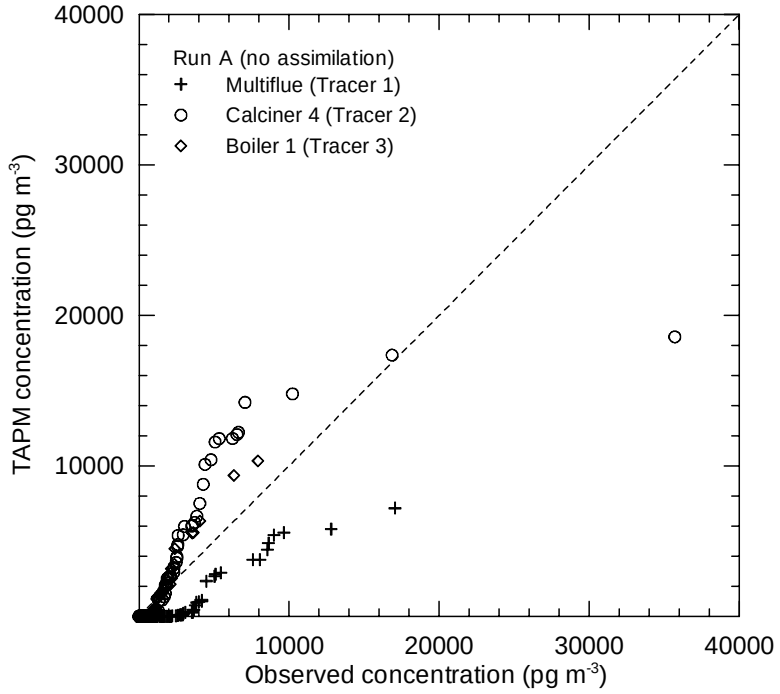

Figure 19: Quantile-quantile plots of the hourly-averaged modelled vs. observed tracer concentrations for various stack sources without wind data assimilation in the model.

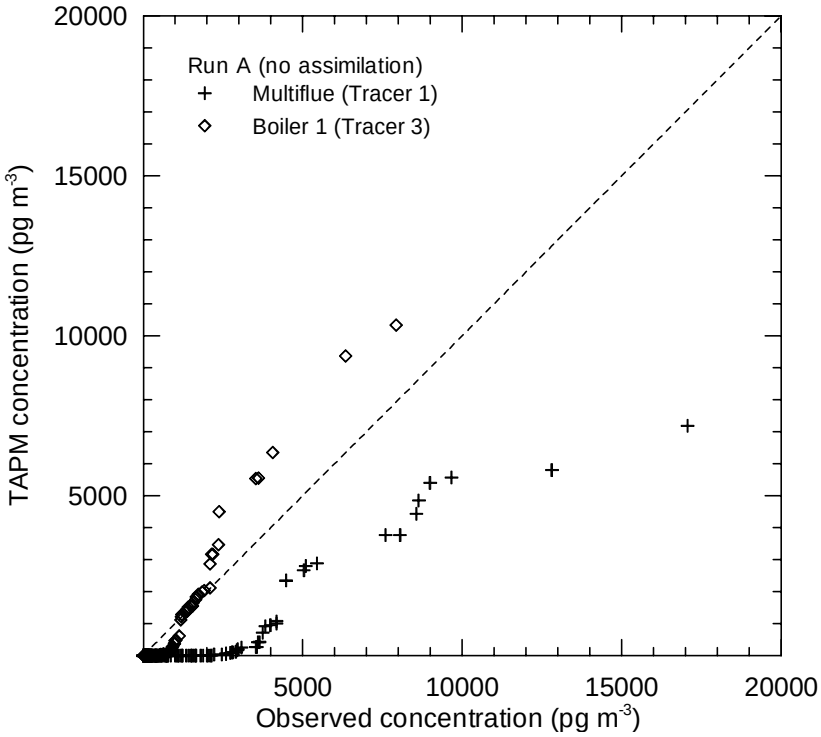

Figure 20: Quantile-quantile plots of the hourly-averaged modelled vs. observed tracer concentrations for two stack sources without wind data assimilation in the model.

Figure 21 presents q-q plots when the wind speed and wind direction observations taken at 10 m at Bancell Road are assimilated (Run B) in the model. It is apparent that the model performance improves for the 100-m Multiflue when wind data are assimilated in the model, including in the lower concentration range. However, the model overpredicts the Calciner 4 and Boiler 1 concentrations to an even greater degree than without wind data assimilation. Modelled to observed ratios of the mean concentration, maximum concentrations, 2nd highest concentration, robust highest concentration (RHC), and the average of the top ten concentrations, are given in Table 6. For Run A (no wind data assimilation), all the performance measures for high concentration events show that the ratios are approximately 0.5 for the 100-m Multiflue, 1 for Calciner 4, and 1.5 for Boiler 1. For Run B (wind data assimilation), these ratios are roughly 1 for the 100-m Multiflue, 1.5 for Calciner 4, and 3 for Boiler 1.

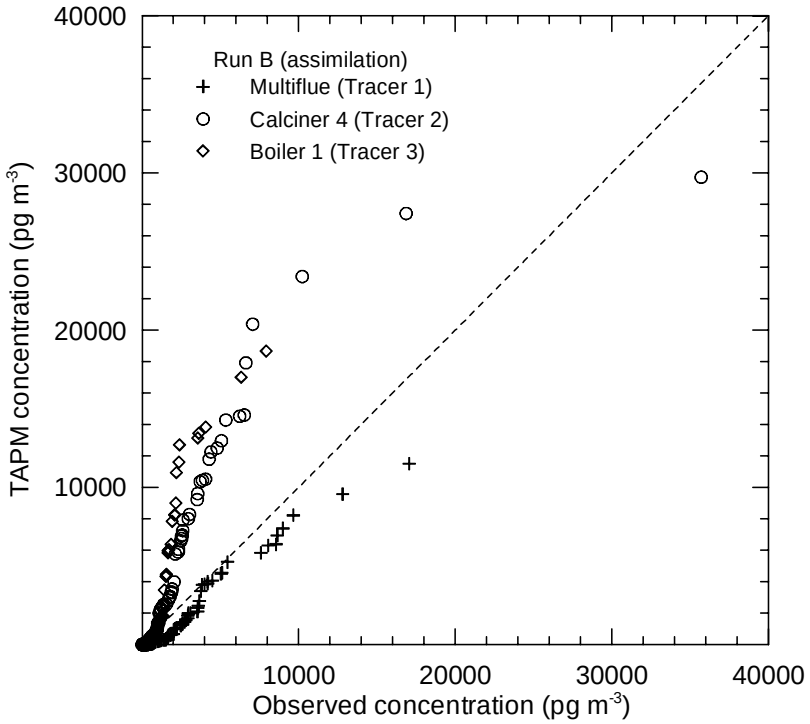

Figure 21: Quantile-quantile plots of the hourly-averaged modelled vs. observed tracer concentrations for various stack sources with wind data assimilation in the model.

Table 6: Ratios of modelled to observed statistics of tracer concentrations for Run A and Run B.

TAPM run	Statistic	Model to observed ratio		
		Multiflue (Tracer 1)	Calciner 4 (Tracer 2)	Boiler 1 (Tracer 3)
Run A (no wind data assimilation)	Mean	0.26	1.18	0.90
	Maximum	0.42	0.52	1.30
	2nd highest	0.45	1.03	1.48
	RHC	0.49	0.92	1.75
	Average of top ten	0.51	1.29	1.48
Run B (wind data assimilation)	Mean	0.63	1.87	2.35
	Maximum	0.67	0.83	2.35
	2nd highest	0.75	1.63	2.68
	RHC	0.72	1.43	3.27
	Average of top ten	0.78	1.80	3.51

In SKM (2003a), the model to observed ratios of the maximum concentration for the Multiflue, Calciner 4 and Boiler 1 obtained using CALPUFF are 0.41, 0.32 and 0.81, respectively, and those obtained using TAPM are 0.41, 0.40 and 1.29, respectively. In the same report, the model to observed ratios of the RHC for these sources obtained

using CALPUFF are 0.44, 0.51 and 0.99, respectively, and those obtained using TAPM are 0.55, 0.91 and 1.57, respectively.

4.4. Use of wind data assimilation

Only a limited quantity of wind data was available for assimilation: the 30-m at Bancell Road were for the period 18 July 2003 – 31 March 2004, and the 8-m RDA data had errors in the low wind speeds and these erroneous data were discarded. Wind data assimilation had mixed impact on pollution predictions. The comparison of the model concentrations with the NO_x at Upper Dam (best available data) showed that wind data assimilation leads to somewhat better results. The ANSTO tracer-modelling results show that for Calciner 4 and Boiler 1, the wind data assimilation worsens the predictions and for the 100-m Multiflue it improves the predictions in areas south/south-west of the Refinery. Besides the issues concerning the quality and completeness of the data from the two sites currently available for wind data assimilation, it is doubtful whether wind data assimilation from only two sites is appropriate for modelling the large complex terrain region around the Wagerup Refinery with a large number of receptor points that will be considered in Phase 3. In complex terrain, there can be significant differences in meteorology from location to location, such as that observed between the RDA and Bancell Road stations which are only about 3 km apart. While wind data assimilation will generally improve modelled concentrations close to the location where the wind data is recorded, it could in some circumstances have a different effect further a field. In a topographically complex region such as Wagerup where there is significant influence of the escarpment on local wind fields, the radius of influence of 5 km (TAPM minimum recommended) for the assimilated winds means that the influence of the assimilated winds can extend into regions where the local wind fields differ from those at the wind data site. More meteorological and pollution observations would be necessary to examine the impact of wind data assimilation on predictions within the larger domain of interest.

4.5. Total suspended particulate (TSP) concentrations

The Residue Disposal Area (RDA) west of the Refinery is a source of dust to the surrounding district. Modelling of dust is much more difficult than that of pollutants from well-defined point sources. This is largely because it is not possible to estimate dust emissions from open residue dumps to the same accuracy as gaseous or aerosol emissions from well-defined point sources, since dust emissions are strongly influenced by multiple factors, including activity, wind and soil conditions. Hence, model evaluation based on dust involves large uncertainties. TAPM can predict dust concentrations given the rates of dust emissions as an input. However, TAPM does not have a dust rise module for estimating dust emissions for given wind speed and soil conditions. Consequently, we do not apply the model for dust concentration predictions directly, but rather test the ability of the model to simulate the winds on occasions when elevated dust concentrations are observed in the area. This comparison is based on the assumption that high winds generally lead to dust rise, overcoming the gravitational and cohesive forces binding dust particles to the surface, and, therefore, cause high ambient dust concentrations. Dispersal of dust is affected by the particle size, shape and density, as well as wind speed and other climatic effects. The emission of dust also depends on soil moisture as well as the effectiveness of dust control systems.

To carry out an analysis of dust concentration with respect to winds, hourly-averaged concentrations of TSP (a measure of dust) measured using a TEOM at Residue South (RS) and Residue South West (RSW), and the hourly-averaged wind speed and wind direction measurements at RDA for the period 1 April 2003–31 March 2004 were used. The concentration data averaged over 6 min periods were used to calculate hourly averages. The locations of the two TSP monitoring sites are shown in Figure 22. The RDA meteorological site (AMG coordinates 394.941 km east and 6357.882 km north) is located about 3 km west of the Refinery (see Figure 1) and the data from this station are primarily used for the management of dust control and sprinkler operation at RDA. Measurements of wind speed and wind direction at about 8 m AGL are made at using a separated cup and vane anemometer. It is more appropriate to use data from this meteorological station for analysis of the TEOM data at the RDA than those from the Bancell Road meteorological station, the latter is further away from the RDA dust sources, south of the refinery and closer to the escarpment.

We also use the TAPM meteorological predictions obtained from Run B at a height of 10 m at the location of the RDA weather station.

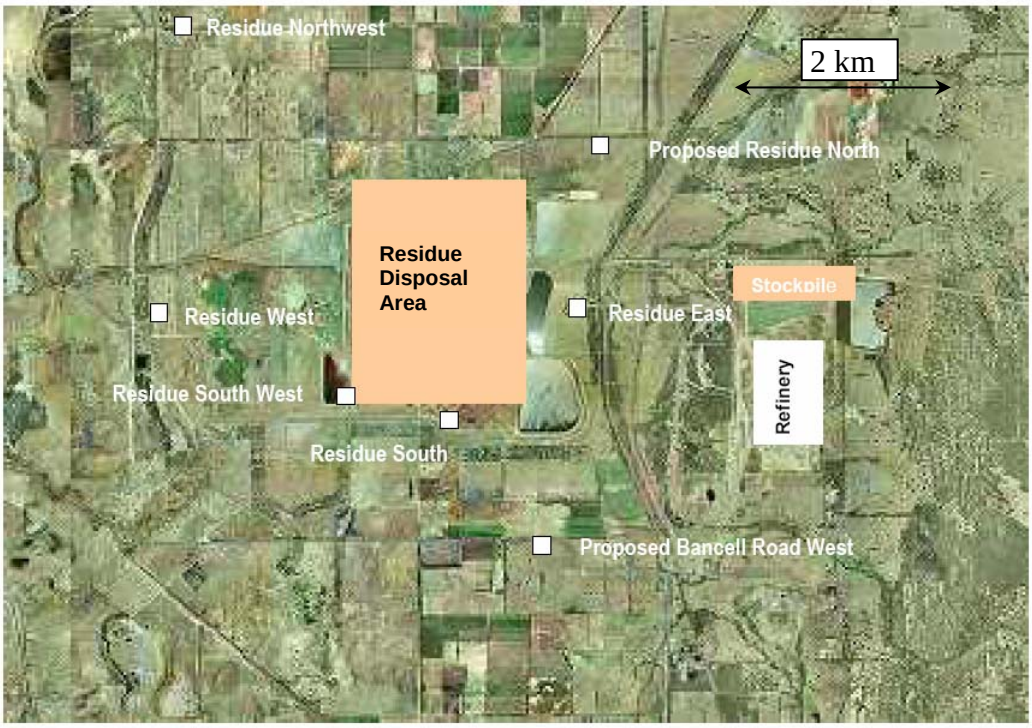

Figure 22: Locations of the Residue South (RS) and Residue South West (RSW) total suspended particulate (TSP) monitoring sites (adapted from SKM, 2003b).

The variations of the hourly-averaged TSP data with the hourly-averaged wind direction at RDA for Residue South and Residue South West, are presented in Figure 23a and Figure 23b, respectively. At both sites, high concentrations of hourly-averaged TSP are observed, on a few occasions exceeding 1000 μg m-3, especially at Residue South West, when the winds are from the Residue Disposal Area (note that the daily average concentrations would be much lower than the hourly-averaged peaks, but no lower than

1/24 of the maximum hourly average). For the RS site, most high TSP levels lie within the wind sector 310°–110°, whereas for the RSW site, most high TSP levels lie within the wind sector 340°–110°, which is consistent with the orientation of these sites with respect to the RDA area in Figure 22.

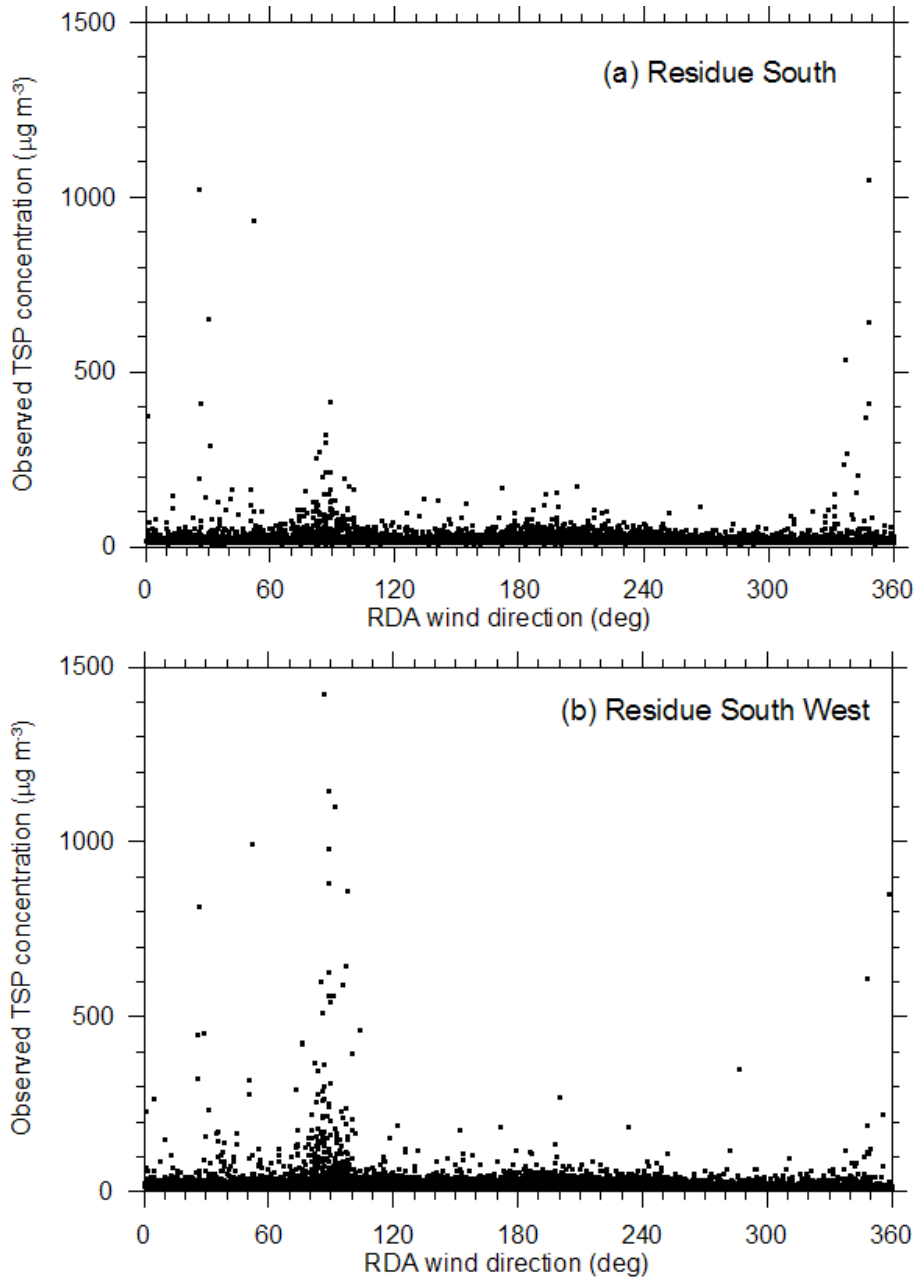

Figure 23: Variation of the hourly-averaged TSP concentration as a function of the RDA wind direction at (a) Residue South (RS) and (b) Residue South West (RSW).

Figure 24a and Figure 24b show the variation of the hourly-averaged TSP concentration with the hourly-averaged wind speed at RDA for Residue South and Residue South West, respectively. Both plots are very similar, and show that there is not a significant

trend in the TSP concentration with speed below about 7 m s^{-1}, but above this value there is an increasing trend in the TSP concentration with wind speed.

The next case considered is for winds exceeding 7 m s^{-1} at the RDA. Those hours for which the observed wind speed at RDA was less than 7 m s^{-1} were removed from the analysis, and the resulting observed and modelled winds *paired in time* were then used for comparison. This means that the comparison is between the observed and modelled winds on an hour-by-hour basis.

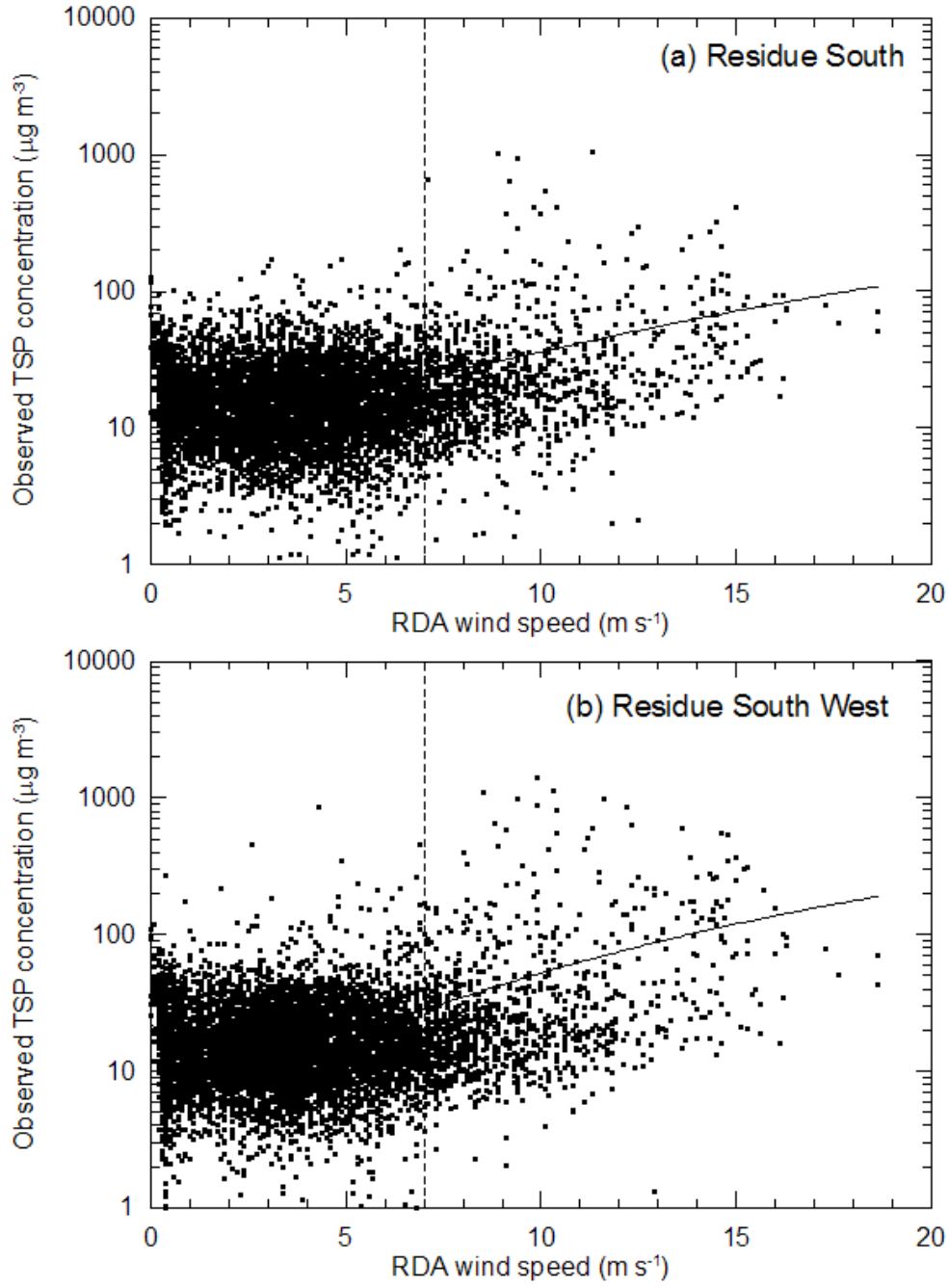

Figure 24: Variation of the hourly-averaged TSP concentration as a function of the RDA wind speed at (a) Residue South (RS) and (b) Residue South West (RSW).

A scatter plot of the modelled versus observed wind speeds at RDA when the observed winds are above 7 m s^{-1} is given in Figure 25a (sample size is 1122). The comparison gives a correlation coefficient (r) with a value of about 0.6 and the slope of the linear fit being 0.75. The value of the highest wind speed predicted by the model (18.5 m s^{-1}) is almost the same as the highest observed wind speed. There is an overall tendency in the model to underestimate high wind speeds. In order to examine whether the model accurately predicts the wind direction under high wind-speed conditions, the model wind directions versus the observed wind directions at RDA are plotted in Figure 25b. The small amount of scatter in this plot shows that the model is able to simulate the wind directions well. To further quantify this comparison, the observed and model probability (or frequency) of occurrence for wind direction is presented in Figure 25c. The modelled probability variation is in good agreement with the observation, and the wind sector 340°–110° for which the high TSP levels at the RS and RSW sites occur is simulated reasonably well by the model, including the peak for the easterly winds.

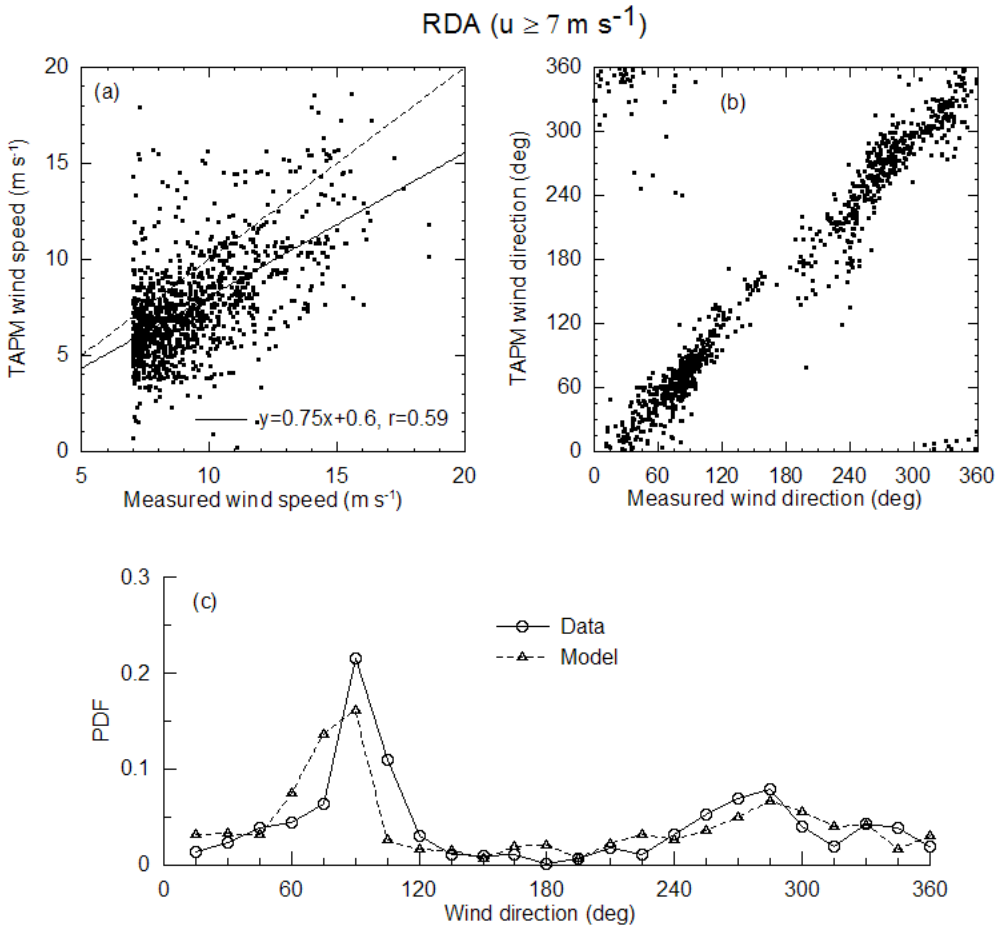

Figure 25: (a) Scatter plot of the observed and modelled wind speeds at RDA, (b) the same as (a) but for wind direction, and (c) the observed and model probability (expressed as probability density function (pdf)) of occurrence of wind direction. Only those hours have been considered for which the observed wind speed is greater than 7 m s^{-1}.

The data for high TSP concentrations were further filtered by considering only those hours for which the observed wind speed at RDA are above 7 m s^{-1} *and* the observed TSP concentration at the RSW is greater than 50 μg m^{-3}. This filtering reduces the sample size to 209. Figure 26a is a scatter plot of the resulting observed and modelled wind speeds at the RDA. The agreement is slightly better than that in Figure 25a, with a

correlation coefficient of about 0.7. The corresponding wind directions are also predicted well by the model (Figure 26b). The observed and model probability of occurrence plots for wind direction in Figure 26c indicate that TAPM performs well in simulating the frequency of occurrence of easterly winds that leads to the high TSP concentrations.

The above analysis shows that overall TAPM is able simulate the high wind-speed events that are responsible for the elevated TSP concentrations around the RDA area with a fair degree of accuracy.

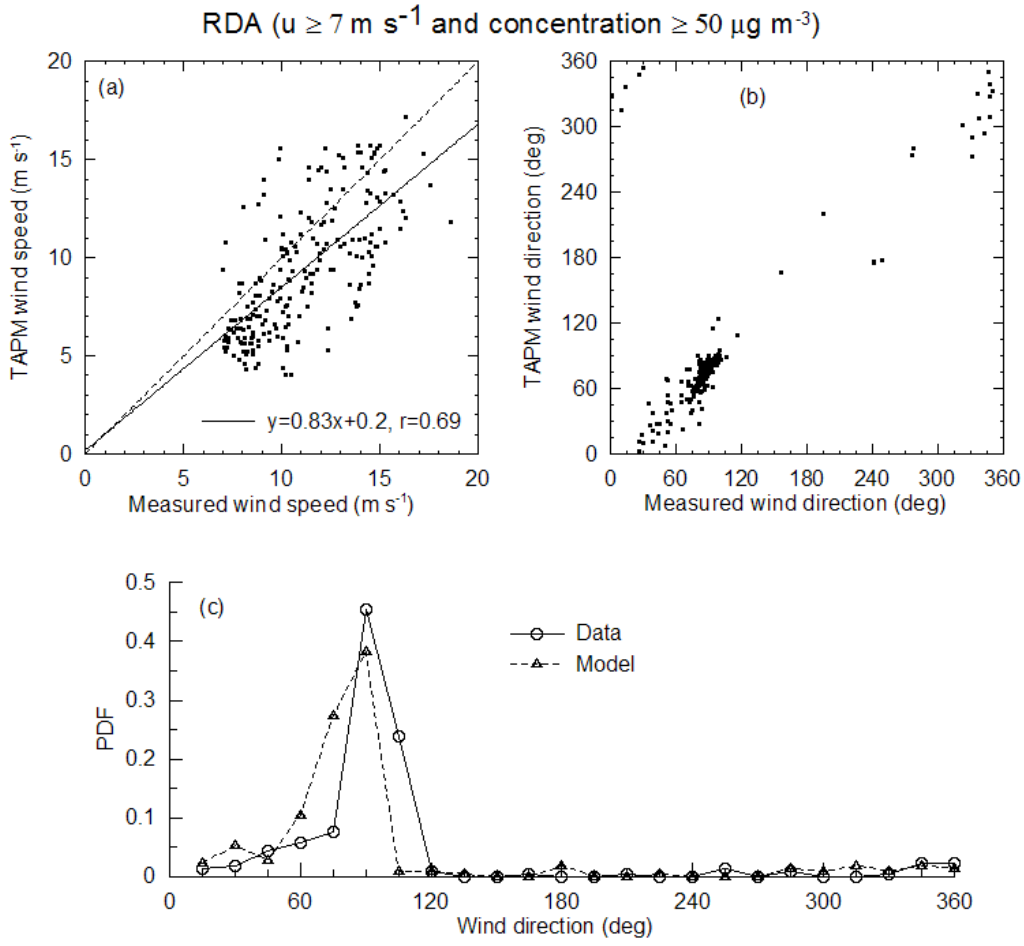

Figure 26: (a) Scatter plot of the observed and modelled wind speeds at RDA, (b) the same as (a) but for wind direction, and (c) the observed and model probability (expressed as probability density function (pdf)) of occurrence of wind direction. Only those hours have been considered for which both observed wind speed is greater than 7 m s^{-1} and the observed TSP concentration at the RSW site is greater than 50 µg m^{-3}.

5. Comparison with other TAPM studies and models

In most previous air pollution evaluation studies for other sites, TAPM has been applied to annual datasets of hourly-averaged concentrations measured at routinely-operated monitoring stations, or to datasets from intensive field studies that involved a dense network of ambient air sampling monitors over shorter periods. The large sample size of such datasets is essential for a robust estimation of evaluation statistics, especially those pertinent to the prediction of the high-end concentration distribution. In the present

study, the evaluation of TAPM using the NO_x measurements around the Wagerup Refinery involved one year of data, and it is possible to compare the model evaluation results with the performance of TAPM elsewhere where the dominant sources are, as in Wagerup, stack (i.e. point) sources. In the present study, the evaluation of TAPM using the ANSTO tracer data is not as robust as that using the NO_x data, because of the much smaller sample size of the former. Therefore, the focus is on the comparison of the TAPM performance obtained for NO_x at Wagerup with that obtained for other areas. A number of statistical measures have been used in the previous TAPM applications, but most focus on those that are applicable to the prediction of high-end concentrations. We use the ratio of the predicted to observed robust highest concentration, RHC_R, as the overall measure for comparing model performance.

Where available and appropriate, we also give RHC_R values for some of the commonly used models, namely AUSPLUME, DISPMOD, CALPUFF, ISCST3, AERMOD and ADMS3, all of which normally require observed meteorology as input. AUSPLUME, a regulatory model developed for and approved by EPA Victoria (EPAV, 2000), is a simple, steady-state, Gaussian plume dispersion model that assumes that the meteorology at the single site is representative of the whole modelled domain. It is a model commonly used in Australia and New Zealand. DISPMOD is a semi-analytical model (Rayner, 1987, 1998; Luhar, 2002) that was developed specifically for air pollution regulation in the Kwinana industrial area by the Department of Environmental Protection (DEP) of Western Australia. It is capable of accounting for coastal processes such as fumigation. CALPUFF simulates the transport and diffusion of a plume via the puff approach in which a plume is described as consisting of a series of puffs, so that flow complexities, such as horizontal wind shear, can be taken into account. It typically uses meteorological data generated by the processor CALMET, which is driven by observed or large-scale model meteorology and is capable of calculating temporally and spatially varying wind fields (see http://www.src.com/calpuff/calpuff1.htm). The regulatory models ISCST3 and AERMOD (both US EPA models, see http://www.epa.gov/scram001/tt26.htm#aermod and http://www.epa.gov/scram001/tt22.htm#isc) are based on the plume approach, whereas ADMS3 (a UK model, see http://www.cerc.co.uk/software/adms3.htm) utilises both plume and puff concepts of dispersion.

The values of RHC_R obtained using TAPM for Wagerup NO_x predictions at Upper Dam are 0.90, 0.87 and 0.90, for Run A, B and C, respectively. The respective values at Boundary Road are 0.71, 0.58 and 1.18. As stated earlier, the data from the Upper Dam monitoring site are of better quality because, as suggested by the variation of the observed concentration with wind direction, the NO_x concentrations at Boundary Road are substantially influenced by sources other than the Refinery sources. The above results demonstrate that there is not a significant difference between the three TAPM runs for Upper Dam, but for Boundary Road Run C (with wind data assimilation) gives the best results.

Hurley et al. (2001, 2002) applied TAPM (v2.0) to an annual (1997) database of sulfur dioxide concentrations monitored at six stations in the coastal industrial area of Kwinana in Western Australia using hour-by-hour emissions inventory for the industrial sources in the region, and found that the value of RHC_R ranged between 0.84–1.45, with a value averaged over all sites of 1.04. For the same dataset, the RHC_R values obtained

using DISPMOD and AUSPLUME ranged between 0.76–1.92 and 0.30–0.77, respectively, with mean values of 1.12 and 0.57, respectively.

An application of TAPM (v2.0) to an annual (1999) database of NO_x concentrations at two monitoring sites in the coastal region of Pilbara in Western Australia (Physick and Blockley, 2001; Physick et al., 2002) showed that the value of RHC_R was 0.70 for one site (Dampier) and 1.75 for the other (King Bay). DISPMOD gave virtually the same values, whereas the AUSPLUME values were 0.42 and 0.63, respectively. Both this and previous examples are coastal, where one would not expect AUSPLUME to perform well as it does not include processes specific to coastal areas, such as shoreline fumigation.

Luhar and Hurley (2003) used TAPM (v2.0) to simulate the arcwise maximum concentrations measured as part of the Indianapolis and Kincaid field experiments using a very dense network of tracer monitors around single stack sources. They obtained RHC_R values of 0.92 and 1.21 with and without wind data assimilation, respectively, for Indianapolis, and 1.18 and 1.48, respectively, for Kincaid. For Indianapolis, the RHC_R values obtained by other researchers (as reported in Luhar and Hurley (2003)) using ISCST3, AERMOD and ADMS3, are 1.14, 0.86 and 1.03, respectively; whereas for Kincaid the respective values are 0.61, 0.52 and 0.70.

In a more recent model comparison study, Hurley and Luhar (2005) found that the RHC_R values for AUSPLUME, CALPUFF and TAPM ranged between 0.17–0.56, 0.54–1.86 and 1.09–1.36, respectively, for Indianapolis, and 0.92–1.29, 0.67–2.10 and 1.08–1.25, respectively, for Kincaid, depending on the selected model options.

In summary, in the previous applications of TAPM mentioned above, RHC_R ranged between 0.7–1.75, with a mean value of 1.23.

Table 7 lists the ratios of modelled to observed robust highest concentration (RHC_R) from various modelling studies, including the present study.

The above comparisons suggest that TAPM's overall performance at Wagerup is on par with its performance elsewhere for annual data measured at sparse monitoring networks. It should be noted, however, that all of above studies were performed in different regions, and the performance of a model may be partly dependent on the complexity of the area being studied. At Wagerup, some uncertainty in the model evaluation is generated by taking the NO_x emission rates to be constant throughout the year whereas in fact they vary, and by the neglect of possible NO_x contribution from sources other than the Refinery.

Table 7: Ratios of modelled to observed robust highest concentration (RHC_R) from various studies.

Location	Model	RHC_R	Reference
Kwinana (WA) (annual SO_2), 6 sites	TAPM (v2.0)	0.84–1.45	Hurley et al. (2002)
	DISPMOD	0.76–1.92	
	AUSPLUME	0.30–0.77	
Pilbara (WA) (annual NO_x), 2 sites	TAPM (v2.0)	0.70–1.75	Physick and Blockley (2001), Physick et al. (2002)
	DISPMOD	0.70–1.80	
	AUSPLUME	0.42–0.63	
Indianapolis (US), arcwise maximum SF_6 concentrations	TAPM (v2.0)	0.92, 1.21*	Luhar and Hurley (2003), Hurley and Luhar (2005)
	ISCST3	1.14	
	AERMOD	0.86	
	ADMS3	1.03	
	CALPUFF	0.54–1.86	
	AUSPLUME	0.17–0.56	
Kincaid (US), arcwise maximum SF_6 concentrations	TAPM (v2.0)	1.18, 1.48*	Luhar and Hurley (2003), Hurley and Luhar (2005)
	ISCST3	0.61	
	AERMOD	0.52	
	ADMS3	0.70	
	CALPUFF	0.67–2.10	
	AUSPLUME	0.92–1.29	
Wagerup (annual NO_x)	TAPM (v2.6) – Upper Dam	0.87–0.90*	Present study
	TAPM (v2.6) – Boundary Road	0.58–1.18*	

* With wind data assimilation.