Meteorological and Dispersion Modelling Using TAPM for Wagerup

Phase 1: Meteorology

Prepared for
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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 (version 2.6) for Wagerup”, addressing three closely defined objectives. This report deals with the first objective (Phase 1: Meteorology), which was to evaluate the capability of CSIRO’s The Air Pollution Model (TAPM) to acceptably produce hourly-averaged meteorological predictions matching available field observations in the close proximity of the Wagerup Refinery. The reports of Phase 2 (Dispersion) and Phase 3 (TAPM modelling for Health Risk Assessment) will be presented subsequently.

TAPM is a prognostic meteorological and air pollution dispersion model developed by CSIRO Atmospheric Research (see http://www.dar.csiro.au/tapm). The main advantage of the prognostic approach is that rather than requiring local meteorology it calculates it. The meteorological component of TAPM predicts the local-scale flow, such as sea breezes and terrain-induced circulations, using the larger-scale synoptic meteorology as boundary conditions. The air pollution component uses the model-predicted three-dimensional meteorology and turbulence.

The period April 2003–March 2004 was selected as the period for model evaluation, because it encompasses a complete, continuous winter season and a complete, continuous summer season, with the best meteorological data currently available. No previous continuous seasons were considered because new meteorological measurement systems were deployed in the year 2003 (e.g. a 30-m tower at Bancell Road, and radiosonde releases), providing extra meteorological data for a more comprehensive model evaluation.

The specific components of the Phase 1 objective included:

- Development of a finer, more accurate land-use database for Wagerup for use as input in TAPM than the default database.
- Derivation of the refinery-generated heat flux, its inclusion in TAPM, and evaluation of its effect on meteorological predictions.
- Analysis of the near-surface meteorological data from the Bancell Road and Residue Disposal Area (RDA) monitoring sites.
- Evaluation of TAPM performance against the locally observed meteorology using an internationally accepted set of statistical and graphical methods.
- Comparison the model profiles of wind speed, wind direction, and temperature with the radiosonde data from the 2003 campaign.
- Evaluation of the sensitivity of TAPM to surface roughness and deep soil moisture content.
- An analysis of underlying factors that influence the degree of disagreement in the model vs. observations comparison.
- Comparison of the model evaluation results with other studies.

As part of the Phase 1 work, the default land-use database used as input in TAPM was replaced by a more refined Wagerup specific land-use database at a resolution of 250 m × 250 m using GIS maps and a recent aerial photo covering an area of approximately 25 km × 25 km centred on the Refinery. The Refinery, the RDA and the adjacent cooling lakes were resolved.

An estimation of the Refinery-generated heat flux was made using Alcoa supplied information on heat balance for Wagerup Refinery based on known energy inputs, outputs and losses. The estimated heat flux value of 150 W m^{-2} was added to the TAPM surface-energy balance equation.

TAPM was run with four nested grid domains at 20, 7, 2, 0.5 km resolution for meteorology (31 × 31 grid points). The lowest ten of the 25 vertical levels were 10, 25, 50, 100, 150, 200, 250, 300, 400 and 500 m. The default databases of topography, monthly sea-surface temperature, soil types, deep soil moisture content, and deep soil temperature were used. The results from the innermost model grid domain (with a resolution of 0.5 km) were used to compare with the measurements.

The use of the derived Wagerup-specific land use, together with the refinery-generated heat flux, in the model improved the temperature and relative humidity predictions at Bancell Road, but only slightly.

A sensitivity test indicated that increasing or decreasing the deep soil moisture content to acceptable bounds in the model does not improve the agreement between the modelled meteorology and the observations.

A sensitivity test indicates that increasing the roughness length for the area to an acceptable limit in the model does not improve the agreement between the modelled meteorology and the observations.

Scatter plots, probability density function (or frequency) plots, and model evaluation statistics, such as observed and predicted means and standard deviations, correlation coefficient, root mean square error, systematic root mean square error, unsystematic root mean square error and index of agreement, were used to test TAPM's performance. The model evaluation was done for whole year, daytime, nighttime, winter period and summer period.

The meteorological measurements used in the test of TAPM against observations were: hourly-averaged wind speed, wind direction and temperature (all measured at both 10 m and 30 m AGL), net radiation, and relative humidity observations taken at Alcoa's Bancell Road monitoring site; the hourly-averaged wind speed and wind direction observations taken at 8 m AGL at the RDA monitoring site; and the radiosonde profiles of wind speed, wind direction, temperature and relative humidity from five morning releases conducted over a 3-day period in July 2003. Statistics and graphs of these tests are presented in this report.

Some particular inaccuracies in the wind speed, wind direction and net radiation measurements at Wagerup, already identified, will cause discrepancies between the TAPM outputs and meteorological observations at Wagerup. These are reviewed in the report.

The agreement between the TAPM predictions and the measurements, as judged by the index of agreement, for Wagerup is the highest for temperature, followed by net radiation, relative humidity, wind direction and wind speed. The model wind predictions are better in the daytime than in the nighttime, and they are better in winter than in summer. The overall wind-speed comparison at Bancell Road is dominated by the strong nighttime easterlies/south-easterlies. The model performance for wind predictions at RDA is better than that at Bancell Road.

The performance of TAPM in predicting the local meteorology at Wagerup is comparable to its performance in predicting the near-surface meteorology elsewhere in the world. TAPM generally predicts stronger wind speeds at Wagerup, and its performance for wind speed for Wagerup is not as good as for other locations.

TAPM's overall performance in predicting local meteorology at Wagerup is as good as and in some cases better than the available published accounts of three other internationally accepted prognostic meteorological models predicting meteorology at other locations.

The performance of the model is partly dependent on the complexity of the area being studied. The Bancell Road site is only about 1 km west from the western foothills of the north-south Darling escarpment, which rises to about 200 m within a distance of about 1.5 km from the foothills. It is possible that the Bancell Road site is sheltered by the escarpment for the easterly/south-easterly winds, and that the model is not able to simulate properly.

The limitations in TAPM predictions arise from these reasons: approximations to the underlying physics; uncertainties in the input data; problems of matching of the scale of the model to the observations. These are basic limitations that arise from current scientific knowledge and computing power.

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 also, NBL, SBL and convective mixed layer.
AGL	Height Above Ground Level
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.
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)
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)
Diagnostic equation	Any equation governing a system that contains no change

	with time, and therefore specifies a balance of quantities in space at a moment of time. *Compare* prognostic equation.
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).
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.
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.
Mesoscale	Pertaining to atmospheric phenomena having horizontal scales ranging from a few to several hundred kilometres (e.g. sea breezes).
Meteorology	The study of the physics, chemistry and dynamics of the

	earth's atmosphere.
Micrometeorology	A part of meteorology that deals with the small-scale motions within the atmospheric boundary layer (ABL).
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.
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. *Compare* diagnostic equation.
RDA	Residue Disposal Area
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.
Surface layer	A layer of air of order tens of metres thick adjacent to the ground where the effects of the frictional drag imposed on the wind by the ground dominate over those of the heating (or cooling) of the ground.
SKM	Sinclair Knight Merz (an environmental consulting company)
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
US EPA	United States Environmental Protection Agency (http://www.epa.gov)

WA	Western Australia
WA DEP	West Australian Department of Environmental Protection
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.

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 1 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 objectives:

- 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*).

This report addresses the objectives of Phase 1 (Meteorology) as set out in the original proposal. Overall, the purpose of Phase 1 is:

"To evaluate the capability of TAPM (version 2.6) with a detailed Wagerup specific land-use specification to acceptably produce hourly-averaged meteorological predictions matching available field observations in the Wagerup region, especially under a range of conditions that include both light and moderate wind speeds".

In the present work, given the occurrence of air quality issues in both winter and summer, the evaluation of TAPM is performed using local meteorological data for 12 months.

The period April 2003−March 2004 was selected as the period for model simulation. This period encompasses a complete, continuous winter season and a complete, continuous summer season, with the best meteorological data currently available. No previous continuous seasons were considered because new meteorological measurement systems were employed in the year 2003 (e.g. a 30-m tower and radiosonde releases), providing extra meteorological data for a more comprehensive model evaluation.

During the period April−September, northerly winds are frequent and the highest number of pollution/odour complaints are received from the local residents. This period is termed the winter season. Most of the complaints are from the Yarloop township, about 3 km south of the Refinery. The six-month period selected is the minimum period to simulate for meteorology at Wagerup, as it provides a sufficient sample size required for a reduced statistical uncertainty in the model-observation comparison study.

The summer period for meteorological model-observation comparison is October–March, so as to include periods during which the meteorology is generally more variable such that complaints are received from areas other than Yarloop (e.g. Hamel, about 5 km north of the refinery), and when issues such as dust from the Residual Disposal Area (RDA) mainly occur.

Section 2 describes the model, TAPM, used in this work. Sections 3, 4 and 5 present technical detail necessary to document the study. Section 6 presents the comparison of TAPM modelled and observed meteorology. The sensitivity of TAPM to surface roughness and deep soil moisture content is presented in Sections 7 and 8, respectively. There are a number of possible sources of disagreement between the model results and the measurements; these are discussed in Section 9. Section 10 gives a comparison of the TAPM results obtained from the present work with other modelling studies, and Section 11 presents the conclusions.

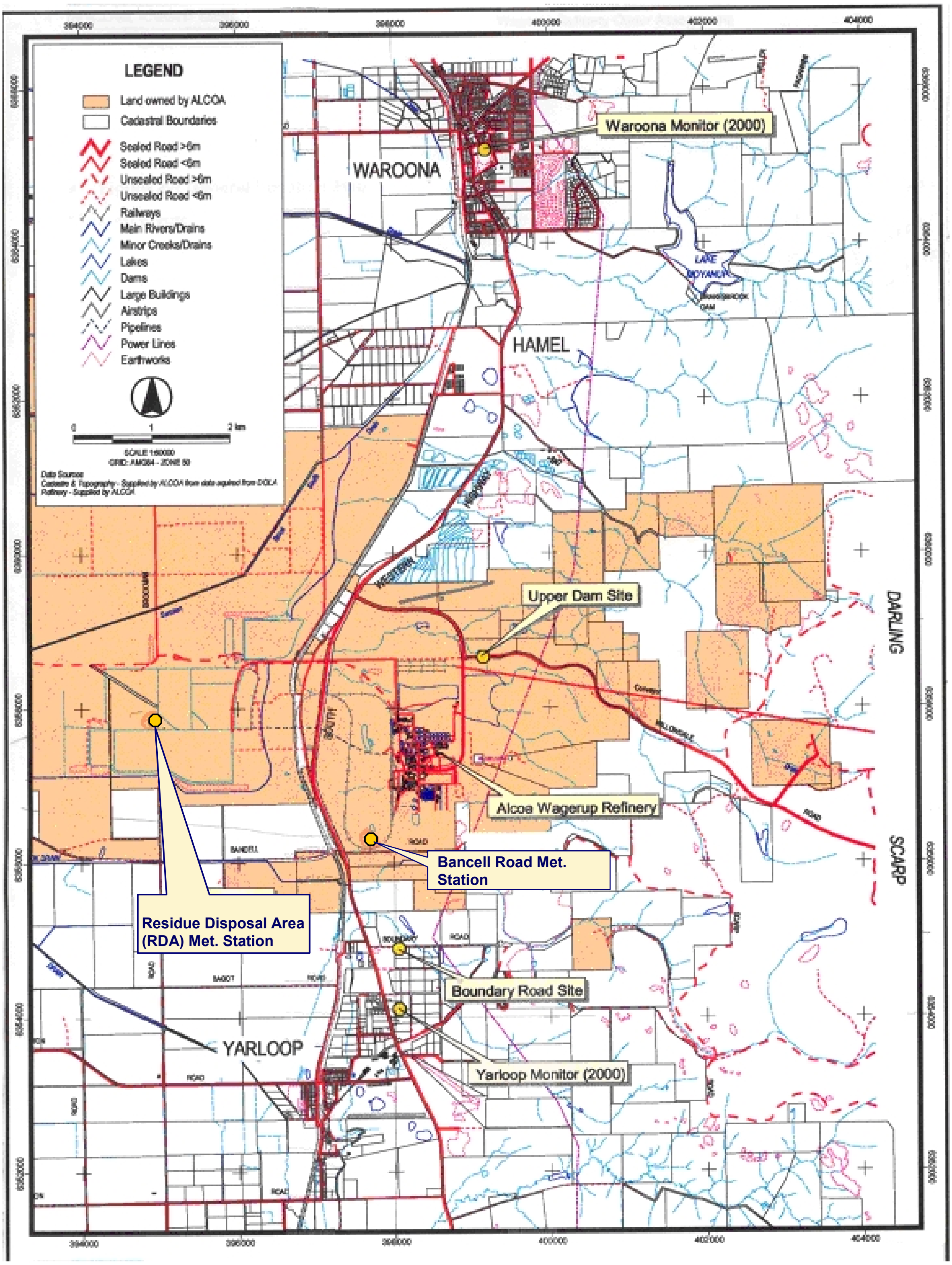

Figure 1: A map of Wagerup area showing the Alcoa Wagerup Refinery, Bancell Road meteorological station, Residue Disposal Area (RDA) meteorological station, Boundary Road air quality monitoring station, and the Upper Dam monitoring site. The Yarloop monitoring site and the Waroona Monitor are non-operative.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

2. Air Pollution Modelling

2.1. Introduction

From the meteorological perspective, air pollution models used for predicting ambient concentrations of pollutants for environmental impact assessments can be categorised into three main groups, as described below. The emphasis here is on the meteorological aspects of these models.

2.1.1 Models using observed meteorological data

Simple Gaussian plume or puff models, and some non-Gaussian analytical models, of air pollution dispersion require meteorological observations for the region being modelled. The meteorological data required typically includes: near-surface (e.g. at 10 m AGL) observations of wind speed, wind direction, and temperature; estimates of mixing heights and atmospheric stability; and optionally extra information to handle more complex effects.

These types of models are computationally fast, and can be used to predict pollution concentrations at very high spatial resolution (e.g. 100-m spaced pollutant grids). They are generally used to represent discrete sources such as industrial emissions (e.g., point, line, or area source emissions), where chemical reactions are either ignored or treated very simply. However, under conditions where complex air flows and diffusion occur (e.g., in coastal regions or complex terrain) these types of models are either not applicable or the simple assumptions and extensions used therein lack portability and generality. Moreover, the meteorological information required by these models is not always available or not available in sufficient detail.

Examples of such models include ISC3 (USEPA, 1995; http://www.epa.gov/scram001/tt22.htm#isc), AERMOD (a USEPA model, see http://www.epa.gov/scram001/tt26.htm#aermod), AUSPLUME (EPAV, 2000), and CALPUFF (Scire et al., 1997, 2000; http://www.src.com/calpuff/calpuff1.htm) using the option of a simple meteorological input.

2.1.2 Models using diagnostic meteorology

In complex terrain, meteorological observations from sparsely located monitoring stations are generally not sufficient for driving air pollution models because these observations may not represent the complex horizontal and vertical structure of the air flow in the region. Under these circumstances, meteorological fields that are derived using diagnostic models can be useful. Diagnostic models are based on an objective analysis of available meteorological data, and provide three-dimensional fields of meteorological parameters computed by appropriate interpolation and extrapolation of available meteorological measurements (e.g., Goodin et al., 1980). They are diagnostic because they cannot be used to forecast the meteorological evolution, but simply provide a best estimate of a steady-sate (or quasi steady-state) condition.

A simple diagnostic model may involve just a simple inverse-distance-square interpolation of the observations (e.g., Luhar and Rao, 1994). (This means that the influence of the observation on the calculated meteorology falls off steeply with distance from the location of the observation.) However, typically a diagnostic model derives mass-consistent flow fields that satisfy the conservation of mass equation and at the same time minimises the differences between the observations and the model predictions (e.g. Ratto et al., 1994). Such models normally involve the use of variational calculus techniques.

The diagnostic approach is computationally fast, but requires surface meteorological observations from a dense network of monitoring stations, which may not be routinely available, and are generally only valid under the neutral atmospheric conditions (i.e. cloudy and/or windy conditions). Also, the meteorological fields obtained as solutions to the diagnostic equations may not be unique, two or more different air flows may satisfy the same set of initial observations. Some diagnostic models can use the output of a large-scale prognostic model, and interpolate it to a finer resolution.

Examples of diagnostic wind field models include NUATMOS (Ross et al., 1988), and the CALMET processor of the CALPUFF model (Scire et al., 1997, 2000).

2.1.3 Models using prognostic meteorology

Prognostic models are based on basic physical principles (or laws), and are the most complex of air pollution models. They are used to forecast the time evolution of the atmospheric system through the space-time integration of the fundamental equations of conservation of mass, heat, motion, water and other substances. Generally, most prognostic models for air pollution applications are of mesoscale range (i.e. horizontal scales from a few to several hundred kilometres), and are much slower to run on a computer than diagnostic models. They are either stand-alone meteorological models driving air pollution dispersion models, or are fully coupled meteorological and air pollution models. They can account for complex terrain and coastal regions. The main advantage of the prognostic approach is that it eliminates the need to have site-specific meteorological observations to drive a pollution model, but can assimilate observations if they are available.

Prognostic air pollution models can handle urban sources on a gridded emissions inventory (e.g., vehicle, domestic, industrial, biogenic emissions), where chemical reactions are treated in a detailed manner using complex coupled chemical reactions (e.g., photochemical smog and particles) (Seaman, 2000). On the other hand, the near-source diffusion of point-source plumes can also be described accurately.

Some limited examples of combinations of the diagnostic and prognostic approaches have also been used in the past. For example, a photochemical urban airshed model that uses output from a diagnostic wind field model, or a puff model using output from a prognostic meteorological model.

Some example of the prognostic models are: the PSU/NCAR mesoscale model (known as MM5), which is mainly a meteorological model without any air pollution component (see http://www.mmm.ucar.edu/mm5/); the HOTMAC/RAPTAD modelling system, which is a is a three-dimensional mesoscale prediction model that forecasts wind, turbulence, humidity, and atmospheric turbulence, coupled with a Lagrangian puff model for the transport and diffusion of air pollutants (see http://www.ysasoft.com/solution/system.htm); and CSIRO's The Air Pollution Model (TAPM) (see http://www.dar.csiro.au/tapm/).

Until recently, the prognostic approach as used in TAPM has been impracticable for use in regulatory modelling on personal computers because of the time and computing resources required, but advances in computing power now make this approach realistic for simulations of extended periods (up to year-long simulations) at high resolution (down to 0.2-km spaced pollutant grids). We examine the performance of the meteorological component of TAPM in this report.

2.2. TAPM

The Air Pollution Model (TAPM) developed by CSIRO Atmospheric Research is a three-dimensional, prognostic meteorological and air pollution model, controlled by a graphical user interface (see Hurley, 2002; http://www.dar.csiro.au/tapm/ for a complete description of the model). The model uses a complete set of 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. TAPM is perhaps the most complex and advanced of the models widely used in Australia for regulatory applications as well as research problems. With TAPM, all input data sets, except emissions, accompany the model 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 meteorological model 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 few of these correspond typically to 0, 75, 200, 425, 650, 875, 1100, 1325 and 1800 m above mean-sea level. TAPM then 'zooms-in' 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 the momentum equations for 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 (not used here) non-hydrostatic components, and a Poisson equation is solved for the non-hydrostatic component. Explicit cloud microphysical processes are included. Wind observations can optionally be assimilated into the momentum equations as nudging terms. 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 turbulence 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.

The air pollution component of TAPM consists of an Eulerian grid-based set of species conservation equations 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, 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 applied to several case studies, including modelling year-long meteorology and air pollution for the industrial area of Kwinana (Hurley et al., 2001); modelling year-long urban meteorology, photochemical smog and particulate matter in Melbourne (Hurley et al., 2003a); and comparison with international model validation data sets (Luhar and Hurley, 2003).

2.3. TAPM setup

The latest version 2.6 of TAPM was used in the present analysis. We ran the model with four nested grid domains at 20, 7, 2, 0.5 km resolution for meteorology (31 × 31 grid points), all centred on 115°54.5′ E, 32°56.5′ S, which is equivalent to 397.951 km east and 6354.639 km north in the AMG[1] (Australian Map Grid) coordinate system, and is almost the location of the Boundary Road air quality monitoring site. 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 8000 m. The default databases of topography, monthly sea-surface temperature, soil types, deep soil moisture content, and deep soil temperature were used. No pollution calculations were performed as part of this Phase.

Figure 2a–d shows the four successive model domains for meteorology, corresponding to a grid resolution of 20, 7, 2 and 0.5 km, respectively (with the default land use). The innermost domain covers an area of 15 km × 15 km. The green-grey shading represents the terrain height at the same resolution as that used for meteorology.

Most TAPM runs were performed on a computer cluster using the AMD Athlon processors with the Linux operating system. The TAPM code was compiled using the Absoft Fortran 90/95 compiler (version 3.0). The remaining runs were performed on an IBM compatible personal computer with an Intel Pentium III processor and Lahey/Fujitsu Fortran 95 compiler (version 5.6) running under the MS Windows environment.

[1] The AMG coordinates specified in this report correspond to the AMG84 coordinate system.

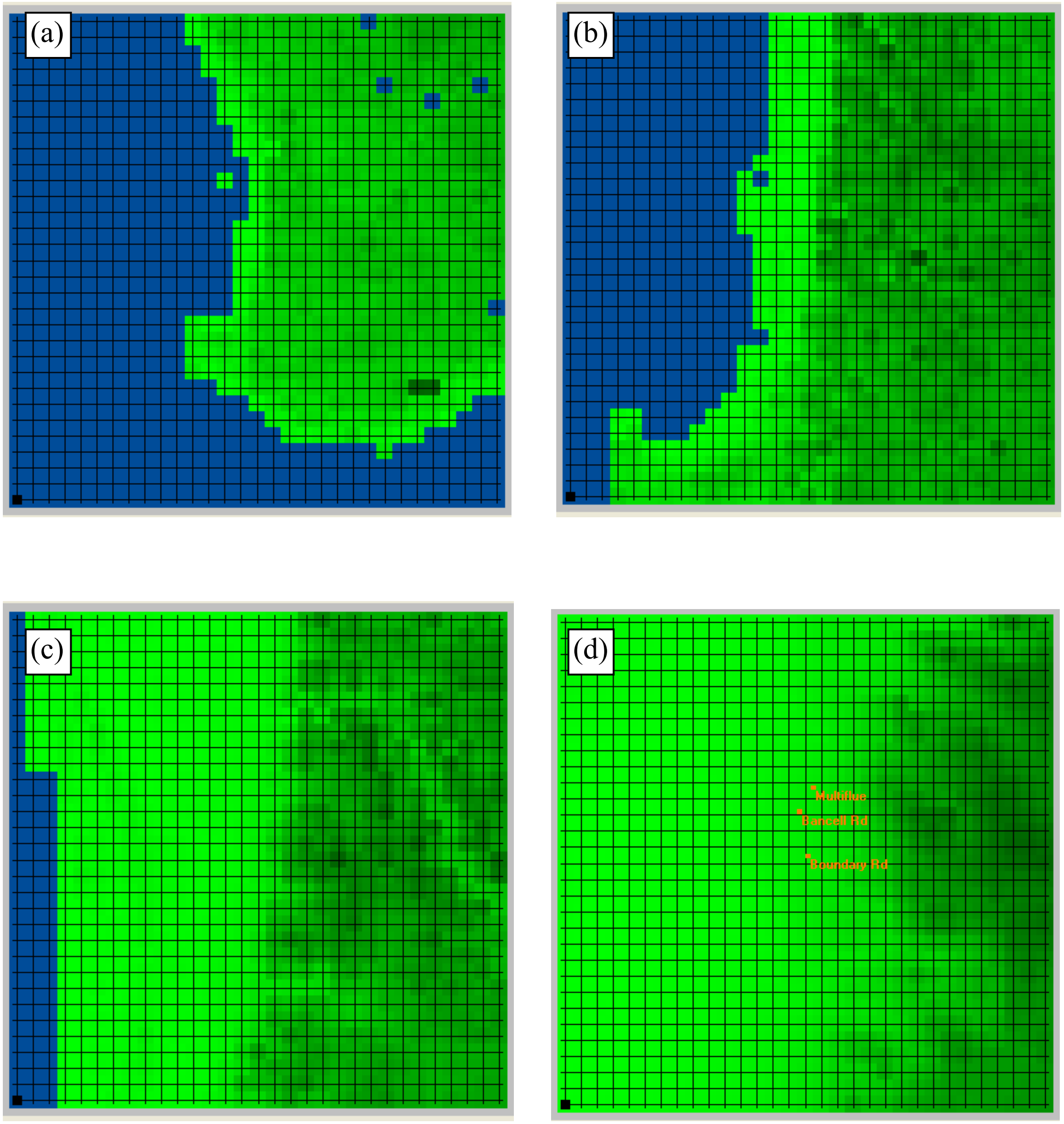

Figure 2: Model grid domains, which are successively nested, for meteorology (31 × 31 grid points) corresponding to a grid resolution of (a) 20, (b) 7, (c) 2 and (d) 0.5 km.

3. Wagerup land-use database

3.1. Default land-use data

Specification of land-use types within the model domain forms an important input to the model. This input, together with other ground-surface properties (e.g. soil type), is used in the surface energy balance scheme of the model for calculating surface fluxes (of heat and momentum, for example) that define the lowest boundary condition in the model. These fluxes influence parameters such as turbulence and stability that in turn influence dispersion characteristics of a plume. The lowest vertical level of the atmospheric domain (i.e. 10 m AGL) in TAPM is parameterised in terms of the Monin-Obukhov surface similarity laws. Table 1 gives the land-use types and the corresponding height of roughness element (h_f) used by TAPM.

TAPM's default database ("vege.aus") of land-use characterisation for Australia is given at an approximate resolution of 5 km × 5 km, which is somewhat coarse. Figure 3 shows the default land use within the innermost model domain (31 × 31 grid points, grid resolution of 0.5 km). The red area corresponds to pasture – dense (seasonal) (Type 23), whereas the blue area corresponds to forest – sparse (woodland) (Type 5). It is apparent that the TAPM default database of land use is limited in resolving the land-use features around the Wagerup Refinery. For example, the Refinery and the lakes around it are not resolved, and neither are the contrasting vegetations.

Table 1: Land-use types and the corresponding roughness element heights used in TAPM (Hurley, 2002).

Category number	Land-use type	Height of roughness element, h_f (m)
-1	Permanent snow/ice	-
0	Water	-
1	Forest – tall dense	42.00
2	Forest – tall mid-dense	36.50
3	Forest – dense	25.00
4	Forest – mid-dense	17.00
5	Forest – sparse (woodland)	12.00
6	Forest – very sparse (woodland)	10.00
7	Forest – low dense	9.00
8	Forest – low mid-dense	7.00
9	Forest – low sparse (woodland)	5.50
10	Shrub-land – tall mid-dense (scrub)	3.00
11	Shrub-land – tall sparse	2.50
12	Shrub-land – tall very sparse	2.00
13	Shrub-land – low mid-dense	1.00
14	Shrub-land – low sparse	0.60
15	Shrub-land – low very sparse	0.50
16	Grassland – sparse hummock	0.50
17	Grassland – very sparse hummock	0.45
18	Grassland – dense tussock	0.75
19	Grassland – mid-dense tussock	0.60
20	Grassland – sparse tussock	0.45
21	Grassland – very sparse tussock	0.40
22	Pasture/herb-field – dense (perennial)	0.60
23	Pasture/herb-field – dense (seasonal)	0.60
24	Pasture/herb-field – mid-dense (perennial)	0.45
25	Pasture/herb-field – mid-dense (seasonal)	0.45
26	Pasture/herb-field – sparse	0.35
27	Pasture/herb-field – very sparse	0.30
28	Littoral	2.50
29	Permanent lake	-
30	Ephemeral lake (salt)	-
31	Urban	10.00

In the following, we derive a better land-use database specific to Wagerup for use in this and subsequent TAPM modelling of Wagerup.

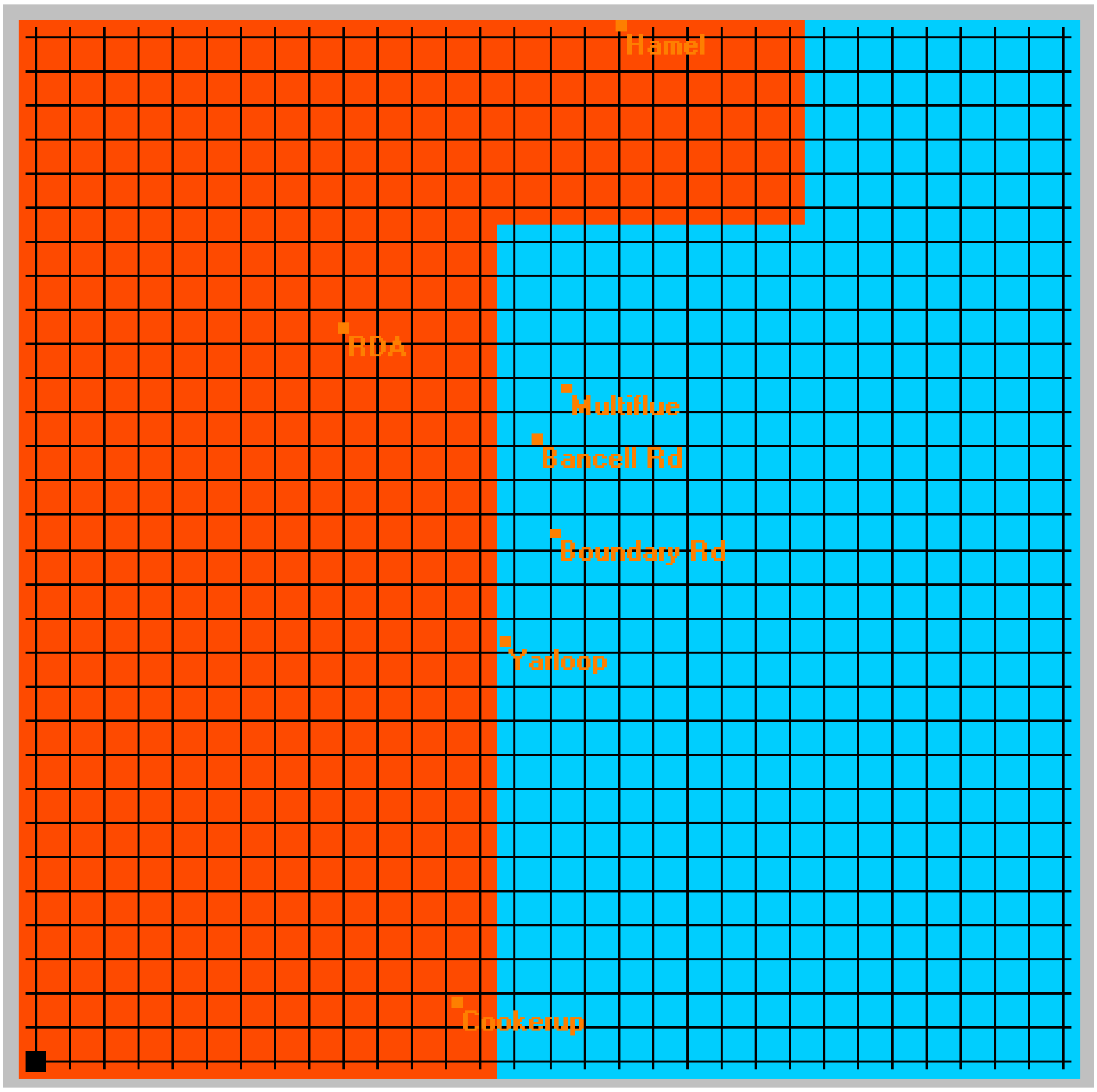

Figure 3: The land-use categories used by TAPM within the innermost model domain (31 × 31 grid points, grid resolution of 0.5 km). The red area corresponds to pasture – dense (seasonal) (Type 23), whereas the blue area corresponds to forest – sparse (woodland) (Type 5).

3.2. Development of a Wagerup-specific land-use database

Alcoa supplied a GIS database of the Wagerup area containing information about land-use zones, roads, plot boundaries, water streams, and topographic contours in the AMG coordinate system (Geo spatial information reproduced with permission of WA Department of Land Information (DLI), P339). In the database, the 'zones' files are land-use planning files from the WA Department of Planning and Infrastructure (via

WA Department of Land Administration (DOLA)), and thus reflect the assigned land uses in town and regional plans. According to the mapping department of Alcoa, these files were up to date as at June 2003 (P. Coffey, personal communication, 17 November 2004). The cadastral data files (relating to land boundaries and subdivisions) were up to date as at January 2004. The other files relating to topography, roads, drainage, etc. are most likely 2003.

The database covered an area of approximately 25 km × 25 km centred on the Refinery. A GIS map of the Wagerup area showing the land-use zones from the database is presented in Figure 4. Because TAPM needs gridded data of land use, the land-use part of the database was gridded at a resolution of 250 m × 250 m using the GIS software ArcView. Table 2 presents the land-use types included in the Wagerup GIS database, and the percentage areal coverage of each land-use type calculated by ArcView as part of the griding process. It is apparent that the land-use is dominated by forestry and general farming.

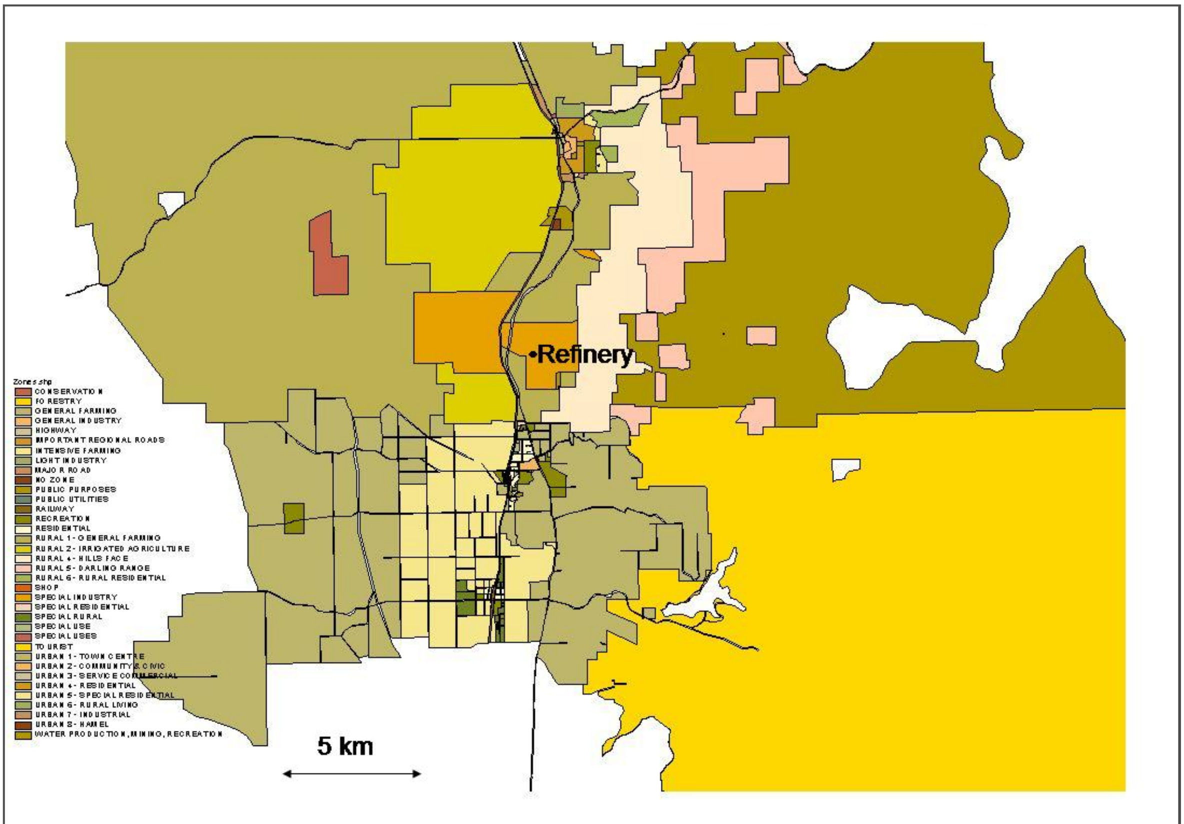

Figure 4: An original GIS map of the Wagerup area showing land-use zones.

The land-use categories of the GIS database in Table 2 were translated to the nearest land-use types in Table 1 used by TAPM. To help with this translation, an Alcoa-supplied aerial image of the Wagerup land surface covering 29.5 km × 25.5 km with the Refinery at the centre was used. This aerial image file, ‘Wg.ecw’ (ER Mapper’s Enhanced Compressed Wavelet file in the MGA94 coordinate system) taken in January 2004 (P. Coffey, personal communication, 17 November 2004), is a very high resolution image of the area, and allows high-level zooming in at a particular sub-area without losing much resolution (see Figure 5). The GIS database categories 1, 2, 3, 4, 8, 24, 25, 27, 28 and 36 were assigned TAPM category 25; the categories 9, 10, 11, 12, 14, 16, 17, 18, 19, 30 and 33 were assigned TAPM category 31; the categories 5, 20 and 23 were assigned TAPM category 4; and the categories 6 and 7 were assigned TAPM category 13. The Refinery and the Residue Disposal Area (RDA) are classified as Special Industry (Category 22) in the GIS database. This specification was edited so that the RDA area was TAPM category 14 (shrub-land – low sparse), and the Refinery area was TAPM category 31. This TAPM category 31 is urban in the default dataset, and is adapted for the Refinery here. TAPM category 31 was selected for the Refinery due to height of buildings and plants and associated heat loss (see Section 4). The RDA water bodies and other lakes around the Refinery were added and assigned TAPM category 0 (water). The translated land-use types for TAPM are given Table 2.

In TAPM, surface moisture, surface temperature and surface fluxes of momentum and heat are calculated separately for bare soil and vegetation cover, and they are then weighted according to the fraction of the surface covered by vegetation in order to derive the effective values of these parameters. These surface values impose the lower boundary conditions in the model. As such, TAPM does not use any effective surface roughness length; separate values are used for bare soil and vegetation cover. For the bare soil component, the model assumes a surface roughness length (z_o) of 0.1 m, whereas for the vegetation component the following expression is used.

$$z_o = \max[0.1,\ \min(h_f/10, 1.0)], \qquad (1)$$

where h_f is the height (m) of the roughness element. Hence, in the model (version 2.5 onwards), the minimum value of z_o is 0.1 m (equal to the bare soil value) and the maximum value is 1.0 m.

The minimum value of z_o = 0.1 m in the model is used to account for the soil texture and any undulations in terrain height within the model grid (i.e. subgrid-scale topographic variations). The upper limit of z_o = 1.0 m is imposed because the Monin-Obukhov similarity laws for wind velocity and temperature profiles used in the model tend to break down when z/z_o becomes small (~5–10), where z is the sampling height or model level (Garratt, 1994). This breakdown occurs because z is so small that it lies within the roughness layer, and not within the overlying surface layer for which the similarity laws are applicable. In the model the lowest level is at 10 m, and, therefore, a maximum value of z_o = 1.0 m is assumed.

Table 2 shows that about 42% of the land-use around the Refinery is dominated by forestry for which a z_o value of 1.0 m is used by TAPM. For this surface type, TAPM assumes that 50% of the ground surface is covered by vegetation and the rest by bare soil (with z_o = 0.1 m). The next dominant land use is farming, which corresponds to TAPM's Pasture/herb-field–mid-dense (seasonal). For this category, TAPM assumes the vegetation roughness length (z_o) to be 0.1 m with 50% of the ground surface covered by vegetation and the rest by bare soil.

Figure 5: An aerial image of the Wagerup area used in deriving the Wagerup-specific land-use data base for TAPM. The image covers a domain of 29.5 km × 25.5 km, and one can zoom-in to examine the surface details more closely.

Table 2: Land-use type specified for Wagerup in the GIS database, its equivalent TAPM land-use type, and the corresponding surface roughness length used in TAPM.

Category number	GIS land-use type	% covered	Equivalent TAPM land-use type	$h_f/10$ (m)	TAPM roughness length (m)
1	Major road	0.07	25	0.045	0.1
2	Rural 1 – general farming	20.17	25	0.045	0.1
3	Railway	0.13	25	0.045	0.1
4	Highway	0.07	25	0.045	0.1
5	Water production, mining, recreation	14.16	4	1.7	1.0
6	Rural 5 – Darling Range	2.19	13	0.1	0.1
7	Rural 4 – hills face	2.47	13	0.1	0.1
8	Rural 2 – irrigated agriculture	3.71	25	0.045	0.1
9	Urban 7 – industrial*	0.02	31 (25)*	1.0	0.1
10	Urban 6 – rural living*	0.09	31 (25)*	1.0	0.1
11	Rural 6 – rural residential*	0.11	31 (25)*	1.0	0.1
12	Urban 5 – special residential*	0.07	31 (25)*	1.0	0.1
14	Urban 4 – residential*	0.13	31 (25)*	1.0	0.1
16	Recreation*	0.29	31 (25)*	1.0	0.1
17	Urban 1 – town centre*	0.02	31 (25)*	1.0	0.1
18	Urban 2 – community & civic*	0.02	31 (25)*	1.0	0.1
19	Public purposes*	0.02	31 (25)*	1.0	0.1
20	Conservation	0.29	4	1.7	1.0
22	Special industry (Wagerup Refinery)	1.30	14 (RDA) 31 (Refinery) 0 (lakes)	0.06 1.0 -	0.1 1.0 -
23	Forestry	41.90	4	1.7	1.0
24	General farming	9.87	25	0.045	0.1
25	Intensive farming	2.67	25	0.045	0.1
27	Important regional roads	0.11	25	0.045	0.1
28	No zone	0.02	25	0.045	0.1
30	Residential*	0.04	31 (25)*	1.0	0.1
33	General industry*	0.02	31 (25)*	1.0	0.1
36	Special rural	0.02	25	0.045	0.1

*These areas, which cover a total of 0.8% of the area used for analysis, fall under the urban category of TAPM (with a roughness length of 1 m). However, because TAPM can only assign additional (anthropogenic) heat flux to the TAPM urban category (31), this TAPM urban category must be used for the refinery to account for the Refinery-generated heat flux. The application of this same category to the Yarloop, Hamel and other residential/urban areas in the model would wrongly add the same heat flux to these areas. Hence, the Yarloop, Hamel and other residential/urban areas are assigned the same land-use categories as their immediate surroundings (i.e., Category 25 – pasture/herb-field - mid-dense (seasonal)). This is considered the most appropriate adjustment within a current limitation of the model.

The translated land use generated was converted from the AMG coordinate system to the Geographic (i.e. latitude-longitude) coordinate system, as required by TAPM, with a uniform spacing of 0.0025°C (about 230 m east and 280 m north). Figure 6 shows the new land-use pattern used by TAPM within the innermost model domain (31 × 31 grid points, grid resolution of 0.5 km) based on the modified, Wagerup-specific land use. It is evident that the new land-use specification is much more detailed than the default one shown in Figure 3, with the Refinery and the lakes around it resolved. In Figure 6, the red area is Pasture – mid dense (seasonal) (Type 25), green is Shrub-land – low mid-dense (Type 13), light blue is Forest – mid-dense (Type 4), dark blue is Water (Type 0), and pink is Urban (Type 31). The pink (urban) areas just south of the Refinery correspond to Yarloop. However, because TAPM can only assign additional (anthropogenic) heat flux to the one urban category, an addition of the Refinery-generated heat flux for the Refinery area in the model would also add the same heat flux to the Yarloop area (see next Section). Hence, the Yarloop area are assigned the same land-use categories as their immediate surroundings (i.e., Category 25 – pasture/herb-field - mid-dense (seasonal)).

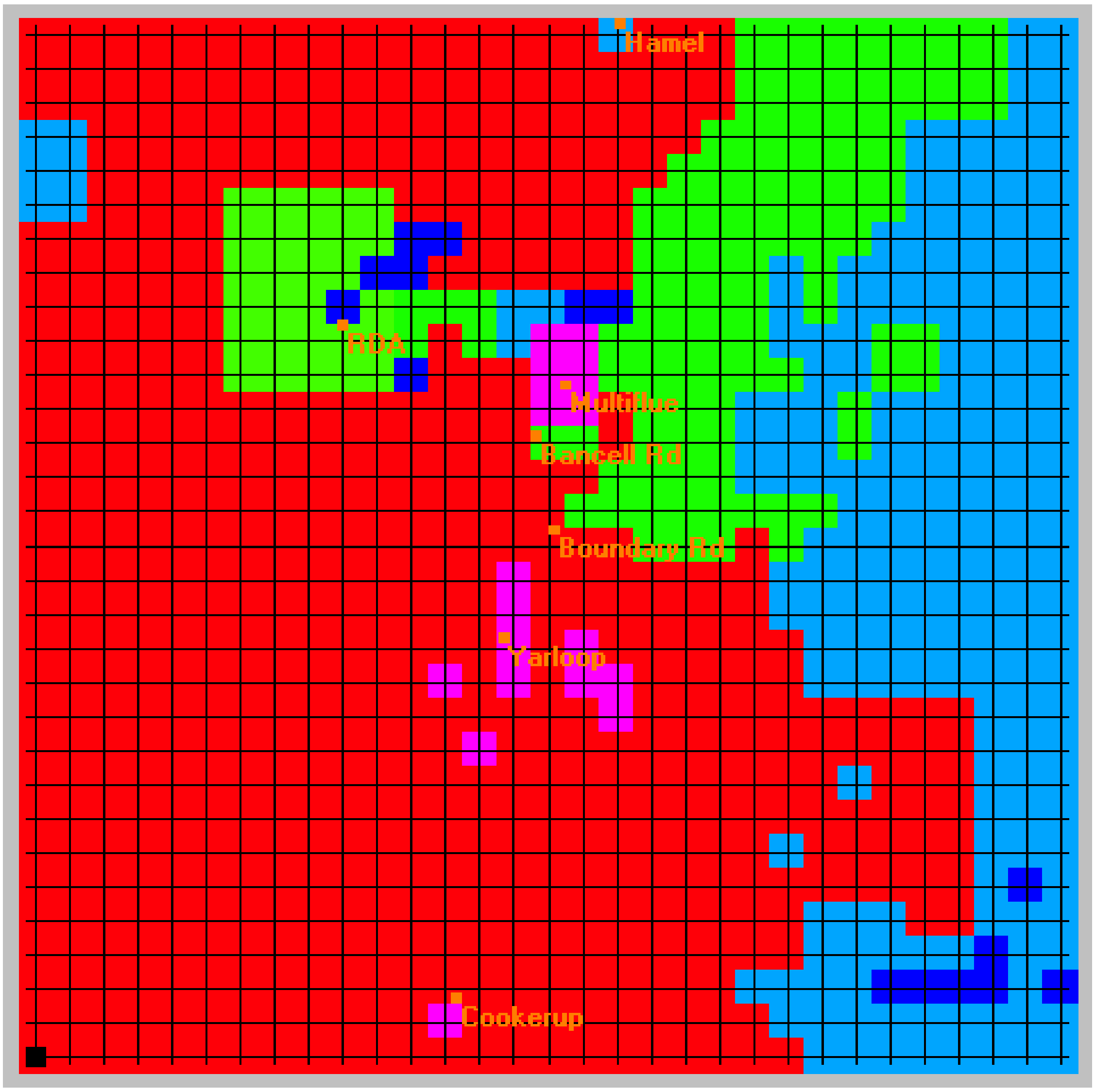

Figure 6: New land-use categories used by TAPM within the innermost model domain (31 × 31 grid points, grid resolution of 0.5 km). The colour coding varies from dark blue (water – Type 0) to pink (urban – Type 31). The red area is pasture – mid dense (seasonal) (Type 25). The final land-use map used in TAPM is Figure 8.

4. Calculation of Refinery-generated surface heat flux

Considerable amount of the total Refinery power input is lost as heat. As a result it is possible that the Refinery area is warmer than the surrounding countryside. This phenomenon is equivalent to an 'urban heat island', albeit on a much smaller spatial scale. Most large cities are anthropogenic sources of heat, and the surface-layer air is generally warmer than that of their surroundings. The intensity of this 'urban heat island' (i.e. the temperature difference between urban and rural areas) is the strongest during the night under cloudless skies and light wind conditions, with a typical value of 5°C. In many cases, heat from the city is sufficient to maintain a shallow convective mixed layer at night, even while a substantial stable boundary layer has developed over the surrounding countryside (Stull, 1988). On the other hand, during the daytime, heat from the urban area can enhance the mixing already present in the mixed layer. The presence of large buildings increases surface drag and mechanical turbulence, and decreases the mean wind speed. All these 'urban heat island' properties have bearings on near-surface vertical mixing and plume dispersion characteristics. In Figure 6 for TAPM, the Refinery area has been classified as an urban land-use category with a roughness element height of 10 m. It covers only 3-4 effective (horizontal) grid points within the domain. TAPM (in default) assumes that this kind of surface consists of 50% hard surface and 50% vegetation/soil with an anthropogenic heat-flux contribution of 30 W m^{-2}.

Because the Wagerup Refinery is a small, concentrated source of heat, the default anthropogenic heat-flux of 30 W m^{-2} used in TAPM for a generic urban land use was not used. In the following, we determine the Refinery-generated heat flux.

Alcoa supplied information on the heat-loss balance for the Wagerup Refinery based on known energy inputs, outputs and losses (Coffey, personal communication, 6 July 2004). In many cases the loss calculations for individual buildings and processes were backed up by temperature and material flow calculations, though in some cases a more simple inputs-less-outputs approach was used. Figure 7 presents an overview of the energy balance, with the percentages shown reflecting the proportion of total energy input (= 809 MW) that are estimated as heat losses. The arrows show the general recirculating liquor flow directions, with off-takes at clarification (bauxite residue to the RDA) and calciners (alumina hydrate to calcined alumina, the product).

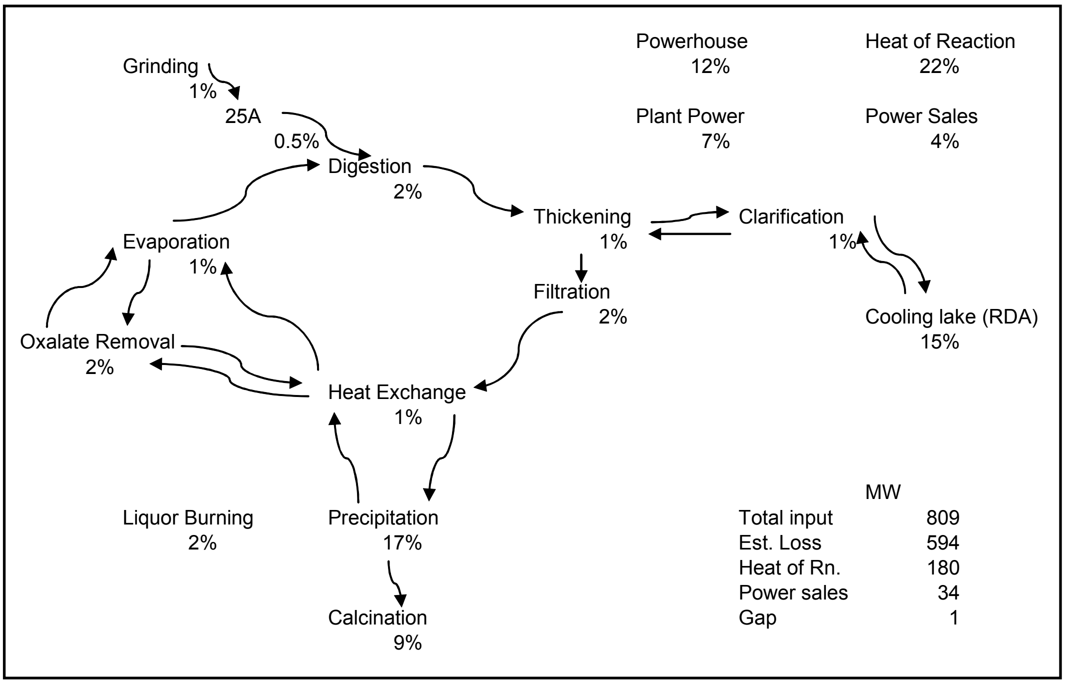

Figure 7: An overview of the energy balance, with the percentages shown reflecting the proportion of total energy input (= 809 MW) that is estimated as heat losses (Coffey, 6 July 2004). The arrows show the general recirculating liquor flow directions (Rn ≡ Reaction).

In Figure 7, the terms ‘heat of reaction’, ‘power sales’ and ‘gap’ are not heat losses but are effective uses or exports of energy, or closure gap (P. Coffey, personal communication, 6 July 2004). Table 3 presents the values of heat loss from various stages of the Wagerup Refinery processes.

Table 3: Heat loss from various stages at Wagerup Refinery.

Stage number	Stage	Heat loss (MW)
1	Grinding	8
2	25A (desilication)	4
3	Residue (cooling lake and super thickener)	123
4	Evaporation	12
5	Digestion	14
6	Thickening	6
7	Clarification	10
8	Filtration	17
9	Oxalate removal	19
10	Heat exchange	5
11	Precipitation	136
12	Calcination	70
13	Liquor burning	16
14	Powerhouse	97
15	Power usage	57
	Total	594

It is clear from Table 3 that the main heat losses are from the powerhouse, from precipitation, at the cooling lake (within the RDA complex which is to the west of the refinery), from Powerhouse, from calciners, and from Power usage (or 'plant power').

Alcoa estimates that greater than 80% of the Powerhouse heat loss is via the stack emissions, about 75% of the heat loss from precipitation is from the cooling towers, and the majority of the heat loss from calciners is likely to be from the stack emissions. Plant power is electricity sent out of the refinery powerhouse to the refinery, and is used in providing motive power (pumps and blowers), lighting, and other services. Some of this ends as effective work done, but one can conservatively assume that much of it too ends up as heat losses distributed more or less across the whole Refinery. The other process buildings have minor heat losses by comparison (P. Coffey, personal communication, 6 July 2004).

TAPM can account for anthropogenic heat only through the specification of a surface heat flux value with the land-use category being urban. We do not treat stack emissions as contributing to surface heat flux. In addition, it is not possible to account for the heat flux from the cooling lake because TAPM treats water bodies as having 'normal' temperature. Therefore, ignoring the heat losses both at the cooling lake and from the stack emissions, the total heat loss is equal to $595 - 123 - 136 \times 0.75 - 70 - 97 \times 0.8 = 224.4$ MW. Given the Refinery area of 1 km × 1.5 km in the TAPM innermost domain, the heat flux due the Refinery heat losses is calculated to be 150 W m^{-2}. This value is much larger than the default value of 30 W m^{-2} used by TAPM for urban land use. Hence, for this Wagerup study we assign an anthropogenic heat-flux value of 150 W m^{-2} to the Wagerup Refinery (urban) category. Because the Yarloop grid points in Figure 6 are classified as urban land use, but Yarloop cannot have an anthropogenic heat-flux value as high as that of the Refinery, we treat Yarloop grid points as the same land use as the surroundings. Figure 8 presents the *final* land-use pattern used in TAPM for the model evaluation.

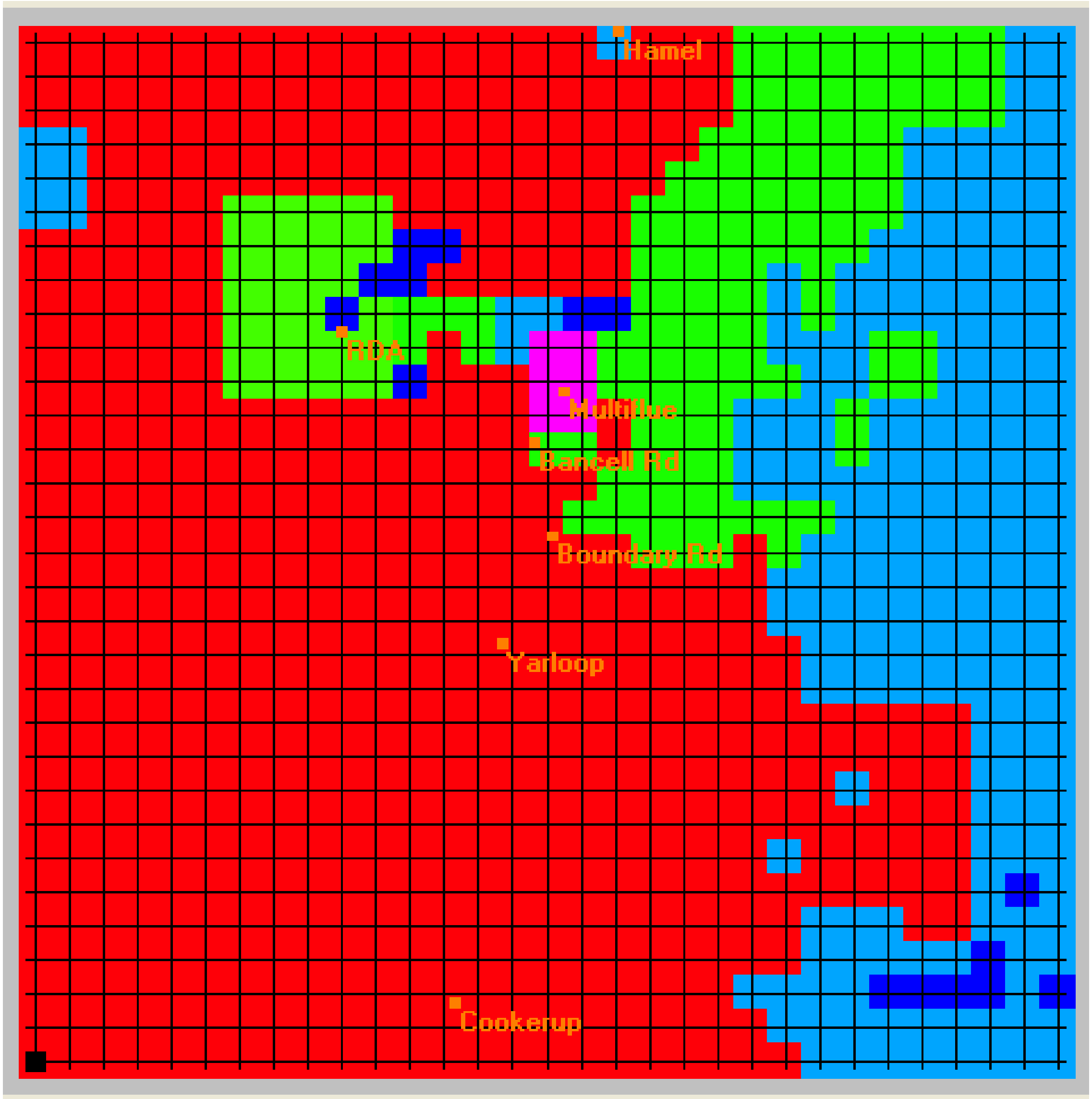

Figure 8: Final land-use categories used by TAPM within the innermost model domain (31 × 31 grid points, grid resolution of 0.5 km). The colour coding varies from dark blue (water – Type 0) to pink (urban – Type 31). The red area is pasture – mid dense (seasonal) (Type 25).

Note the use of 150 W m^{-2} as the Refinery-generated heat flux in the model does not mean that this is the minimum value of the sensible heat flux used by the model for the Refinery area. The Refinery-generated heat flux is added as a term in the surface energy balance equation, which also takes into account the cooling of the ground in the nighttime. Hence, the minimum surface sensible heat flux is always lower than the Refinery-generated heat flux.

5. Meteorological data

5.1. Surface data

Alcoa's Bancell Road meteorological station (AMG coordinates 397.740 km east and 6356.260 km north) is their primary weather station, and is located about 1 km south of the Refinery (

Figure 1). Table 4 gives the type of continuous measurements taken at this station. The net radiation measurements and the measurements at 30 m started from 18 July 2003 when the then existing 10-metre meteorological mast was relocated, and replaced by a 30-metre mast.

Table 4: Details of meteorological monitoring at Wagerup

Instrument list at Bancell Road	Height AGL (m)
Solid state sonic wind sensor	10
Solid state sonic wind sensor	30
Sensor, differential temperature	10
Sensor, differential temperature	30
Net pyrradiometer	1
Barometric pressure gauge	1
Solar radiation sensor	1
Temperature and relative humidity sensor	1
Rain gauge	0
Instrument list at RDA	
Separated cup and vane anemometer	8

The 10-m wind sensor on the 30-m mast is sheltered from due easterly winds by the mast (see Section 6.5 for more details). The effect of this sheltering is clearly visible in a wind speed vs. wind direction plot when compared with that for the 30-m wind data. An SKM (2003) audit report on the Bancell Road meteorological observations states the 10-m wind sensor does not meet the Australian Class 1 station standard due to the sheltering by the mast and by the nearby trees (it is understood that the trees have since been cleared), and recommends using only the 30-m wind data as the primary source of wind information. The 30-m sensor is located on the top of the mast and meets the exposure standards.

The RDA site (AMG coordinates 394.941 km east and 6357.882 km north) is Alcoa's secondary weather station located about 3 km west of the Refinery (

Figure 1). Measurements of wind speed and wind direction at about 8 m AGL are made using a separated cup and vane anemometer, and the data from this station are mainly used for the management of dust control and sprinkler operation. The RDA wind mast is mounted on a small building, which in turn is on an embankment. It is stated in an SKM review (file "SKMReviewWagerup RDA Weather Station.doc", P. Coffey, personal communication, 10 August 2004) that the RDA site does not conform to appropriate Australian standard for anemometer siting because it is mounted less than 10 m high, and that acceleration of measured wind may be caused by the building and RDA embankment. There are also stalling issues with the RDA anemometer when the winds are low (see Section 6.6.1).

Because of the sheltering of the 10-m wind sensor by the measurement tower for easterly winds at Bancell Road, only a limited model comparison analysis will be performed using the 10-m data. The measured winds at 30-m at Bancell Road and those at 8 m at RDA will be used for a full model evaluation exercise.

5.2. Radiosonde data

A series of GPS-tracked radiosonde releases were conducted by Alcoa in 2003 to enable characterisation of the lower portion of the atmospheric boundary layer (ABL) in the morning at Wagerup.

In June and July 2003, Alcoa conducted radiosonde measurements of meteorology in an area about 350 m south-east of Bancell Road, at an approximate location of 115.91° E and 32.93° S (corresponding to 398.095 km east and 6355.935 km north in the Australian Map Grid (AMG) coordinate system). The sonde flights were undertaken in the early morning and late morning using Vaisala RS80 Radiosondes and the signal was received by a DigiCORA III radio sounding system (Pitts, 2004). The sonde ascent rate was generally 5 m s^{-1} with data recorded every two seconds. The sonde recorded air pressure, dry bulb temperature and the relative humidity. These measurements were then used to calculate the dew point temperature and the geo-potential height. Wind speed and wind direction were determined using the GPS-obtained position of the sonde. Table 5 gives the sonde release dates, launch times and the corresponding weather conditions.

Table 5: Radiosonde releases undertaken in 2003 at Wagerup (Pitts, 2004)

Date	Sonde release time (WST)	Weather conditions
11 June	1152	A weak cold front south of WA, light south-westerly synoptic flow, clear skies. A test day.
13 July	0801	An approaching cold front west to WA, strengthening north-westerly synoptic flow, clear skies.
19 July	0727and 1006	An approaching weak cold front, weak north to north-westerly synoptic flow, clear skies.
29 July	0738 and 1006	A high to the east of WA and an approaching cold front to the west, moderate to strong north, north-easterly flow, cloud increasing throughout the morning.

11 June was a test day. We use data from 13 June, and 19 and 29 July for comparison with the meteorological modelling results in Section 6.9.

6. Comparison of model results with observed meteorological data

6.1. Model runs done

For the meteorological modelling reported in this document, TAPM was run for one year from April 2003–March 2004 in three configurations:

- TAPM with the default database for land-use characteristics,
- TAPM with the derived Wagerup-specific land-use data base, and
- TAPM with the derived Wagerup-specific land-use data base together with a refinery-generated surface heat flux of 150 W m^{-2}.

The model results used for evaluation in this report are all from the last model configuration, except in Section 6.3 where some results from the default (first) and last configurations are compared.

The hourly-averaged model meteorological predictions on the innermost grid domain were extracted at the grid point nearest to each of the monitoring sites (Bancell Road, RDA and sonde site) for comparison with the data.

6.2. Comparison method used

Two types of graphical comparison, scatter plots and frequency of occurrence, are used to compare the model results with the observations. A scatter plot is useful for visually inspecting the relationship between model results and measurements paired in space and/or time. Least-squares fits can be superimposed on scatter plots to examine mean trends. In a probability distribution function (pdf) plot of a meteorological variable, the normalised frequency of occurrence of a variable value is plotted against the value itself. The values of a given meteorological variable were binned and the number of values in a particular bin were normalised by the total number of values to obtain the probability. The bin size for a given variable was constant and is equal to the separation between two successive points.

In order to quantitatively measure model performance, it is desirable to calculate a set of statistical measures that enable comparison between observations and model predictions. These calculated statistics can then be compared with those obtained from other studies in order to decide whether the present results are satisfactory or not. The following statistical measures are used here for model evaluation (Willmott, 1981; Pielke, 1984):

- Predicted mean $P_{mean} = \frac{1}{N}\sum_{i=1}^{N} P_i$, where P_i are the predictions.
- Observed mean $O_{mean} = \frac{1}{N}\sum_{i=1}^{N} O_i$, where O_i are the observations.
- Predicted standard deviation $P_{std} = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}\left(P_i - P_{mean}\right)^2}$.

- Observed standard deviation $O_{std} = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}\left(O_i - O_{mean}\right)^2}$.

- Correlation coefficient $r = \frac{\sum_{i=1}^{N}(O_i - O_{mean})(P_i - P_{mean})}{\sqrt{\sum_{i=1}^{N}(O_i - O_{mean})^2}\ \sqrt{\sum_{i=1}^{N}(P_i - P_{mean})^2}}$.

- Root Mean Square Error $RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(P_i - O_i\right)^2}$.

- Systematic Root Mean Square Error $RMSE_S = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\hat{P}_i - O_i\right)^2}$.

- Unsystematic Root Mean Square Error $RMSE_U = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\hat{P}_i - P_i\right)^2}$.

- Index of Agreement $IOA = 1 - \frac{\sum_{i=1}^{N}\left(P_i - O_i\right)^2}{\sum_{i=1}^{N}\left(\left|P_i - O_{mean}\right| + \left|O_i - O_{mean}\right|\right)^2}$.

Note that N is the number of observations and $\hat{P}_i = a + bO_i$ is the linear regression fitted formula with intercept (a) and slope (b).

The Root Mean Square Error (RMSE) is a measure of the actual size of the error produced by the model, and is also called the standard error of estimate. Low RMSE values for a model indicate that the model is explaining most of the variation in the observations. Ideally, in a model lacking bias, $RMSE_S$ should approach zero, and consequently $RMSE_U$ should be close to RMSE. Practically, for a good model, the unsystematic portion of the RMSE should be larger than the systematic one. The $RMSE_S$ assesses whether the model errors are predictable, whereas the $RMSE_U$ identifies those errors that are not predictable mathematically.

The correlation coefficient (r) describes the proportionality changes with respect to the means of two quantities. The Index of Agreement (IOA) is a measure of the degree to which the observed variable is accurately estimated by the model variable. Unlike correlation coefficient, IOA is sensitive to differences between the observed and model means, as well as to certain changes in proportionality, and is a more consistent measure of performance than the correlation coefficient. An IOA value of 0 means no agreement where as a value of 1 means perfect agreement.

A model is predicting with skill if the standard deviations of the predictions and observations are approximately the same, and RMSE is less than the standard deviation of the observations.

The predicted hourly-averaged meteorological variables and the corresponding observed data were paired in space and time in calculating the evaluation statistics.

In the subsequent analysis, we cannot use the wind direction values directly for calculating evaluation statistics due to the discontinuity at north, and therefore, the wind components (*U, V*) are used instead. A positive *V* indicates a southerly wind component, whereas a negative *V* indicates a northerly wind component. Similarly, a positive *U* indicates a westerly wind component, whereas a negative *U* indicates an easterly wind component.

6.3. Comparison of model performance with different land-use and Refinery heat-flux configurations

In this Section, some results from the default (first) and last model configurations are compared. The objective here is to examine any differences in the model results caused by the use of the derived Wagerup-specific land use coupled with the added surface heat flux generated by the refinery in TAPM, and present the extent and importance of these differences. The largest differences are expected to occur in the nighttime when the surface heat fluxes are small. For comparison, we select the winter months June–August 2003 when the northerly winds are more frequent than at other times. Under such winds, the air over the Refinery is directly advected to the Bancell Road monitoring site so that there is a maximum potential for the local Refinery land use (and the associated heat flux) to affect the measurements. The measured meteorological parameters that are likely to be influenced by the local surface characteristics more than others are temperature and relative humidity close to the ground.

Figure 9a and Figure 9b present scatter plots of the observed data vs. model predictions of temperature at 10 m AGL for Bancell Road obtained using the default model land use and the Wagerup-specific model land use (with added heat flux), respectively, for nighttime (2000–0700 h). Figure 9c and Figure 9d are the corresponding plots for relative humidity obtained at a height of about 1 m AGL. The differences between Figure 9a and Figure 9b are not large but it is clear that the use of the Wagerup-specific land use in the model does improve the temperature predictions compared with the data. The value of the correlation coefficient increases from 0.68 to 0.73 and that of the slope of the least-squares linear fit from 0.51 to 0.58. The model predictions of relative humidity also improve by a similar magnitude when the new land use is used in TAPM (see Figure 9). A more complete comparison of the model results with the data is made in the following Sections.

In order to test the sensitivity of the meteorological variables to the amount of refinery-generated surface heat flux, two additional model simulations were made for the winter month of August 2003 with the refinery-generated heat flux values of 120 and 185 W m^{-2}. It was found that the modelled meteorological predictions (i.e. winds, temperature and relative humidity) at Bancell Road were virtually insensitive to the value of the refinery-generated heat flux within the range 120–185 W m^{-2}. Meteorological predictions calculated over the Refinery surface also showed insensitivity to the refinery-generated heat flux value. Some of the variables directly affecting pollution dilution, such as the mixing height and convective velocity, that were calculated at locations within the Refinery showed some variation with the refinery-generated heat flux value. For example, the minimum nighttime mixing height over the Refinery typically increased by 10–20% within the heat flux range 120–185 W m^{-2} (the daytime sensitivity of the mixing height was negligible).

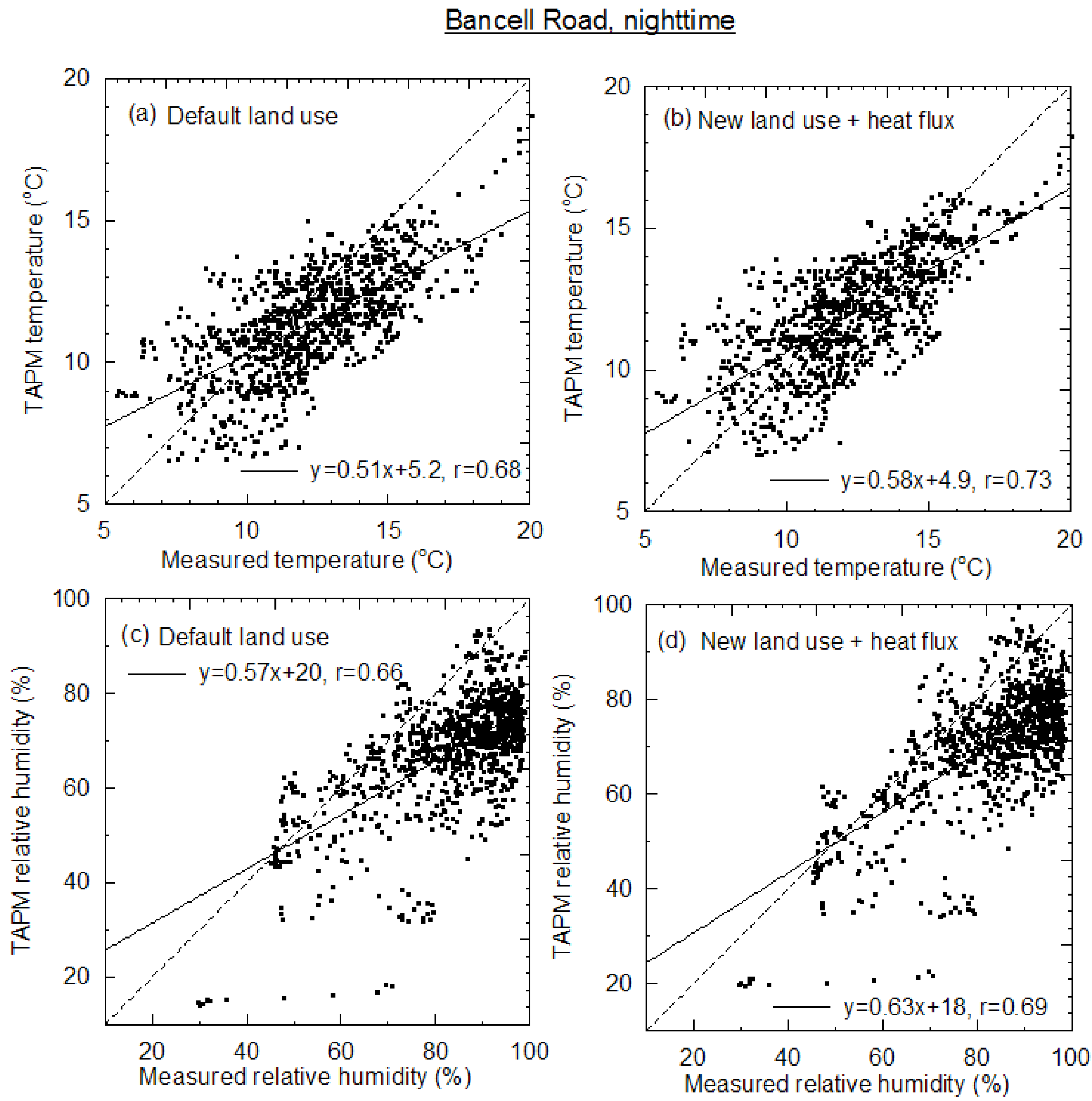

Figure 9: Scatter plots of the observed data vs. model predictions for Bancell Road obtained using the default model land use and the Wagerup-specific model land use for nighttime (2000–0700 h). Plots (a) and (b) are for temperature, whereas (c) and (d) are for relative humidity. The temperature values are at 10 m AGL and the relative humidity values at 1 m AGL.

The Refinery area is small compared to distances of interest for meteorological and dispersion calculations. The atmospheric influence of the Refinery surface properties diminishes with distance from the Refinery and/or as the altitude increases. Although a meteorological site may be directly downwind of the Refinery, it is possible that the sensor does not fully sample the Refinery surface properties because of the advection of air to the sensor from the surfaces upwind and downwind of the Refinery. The maximum influence of the Refinery surface characteristics would generally be on the properties of air just above that surface. This implies that the influence of the Refinery surface may be more identifiable in the diffusion of low-level plumes as they are emitted from within the Refinery than in the meteorological observations at Bancell Road. The enhanced Refinery-generated heat flux will change the atmospheric stability of the air passing above the Refinery surface from stable towards neutral and increase the mixing height (as mentioned above) in the nighttime, generating a higher vertical turbulence intensity, thus causing a higher initial dispersion of plumes emitted from the Refinery. This higher initial dispersion may affect concentrations outside the Refinery domain. In Phase 2, we plan to investigate the influence of the refinery generated heat flux via a comparison of observed ambient concentrations of NO_x with the model calculated concentrations.

6.4. Model evaluation with the Wagerup-specific land-use and Refinery heat-flux configuration – Bancell Road (30 m)

All the model results presented hereafter were obtained using TAPM with the derived Wagerup-specific land-use data base together with a refinery-generated surface heat flux of 150 W m^{-2}. Wind speed, wind direction and temperature modelled at a height of 25 m were used to compare with the corresponding observations at 30 m. The net radiation (R_n) observations at 1.5 m AGL were used to compare the model results at screen level (1.5 m AGL). Note that the R_n measurements and meteorological observations at 30 m at Wagerup commenced in the middle of July 2003. The Alcoa-supplied hourly-averaged winds at Bancell Road were compared with the hourly averages determined from the Alcoa-supplied 6-minute data, and no significant differences were found between the two datasets. (This comparison could not be done for the RDA meteorological site as there were no 6-minute data available.)

6.4.1 All data

Figure 10 shows scatter plots of model predictions vs. observed data for wind speed, wind direction, temperature, net radiation, and relative humidity at Bancell Road. The net radiation and relative humidity are measured at about 1 m AGL. For wind speed, the value of the correlation coefficient is 0.51, and Figure 10a shows that the model is biased towards predicting stronger winds than observed (this will be discussed later). Wind direction is generally predicted well, except for a few points for which the model is predicting an easterly flow while the observations are more variable and are from between southerly and westerly directions. The temperature observations are predicted very well by TAPM with a correlation coefficient of 0.95. In Figure 10e, the relative humidity comparison has a correlation coefficient of 0.82.

In Figure 10d for net radiation, the model gives a correlation coefficient of 0.93, but the model overestimates some of the high values of the observed net radiation. A photograph of the net radiation measurement site given in the SKM (2003) report suggests the net radiometer has been placed over a small area (roughly 1 m × 1.5 m) with woodchips and bark, which in turn is surrounded by an area with bare sand. This surface is not truly representative of the natural surface of the area. Also, there may be a lack of routine calibration and the maintenance procedures for the radiometer affecting the measurements. A maintenance check in August 2004 reported clarity problems with lenses that would cause lower values of net radiation than actual values (O. Pitts, 31 July 2004, comments on the CSIRO's Phase 1: Meteorology draft report). It is also possible that TAPM may be underestimating the number of cloudy/foggy days, and therefore, overestimating the net radiation. Additionally, the inputs (e.g. albedo and emissivity) used in the surface radiation budget in TAPM are based on average surface conditions, and may not match the surface properties under a net radiometer.

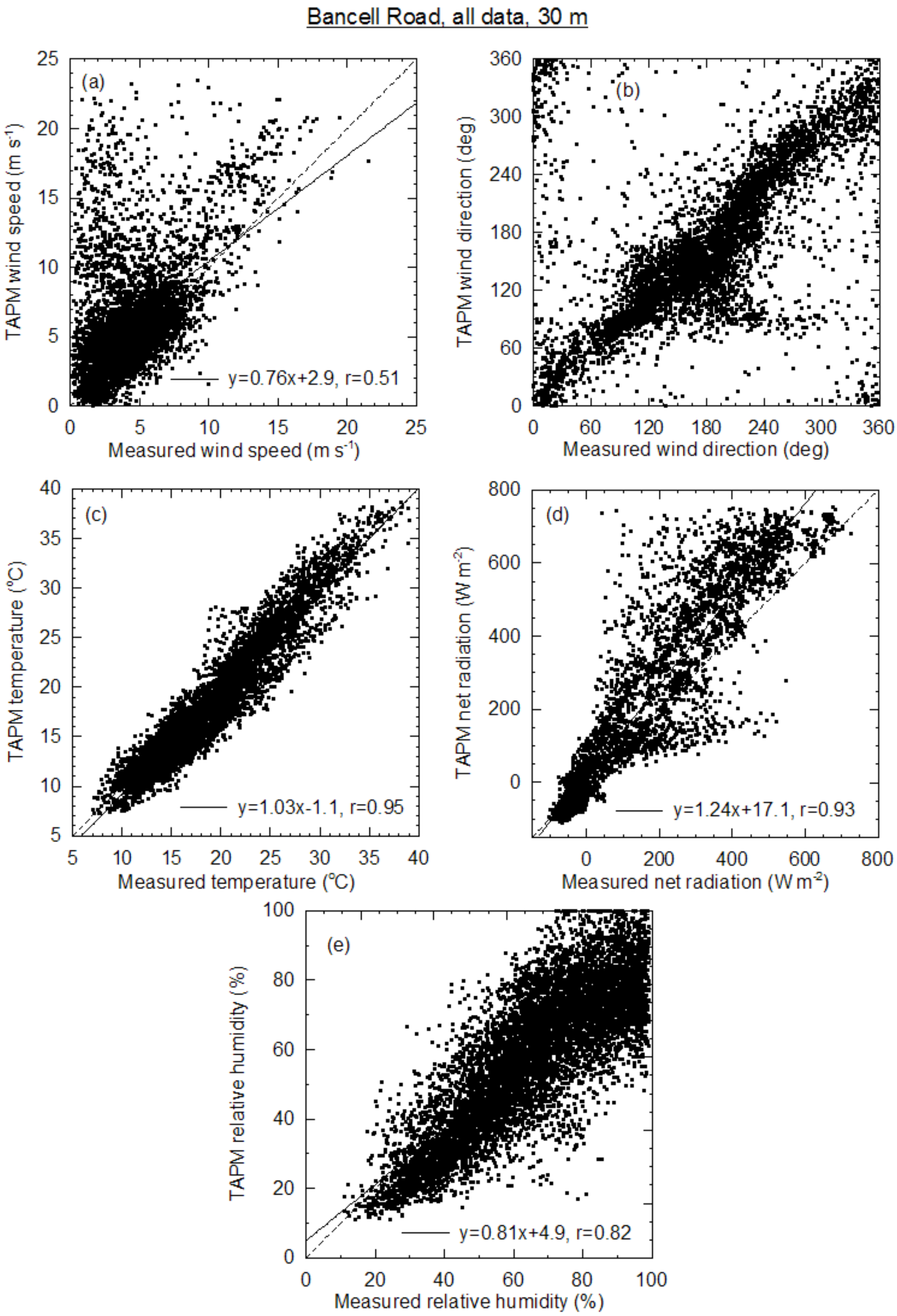

Figure 10: Scatter plots of model predictions vs. observed data for (a) wind speed, (b) wind direction, (c) temperature, (d) net radiation, and (e) relative humidity at Bancell Road. The net radiation and relative humidity are measured at about 1 m AGL, while the other parameters are measured at 30 m AGL.

Figure 11 presents the variation of wind speed with wind direction at 30 m AGL at Bancell Road based on (a) observed data and (b) model predictions. The observational data and the model predictions agree with regard to the fact that the strongest winds are from the east (which mostly occur under nighttime conditions), but the model easterlies are stronger and seem to be more frequent than the observations. There could be sources of error in the model and input used (e.g. terrain resolution). The synoptic analyses are a critical input to the model, and there are possibilities of differences/errors there.

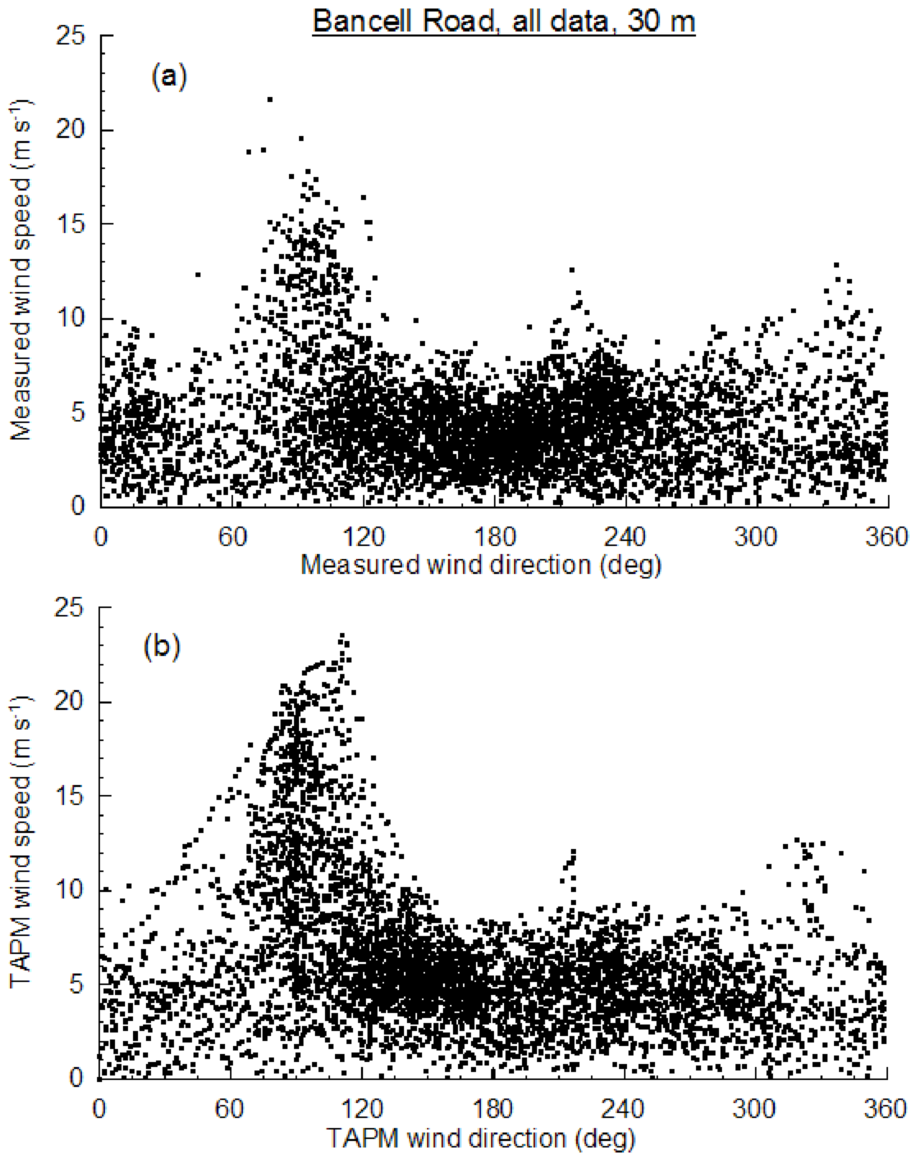

Figure 11: Variation of wind speed with wind direction at 30 m AGL at Bancell Road: (a) observations and (b) model predictions.