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Preliminary Testing of an Urban Air Quality Model for Ozone Forecasting over the Sydney Basin

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FThe aim of this study was to carry out a preliminary test of the air quality modelling system (HIRES-AIRCHEM) developed at The University of New South Wales, particularly with regard to the forecast ozone distribution. This was achieved by assimilating the New South Wales State Environment Protection Authority (EPA) emissions inventory, consisting of road and non-road sources, and running the system over the Sydney metropolitan area for the four day period 25-28 February 1998. During this period ozone readings exceeded the EPA's goal of 8pphm on several occasions. The model forecasts of ozone distribution verified well with the EPA's ozone readings. This result has important implications for possible future use of the system as a tool for routinely predicting and assessing air quality.

Key Words : Drainge flow, Sea breeze, Ozone

1. Introduction

Sydney is affected episodically by high ozone levels. Drainage flows and sea breezes are regular meteorological features of the Sydney basin (see location map Fig. 1). When combined with emissions from motor vehicles and a high number of daily average sunshine hours during the warm season, the Sydney basin is an area prone to photochemical smog. A typical synoptic pattern representing light morning offshore drainage flows followed by afternoon sea-breezes is shown in Figure 2. Ozone, in particular, is a very important photochemically produced pollutant. The authors have previously reported on the results of a modeling study of ozone over the Sydney basin[2]. In that study an Environment Protection Authority (EPA) ozone analysis was assimilated into the initial state of the high resolution NWP model (HIRES) developed by one of the authors (LML) and coupled to an air chemistry model (AIRCHEM) which includes reactions due to photochemical processes.

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The results, showing the ozone distribution over the metropolitan area after five days, were encouraging. However, a more stringent test of the air quality modelling system was needed, covering a longer

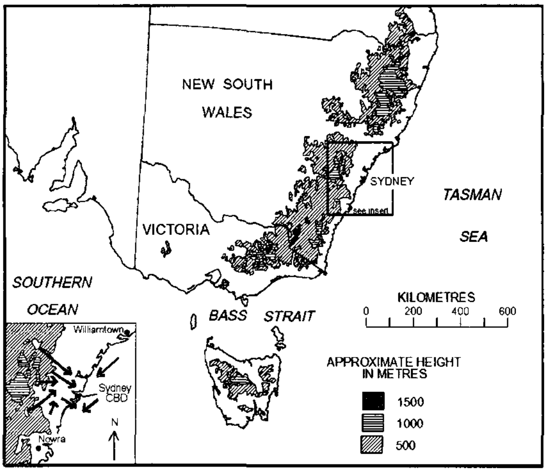


Fig. 1. Location map of southeastern Australia including topographical contours. In the inset the arrows indicate the drainage flows (NW to SW) over the Sydney basin and the sea-breeze direction (NE).

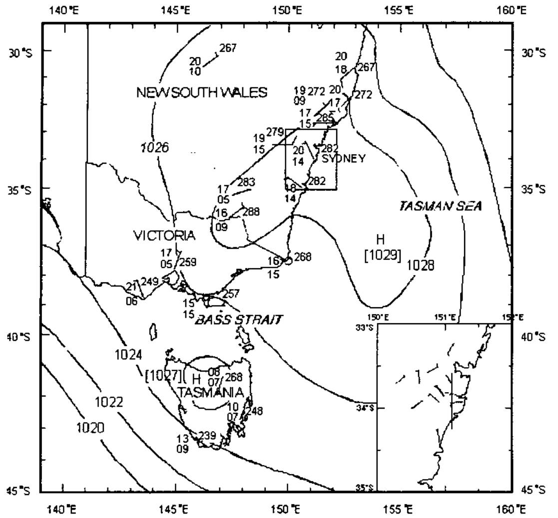


Fig. 2. A typical synoptic SLP pattern with high pressure centred off the coast representative of pollution episodes. The small wind barbs in the inset indicate light morning drainage flows. The large wind barb indicates a light northerly (10 km/h) at approximately 900 m above the surface.

period and including the production of ozone from all sources (e.g. industrial, motor vehicle traffic). In other modelling studies not involving the air chemistry component but rather the model capability of predicting the inter-regional and local transport of smoke particulates from bushfire sources into metropolitan areas, the results verified well with observations[2,3].

During the 1997/98 warm season (October to March inclusive), ozone levels approached or exceeded the New South Wales Environment Protection Authority's long term reporting goal of 8 pphm for a 1-hour average on a total of 38 days. In this study the authors report on the results of a modelling study of ozone over the Sydney metropolitan area covering the four day period, 25-28 February 1998.

2. Model and data

The air chemistry model, known as AIRCHEM, has a set of advection (transport), diffusion, deposition and chemical reaction components. Details of the advection component are discussed later in this Section. The diffusion scheme used most in AIRCHEM is a standard, variable coefficient, three-dimensional diffusion equation. The modelling of wet and dry deposition processes is represented by a linear mode with the wet and dry deposition coefficients being functions of the chemical species and of spatial location and time. The chemical scheme contains 100 species with all types of chemical and photochemical reactions possible.

AIRCHEM is coupled to an atmospheric model, known as HIRES. HIRES-AIRCHEM has a full atmospheric dispersion model comprising input fields, output fields and additional modules for diffusion, wet and dry deposition and chemical reactions (Fig. 3). The particle dispersion model is a standard Lagrangian stochastic dispersion model based on the Ito-type stochastic differential equation, and well- mixed theory. HIRES-AIRCHEM can be applied either to analysis of air quality problems that require a diagnostic capacity, or as a predictive scheme that allows forecasts out to hours or days in advance.

AIRCHEM was initialized and verified with maximum 24-hour averaged daily ozone data at sites indicated in Figure 4 from the archives of the NSW EPA. Also, an EPA emissions inventory of industrial and vehicular pollution sources was assimilated at hourly intervals. The emissions data contains surface emissions analyzed onto a 3 km $\times$ 3 km grid and elevated point source emissions for 19 chemical species. The 19 chemical species are:-

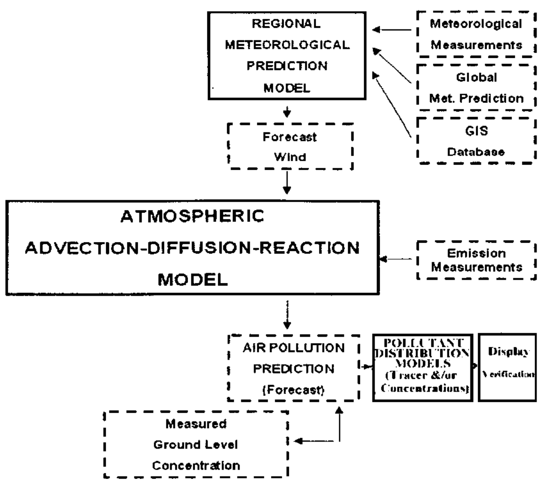


Fig. 3. Schematic of the HIRES-AIRCHEM prediction system and the forecast wind input into the atmospheric advection-diffusion-chemical reaction model.

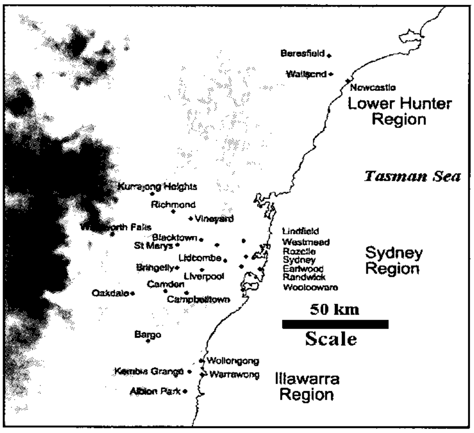


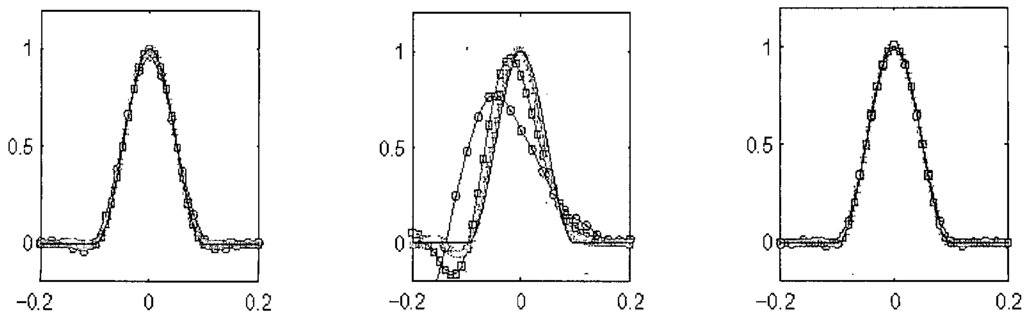
Fig. 4. Locations of the New South Wales EPA ozone measuring sites in the Newcastle, Sydney and Wollongong regions.

Nitric oxide (NO)
Nitrogen dioxide (NO2)
Carbon monoxide
Particulate matter (used as tracer, not part of the chemistry)
Ethene
Alkenes (lumped ROC grouping)
Alkanes (lumped ROC grouping)
Toluene (including monoalkyl benzenes)
Aromatic species (lumped ROC grouping including di- and tri-alkyl benzenes)
Formaldehyde
Higher aldehydes (lumped ROC grouping)
Ketones
Methanol
Ethanol
Isoprene
Cineol
Pinene
Total reactive organic compounds (diagnostic only)

HIRES was initialized with the boundary and initial conditions provided from the Australian Bureau of Meteorology's Australian Region LAPS model. HIRES is based on diabatic nonlinear dynamical initialization in order to control the generation of spurious gravity waves and to minimize spin-up problems, and is then passed on to the prediction component of HIRES. This component has a range of options but in the present application it is a non-hydrostatic, primitive equation model that uses the energy conserving form of the primitive equations for momentum, mass, moisture, and thermal energy.

The time-stepping scheme is a split semi-implicit time-differencing scheme. Advective spatial differencing is fifth order on the advective terms (Fig. 5a). Fifth order is optimal as it is a significant improvement on lower order difference schemes such as the widely used second order centred scheme (see Fig. 5b). The desired physical mode (the solution we actually want) is most clearly seen as the single black line in Figure 5(b). Furthermore, there are diminishing returns for higher than fifth order schemes such as 9th order upwind (see Fig. 5c). Finally, the fifth order upwind scheme is corrected slightly, to be made positive-definite using a standard interpolation technique. By using energy-conserving spatial differencing, computational stability is achieved for the advection terms. The pressure gradient term is discretized using fourth order differencing.

All available high resolution data including radar



(a) 5th order upwind (b) 2nd order centred (c) 9th order upwind

Fig. 5. A split semi-implicit time-differencing upwind scheme.

derived winds and satellite derived winds and sea surface temperatures, which are important for accurate sea-breeze depiction, have been assimilated over a 6 hour period prior to each 24 hour forecast. A triple nesting procedure was employed that initially interpolated the LAPS fields onto the HIRES domain covering the Australian region and surrounding oceans from which the forecasts at 15 km horizontal were generated. The forecasts were then successively nested onto 5 km and 1 km domains, finally producing forecasts over the area of concern (Fig. 6). The vertical turbulent exchanges in the boundary layer are parameterized using the Louis scheme. A summary of the HIRES model details is shown in Table 1.

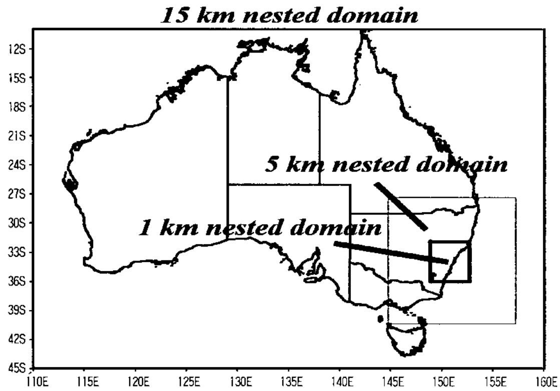


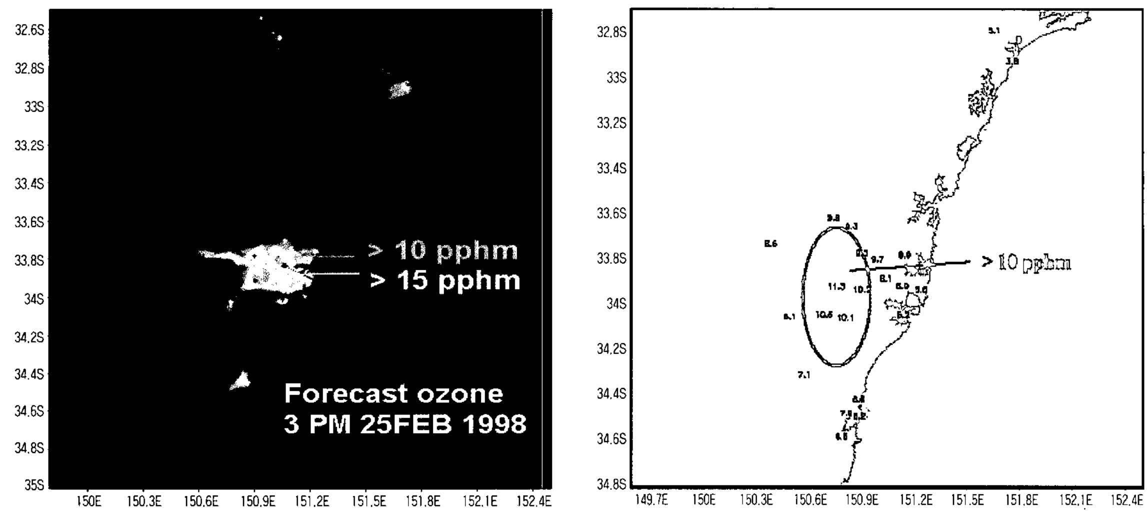
Fig. 6. Map showing the 3 nested grid domains.

Table 1. Details of the model HIRES

Model feature	HIRES
Horizontal resolution	15, 5 and 1 km
Numerical scheme	Split semi-implicit (5th order advection)
No. of vertical levels	40
Assimilation scheme	6-h cycling
Initialization	Dynamic
Orography	2 minute resolution
Boundary layer scheme	Mellor-Yamada, level 2.25
Radiation scheme	Fels-Schwarzkopf
Convective scheme	Louis
Sea surface temperatures	5-day average
Lateral boundary conditions	From BMRC LAPS model

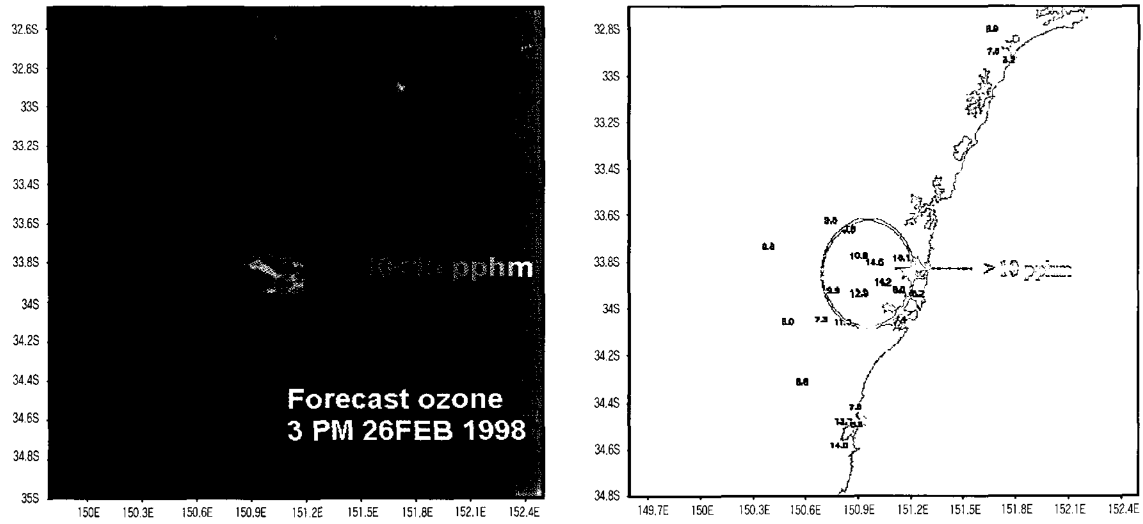
3. Results

There is generally good agreement between the patterns of ozone concentration produced from the model results and those based on the values at the NSW EPA monitoring sites covering the Sydney metropolitan area. Figure 7(a), 7(b), 8(a) and 8(b) show the ozone distribution across the Sydney metropolitan area for the four day period 25-28 February 1998. During this period ozone readings exceeded the EPA's goal of 80ppb on several occasions. The model forecasts of ozone distribution verified well with the EPA's ozone readings. into the model forecast. Verification is provided by the values on the map, representing observed ozone readings.



(a) (b)

Fig. 7. (a) HIRES-AIRCHEM model forecast (+18 hr) ozone distribution (pphm) for 3 pm 25 February, 1998. (b) Maximum ozone values recorded by the New South Wales EPA for 25 February, 1998.



(a) (b)

Fig. 8. (a) HIRES-AIRCHEM model forecast (+42 hr) ozone distribution (pphm) for 3 pm 26 February, 1998. (b) Maximum ozone values recorded by the New South Wales EPA for 26 February, 1998.

4. Conclusions

These results are encouraging, particularly as the four day period covered by this study contained observed ozone values that exceeded local environmental goals for peak concentrations. This modelling example provides a stringent test of the HIRES-AIRCHEM modelling system. More results are shown at the meeting including forecasts without the assimilation of EPA sources that, as expected, are poor when compared to observed values. These results have important implications for possible future use of the system as a tool for routinely assessing air quality in the Sydney basin. While the results of this study represent an extensive test of the air quality modelling system, the authors intend to continue experimenting with improved emissions inventories as they become available on more recent episodes of high ozone concentration.

Acknowledgements

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