

A dispersion modelling analysis of tropospheric ozone potential for Canterbury

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A technical report prepared for Environment
Canterbury by

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This report outlines the methodology for preparation of a spatial map of *tropospheric* (i.e. near ground level) ozone concentrations in the Canterbury Region. The map is constructed from the calculations made over a period of 3.5 months in the summer 1998 by The Air Pollution Model (TAPM). The only source of emission considered in this work is the city of Christchurch.

Note: Concentrations are reported in mixing ratio units of parts-per-billion (ppb). With this unit, alert category (66% - 100% of the guideline value of the National ambient air quality, Ministry for the Environment, 2002) is reached at 47 ppb (1 hour-average), and action category is above 70 ppb (1 hour-average).

The objectives of this report are:

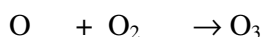
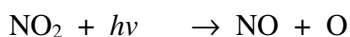
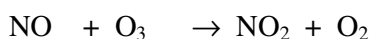
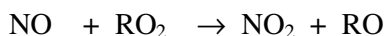
- To perform a cursory analysis of measured concentration of ozone and its precursor gases (NO_x) for the limited summer time periods when ozone was measured by Environment Canterbury.
- To use the estimates of emission of precursor molecules in simulating the formation of ozone and its dispersion with TAPM.
- To provide a map of ozone concentration indicating where the highest values are likely to occur in order to assist site selection for monitoring purpose.

1. Introduction

Elevated ground-level ozone (O₃) can be caused by photochemical reactions (reactions induced by sunlight) of precursor gases (i.e. primary pollutants). This type of pollution is commonly referred to as photochemical smog. Photochemical smog has been observed in many urban areas around the world and continues to be a serious problem in many megacities.

Photochemical reactions are not the only way ozone can be present close to the ground. Strong downdrafts due to thunderstorm activity and long range transport are two of many reasons that can also cause elevated levels.

Photochemical smog involves gas phase reactions between nitrogen oxides (NO_x = NO + NO₂) and reactive organic gases (ROGs, defined as total organic gases minus methane). In this report, the term ROG and VOC (Volatile Organic Compounds) will be used interchangeably. Ozone in photochemical smog forms by the following reactions.



Where (all chemical species are in gas phase):

NO = nitric oxide

NO₂ = nitrogen dioxide

RO₂ = organic peroxy radical

RO = organic oxy radical

O₂ = molecular oxygen

O = atomic oxygen

hν = photon of light

Other gases that are emitted into the urban atmosphere include carbon monoxide (CO), and sulfur oxides (SO_X = SO₂ + SO₃), yet, NO_X and ROG are the main precursors ozone in photochemical smog.

2. Previous work in Canterbury

Previous investigations of ozone in urban areas of New Zealand have mostly focused on its largest city, Auckland. However, there is some information available for Christchurch and its environs. Farkas (1978) monitored ozone at four locations from January to April of 1978 where he recorded a maximum (5-minute average) elevated concentration of 82 ppb at Kainga (Figure 1). In 1997 ozone concentrations were measured during February at Lincoln University; 5-minute average values ranged from 18 ppb to 38 ppb (Stephen 1997). Environment Canterbury has also initiated temporary monitoring sites; first time in the summer of 1998 and then in the summer of 2002–2003. Monitoring sites were chosen down wind of Christchurch, at Lincoln to the south west and Kainga to the north according to the recommendation of McKendry (1996). Analysis by McKendry (1996) was conducted purely from a meteorological standpoint – by finding the number of days where the meteorology over the region could lead to elevated ozone levels, which is mainly a combination of low wind speed and high ambient temperature. It should be noted that ozone is not considered a problem pollutant at the moment. However, population growth and increased emissions can alter this notion.

3. Analysis of measurements at Lincoln and Kainga

In this section a cursory examination of Environment Canterbury datasets is performed. In 1998 monitoring was carried out at sites in Lincoln and Kainga from January to April. In 2002/2003 monitoring was carried out in Lincoln only from December to March.

Indicators of photochemical reactions are a morning peak in precursors, an afternoon peak in ozone measured downwind of the precursor source area, when the combination of low wind speed and high temperatures have allowed these reactions to occur.

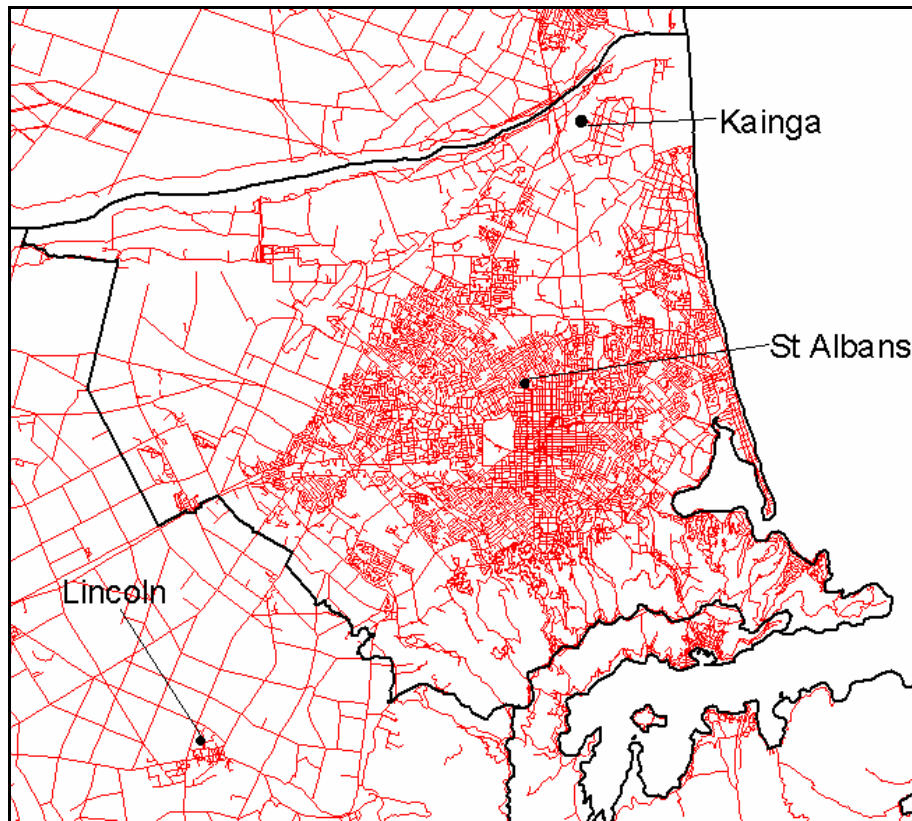


Figure 1: Map of the Christchurch region showing the location of monitoring sites.

Figure 2 illustrates the diurnal variation of ozone at Kainga and Lincoln. The time-series shows averaged values throughout the measurement period at each hour. Averaging by hour, *smooths* out daily variations in meteorology and emissions, allowing a simpler analysis of underlying causes. In addition, the range of measured values is also indicated at each hour. Both sites show a clear diurnal pattern for ozone, strongly suggesting a photochemical origin for its presence (Figure 2). Possibly due to scavenging by the surface, ozone concentrations decrease slowly after midnight until sunrise when there is a gradual increase in concentrations until a peak is reached *on average* at 25 ppb between 2 to 3 pm. This is also consistent with findings from other locations in the world where maximum ozone levels are recorded in the afternoon. From then on, concentrations gradually start decreasing as the sunset approaches and the sunlight intensity diminishes.

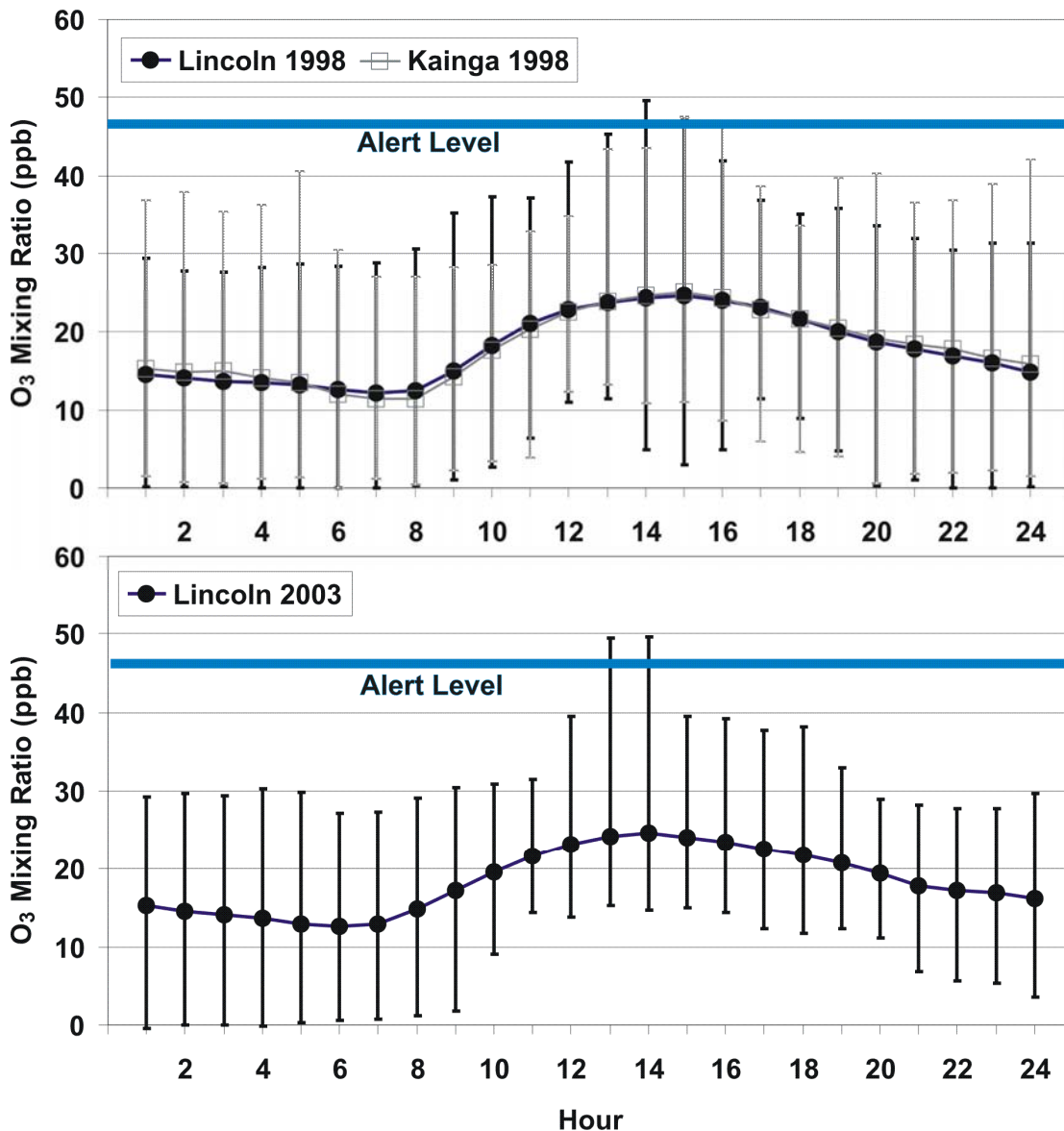


Figure 2: Time-series for ozone. The filled circle and square indicate the average value at that hour for the entire measuring period, while the lines show the range.

It is also interesting to see that minimum values closely trace the average. It has to be noted that in comparison with northern hemisphere locations, background ozone levels, as indicated by these minima, are much lower here.

Also suggestive of a photochemical origin of ozone is the diurnal pattern of one of the precursor species for ozone during the same summertime measurement periods. Figure 3 presents a time-series of the oxides of nitrogen (NO and NO_x) measured at Coles Place (St. Albans) and Packer Street (about a kilometer away). A clear maximum *average* value is evident early in the morning at both sites; however Packer Street values tend to be higher. Such a peak is probably due to emissions from motor vehicles and corresponds to the early morning rush hour. There is no peak for the evening rush hour since the instability of the atmosphere and the wind speeds tend to be higher over Christchurch during these summer months thereby flushing away the pollutants.

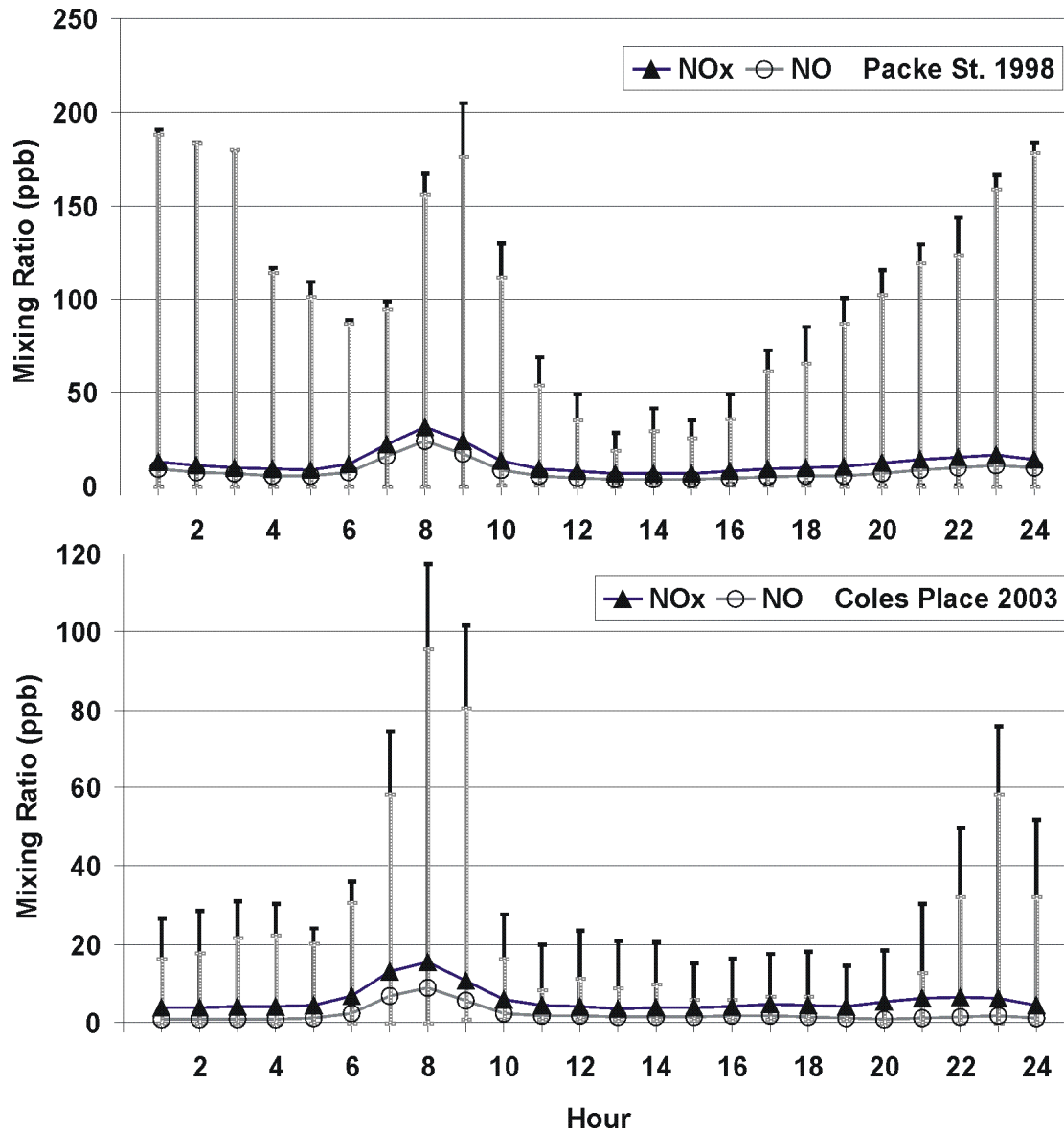


Figure 3: Time-series for oxides of nitrogen. The circle and the triangle indicate the average value at that hour for the entire measuring period, while the lines show the range.

4. Introduction to TAPM and modelling set-up

4.1. General comments

The Air Pollution Model (TAPM; Hurley, 2002) was used to simulate formation of ozone from the precursor species in Canterbury. TAPM has been extensively tested in different regions of the world including the Canterbury Region. The model has shown considerable skill at simulating meteorology and dispersion of air pollutants – given reasonably accurate emission inventory data is supplied (Zawar-Reza and Titov, 2005). TAPM can be used to

simulate meteorology and dispersion for either long-term (seasonal or yearly) or short-term (order of days).

The model is set up at a spatial resolution of 1.5 km (i.e. meteorology and dispersion is simulated every 1.5 km). To test the model's skill in predicting ozone concentration, analysis of a test case day is provided for 31 December 2002 in section 5, since on this day the model reasonably captures the observed meteorological conditions.

4.2. Emission scenario

Ozone formation in the troposphere is highly dependent on the concentration of precursor species such as NO_x and VOC. Emission estimates for NO_x for this work were derived from the Christchurch emission inventory for 2002 (Scott and Gunatilaka, 2004), and for VOC the 1999 inventory was used (Wilton 2001), as these were not reported in the 2002 inventory. Figure 4 shows the values used as input into TAPM. There are no emission estimates available outside of the urban area, therefore this aspect was neglected in these series of simulations. Emission estimates are for a typical winter's day for the city as a whole (i.e. there is no spatial heterogeneity in the emission field input into the dispersion model). The emission rates tend to be much higher during the daytime due to transport and industrial activity. Given these sources, estimates are not expected to be much different for a summer's day. The temporal resolution varies from 4 to 8 hours, and there is no distinction between weekday and weekend scenarios.

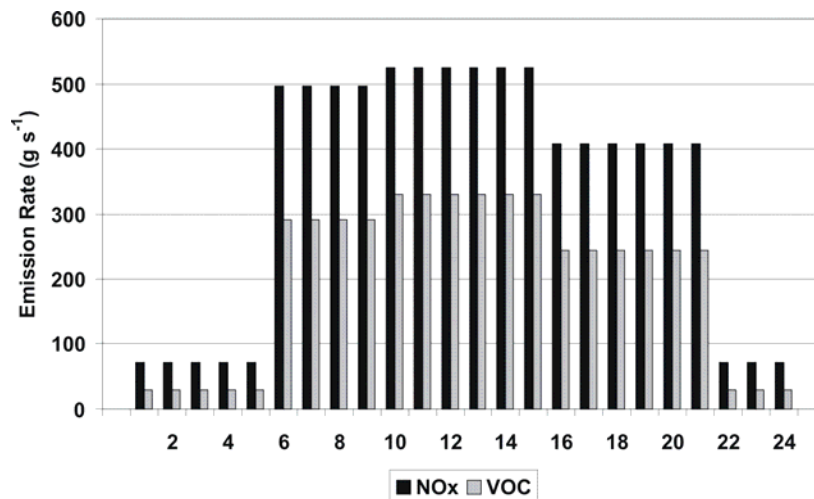


Figure 4: Emission rates for NO_x and Volatile Organic Compounds (VOC).

5. Modelling results

5.1. Assessment of model output

Figures 5 and 6 illustrate TAPM results of simulated meteorology for 30th and 31st of December 2002 compared to observations made at St. Albans and Lincoln monitoring stations (Figure 1). In the *modelling circles*, the first day of a simulation is usually ignored since the model is considered to be *adjusting* to the terrain. Therefore our analysis will focus on the 31st.

At the St. Albans station, a north-westerly wind is detected shortly before 6 am on the 31st, while TAPM predicts the initiation of this wind a few hours earlier at 10 pm the previous day. Yet the fact that both surface winds are north-easterly during the day – when ozone is forming – is encouraging. The light south-westerly ceases at 11 am at St. Albans and the model prediction is two hours behind. Since ambient temperature controls the rate of ozone formation, it is encouraging to see that TAPM predicts the maximum temperature well. Both model and the observations show that air temperature reached a maximum of 25°C.

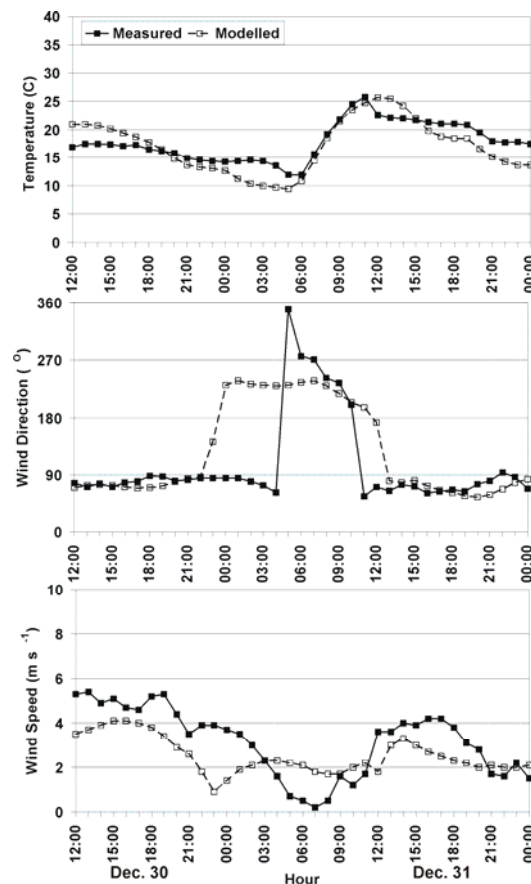


Figure 5: Measured and modeled meteorological variables at St. Albans for 30th and 31st of December 2002.

Figure 6 shows the modelled meteorological results for Lincoln site. Modelled maximum temperature is slightly under-predicted – by 2°C. Observations show that a southerly wind

is gradually replaced by north-easterly around 2 pm, while the model predicts this change abruptly two hours later.

Although TAPM is able to simulate the coarse features of the meteorology well, the results can be improved if the model is *forced* to reproduce observations. Such a technique is called data-assimilation, whereby measurement of wind speed and direction at Lincoln and St. Albans are ingested into TAPM, and TAPM adjusts the local wind field around these stations according to the measurement. This technique is experimental and its use is highly controversial. Its inclusion in this report in section 5.2 is to demonstrate the sensitivity of the ozone plume to local wind field condition/variation. Data-assimilated results should in no way be regarded as *better*, since there are also inherent errors in measurements (i.e. like disturbances caused by flow around houses which can contaminate observational data). The ozone map presented in the section 5.4 does not employ data-assimilation.

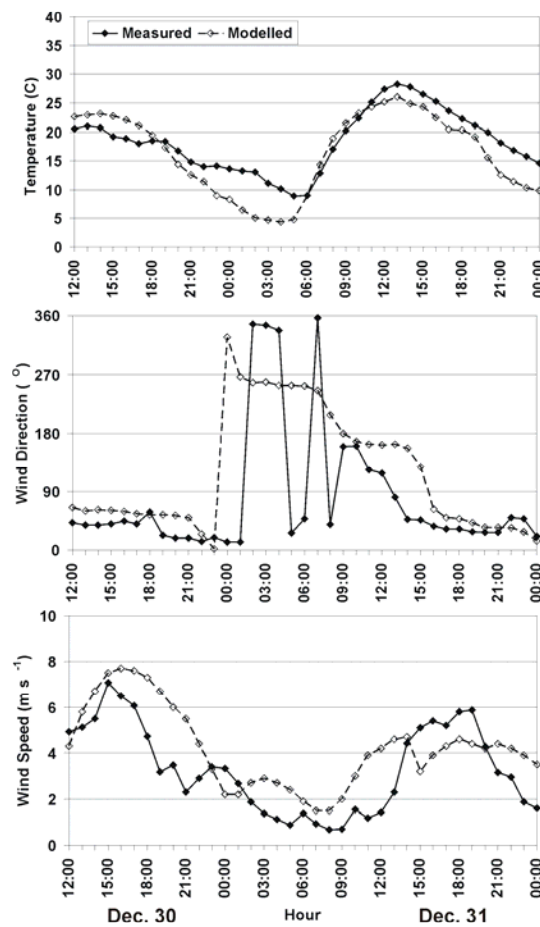


Figure 6: Measured and modeled meteorological variables at Lincoln for 30th and 31st of December 2002.

5.2. Simulated ozone plume behaviour

This section shows the evolution of spatial patterns of ozone plume for the same two day period for the normal and data-assimilated simulations.

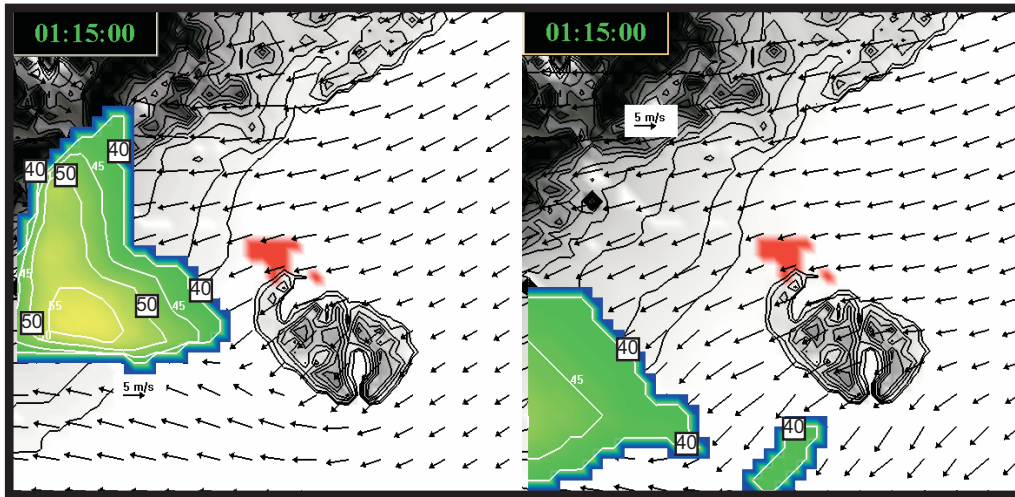


Figure 6: Modelled (left panel) and data-assimilated (right panel) simulations of the ozone plume for December 30 at 1500 NZST. Values shown indicate hour average ozone concentrations in parts-per-billion (ppb) with a contour interval of 5 ppb.

Since the air flow over Canterbury was predominantly north-easterly, the ozone plume is situated to the south-west of the city by 1500 NZST (3 pm). The simulation that is driven by observations shows that the plume has travelled further to the south – the peak values are outside of the window. Since the air flow has a more easterly component at the southern fringes in the modelled run, the ozone plume is situated closer to the Southern Alps.

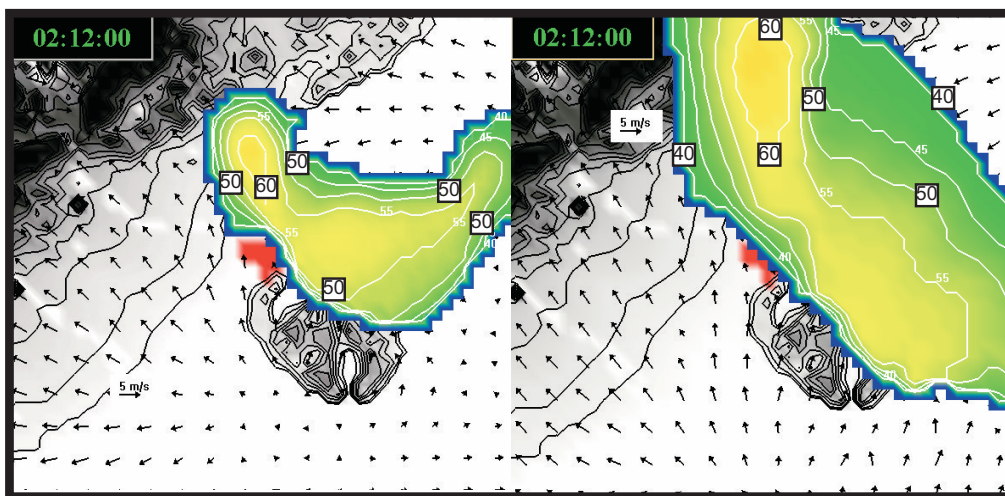


Figure 7: Modelled (left panel) and data-assimilated (right panel) simulations of the ozone plume for December 31 at 1200 NZST. Values shown indicate hour average ozone concentrations in parts-per-billion (ppb) with a contour interval of 5 ppb.

The next day, the ozone plume has formed to the north and east of the city since the precursor chemicals (primary pollutants) were transported to that region in the previous hours (Figure 7). There is a distinct ozone maximum at 60 ppb over land in both simulations. The winds at this time are becoming north-easterly, therefore the ozone plume is back-tracking towards Christchurch. Since ozone precursors also tend to destroy the molecule (scavenging); it is interesting to see that the plume is splitting into two as it is approaching the city – where the emissions occur (Figure 7).

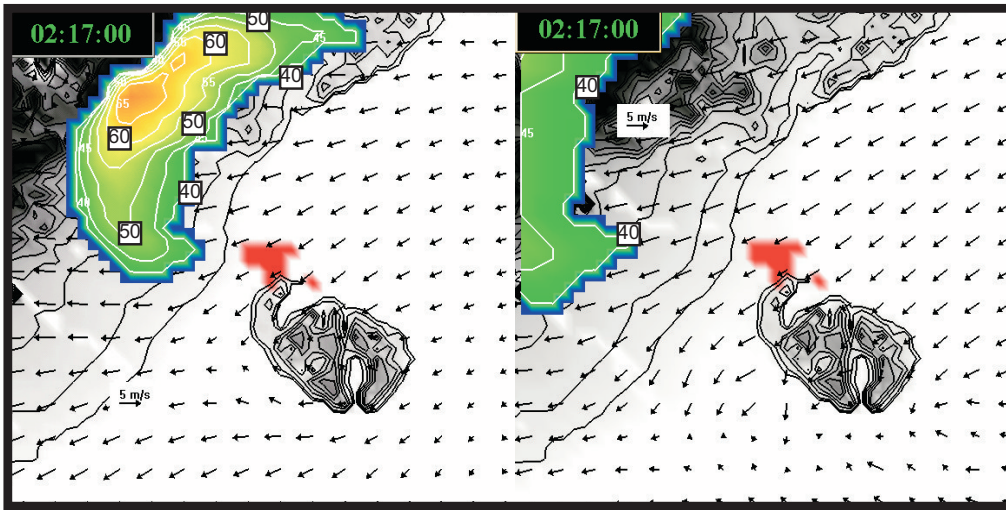


Figure 8: Modelled (left panel) and data-assimilated (right panel) simulations of the ozone plume for December 31 at 1700 NZST. Values shown indicate hour average ozone concentrations in parts-per-billion (ppb) with a contour interval of 5 ppb.

Five hours later, the ozone plume is situated at the fringes of the Southern Alps (Figure 8). Since the air flow is slightly higher with the data-assimilated run, the plume has penetrated further into the mountains.

5.3. Statistical analysis

To obtain more robust statistics for the models ability to simulate ozone concentration, a long-term simulation is also performed from 15th of January to 16th of April in 1998.

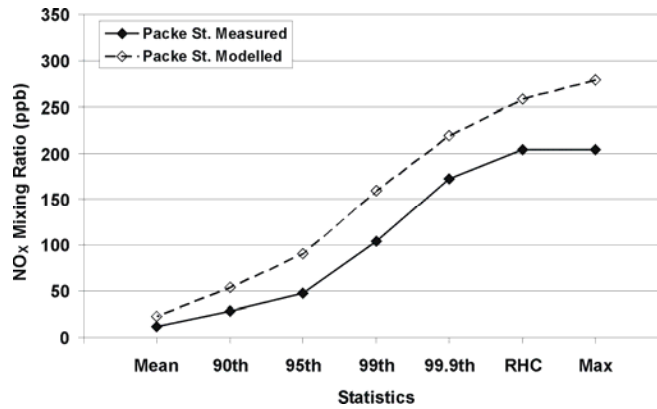


Figure 9: Statistics for measured and modeled concentration of NOx at Packe Street from 15th of January to 16th of April 1998. RHC is the Robust Highest Concentration according to Cox and Tikvart (1990); values for arithmetic mean, percentiles and maximum concentration are also provided.

Figure 9 shows statistics calculated for the entire period of simulation for NOx. The model tends to overestimate NOx concentrations. This is most likely the result of poor emission estimates. The mean is overestimated by 11 ppb, while the 90th percentile is overestimated by 25 ppb.

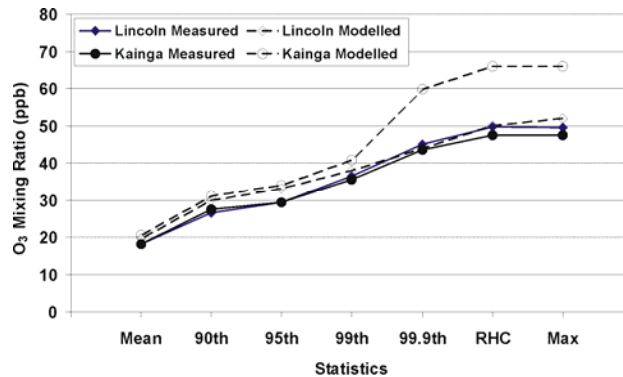


Figure 10: Statistics for measured and modeled concentration of ozone at Lincoln and Kainga from 15th of January to 16th of April 1998. RHC is the Robust Highest Concentration according to Cox and Tikvart (1990); values for arithmetic mean, percentiles and maximum concentration are also provided.

Given that NOx is overestimated, the ozone statistics shows a good skill by TAPM. There is still a tendency to overestimate ozone, yet the statistics are robust up to the 99th percentile range. TAPM tends to overestimate ozone at Kainga above 99th percentile.

5.4. Spatial map of ozone

Given that TAPM is able to estimate ozone formation with reasonable skill, a map of ozone levels near the ground can be made from the long-term runs with confidence. Figure 11 illustrates the spatial variability for 9th highest simulated ozone concentration that occurred during the 1998 summer modelled period. The dark blue circular area in the centre of the map (below 40 ppb) is the urban area of Christchurch; ozone doesn't reach elevated levels here since the precursor species destroy the molecule, therefore even if ozone rich air is advected over the city, ozone levels will drop. Areas to the west and south-west of the city are prone to alert levels of ozone (between 45 to 52 ppb), while areas to the east (over the sea), and the coastal areas of Waimakariri and Hurunui districts can experience elevated levels of ozone (55 to 60 ppb).

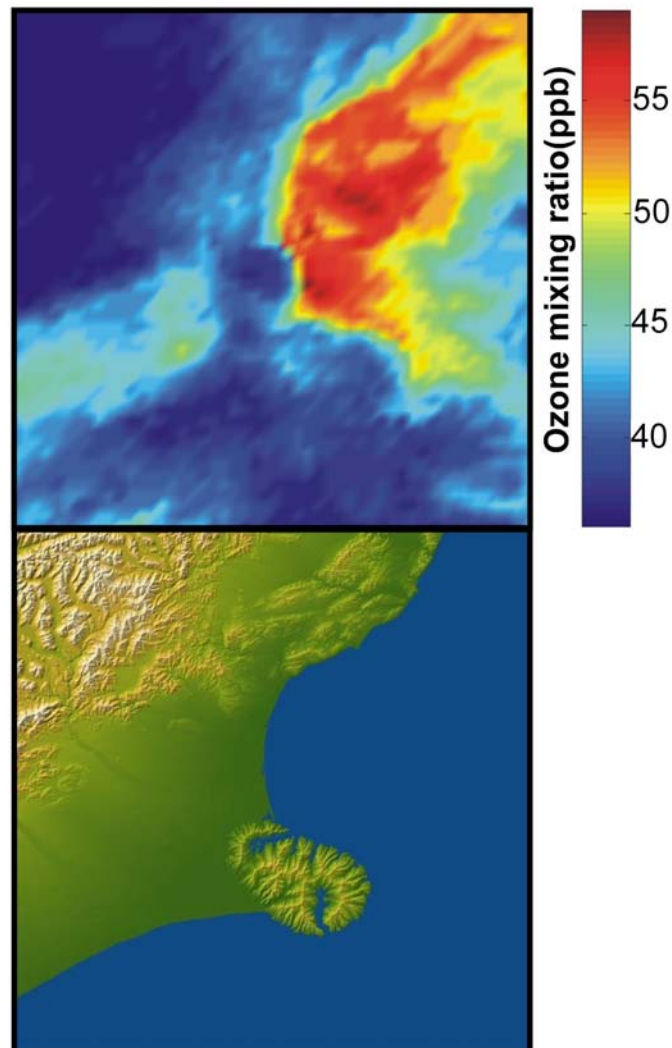


Figure 11: Map of the 9th highest hourly-averaged simulated concentration of ozone during 15 January to 16 April in 1998 (top panel). Topography of the modeled domain indicating the geographical extent of the simulation is shown in the bottom panel. [Note: alert category for ozone level is above 47 ppb].

6. Conclusion

With the aid of the dispersion model TAPM, a cursory analysis of summertime ozone concentration over the Canterbury Region is performed. TAPM shows a reasonable skill at simulating ozone variation measured at summer monitoring stations set up by Environment Canterbury at Kainga and Lincoln. The modelling study suggests that for monitoring purposes, monitoring stations should be based:

- Outside the urban area of Christchurch, since ozone levels are not usually elevated due to scavenging by precursor species.
- In area to the south-west of Christchurch, and
- In the coastal zone of Waimakariri and Hurunui districts where the highest concentration of ozone occurred in the long-term simulation.

7. Limitations of this analysis

Ozone in the troposphere is formed via a complex cascade of gas phase chemical reactions which are highly dependent on and sensitive to the amount of precursor species such as NO_x and VOC. The scenario and rates of emissions used for this analysis are very simplified. The emission of precursor species is very coarse temporally and spatially, and the only source considered is the urban area of Christchurch. Biogenic emissions (i.e. from vegetation in the rural areas) can enhance, and rural emission of precursor species can inhibit, the rate of ozone formation as the ozone plume travels over Canterbury. Therefore, the map that is provided here should be looked upon as a first step analysis for ozone potential, and not a comprehensive view.

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