MODELLING SURFACE OZONE DURING THE 2003 HEAT WAVE IN THE UK

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Abstract: The EMEP Unified model, normally applied to the European domain at 50 km horizontal resolution, has been applied to the UK at a finer resolution of 5 km. This new application is called EMEP4UK. The EMEP4UK model is driven by meteorology from the Weather Research and Forecast model (WRF) and emissions from the National Atmospheric Emissions Inventory (NAEI). The WRF model has been nudged every six hours using NCEP/NCAR GFS reanalysis in order to properly represent the 'real' meteorology observed during a particular time period. The present paper focuses on the simulation of surface ozone concentrations during August 2003, when large parts of Europe, including the UK, experienced extremely high temperatures and surface ozone concentrations.
The evaluation in this paper focuses on comparison of model results with measurements taken during the TORCH campaign in August 2003, based in Writtle, SE England. EMEP4UK was able to accurately simulate most of the ozone peaks which occurred during 2003 and in particular those during August. Measured maximum hourly means reached 130 pbb, while modelled values reached 120 ppb. We conducted a series of model sensitivity runs, varying individual model parameters (e.g., temperature, isoprene, precursor emissions, and ozone deposition) in order to isolate the sensitivity of ozone concentrations during the heat wave to each of these. The two factors which control surface ozone concentration at Writtle have been found to be ozone dry deposition and NO_x emissions.

Key words: *Ozone, heat-wave, air pollution, health.*

1. INTRODUCTION

In the UK, high ozone episodes are often caused by a elevated temperatures associated with summertime anticyclonic conditions. In August 2003, a blocking high centred over Scandinavia caused very high temperatures (>35°C) for several consecutive days over parts of the UK. This was associated with a series of ozone peaks, well above 90 ppb, in the south of England. The heat-wave period was contemporary with the TORCH campaign (Lee et al., 2006), which provided detailed measurements of concentrations of ozone and a wide array of its precursors, including isoprene, at a site about 70 km NE of London. The high temperatures and high levels of ozone experienced during the 2003 heat wave had a large effect on human health. In this study we investigate the causes of the elevated ozone levels using a high resolution (5 km) chemical transport model over the UK domain. We first show that the model is able to simulate hourly ozone measurements realistically from a range of sites over SE England during August 2003. We then conduct a series of sensitivity runs to show the influences of a variety of different factors (emissions of biogenic isoprene, anthropogenic NOx and VOCs, temperatures, ozone dry deposition) that contribute to the ozone episode.

2. MODEL DESCRIPTION

The EMEP4UK (Vieno et al., 2008) model framework is a collection of model pre-processors and post-processors which work together to produce a detailed representation of the physical and chemical state of the atmosphere over Europe and in particular over the UK.

The chemical scheme is identical to the EMEP Unified Model and a full description can be found in Simpson et al. (2003). The chemical mechanism used is based upon the ozone chemistry from the Lagrangian photo-oxidant model (Andersson-Sköld and Simpson, 1999, Simpson at al., 1993), but with additional reactions introduced to extend the model's capabilities to acidification and eutrophication. Two types of emissions are present in the model: anthropogenic and biogenic. For the UK, anthropogenic emissions of NO_2, NH_3, SO_2, $PM_{2.5}$, PM_{CO} (coarse particulate matter), CO, and Non Methane VOC (NMVOC) are derived from the UK's National Atmospheric Emissions Inventories (NAEI). Elsewhere, EMEP emissions are used (www.emep.int). NMVOC are speciated into C_2H_6, NC_4H_{10}, C_2H_4, C_3H_6, OXYL (o-xylene), HCHO, CH_3CHO, MEK (methyl-ethyl-ketone), C_2H_5OH, CH_3OH and un-reactive VOC using prescribed values as shown in Simpson et al. (2003). Biogenic emissions of isoprene and monoterpenes are based on Guenther et al., 1993. Biogenic emissions of di-methly-sulphide (DMS) are input as monthly average emission files, derived from Tarrasón et al. (1995). These DMS emissions are treated as SO_2 on input to the calculations.

Dry deposition is calculated using a resistance analogy to calculate the deposition velocity, whereas wet deposition uses scavenging coefficients applied to the 3D rainfall. Ozone can be dry deposited in two ways; either directly in the leaf stomata or to the ground surface (Simpson et al., 2003).

EMEP4UK is driven by the Weather Research Forecast (WRF) model (http://www.wrf-model.org/) with a resolution of 5×5 km^2. WRF is run including data assimilation (Newtonian nudging) of the numerical weather prediction model

meteorological reanalysis from the US National Center for Environmental Prediction (NCEP)/National Center for Atmospheric Research (NCAR) Global Forecast System (GFS).

WRF is applied here with a nesting domain approach with an outer domain of 50 × 50 km^2, an intermediate domain of 10×10 km^2 and an inner domain of 5 × 5 km^2, to provide meteorological data at the required horizontal and vertical resolution. A coarse domain of 50 × 50 km^2 is used to drive the EMEP Unified Model across the European domain to calculate the chemical initial conditions and boundary conditions for the EMEP4UK model. The EMEP4UK model domain, at a resolution of 5×5 km^2, covers the British Isles and parts of France, Denmark, Holland and Belgium. The model is vertically divided into 20 layers using terrain following coordinates. The vertical column extends from the surface up to 100 hPa (~16 km).

3. METHODS

Model simulated surface ozone concentrations are compared with observations from the Automatic Urban and Rural monitoring network (AURN). Here, results from only two stations are reported; Wicken Fen shown in Figure 1 (East Anglia, England – rural site) and London Eltham shown in Figure 2 (urban background). A full model validation paper, comparing all available sites, is in preparation.

Six sensitivity experiments, focused on the TORCH campaign site (Writtle – East Anglia, England), were carried out to investigate the nature of the elevated ozone during the 2003 August heat-wave. Relative to the base case, these experiments changed the following model processes:

1. Doubled UK biogenic isoprene emissions;
2. Switched off UK biogenic isoprene emissions;
3. Halved anthropogenic UK NO_x NAEI emissions;
4. Halved anthropogenic UK NMVOC NAEI emissions;
5. Reduced surface temperatures by 5° C (across the whole 5 × 5 km^2 domain - with unchanged vertical potential temperature)
6. Switched off dry deposition of ozone (both stomatal and non stomatal deposition)

4. RESULTS AND DISCUSSION

The hourly EMEP4UK model predicted ozone surface concentrations for August 2003 agree very well with observations at both the rural site Wicken Fen and the urban background site of London Eltham, as shown in Figure 1 and Figure 2, respectively. In the Londnon Eltham site, a night time depletion of ozone is predicted by the model (e.g. on the 11th and 27th August) but not seen in the observations.

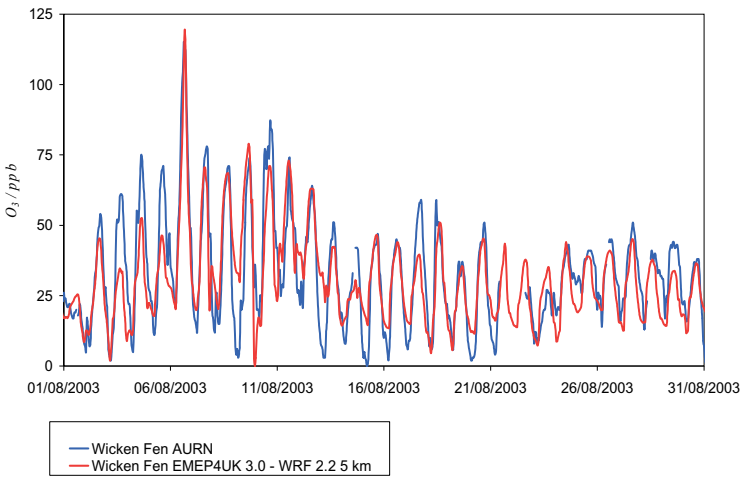

Figure 1. Hourly time-series of modelled (red) and measured (blue) surface ozone during August 2003 at Wicken Fen. Units are ppb.

The EMEP4UK model is also able to represent ozone at the TORCH campaign site (Writtle) as shown in Figure 3. However, for the 2nd, 3rd, 9th and 11th of August 2003 the model somewhat underestimates the measured surface ozone concentration. This appears to be related to the EMEP4UK model simulated surface NO_2 concentrations, which are also compared with observations and shown in Figure 4. NO_2 is overestimated by the EMEP4UK model at this location for the 2nd, 3rd, and 9th of August 2003. This overestimation of NO_2 is probably the cause of underestimation of ozone on these days. The model 5×5 km^2 grid square is probably not always representative of the TORCH site. Interestingly, the model performs much better on these days at the Wicken Fen site which is only approximately 10 km away from Writtle, suggesting it that local factor are causing the model-observation discrepancies.

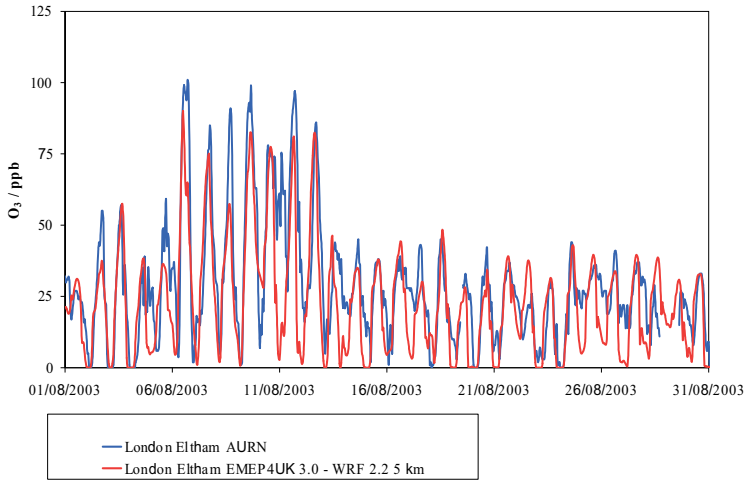

Figure 2. As Figure 1, but for London Eltham.

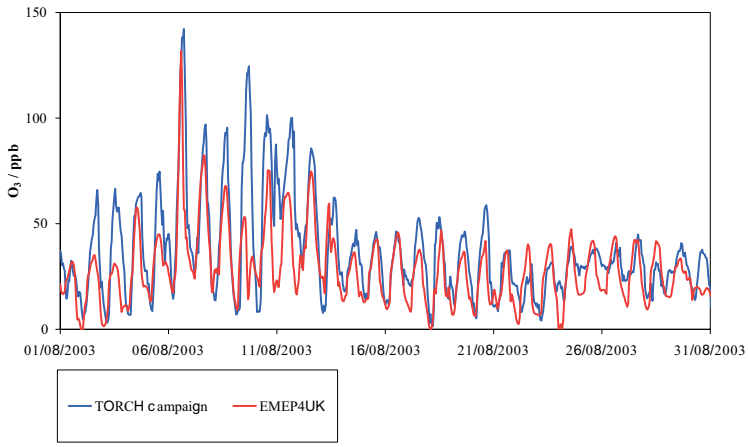

Figure 3. As Figure 1 but for the site of the TORCH campaign (Writtle). Units are ppb.

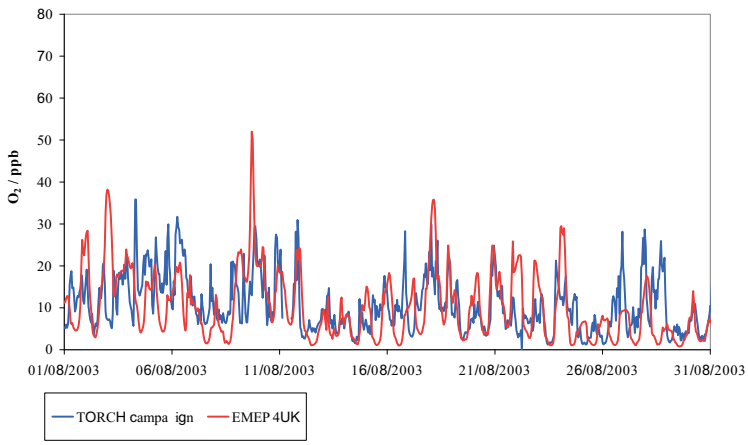

Figure 4. As Figure 3 but for NO_2 surface concentrations at Writtle. Units are ppb.

The results of the six sensitivity experiments are summarised in Figure 5. The response of ozone to isoprene emissions appears to be approximately linear, with doubling of emissions having roughly the opposite effect of switching the emissions off completely. Isoprene emissions contribute up to ~10 ppb ozone on some days. When

compared with observations, the EMEP4UK model predicted isoprene concentration in better agreement with double isoprene emissions (not shown here). Halving anthropogenic NMVOC emissions decreases surface ozone by as much as ~15 ppb. A similar signal is observed when the surface temperature is reduced by 5°C.

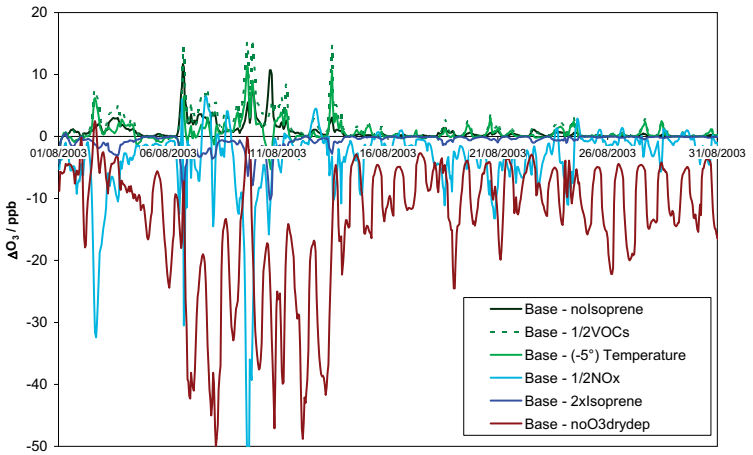

Figure 5. Differences in ozone surface concentration referred to a base run of the EMEP4UK model for August 2003 at Writtle (cf. base run in Figure 3).

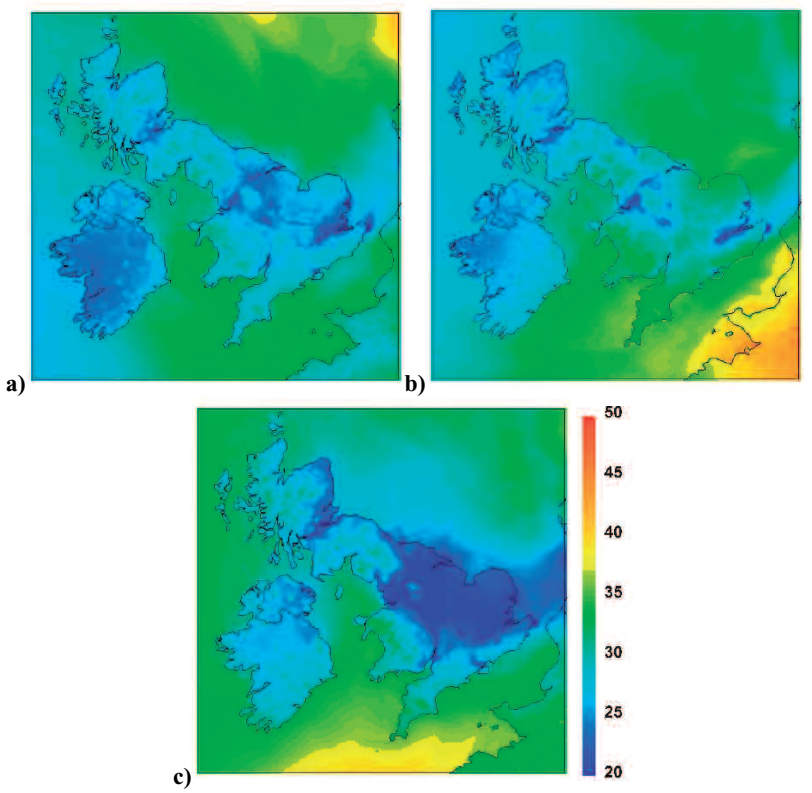

Figure 6. Monthly 2003 surface Ozone concentration calculated by the EMEP4UK model for:
a) July, b) August and c) September. Units are ppb of O_3.

Ozone surface concentration is strongly affected by NO_x emissions and dry deposition. Halving NO_x emissions enhances the surface concentration of ozone by up to 70 ppb on one day during the heat-wave (10 August), whilst on other days it has little impact. Since10 August also represented one of the key periods of O_3 discrepancy, this sensitivity test further supports the conclusion (noted above) that the deviations were particularly related to uncertainties in local patterns of NO_x emission. When NO_x emissions are reduced, NO_x does not accumulate as fast during night time and late afternoon and therefore the ozone production is not limited or depleted so fast by direct

reaction of ozone with NO (titration). Dry deposition also strongly controls surface ozone. Ozone dry deposition shows a large diurnal cycle because the stomata deposition is a strong function of temperature. Surface ozone is increased by to 50 ppb when dry deposition is switched off completely.

Figure 6 shows maps of monthly mean surface ozone over the UK for July, August and September 2003. The NO_x signal in these ozone fields is clearly evident along road corridors, especially in July and August. This highlights the importance of detailed emissions to properly simulate the spatial pattern of ozone over the UK and more generally wherever discrete emissions are present (i.e. road, point sources etc.).

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