Environment Agency

Evidence

# Comparison of simple and advanced regional models (CREMO)

## Ozone Diagnostics

Report – SC060037/c

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E: enquiries@environment-agency.gov.uk.

**Author(s):**
Garry Hayman (Hayman Atmospheric Consulting)
Ranjeet Sokhi and Charles Chemel (University of Hertfordshire)
Stephen Griffiths (E.ON New Build and Technology)
Keith Vincent (AEA Technology)
Tony Dore (Centre for Ecology and Hydrology)
Paul Sutton and Raymond Wright (RWE npower)

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**Research Contractor:**
Centre for Atmospheric and Instrumentation Research University of Hertfordshire College Lane, Hatfield, AL10 9AB, UK. Tel: +44 (0) 1707 284520
Email: r.s.sokhi@herts.ac.uk

**Environment Agency's Project Manager:**
Bernard Fisher, Evidence Directorate

**Collaborator(s):**
Hayman Atmospheric Consulting
22 The Old Pound
Wootton
Abingdon
Oxfordshire, OX13 6BQ
garry_hayman@btinternet.com

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Miranda Kavanagh

**Director of Evidence**

# Executive summary

Ozone is a secondary pollutant formed in the lower atmosphere from the sunlight-initiated oxidation of volatile organic compounds (VOCs) in the presence of oxides of nitrogen (NOx). Exposure to ground-level ozone has effects on human health, crops and vegetation, and materials such as rubber, paints and plastic. Air quality standards have been established to mitigate effects on human health and vegetation, but these standards are widely exceeded across the UK and Europe.

UK measurements of ambient ozone concentrations show substantial variability from hour to hour, day to day and from season to season. In addition, the three major factors controlling ozone concentrations operate at different spatial scales. A number of statistics (derived from hourly ozone concentrations) are used to assess the impacts of ozone and there is no single or preferred ozone statistic (known as an ozone metric) which can be used to quantify all the ozone impacts. This report provides a summary of the diagnostics used in the UK and elsewhere to assess the impact of ozone and contains a recommendation on the preferred diagnostics to use in the 'Comparison of simple and advanced regional models' (CREMO) project.

# Contents

# 1 Introduction

Among its objectives, the project ‘Comparison of simple and advanced regional models’ (CREMO) commissioned by the Environment Agency seeks to:

- provide a technique for assessing the contribution of industrial emissions of oxides of nitrogen (NOx) and volatile organic compounds (VOCs) to ambient levels of ozone under realistic meteorological conditions based on the USEPA Community Multiscale Air Quality (CMAQ) model;
- compare the model results with observations and results from simpler methods.

This report provides a summary of the diagnostics used in the UK and elsewhere to assess the impact of ozone and contains a recommendation on the preferred diagnostics to use in the CREMO project.

# 2 Ground-level ozone

Ozone is not emitted directly into the atmosphere, but is a secondary pollutant formed in the lower atmosphere from the sunlight-initiated oxidation of volatile organic compounds (VOCs) in the presence of oxides of nitrogen (NO and $NO_2$, collectively NOx). Elevated concentrations of ozone are especially generated over the UK when slow-moving or stagnant high pressure (anticyclonic) weather systems, occurring in the spring or summer, bring in photochemically reacting air masses from mainland Europe.

Exposure to ground-level ozone has effects on:

- human health (EPAQS 1994, WHO 2006, AQEG 2009). The human health impacts arise from ozone's irritant properties and the induction of an inflammatory response in the lung.
- crops and vegetation (RoTAP 2012). Crop yields and tree growth are reduced and the composition of natural plant communities is affected.
- materials such as rubber, paints and plastics (UNECE 2004)

Air quality standards have been established to mitigate effects on human health and vegetation (Table 2.1). These air quality standards are widely exceeded across the UK and Europe (EEA 2007, 2008, 2009).

UK measurements of ambient ozone concentrations show substantial variability from hour to hour, day to day and from season to season. There are three major factors controlling ozone concentrations, which operate at different spatial scales:

(i) The **hemispheric** background ozone concentration has been gradually increasing, thereby influencing the background or background levels of ozone brought into the UK from the Atlantic Ocean.

(ii) Short-term elevations in ozone concentrations result from additional formation of ozone from **regional-scale** photochemical processing of emitted NOx and VOCs especially during summertime, with such events tending to be more frequent and intense towards the south of the UK. The severity of such episodes has progressively decreased from the early 1990s as a result of European reductions in anthropogenic emissions of NOx and VOCs.

(iii) The control of NOx emissions in the UK has reduced **local-scale** scavenging of ozone by reaction with emitted NO, contributing to a general increase in ozone concentrations. This has most relevance to urban areas (or large point sources), where NOx emissions are higher.

Ozone, with a hemispheric background concentration of the order of 30–40 parts per billion (ppb) (HTAP 2007), exhibits a very different concentration distribution to those found for primary pollutants (that is, those emitted directly into the atmosphere). The concentration distributions of primary pollutants typically have highly skewed distributions of hourly concentrations, with the mode at low concentrations and a small number of hours with high concentrations. Furthermore, identical annual mean concentrations of ozone can be made up from very different frequency distributions.

**Table 2.1 Air quality standards for ozone**

| Organisation | | Protection | Air quality standard | |
|---|---|---|---|---|
| | | | **Averaging period** | **Value** |
| WHO | WHO (2006) | Human health | Maximum of 24 daily running eight-hour mean concentrations[1] | 100 µg $m^{-3}$ not to be exceeded on more than three days per calendar year |
| European Union | EC (2008) | Human health | Maximum of 24 daily running eight-hour mean concentrations | <u>Target value</u>: 120 µg $m^{-3}$ not to be exceeded on more than 25 days per calendar year, as an average over three years (to be attained by January 2010)<br><u>Long-term objective</u>: 120 µg $m^{-3}$ not to be exceeded. |
| | | Vegetation | AOT40 (accumulated ozone exposure over a threshold of 40 ppb) based on daylight hours from May to July | <u>Target value</u>: AOT40 ≤ 18,000 µg $m^{-3}$ hours, as an average over five years (to be attained by January 2010)<br><u>Long-term objective</u>: AOT40 ≤ 6,000 µg $m^{-3}$ hours |
| UK Air Quality Strategy (Objective) | Defra (2007a) | Human health | Maximum of 24 daily running eight-hour mean concentrations | 100 µg $m^{-3}$ not to be exceeded more than 10 times in a calendar year |

Notes: [1]Running eight-hour mean ozone concentrations are calculated by first deriving the hourly average ozone concentrations over fixed periods from 00.00 to 00.59 onwards. These hourly averages are then taken consecutively in groups of eight and the eight-hour averages for the periods: 00.00–07.59, 01.00–08.59, etc. onwards, are then calculated. The running eight-hour mean concentration is assigned the time of the last hour of the running mean using Greenwich Mean Time (GMT). There are 24 of these running eight-hour mean concentrations per day. The maximum of these 24 mean concentrations is used in many ozone metrics (see Table 2.2).

## 2.1 Ozone concentration metrics

The annual mean concentration by itself does not capture all the features relevant to assess the impact on human health and ecosystems. In addition these impacts operate over different time periods; short periods of exposure to high concentrations are of most relevance to human health while longer-term exposure is of concern for the impact on crops, trees and natural ecosystems.

For these reasons, a number of statistics (derived from hourly ozone concentrations) are used to assess the impacts of ozone and there is no single or preferred ozone statistic (known as an ozone metric) which can be used to quantify all the ozone impacts. Table 2.2 lists a number of concentration-based metrics currently used to assess the impacts on human health and ecosystems. The UK Air Quality Expert Group (AQEG) has not yet been able to propose a method of simplifying the analysis and interpretation of ozone metrics.

Several of the metrics listed in Tables 2.1 and Table 2.2 are based on the annual average of the daily maximum of the running eight-hour mean concentration (see note 1 to Table 2.1). These metrics are calculated using cut-off concentrations of zero (that is, including all days), 70 µg $m^{-3}$ and 100 µg $m^{-3}$. The metrics have been recommended and used for health impact quantification by the UK Interdepartmental Group on Costs and Benefits (Defra 2007b). For the metrics with cut-offs, the cut-off concentration is subtracted from the daily maximum of the running eight-hour mean concentration and the value set to zero if the result is zero or negative. The average across all of the days in the year is then calculated.

These metrics have been recommended as appropriate for the assessment of the impact of the daily variation in ozone concentration on human health. The range of cut-off concentrations reflects uncertainty as to whether there is a threshold for ozone (COMEAP 1998). The World Health Organization (WHO) concluded that there was evidence that associations existed below the current guideline value (120 µg $m^{-3}$), but its confidence in the existence of associations with health outcomes decreased as the concentrations decreased (WHO 2004). The cut-off at 70 µg $m^{-3}$ is not based on direct evidence of a threshold for health effects at this value. It was recommended (UNECE/WHO 2004) for use in cost–benefit analysis and integrated assessment modelling on the basis of a combination of the uncertainty in the shape of the concentration response function at low ozone concentrations, the seasonal cycle and geographical distribution of ozone concentrations, and the range of concentrations for which European-scale ozone modelling was able to provide reliable estimates (Defra 2007b).

The assessment of the impact on crops and trees has been based on the concentration-based metric, the accumulated ozone exposure above a threshold (AOTxx where xx is the concentration threshold in ppb). The AOT40 metric has been most commonly used and is defined as:

> *AOT40 (expressed in µg $m^{-3}$ hours) is the sum of the difference between hourly concentrations greater than 80 µg $m^{-3}$ (=40 ppb) and 80 µg $m^{-3}$ over a given period using only the one-hour values measured (or modelled) between 08:00 and 20:00 Central European Time[1] each day.*

Several important limitations and uncertainties have been recognised when using AOTxx (UNECE 2010). In particular, the real impacts of ozone depend on the amount of ozone reaching the sites of damage within the leaf, whereas critical levels based on AOT40 only consider the ozone concentration at the top of the canopy. The impacts of ozone on crops are now being assessed using flux-based measurements (RoTAP 2012, UNECE 2010).

[1] The UNECE mapping manual (UNECE 2004) defines daylight hours to be when the global radiation exceeds 50 W $m^{-2}$.

**Table 2.2 Metrics or statistics used to assess the impacts of ground-level ozone[1]**

| Metric | Relevance | Key influences |
|---|---|---|
| Annual average | Basic metric used to show long-term trends. | Includes all hours in the year. Strongly influenced by the magnitude of local NOx emissions and by topography through nocturnal depletion. |
| Annual average of the daily maximum of the running eight-hour mean | Used as the 'basic metric' to assess health impacts. | Strongly influenced by magnitude of local NOx emissions. |
| Annual average of the daily maximum of the running eight-hour mean with a 70 µg $m^{-3}$ cut-off | Health impact (effectively equivalent to SOMO35 – the sum of the daily maximum of the 8-hour running means over 35 ppb) | Influenced by magnitude of local NOx emissions and by photochemical episodes. |
| Annual average of the daily maximum of the running eight-hour mean with a 100 µg $m^{-3}$ cut-off | Health impact | Strongly influenced by peak ozone concentrations (that is, photochemical episodes) and to a lesser extent by magnitude of local NOx emissions |
| Maximum one-hour average (peak hour in the year) | Used as the basis for some epidemiological studies, although it has been suggested that the eight-hour metric is more representative.<br><br>Also an indicator of short-term peaks, but note low statistical power, since it is the value for one single hour. | Metric most sensitive to magnitude of regionally generated photochemical episodes and thus likely to show a response to reductions in relevant precursor emissions. |
| Number of days with daily maximum of running eight-hour mean exceeding 100 µg $m^{-3}$ | Equates to the number of exceedences of the UK ozone standard (the Air Quality Strategy objective is no more than 10 exceedences per year). | Strongly influenced by photochemical episodes and to a lesser extent by magnitude of local NOx emissions. |
| Number of days with daily maximum of running eight-hour mean exceeding 120 µg $m^{-3}$ | Equates to the number of exceedences of the EU Target Value (no more than 25 days, averaged over three years) and Long Term Objective (no exceedences) from the air quality directive. | Strongly influenced by photochemical episodes and to a lesser extent by magnitude of local NOx emissions. |
| SOMO35 | Used as a metric by International Institute for Applied Systems Analysis (IIASA) for Clean Air for Europe (CAFE) and NECD revision. | Influenced by magnitude of local NOx emissions and by photochemical episodes. |

| Metric | Relevance | Key influences |
|---|---|---|
| AOT40 | Used as a metric to assess the impact on vegetation within the UK and Europe. | Influenced by magnitude of local NOx emissions and by photochemical episodes. |

Notes: [1]Based on Table 1.1 of AQEG (2009)

## 2.2 Ozone metrics used in policy assessments

In the Clean Air for Europe (CAFE) programme (see, for example, Amman *et al*. 2005), the SOMO35 and AOT40 metrics were used to derive the impacts of ozone on human health and vegetation, respectively. The scenario analysis undertaken for the Review of the UK Air Quality Strategy (Hayman *et al*. 2006) used the following ozone metrics:

Health-based metrics:

a. Annual mean of the maximum daily running eight-hour average ozone concentration (that is, with no cut-off) (units: $\mu g\ m^{-3}$).
b. Annual mean of the difference between the maximum daily running eight-hour average ozone concentration and a 35 ppb (or 70 $\mu g\ m^{-3}$) cut-off (units:$\mu g\ m^{-3}$). This is related to SOMO35 (units: ppb hours or ppm hours).
c. Annual mean of the difference between the maximum daily running eight-hour average ozone concentration and a 50 ppb (or 100 $\mu g\ m^{-3}$) cut-off (units:$\mu g\ m^{-3}$).
d. Number of days when the maximum of the 24 possible eight-hour running mean concentrations in each day exceeds 100 $\mu g\ m^{-3}$ (metric in the UK Air Quality Strategy) (units: number of days).

Non health-based metrics:

e. Annual mean concentration (units: $\mu g\ m^{-3}$).
f. AOT40 for crops (units: $\mu g\ m^{-3}$ hours or ppb hours).
g. AOT40 for forests (units: $\mu g\ m^{-3}$ hours or ppb hours).

# 3 Recommended diagnostics

From the previous discussion it is clear that no single ozone metric adequately describes the range of impacts of ozone. For this reason, it is recommended that the analysis of the modelling results for ozone should include use the metrics listed below. The rationale for their selection is given.

- Annual mean ozone concentration: a general indicator, sensitive to local NOx emissions.
- Annual mean concentrations of $NO_2$, NOx and Ox = (NOx) + ($O_3$): as there is strong coupling between $O_3$ and NOx.
- Maximum running eight-hour mean concentration: this will be sensitive to peak concentration and the photochemical production of ozone.
- SOMO35: widely used as a metric to assess the impact on human health in policy development. Note that this is effectively equal to the UK metric used in the Air Quality Strategy (see metric b) above).
- AOT40: widely used as a metric to assess the impact on vegetation in policy development.

Further insight can be gained by averaging the hourly concentrations by hour of the day, day of the week and month of the year.

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