Appendices

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Appendix 1
Detailed Project Objectives

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AEA Technology
National Environmental Technology Centre

Modelling of Tropospheric Ozone Formation (EPG 1/3/143)

(available from http://www.aeat.co.uk/netcen/airqual/reports/research99_0/333.html)

Background to the Project

Current Policy Status:

Negotiations have started withing the UNECE Convention on Long Range Transboundary Air Pollution (LRTAP) to conclude a protocol to address acidification, eutrophication and photochemical oxidants (ozone). The protocol is likely to contain emissions ceilings for each party to the convention covering nitrogen oxides, sulphur dioxide, volatile organice compounds (VOCs) and ammonia. Targets for reductions in ozone exposure to humans and to vegetation are based upon the AOT60 and AOT40 parameters respectively (accumulated ozone above a given threshold).

In addition, the European Commission is expected to come forward with a directive proposal setting national emissions ceilings (the so called NECD) again to address the environmental problems of acidification, eutrophication and damage to human health and vegetation from exposure to ozone. This is expected in March 1999 as is a directive proposal setting air quality standards for ozone. This daughter directive js likely to contain an air quality objective of 60 ppb as an eight-hour mean (*i.e.* the WHO guideline) with 20-25 days permitted exceedence (*i.e.* days when the maximum 8-hour measurement exceeds 60 ppb). In addition, the directive will contain an obligation for Member States to implement short term action plans (or at least demonstrate that such plans would be ineffective) should hourly ozone levels exceed 120 ppb.

The UK National Air Quality Strategy contains a provisional objective for ozone'.'Jhis is set at 50 ppb as an 8-hour rolling mean (EPAQS standard) but allows exceedence on up to 10 days per year. This equates to exceedences on up to 5 days per year of the less stringent WHO guideline. It is intended that the provisional objective will be the subject of the next review of the NAQS in two years time.

Future Policy Developments:

The NECD directive is likely to be reviewed in 2003/4 as are the UNECE multi-pollutant protocol and the forthcoming ozone daughter directive. The NECD review will look at improving the level of environmental protection from ozone (and acidification/eutrophication) and the daughter directive review will aim to reduce the number of exceedences of the WHO guideline.

Project Aim

The aim of the proposed work is develop and apply predictive models to the formation of tropospheric ozone on a range of different geographical scales (global, regional, national). This is to underpin the formulation of policy with regard to air quality and ambient levels of ozone in the United Kingdom.

Detailed Project Objective

1. Global/Regional Modelling

(a) The contractor should develop a modelling capacity to investigate the impacts of ozone precursor emissions emitted on the global scale on ozone levels in Europe and the United Kingdom. Information on European ozone concentrations should be available at a resolution of at least 50km.

(b) Furthermore, the model should be able to produce annual and monthly spatially disaggregated estimates of acid deposition, secondary aerosol concentrations (both sulphate and nitrate) and accumulated ozone above thresholds of 60 ppb and 40 ppb (*i.e.* AOT40s and AOT60s) at the same spatial resolution.

(c) The contractor should investigate the feasibility of using land use dependent ozone deposition based upon the concept of stomatal conductivity (Mike Ashmore et al). This incorporates the influence of climatic factors on ozone take up by vegetation and may lead to more accurate model predictions.

(d) The contractor should construct several realistic emissions scenarios for European and non-European Countries. These should be (i) current (1997), (ii) Current Reduction Plans for 2010, 2015 and 2020 (incorporating all countries' expected emissions reductions measures).

(e) For each of the scenarios in (d) the contractor should estimate the global and European contributions to acidic deposition and secondary aerosol and estimate AOT40 and AOT60 values on a grid cell basis. Data should be provided on an annual and monthly basis.

2. Urban Ozone/Nitrogen Dioxide

It is possible that at as emissions of nitric oxide are reduced in urban areas (*via* implementation of various vehicle emissions directives *etc.*) levels of ozone may increase. This may have implications for the assessment of human health risks as ozone may be a pollutant where there is no lower threshold for effect.

Nitrogen dioxide is a pollutant currently included in the National Air Quality Strategy. Of the two objectives in the NAQS the annual objective of 21 ppb is the most challenging in terms of reducing exceedences. The chemistry of nitrogen dioxide, nitric oxide and ozone are inextricably linked and changes in the ozone concentrations from local, national, regional and indeed global changes in emissions must be taken into account in estimating future levels of NO_2.

The contractor should be prepared to apply the results of this research regarding ozone changes (on the global, regional and national scales) to the consideration of future ozone and nitrogen dioxide concentrations in urban areas which are treated explicitly in DETR contract No. EPG 1/3/128 (DETR Nominated Officer is Dr Stephanie Coster).

3. Scenario Analysis

A tool is required which will allow the Department to 'analyse the benefits (*i.e.* changes in ozone climate) of implementation of possible European abatement strategies. Such a tool should

be able to quantify changes in ozone levels relative to health based air quality standards in a spatially resolved manner across the UK.

(a) To develop a model which can provide a representative description of the current and future ozone climate of the United Kingdom. The model should

- reproduce current and historical ozone concentration fields based upon representative meteorology.
- be able to predict future ozone concentration fields resulting from various policies to reduce ozone precursor emissions in the UK and Europe.
- should provide results at a spatial resolution no worse than 10 km x 10 km.
- be able to estimate maximum hourly concentrations of ozone .
- be able to estimate the numbers of days on which EPAQS and WHO standards are exceeded (8-hour means equal to 50 ppb and 60 ppb respectively)
- incorporate anticipated changes in the distribution of urban ozone in the UK
- produce output in a form which will allow health based assessments to be undertaken of benefits resulting from particular emission reduction scenarios in the UK and Europe.

(b) Apply the model in a) to the estimation of health benefits (including exceedences of WHO and EPAQS air quality standards and maximum hourly concentrations) for up to 10 emissions scenarios to be chosen and developed in conjunction with the Department.

4. "Real-time" Ozone Forecast Model – "Short term Action Plans"

It is likely that forthcoming directive proposal regarding air quality standards for ozone will contain an obligation for the Member States to implement short-term action plans should hourly levels exceed 120 ppb. If levels exceed this threshold and no plans are activated then Member States will be required to justify that such plans would be ineffective.

The Department requires, therefore, a capacity to forecast ozone levels at a high spatial and temporal resolution. This forecasting tool should also be able to investigate the effects of various emissions control measures in the various source sectors on the forecast levels of ozone. These control measures could be both spatially and temporally varying.

Ideally, any model should have the capacity to fulfill or take account of the criteria below, however, it is appreciated that such requirements may be technically out of reach or too onerous financially or time wise. The contractor should therefore propose the most practical solution available.

- Present hourly concentrations at a minimum 10 km grid square resolution for the whole of the UK.
- Work with the current NAEI contractor (and other organisations such as the London Research Centre) to develop speciated VOC emissions inventories on a 1 km grid square resolution. These inventories should also be resolved temporally to a minimum resolution of 1 hour. Similar inventories should also be prepared for NO_x and CO emissions.
- Be capable of investigating the effect specific measures to reduce ozone precursor emissions (from a variety of sources with differing mixes of VOCs) at specific locations and times of the day.

- Investigate the feasibility of obtaining and utilising improved spatially and temporally disaggregated emissions data (ozone precursors) for Northern European countries such as Belgium, Netherlands, France and Germany.
- The model should be validated against monitoring data gathered during recent pollution episodes.

5. Improvements to Photochemical Reaction Schemes

The programme of work will focus primarily on the maintenance and updating of the Master Chemical Mechanism (version 2: MCM 2.0) as a benchmark mechanism for chemical and photochemical processes in the troposphere, and on the construction and updating of schemes for use in the models.

(1) The Master Chemical Mechanism will be maintained and updated as follows:

- The degredation schemes for aromatic hydrocarbons will be updated in line with new kinetic and mechanistic data, as they become available. The particular features of aromatic degradation which have the most influence on ozone formation will be identified by performing appropriate POCP sensitivity studies.
- The representation of a number of gas-phase chemical processes will be updated in line with recently published kinetic and mechanistic data. This will include the following: (i) the reactions of OH with PAN species, (ii) the reactions of oxy radicals formed from degradation of esters and alkenes and (iii) the formation of excited oxy radicals from the reactions of some peroxy radicals with NO.
- Photolysis rates of ozone and other inorganic and organic species will be updated in line with latest absorption cross-section and quantum yield data.
- The feasibility of incorporating or improving the description of the formation of secondary sulphate and nitrate aerosol will be assessed, with the additional aim of improving the representation of heterogeneous chemical processes of particular importance (*e.g.* the reaction of N_2O_5 with water).
- The updated MCM will be implemented into the Photochemical Trajectory Model (PTM), along with the latest amendments to the NAEI categorisation of sources (Digest of 1996 Emissions). A limited degree of validation of the updates to the MCM/PTM will be performed using a combination of ambient observational data and environmental chamber data.
- The MCM website at Leeds University will be maintained and revised to include the updated MCM when completed.

(2) Chemical schemes for use in the models will be constructed or updated. The performance of these schemes will be compared with that of the MCM using simple box models.

6. Policy Support – National plan for VOCs/Ozone (Chapter 6)

After the 2nd NO_x protocol has been agreed (and the National Emissions Ceilings Directive adopted) there is likely to be a requirement for the Department to produce a National Plan to implement the emissions ceilings in the UK.

The Department is likely to require policy support to cover the following aspects:

- How to maximise the ozone benefits accruing from the implementation of the rational Emission Ceilings Directive in the UK (*e.g.*, VOC management areas, controls on specific VOCs in certain locations, POCPs, *etc.*)
- Provide support in the update of the UK Strategy to Reduce Emissions of Volatile Organic Compounds.

Appendix 2
Comparison of OSRM Calculations with Observed Ozone Concentrations

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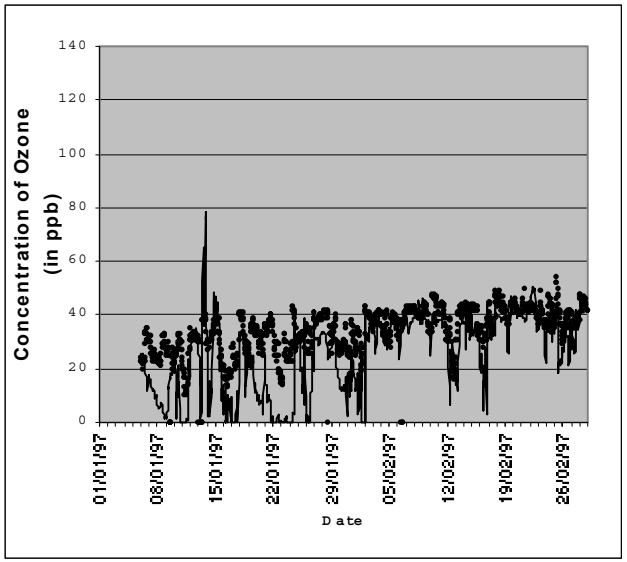

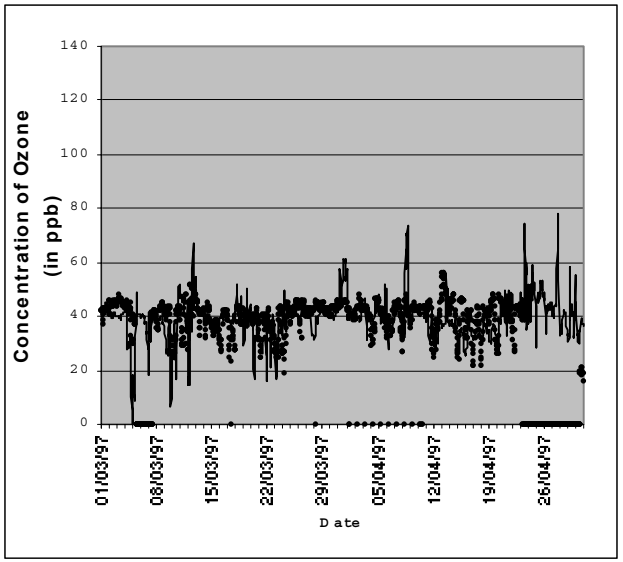

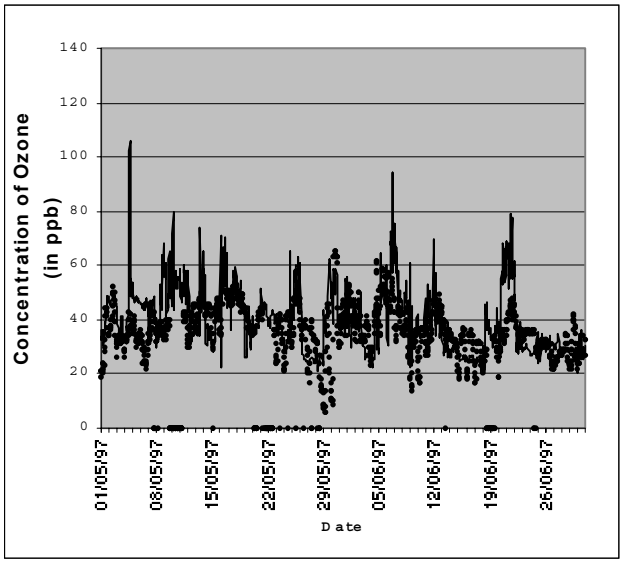

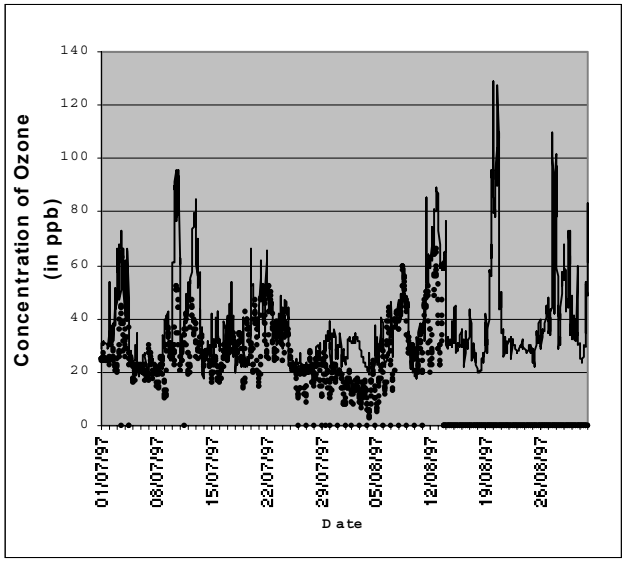

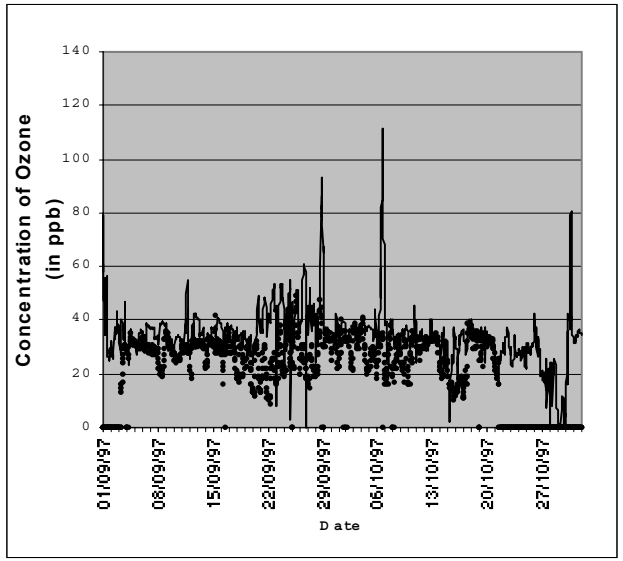

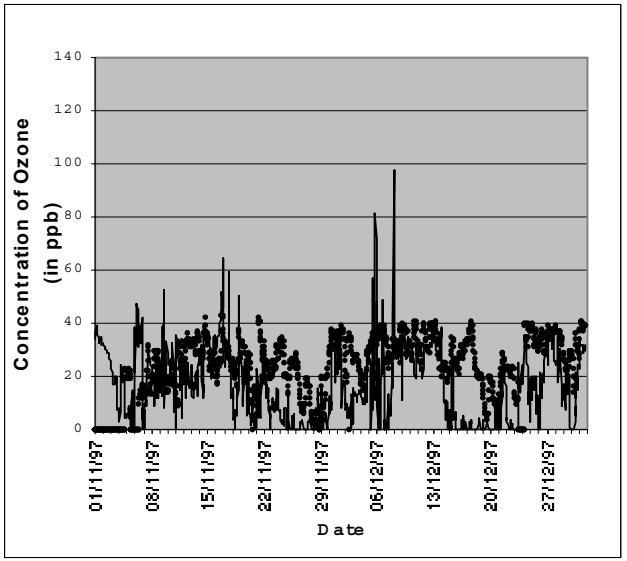

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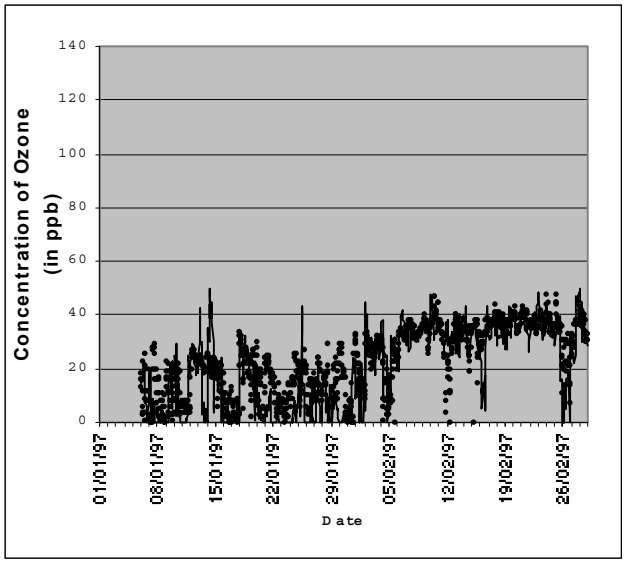
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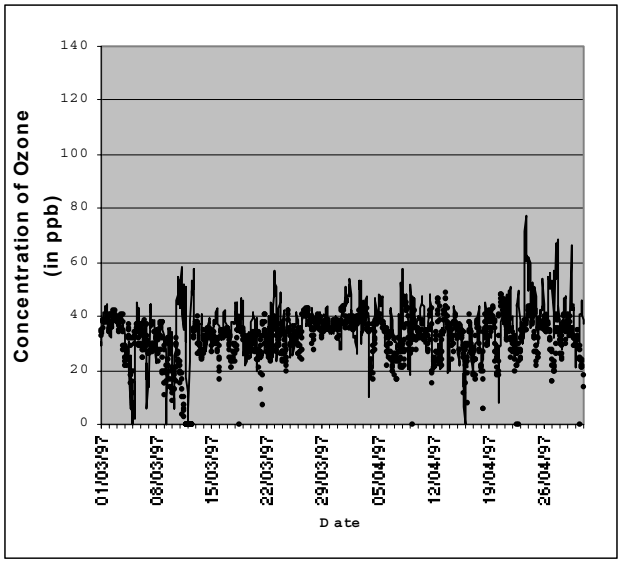
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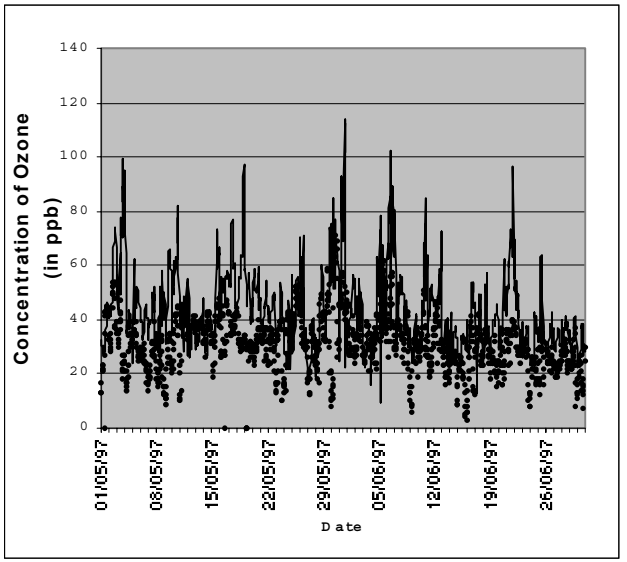
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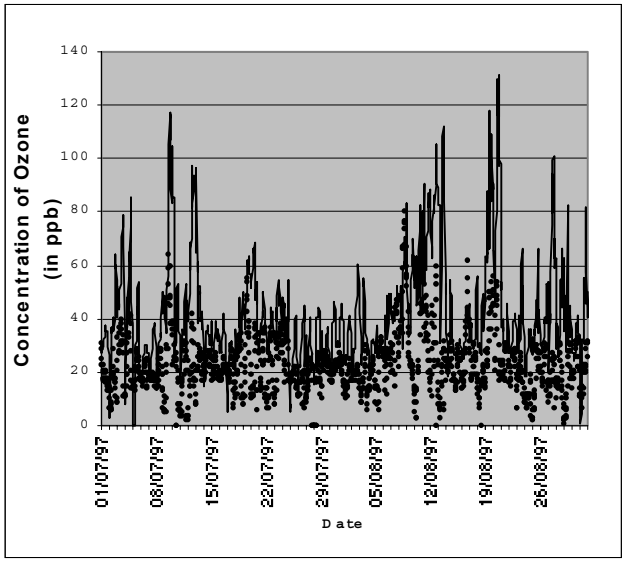
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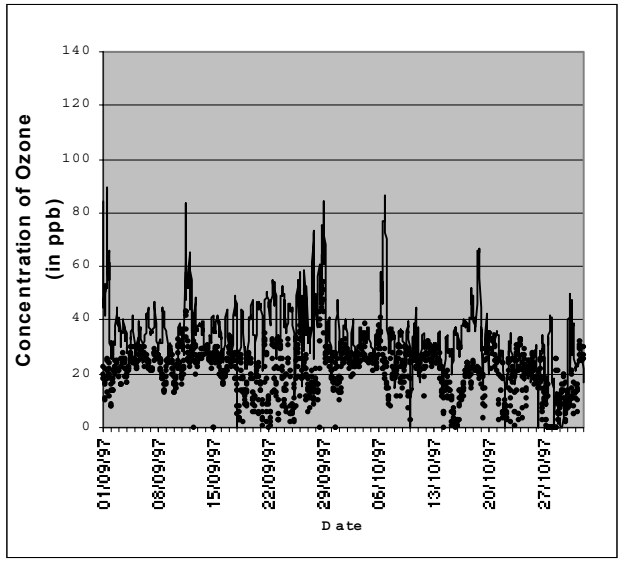
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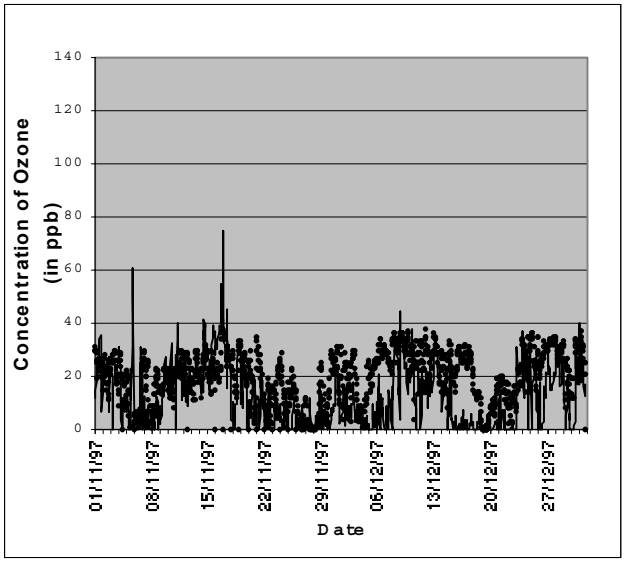
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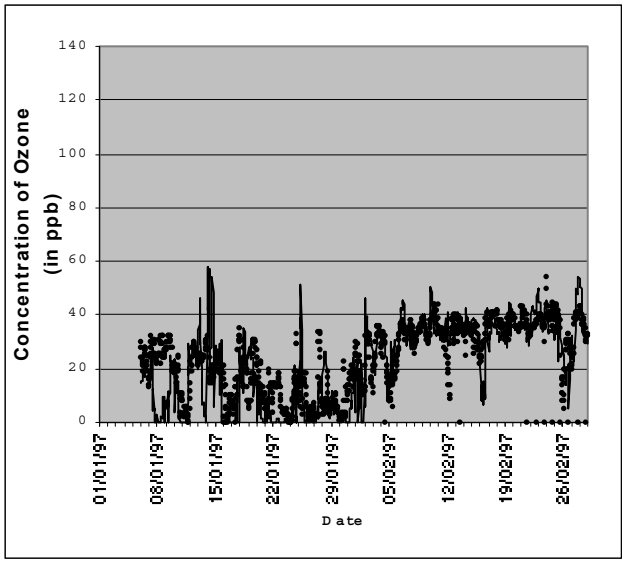

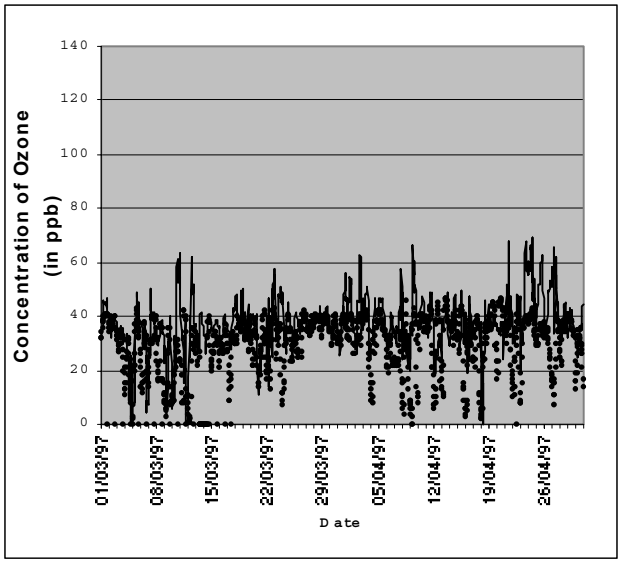

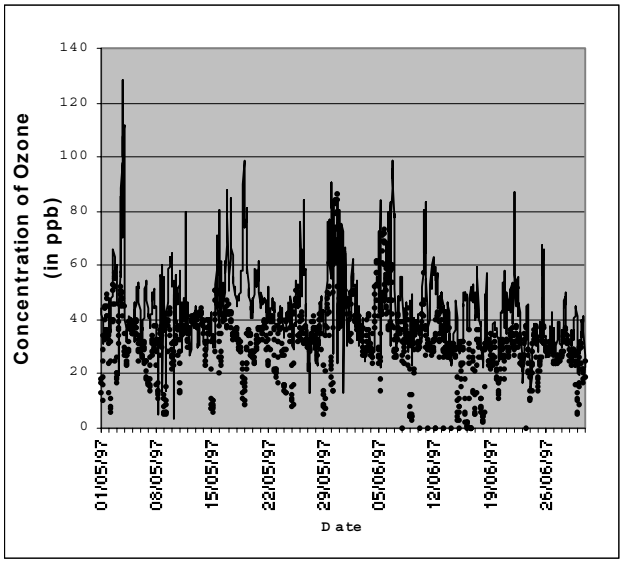

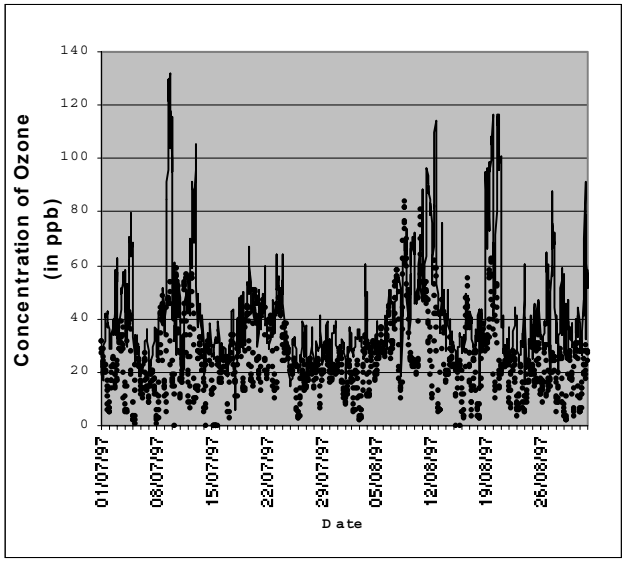

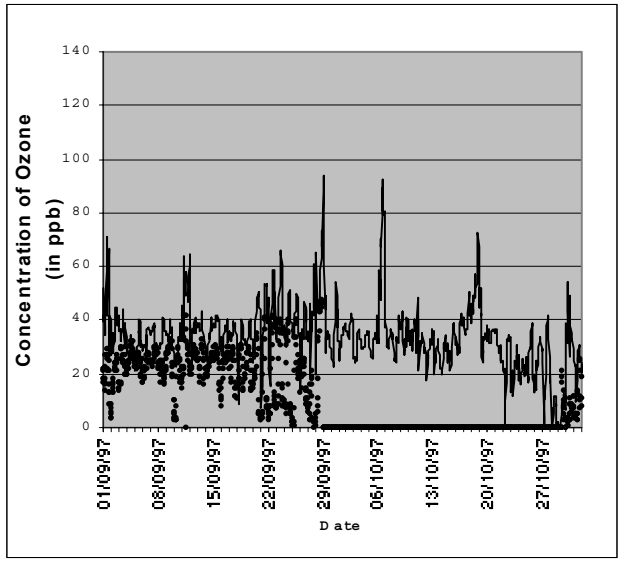

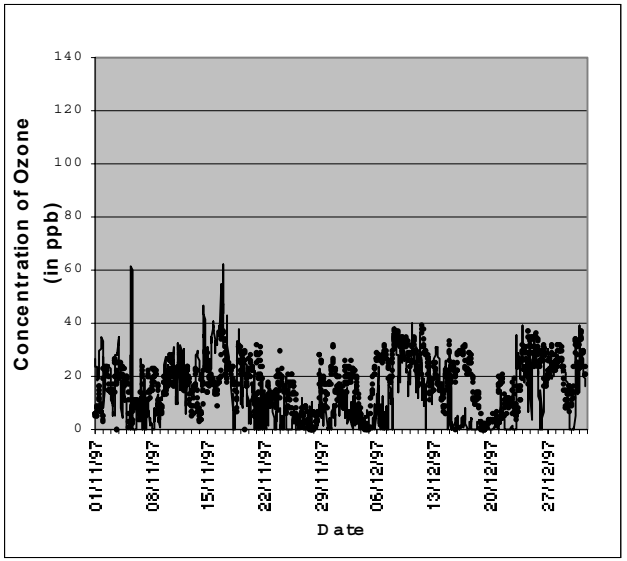

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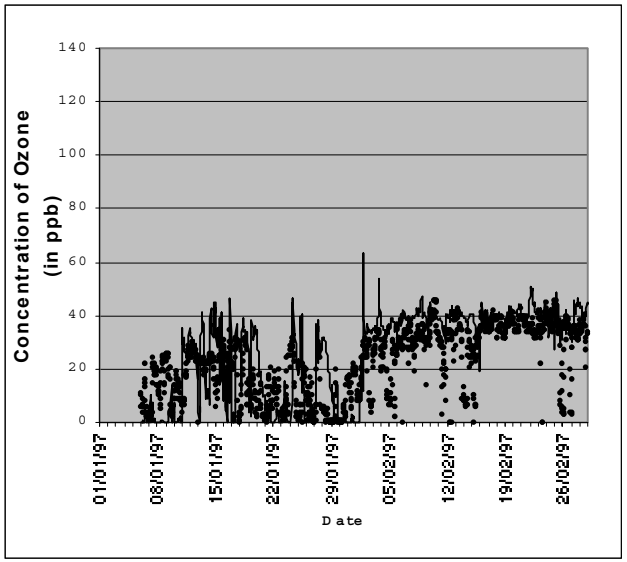
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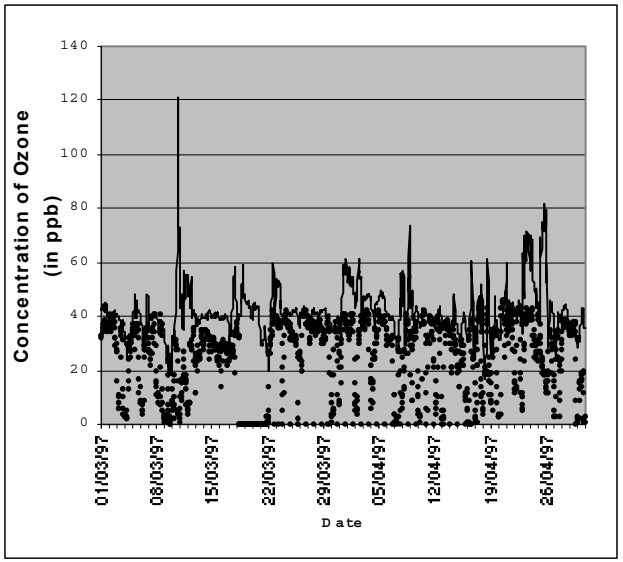
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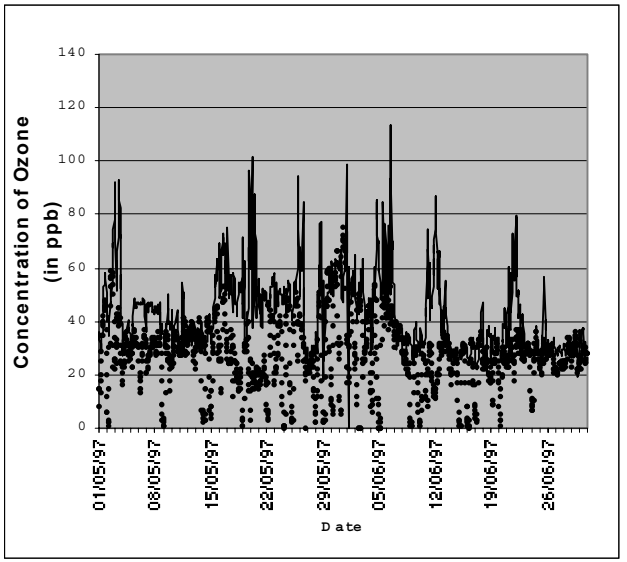
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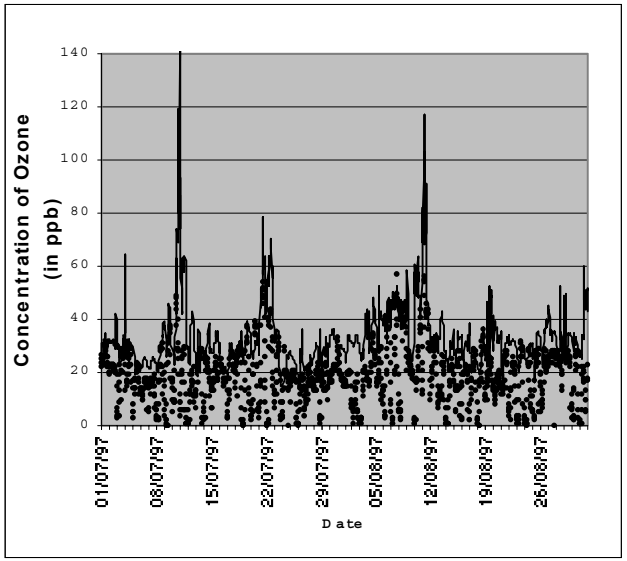
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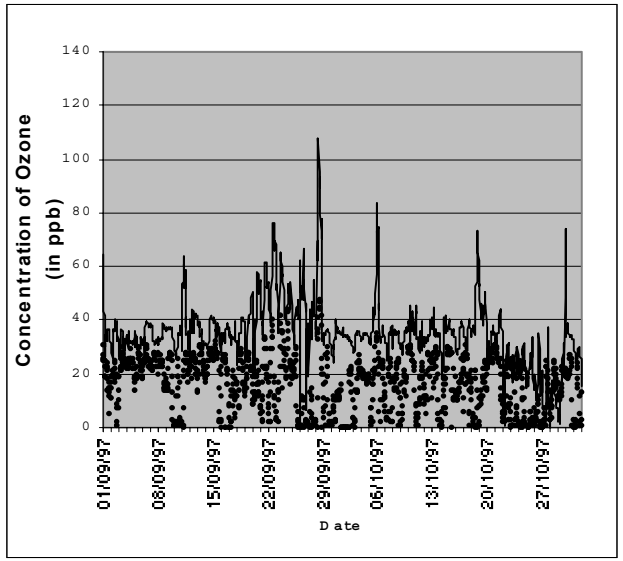
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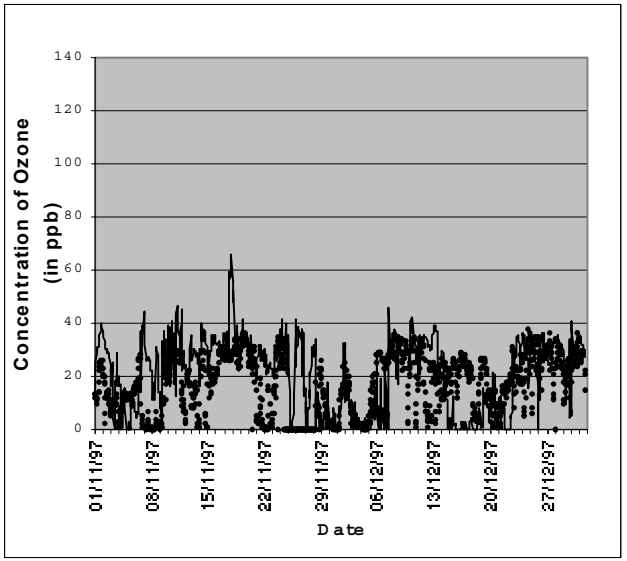
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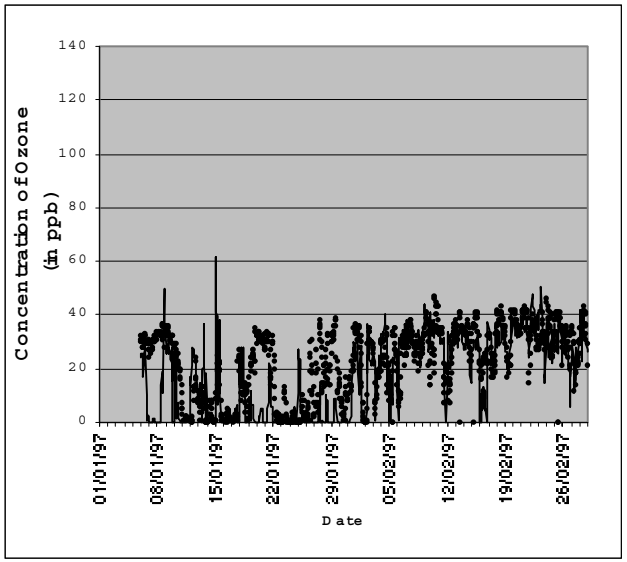

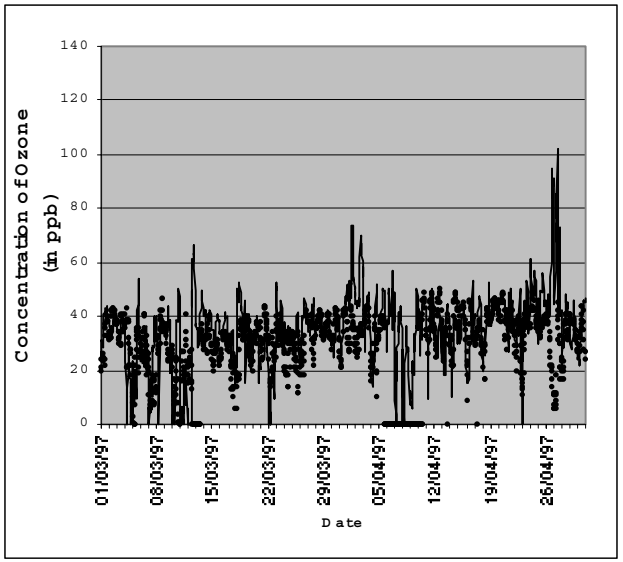

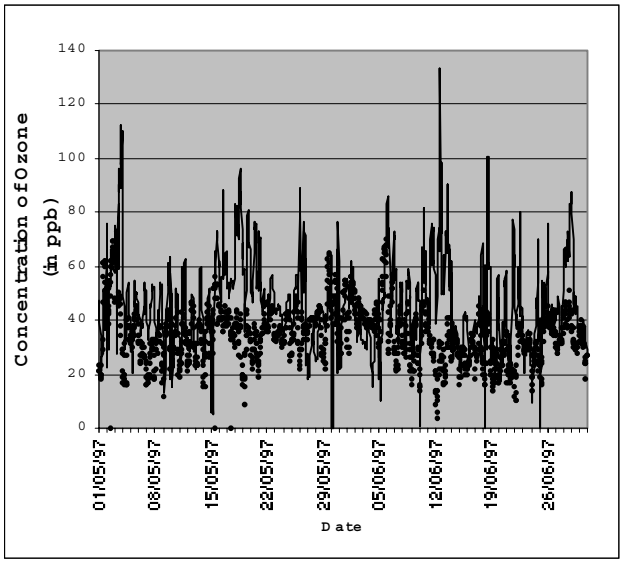

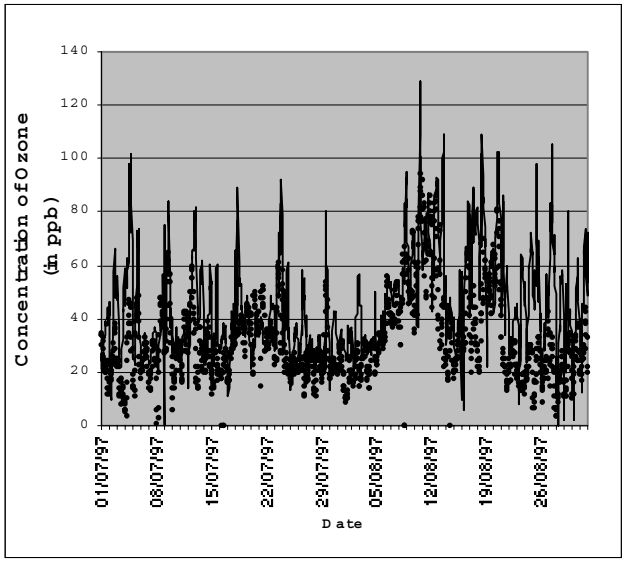

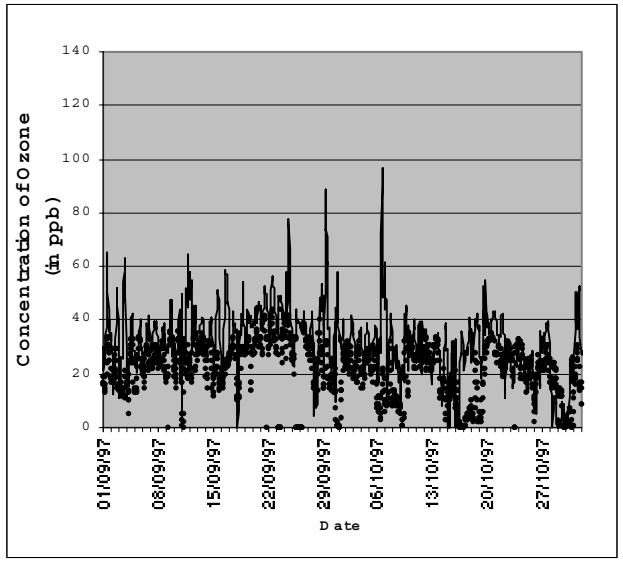

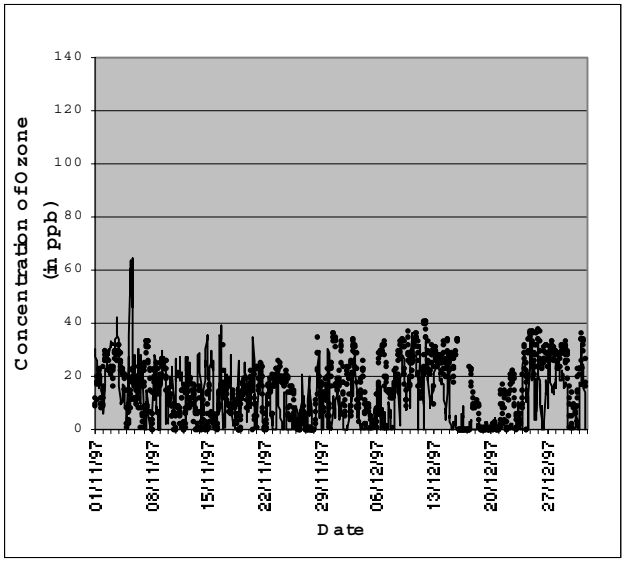

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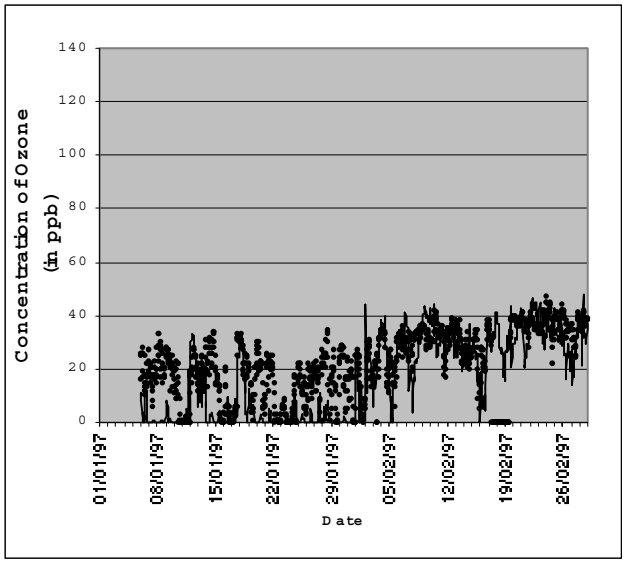
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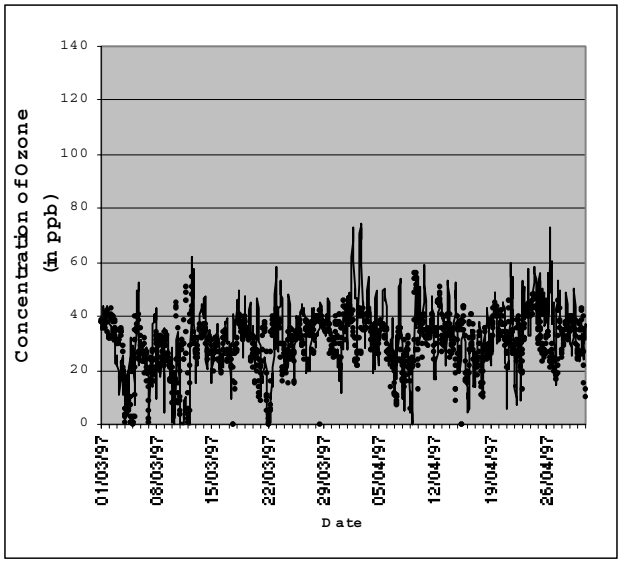
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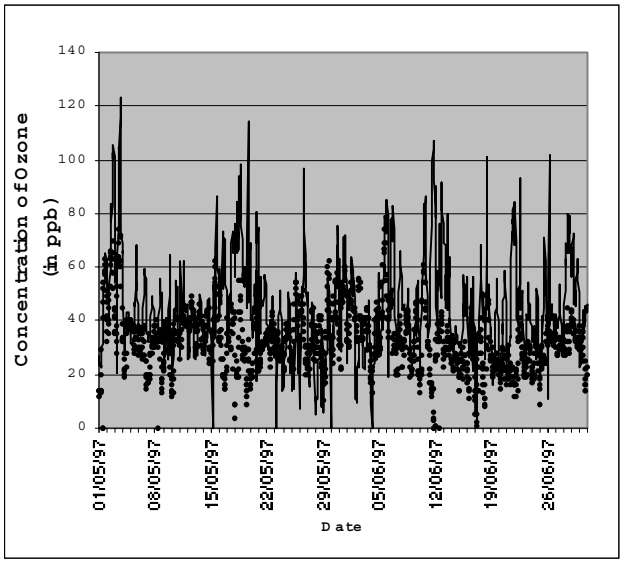
Concentration of Ozone (in ppb)
140
120
100
80
60
40
20
0
01/05/97
08/05/97
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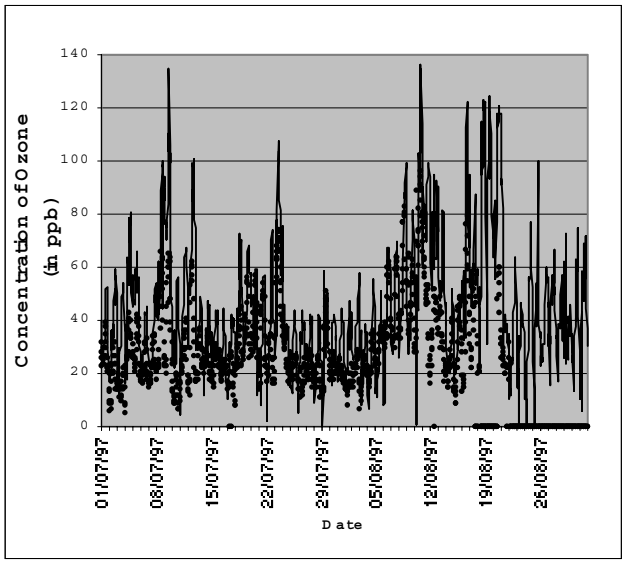
26/06/97
Date


Concentration of Ozone (in ppb)
140
120
100
80
60
40
20
0
01/07/97
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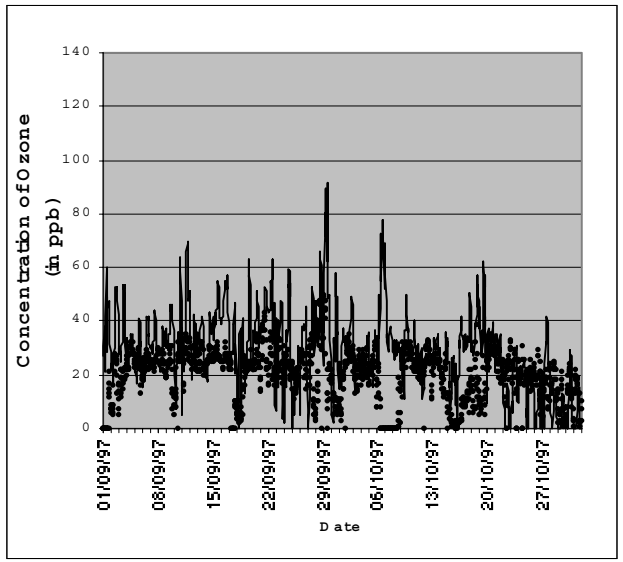
Date


Concentration of Ozone (in ppb)
140
120
100
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60
40
20
0
01/09/97
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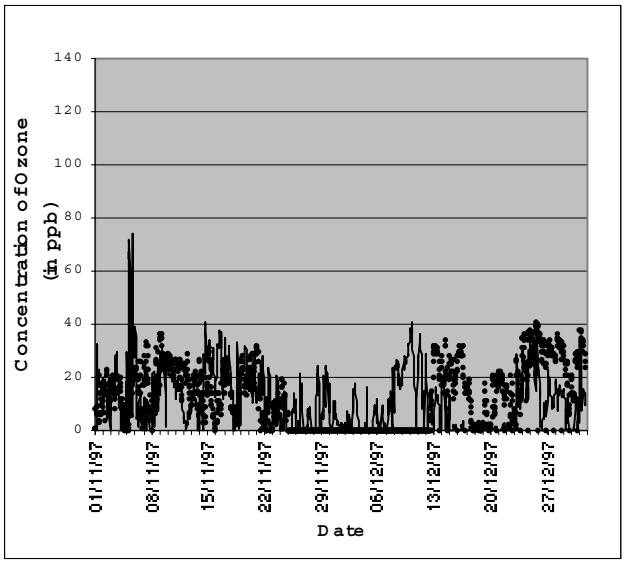
27/10/97
Date


Concentration of Ozone (in ppb)
140
120
100
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60
40
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0
01/11/97
08/11/97
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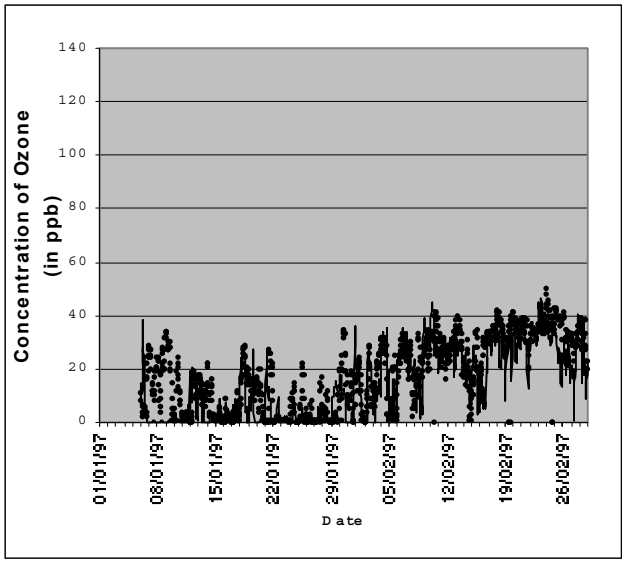
20/12/97
27/12/97
Date

Bottesford


Concentration of Ozone (in ppb)
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80
100
120
140
01/01/97
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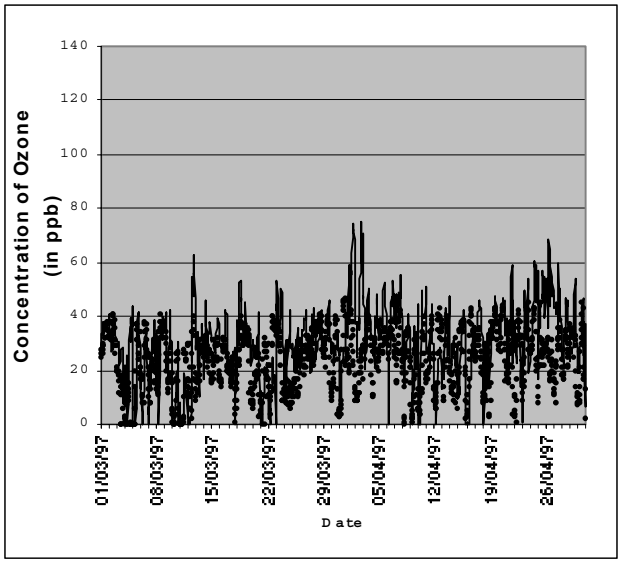
Date


Concentration of Ozone (in ppb)
0
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40
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100
120
140
01/03/97
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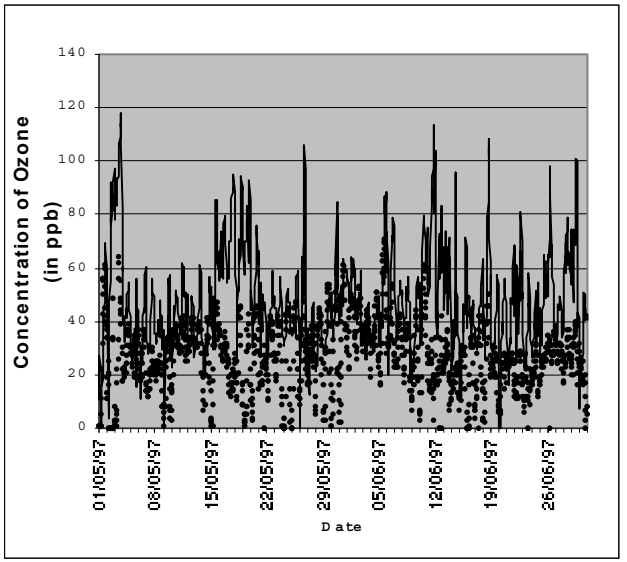
Date


Concentration of Ozone (in ppb)
0
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140
01/05/97
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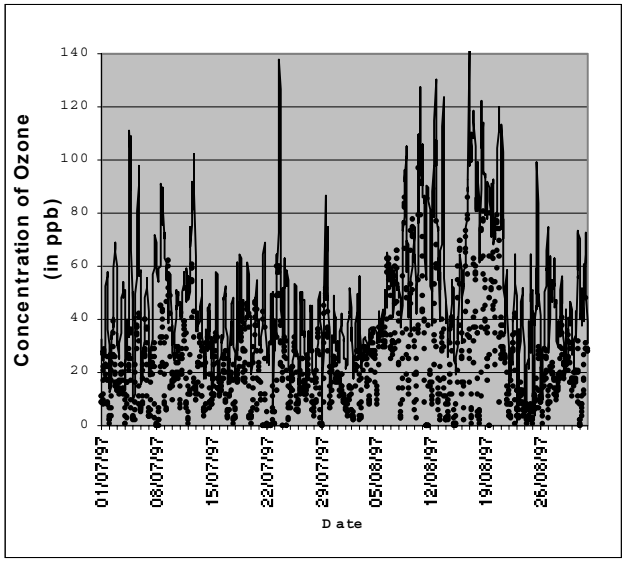
Date


Concentration of Ozone (in ppb)
0
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01/07/97
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26/08/97
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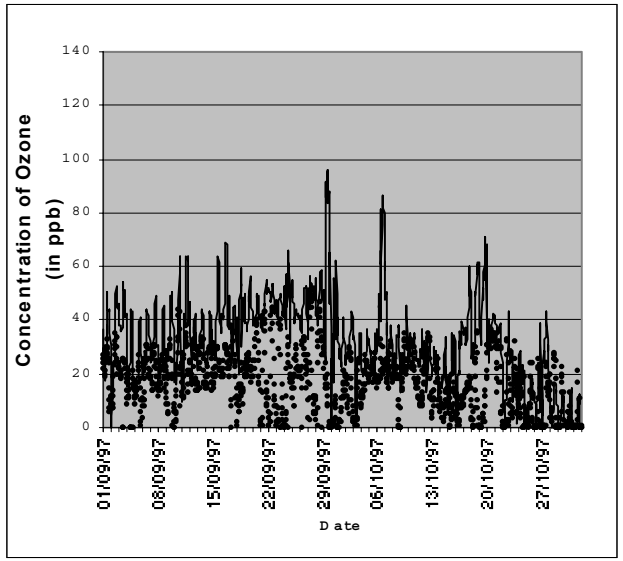
Concentration of Ozone (in ppb)
0
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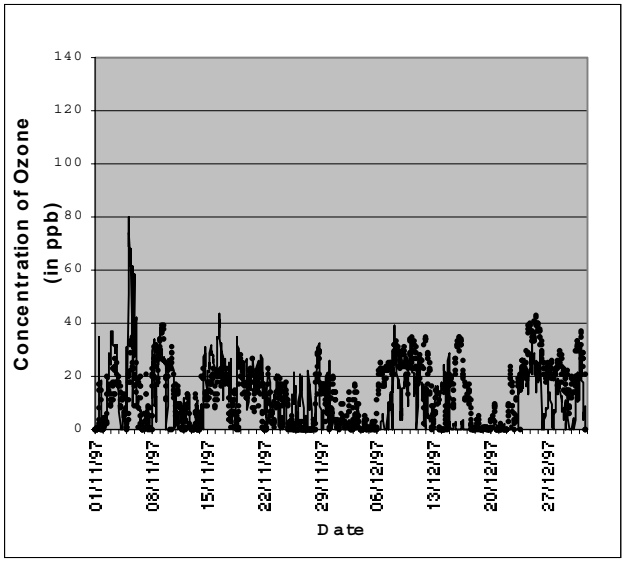
27/10/97
Date


Concentration of Ozone (in ppb)
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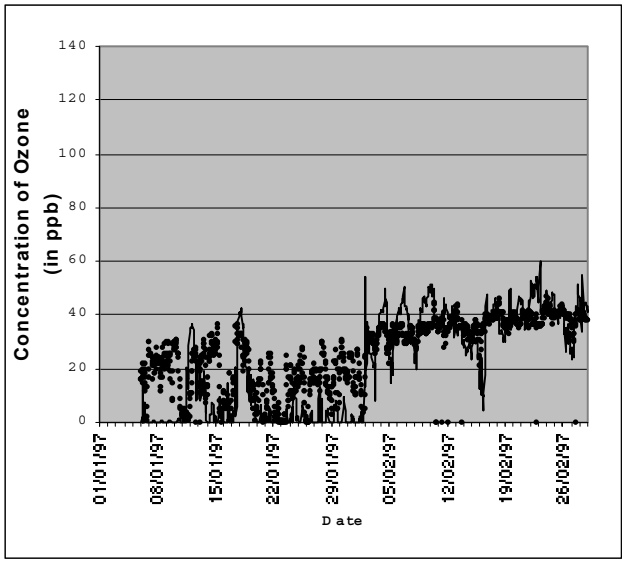
27/12/97
Date

Aston Hill


Concentration of Ozone (in ppb)
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26/02/97
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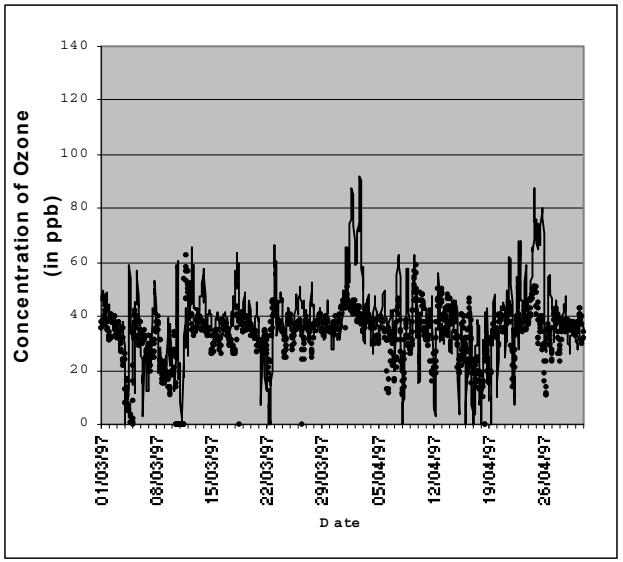
Concentration of Ozone (in ppb)
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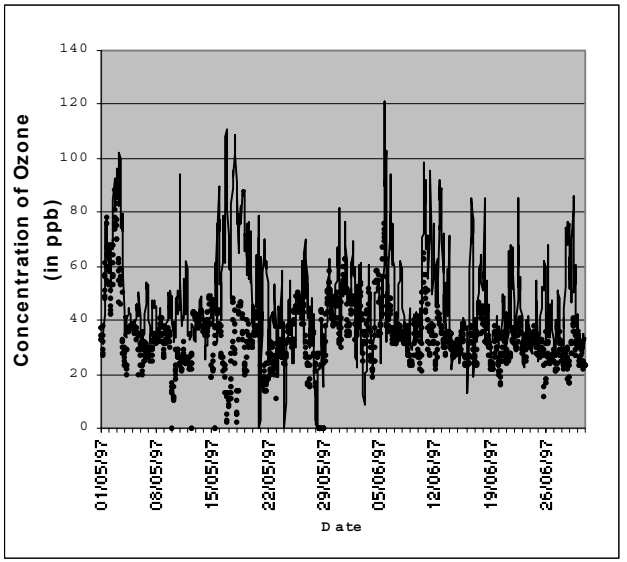
Concentration of Ozone (in ppb)
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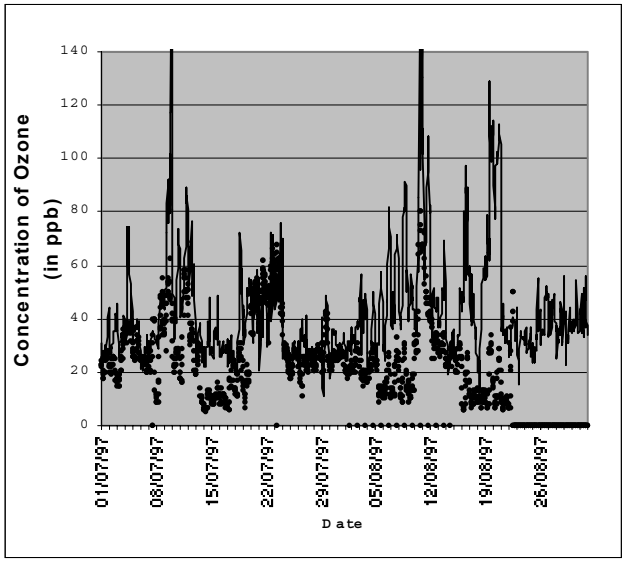
Concentration of Ozone (in ppb)
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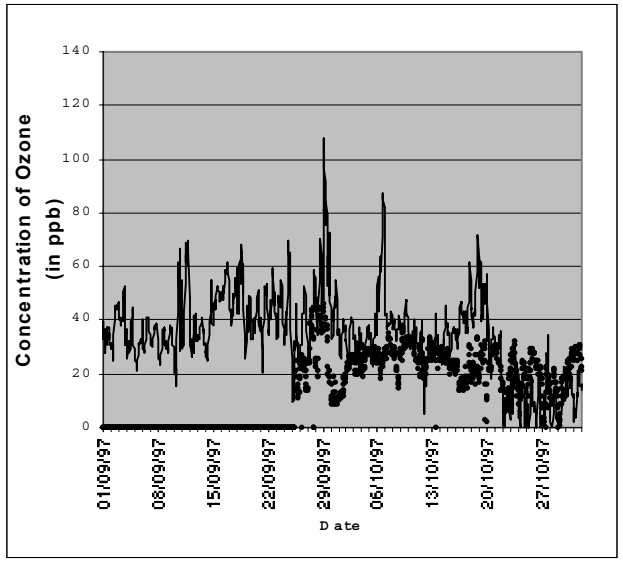
Concentration of Ozone (in ppb)
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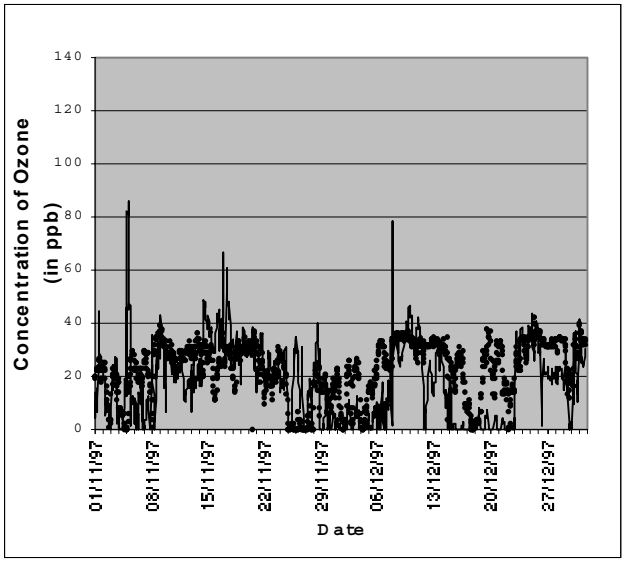
Concentration of Ozone (in ppb)
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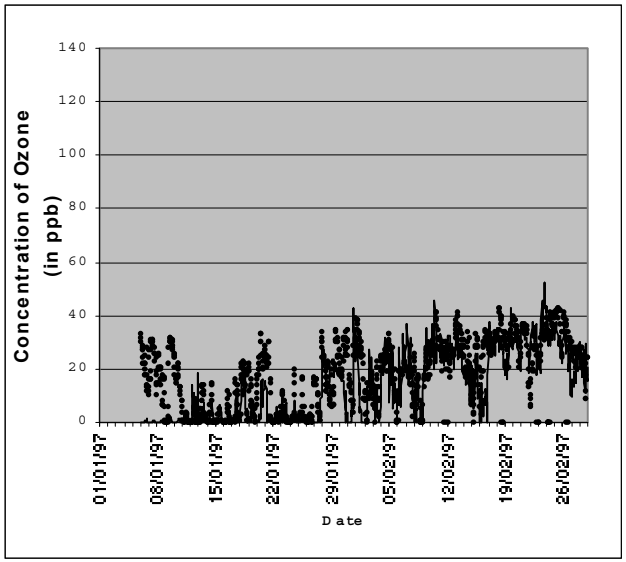
Sibton


Concentration of Ozone (in ppb)
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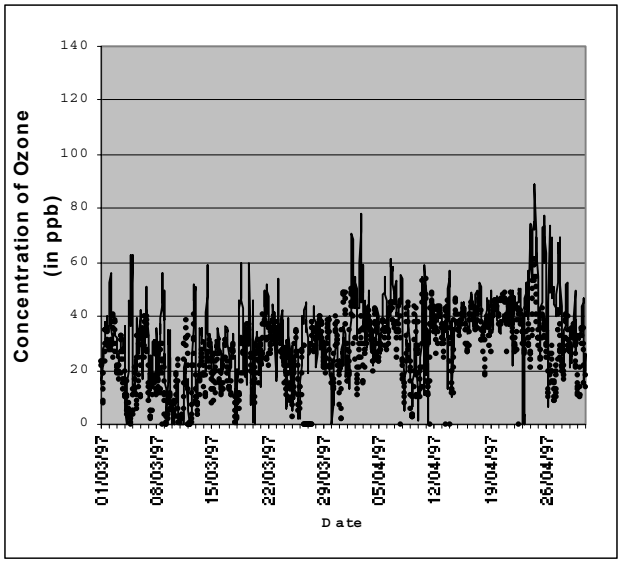
Concentration of Ozone (in ppb)
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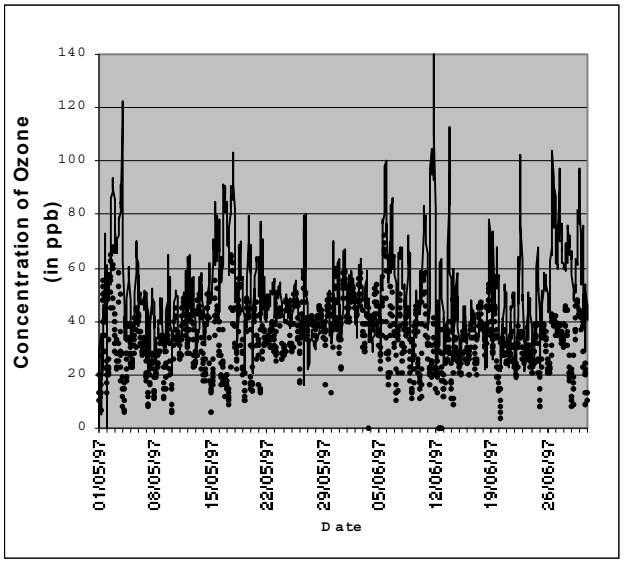
Concentration of Ozone (in ppb)
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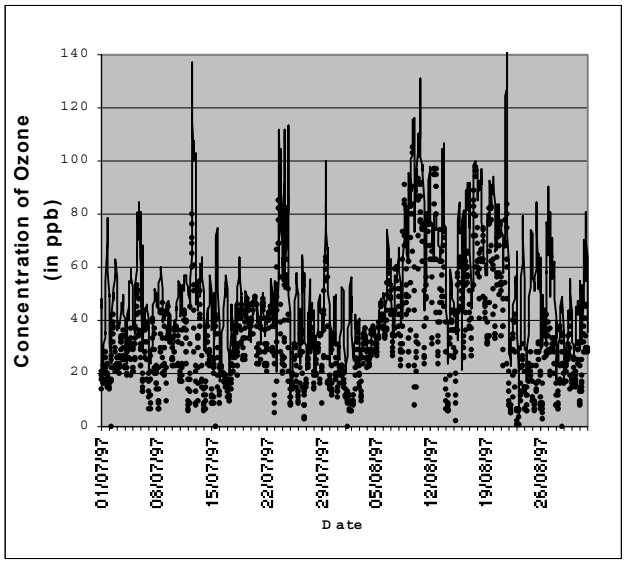
Concentration of Ozone (in ppb)
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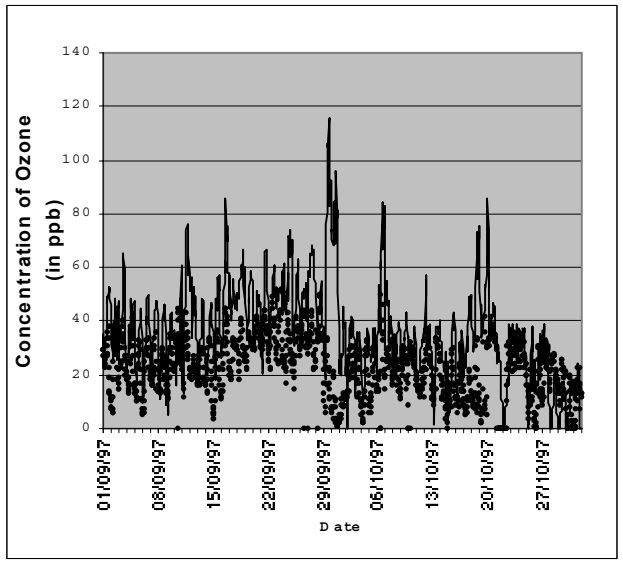
Concentration of Ozone (in ppb)
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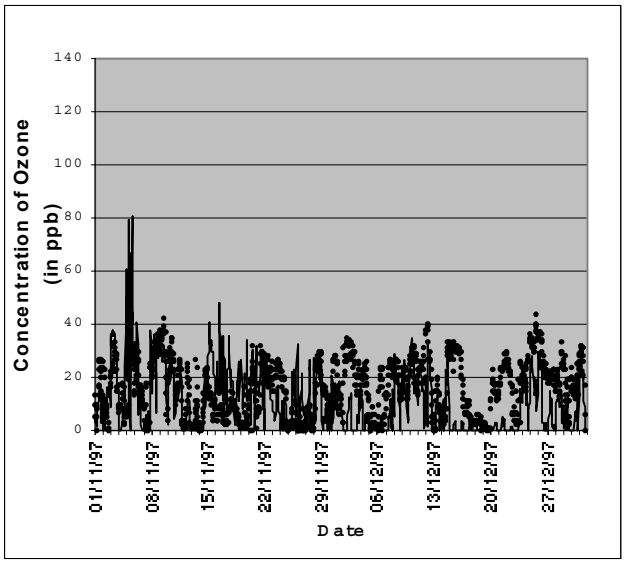
Concentration of Ozone (in ppb)
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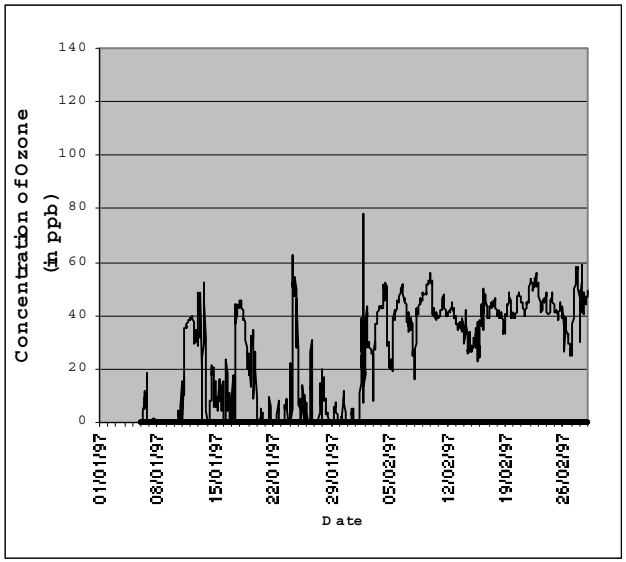
Date

Narberth


Concentration of Ozone (in ppb)
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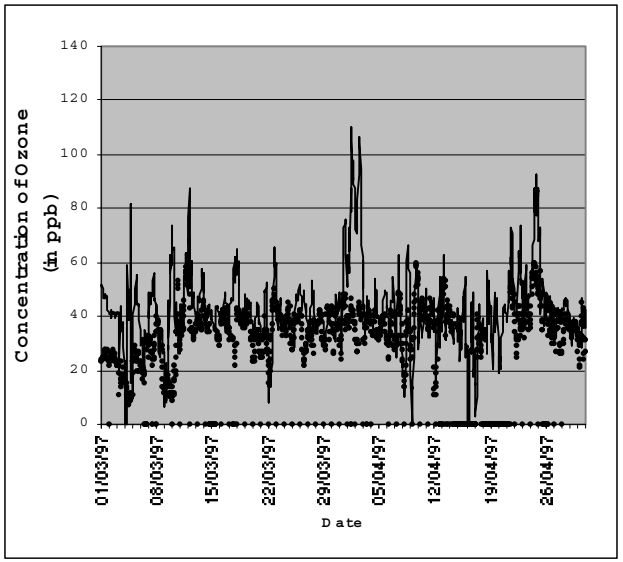
Concentration of Ozone (in ppb)
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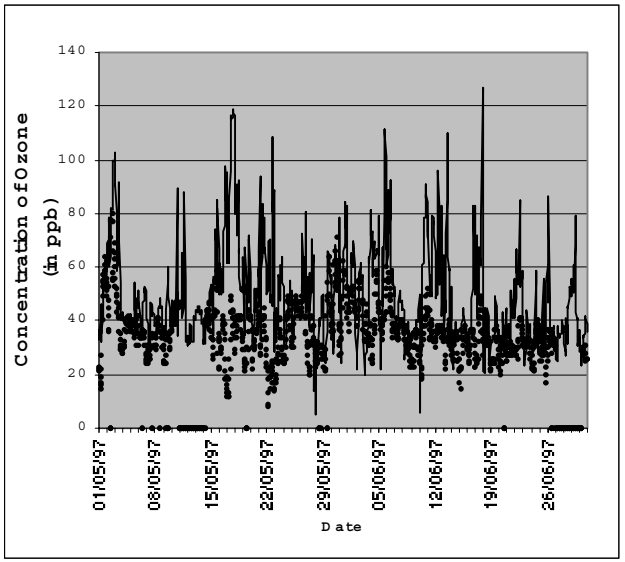
Concentration of Ozone (in ppb)
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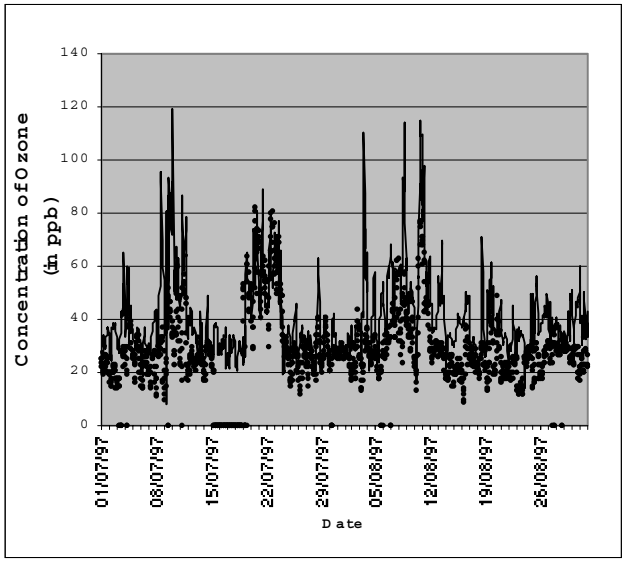
Concentration of Ozone (in ppb)
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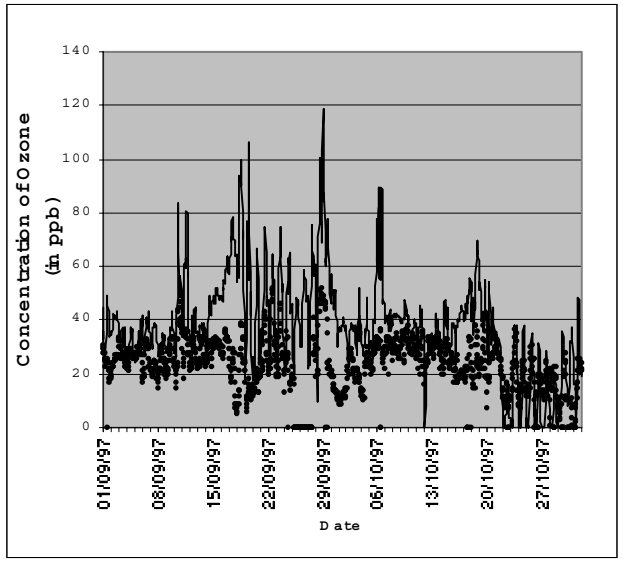
Concentration of Ozone (in ppb)
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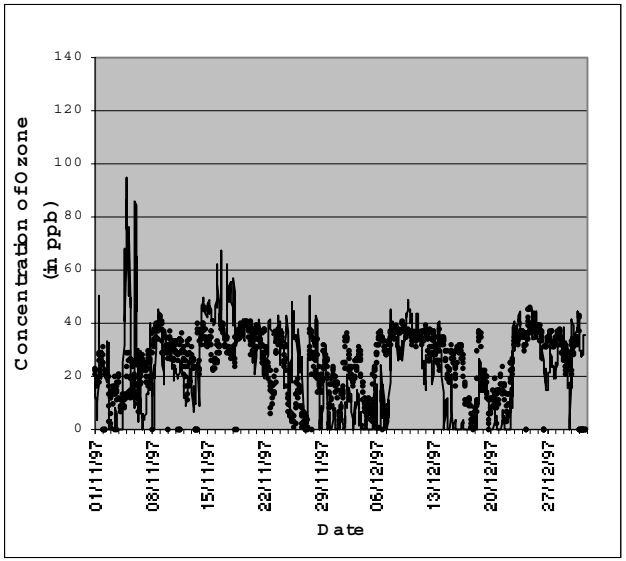
Concentration of Ozone (in ppb)
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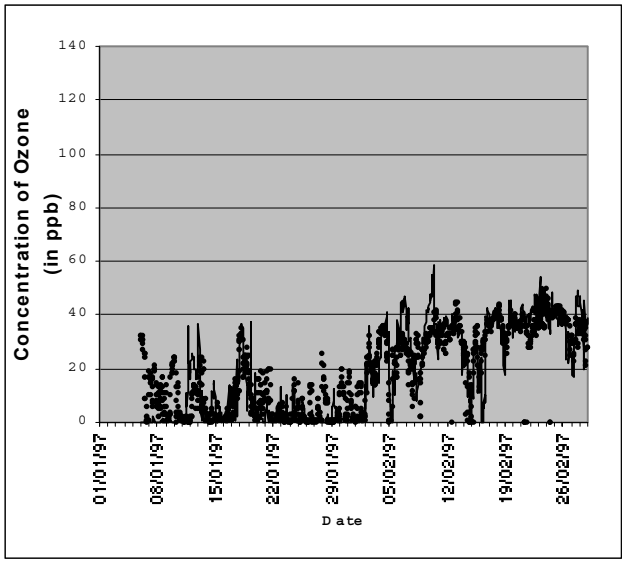
Date

Harwell


Concentration of Ozone (in ppb)
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01/01/97
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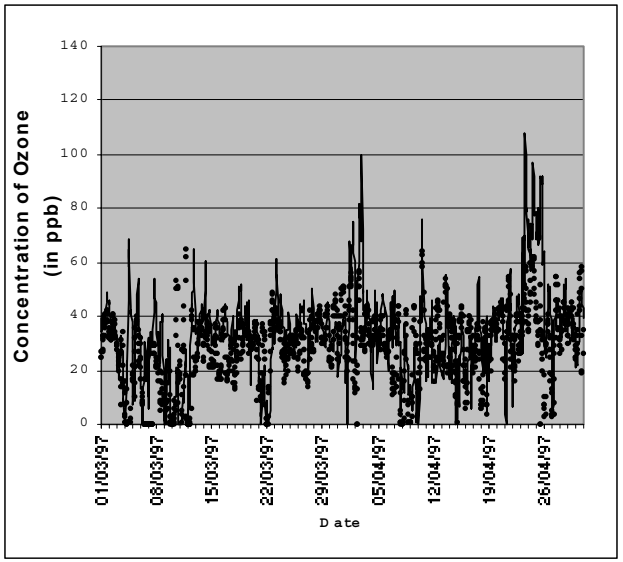
Concentration of Ozone (in ppb)
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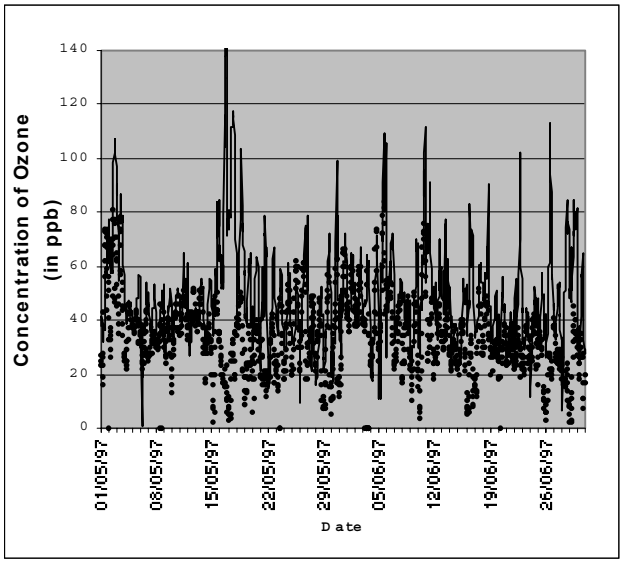
Concentration of Ozone (in ppb)
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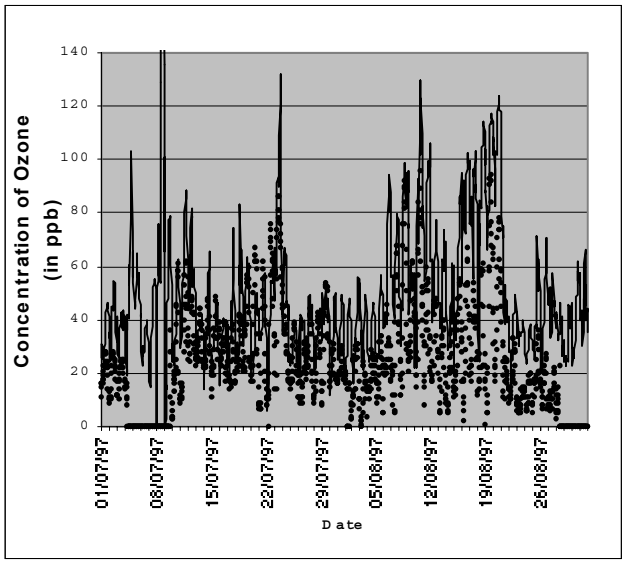
Concentration of Ozone (in ppb)
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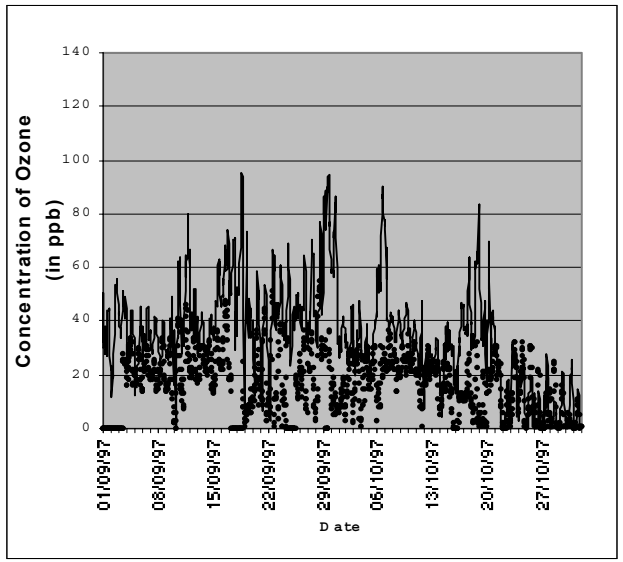
Concentration of Ozone (in ppb)
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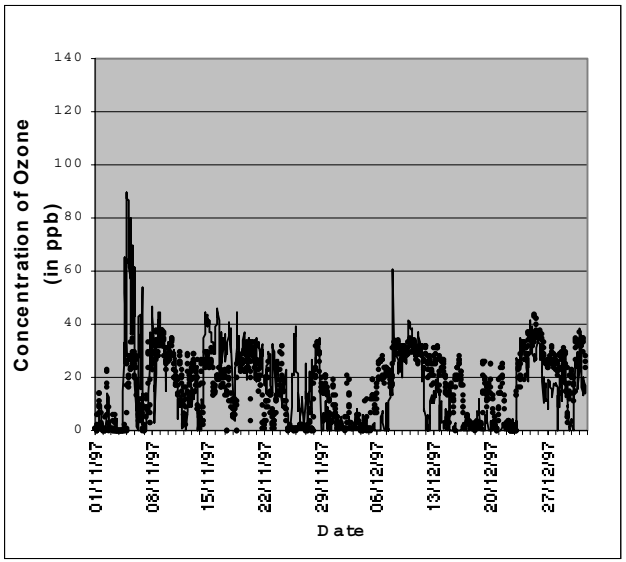
Date


Concentration of Ozone (in ppb)
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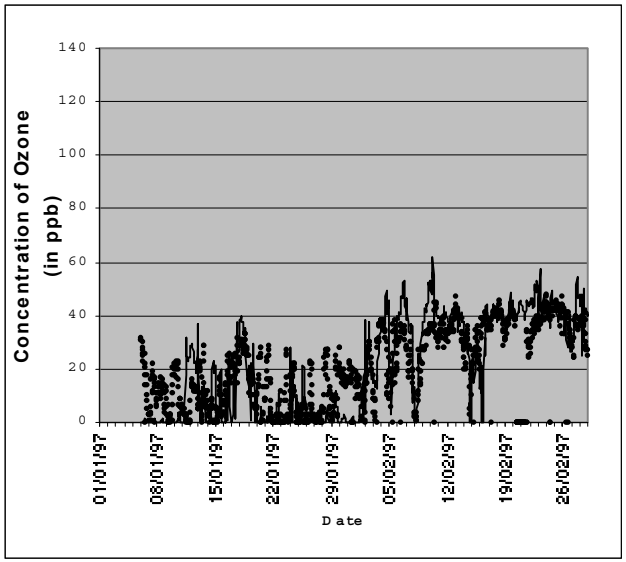
27/12/97
Date

Somerton


Concentration of Ozone (in ppb)
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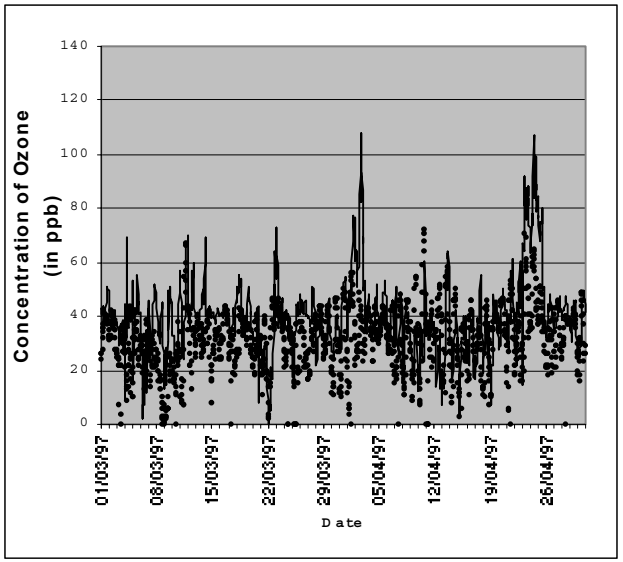
26/02/97
Date


Concentration of Ozone (in ppb)
0
20
40
60
80
100
120
140
01/03/97
08/03/97
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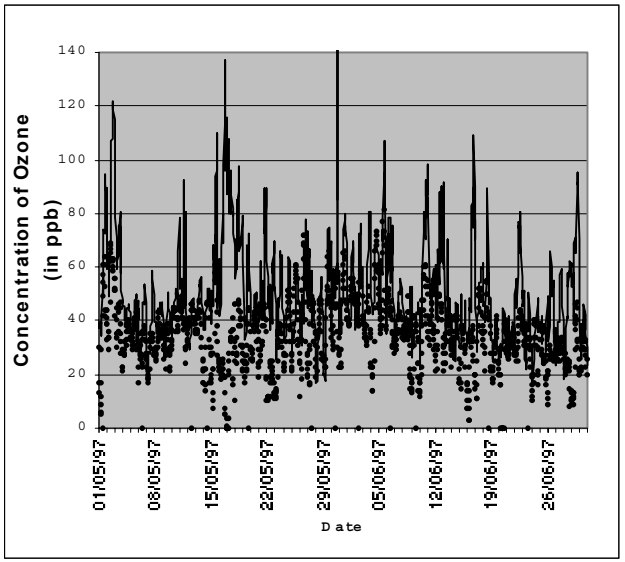
22/03/97
29/03/97
05/04/97
12/04/97
19/04/97
26/04/97
Date


Concentration of Ozone (in ppb)
0
20
40
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80
100
120
140
01/05/97
08/05/97
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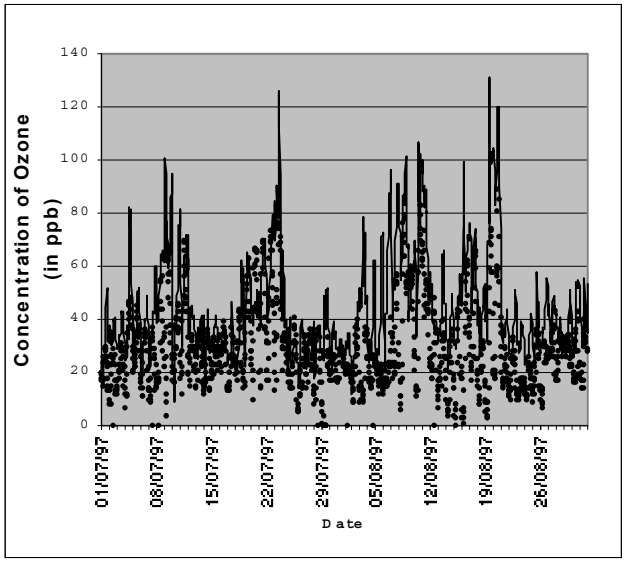
19/06/97
26/06/97
Date


Concentration of Ozone (in ppb)
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40
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100
120
140
01/07/97
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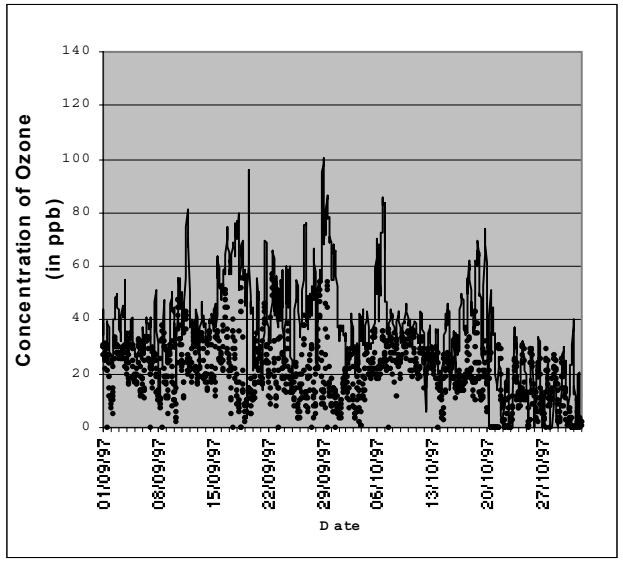
19/08/97
26/08/97
Date


Concentration of Ozone (in ppb)
0
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140
01/09/97
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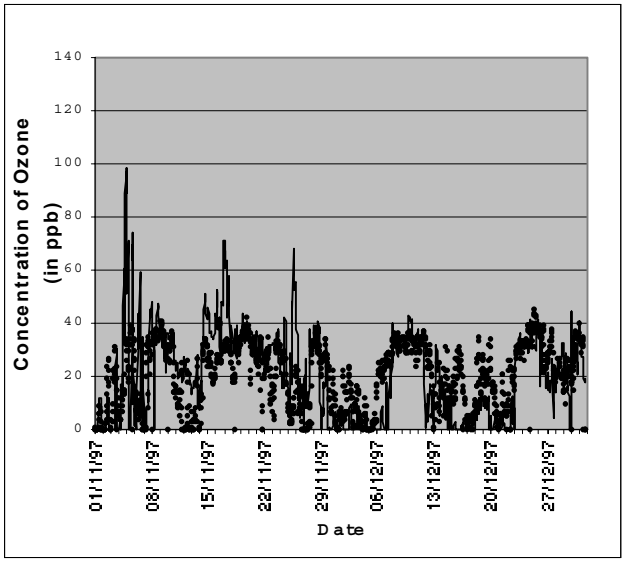
13/10/97
20/10/97
27/10/97
Date


Concentration of Ozone (in ppb)
0
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01/11/97
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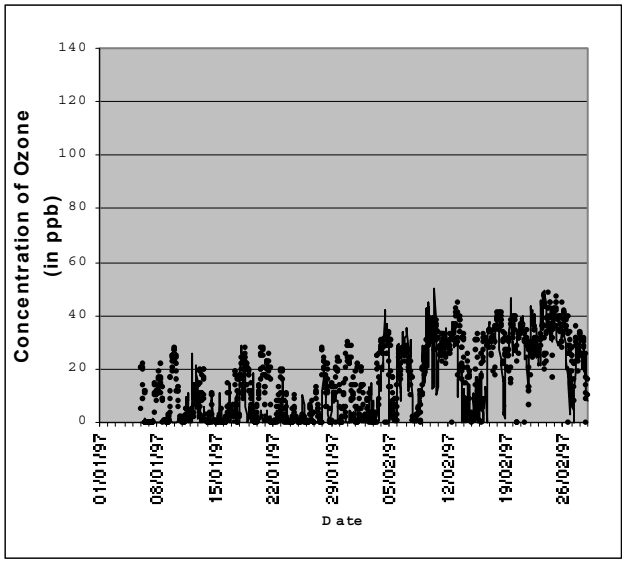
20/12/97
27/12/97
Date

Rochester


Concentration of Ozone (in ppb)
0
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120
140
01/01/97
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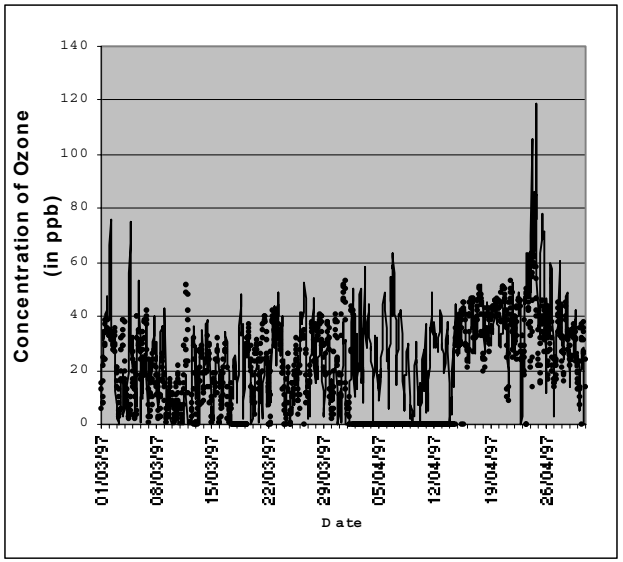
12/02/97
19/02/97
26/02/97
Date


Concentration of Ozone (in ppb)
0
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140
01/03/97
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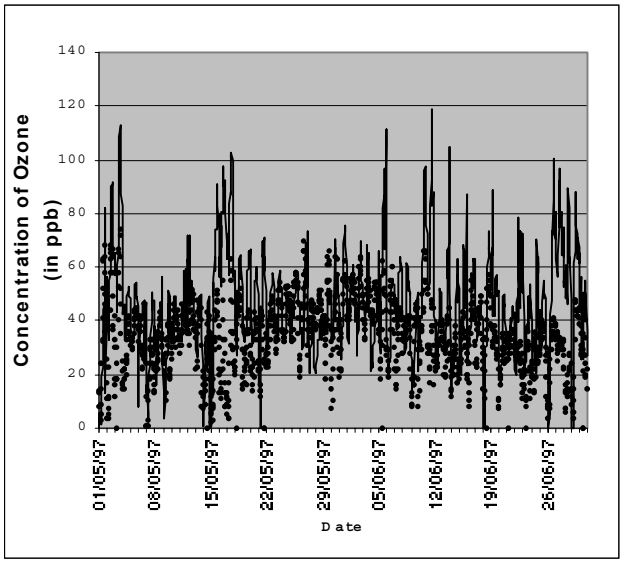
26/04/97
Date


Concentration of Ozone (in ppb)
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01/05/97
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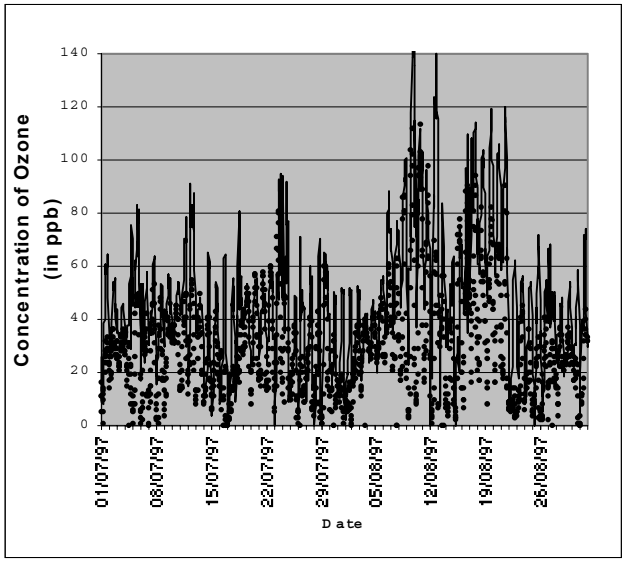
26/06/97
Date


Concentration of Ozone (in ppb)
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01/07/97
08/07/97
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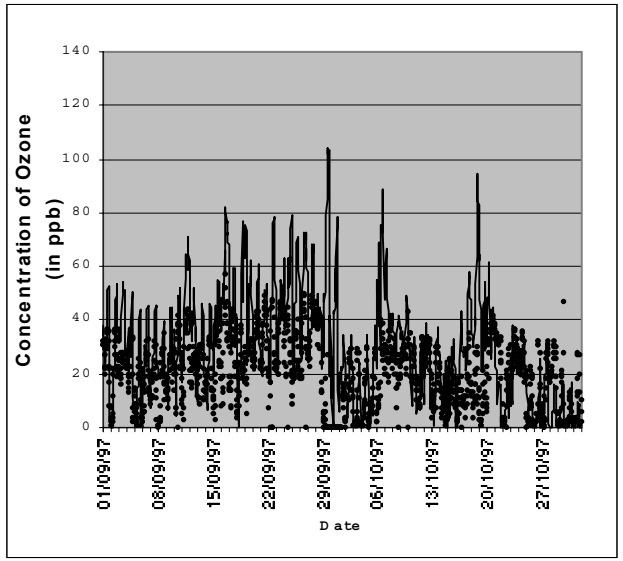
12/08/97
19/08/97
26/08/97
Date


Concentration of Ozone (in ppb)
0
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01/09/97
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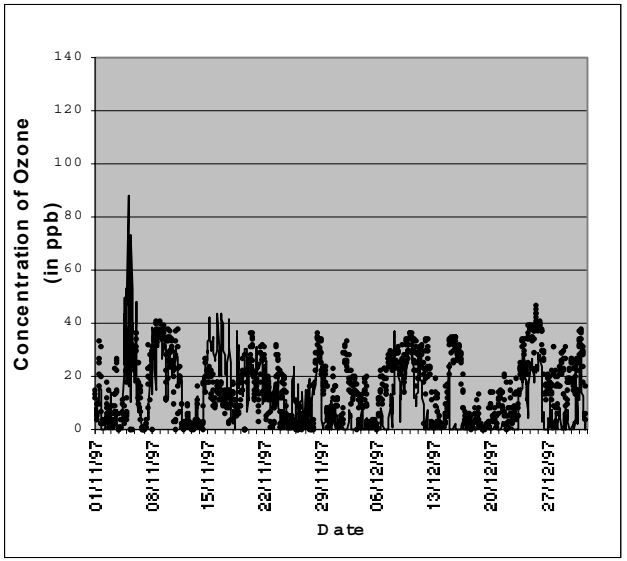
13/10/97
20/10/97
27/10/97
Date


Concentration of Ozone (in ppb)
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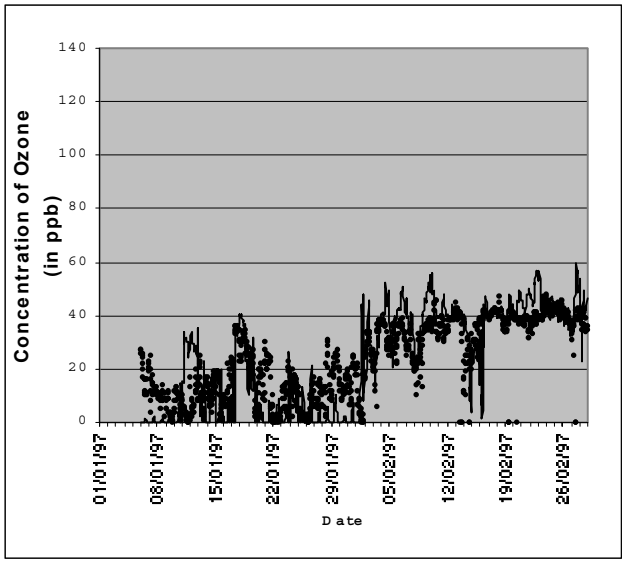
01/11/97
08/11/97
15/11/97
22/11/97
29/11/97
06/12/97
13/12/97
20/12/97
27/12/97
Date

Yarner Wood


Concentration of Ozone (in ppb)
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01/01/97
08/01/97
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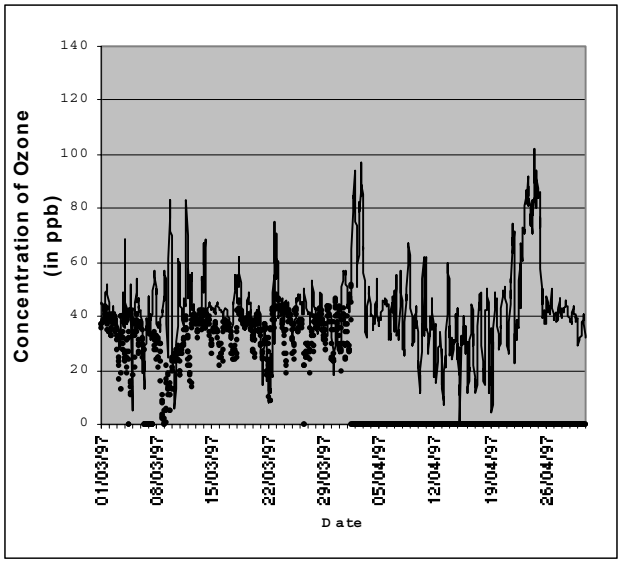
05/02/97
12/02/97
19/02/97
26/02/97
Date


Concentration of Ozone (in ppb)
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01/03/97
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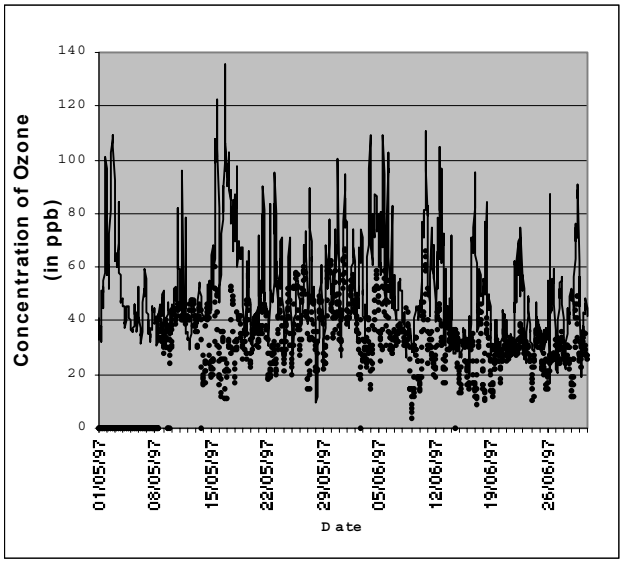
12/04/97
19/04/97
26/04/97
Date


Concentration of Ozone (in ppb)
0
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120
140
01/05/97
08/05/97
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22/05/97
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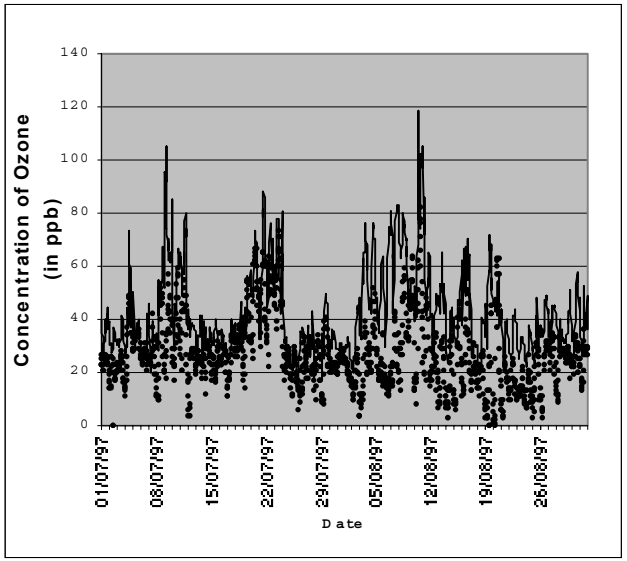
05/06/97
12/06/97
19/06/97
26/06/97
Date


Concentration of Ozone (in ppb)
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01/07/97
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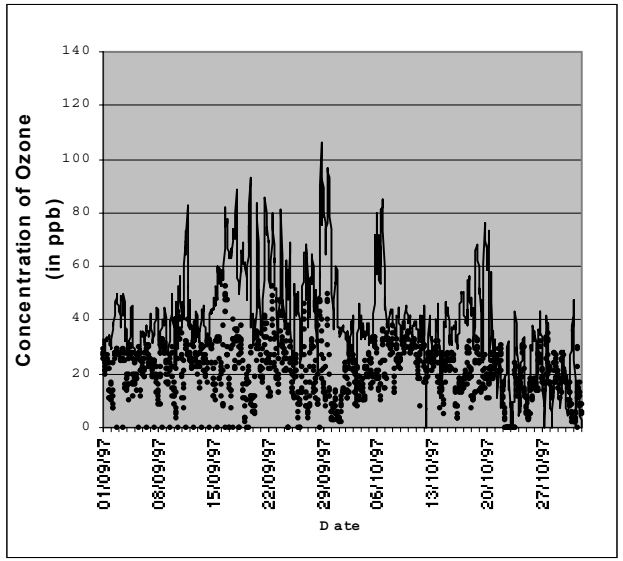
19/08/97
26/08/97
Date


Concentration of Ozone (in ppb)
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01/09/97
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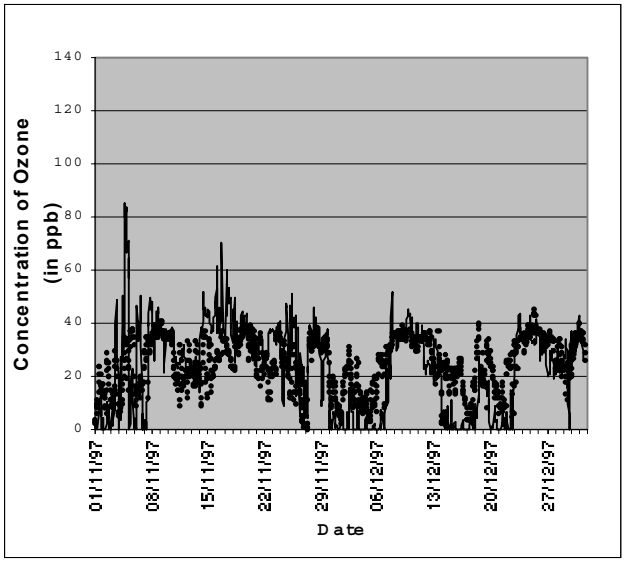
20/10/97
27/10/97
Date


Concentration of Ozone (in ppb)
0
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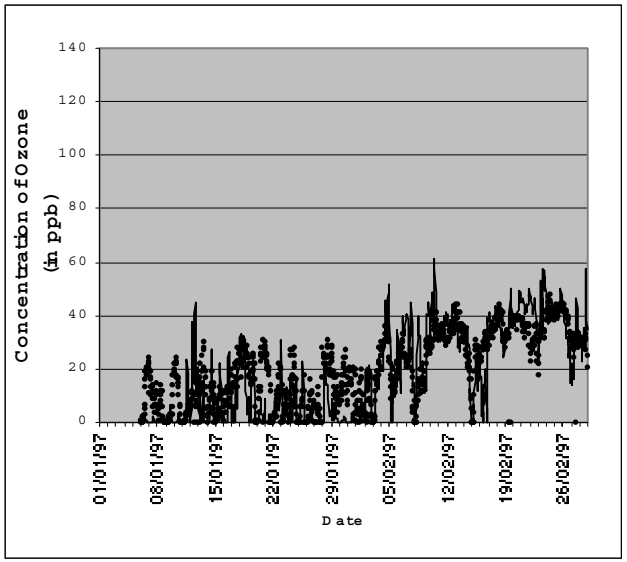
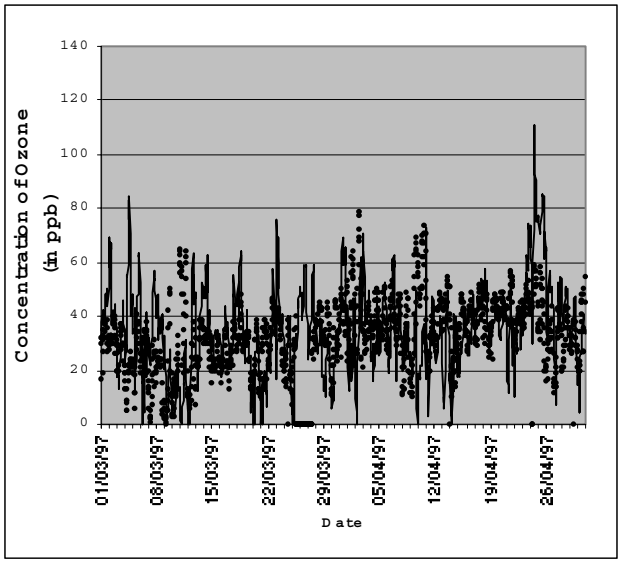
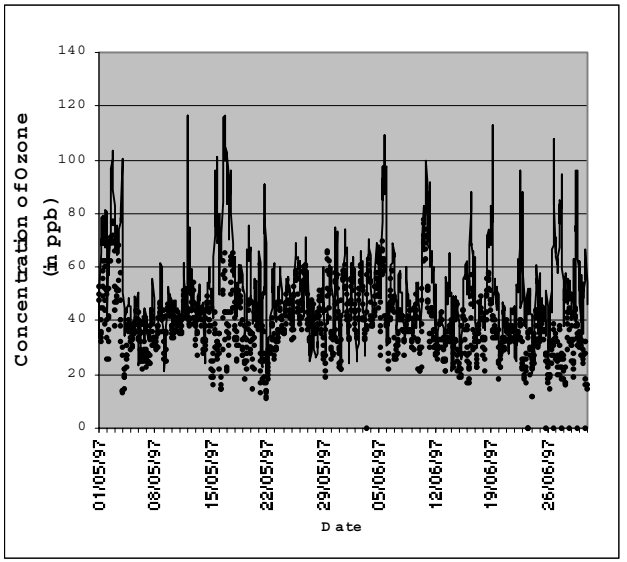
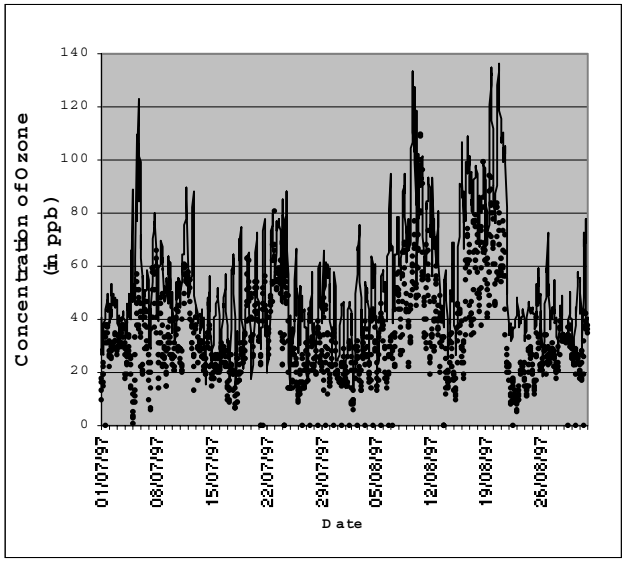
80
100
120
140
01/11/97
08/11/97
15/11/97
22/11/97
29/11/97
06/12/97
13/12/97
20/12/97
27/12/97
Date

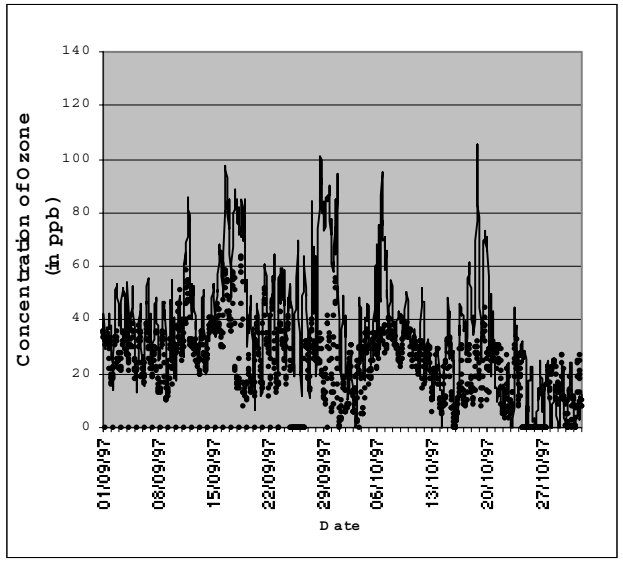
Lullington Heath

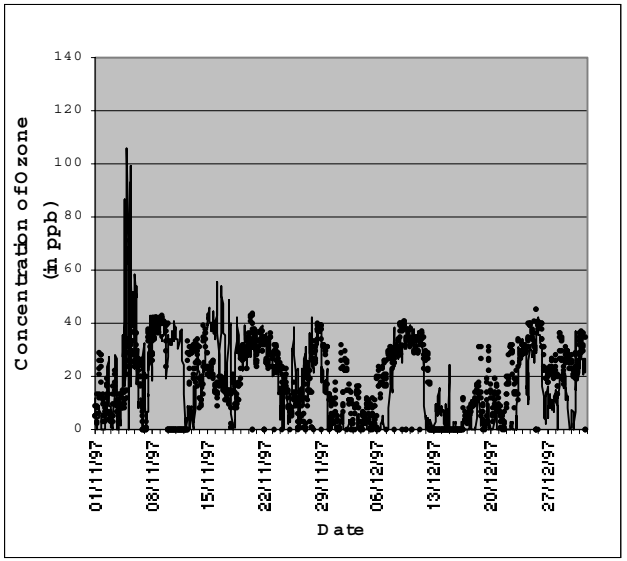




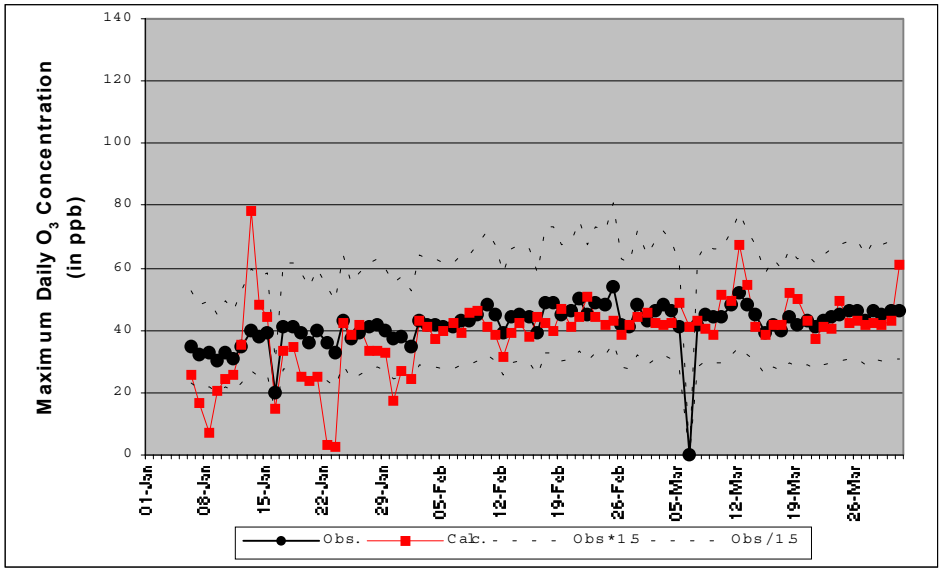


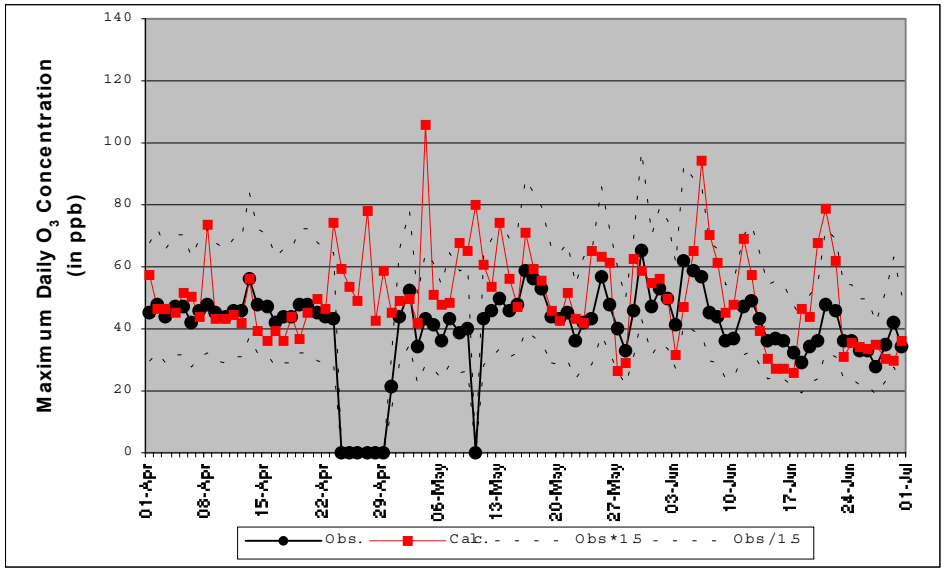


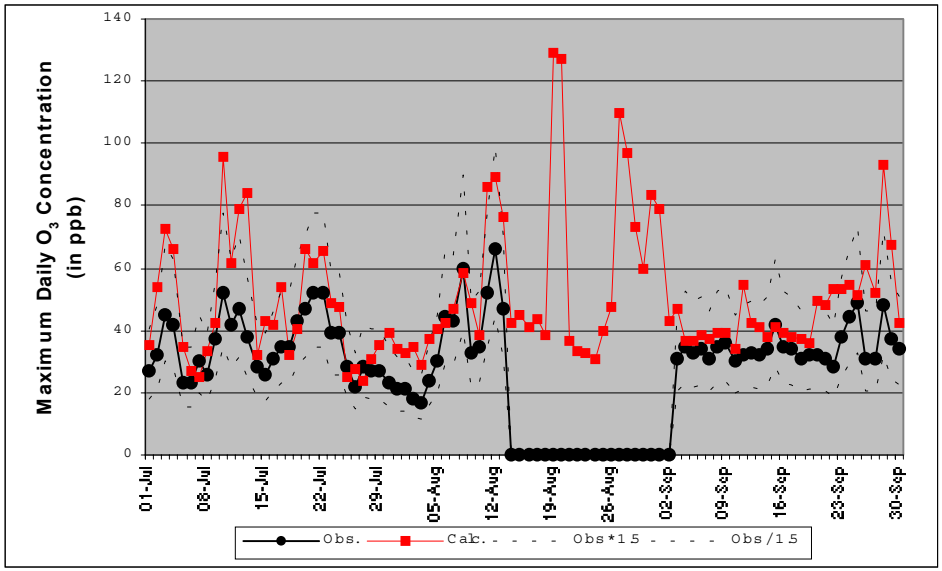


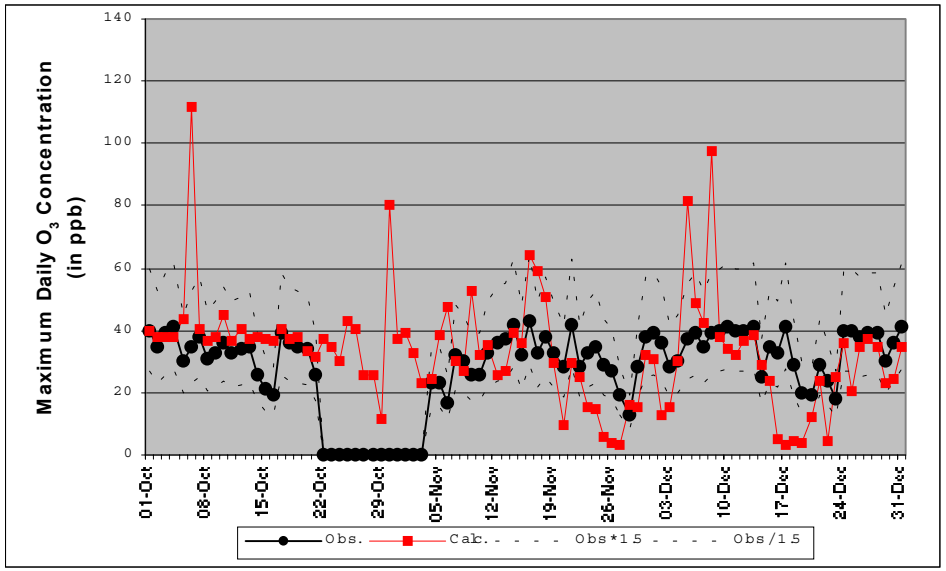


Strathvaich Dam

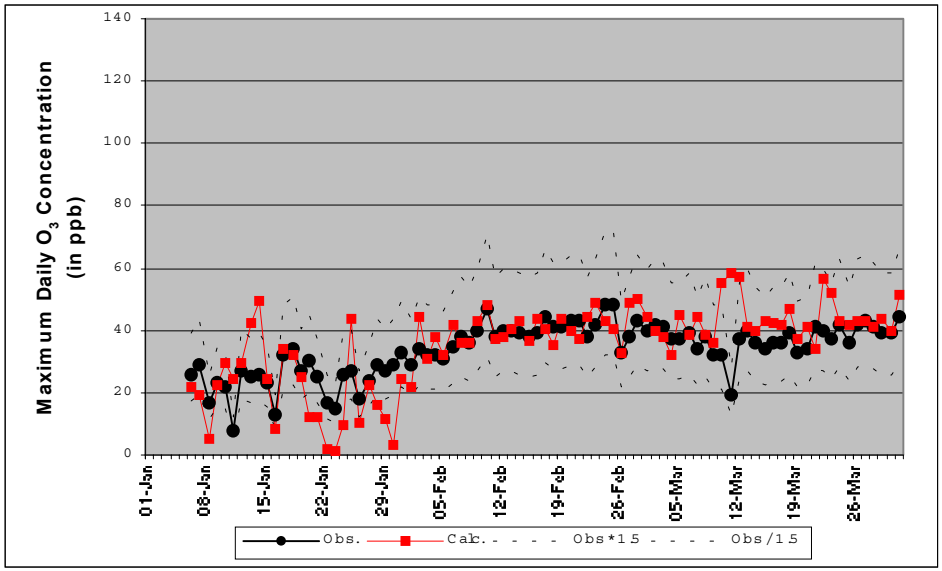


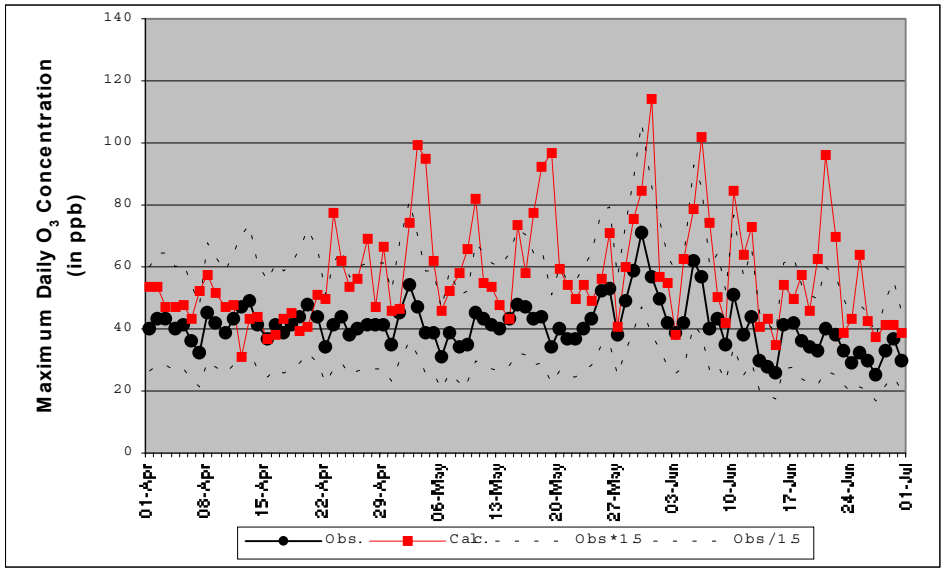


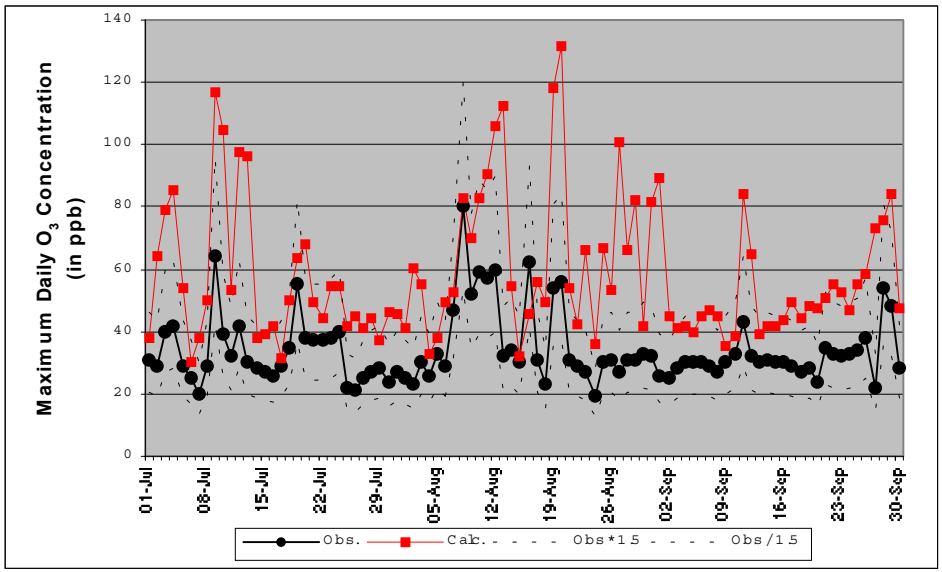




Bush Estate


Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Jan
08-Jan
15-Jan
22-Jan
29-Jan
05-Feb
12-Feb
19-Feb
26-Feb
05-Mar
12-Mar
19-Mar
26-Mar
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Apr
08-Apr
15-Apr
22-Apr
29-Apr
06-May
13-May
20-May
27-May
03-Jun
10-Jun
17-Jun
24-Jun
01-Jul
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
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80
100
120
140
01-Jul
08-Jul
15-Jul
22-Jul
29-Jul
05-Aug
12-Aug
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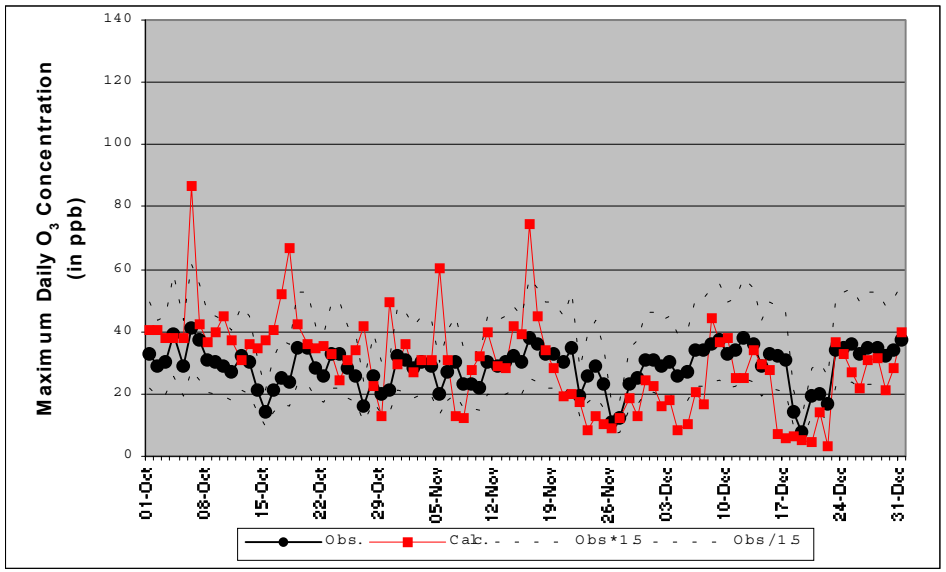
26-Aug
02-Sep
09-Sep
16-Sep
23-Sep
30-Sep
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
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20
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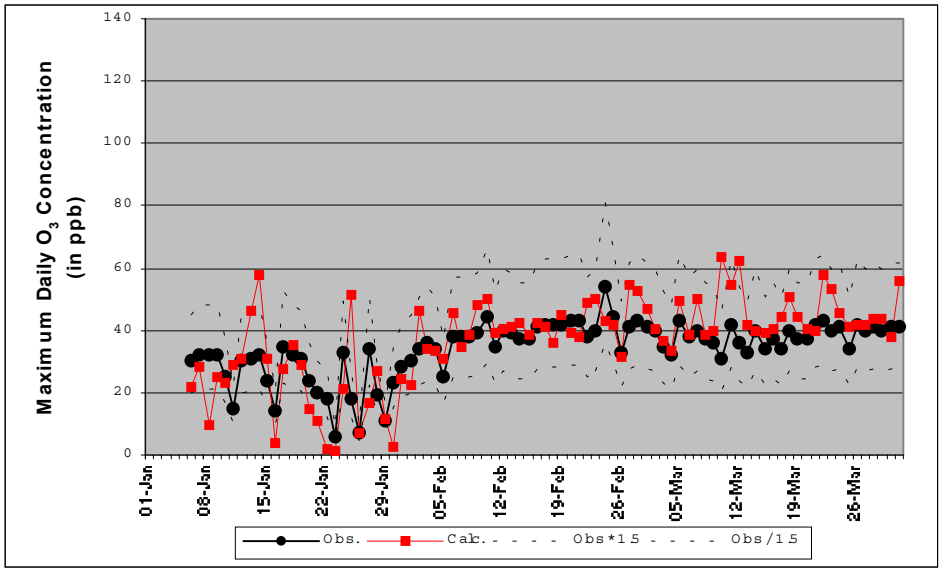
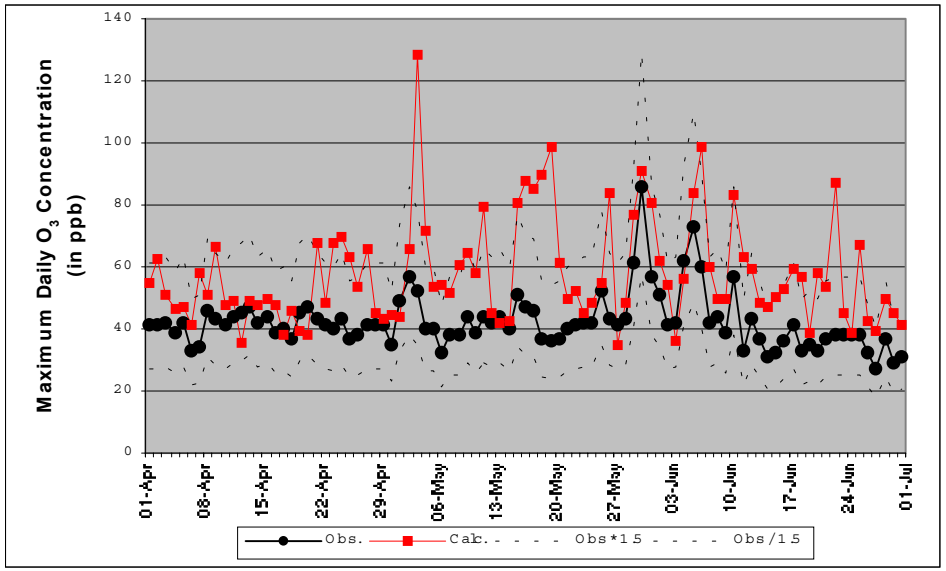
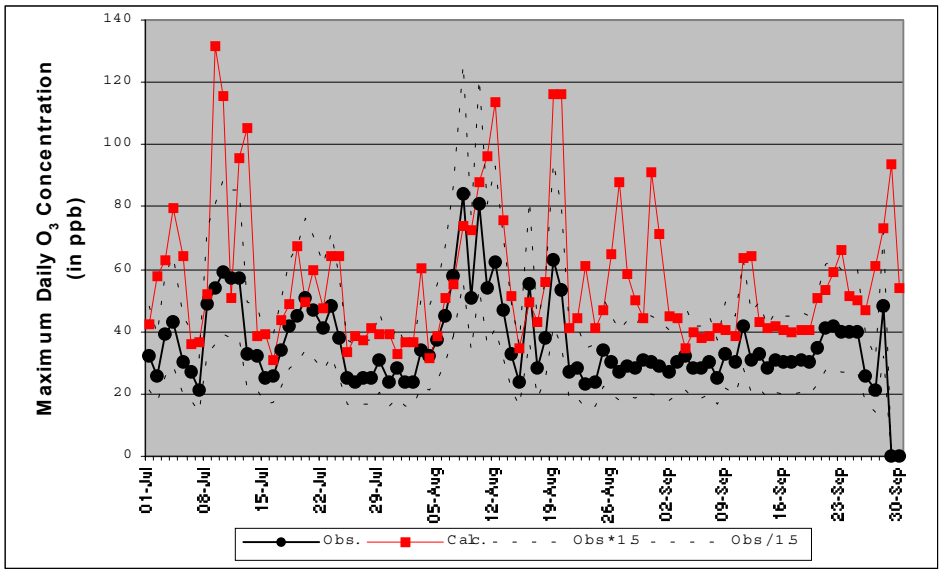
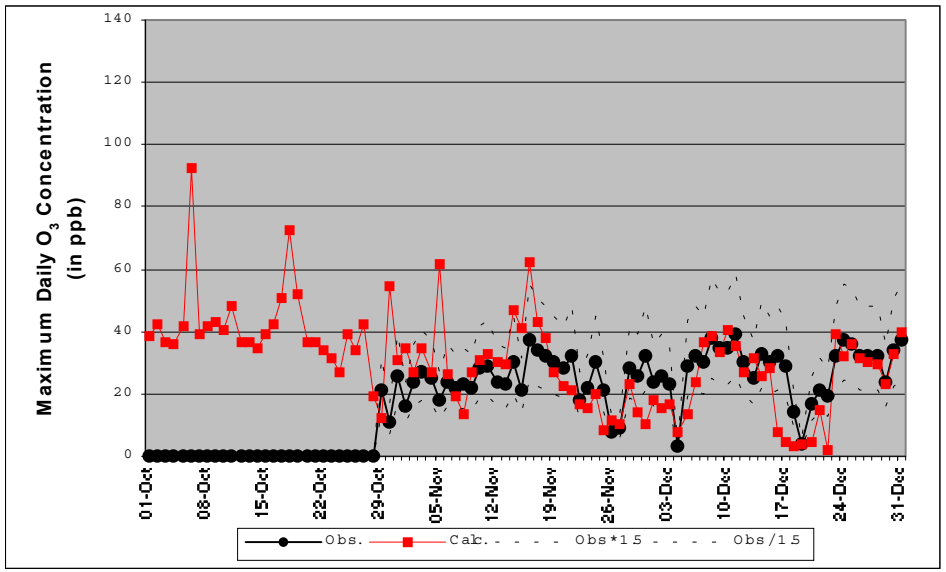
60
80
100
120
140
01-Oct
08-Oct
15-Oct
22-Oct
29-Oct
05-Nov
12-Nov
19-Nov
26-Nov
03-Dec
10-Dec
17-Dec
24-Dec
31-Dec
Obs.
Calc.
Obs*1.5
Obs/1.5

Eskdalemuir

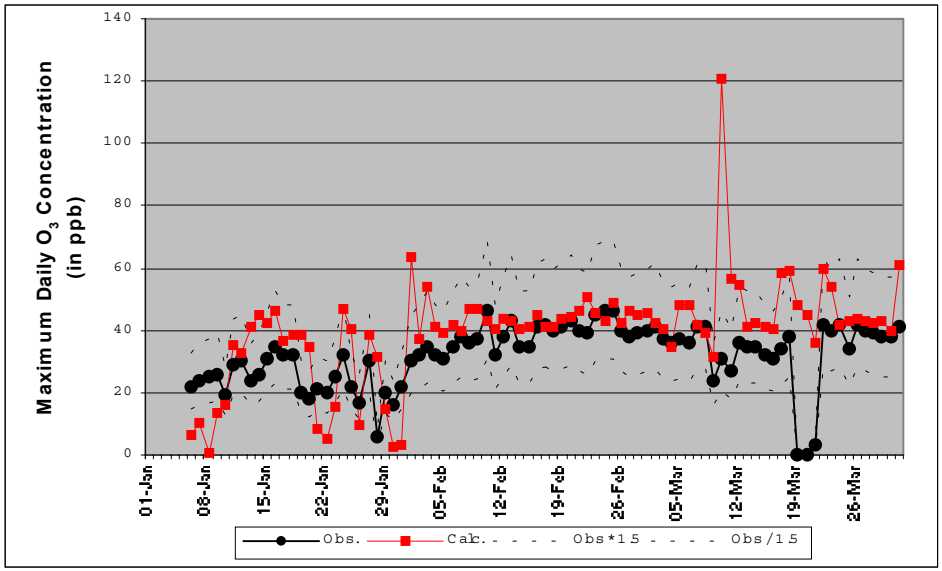








Lough Navar


Maximum Daily O_3 Concentration (in ppb)
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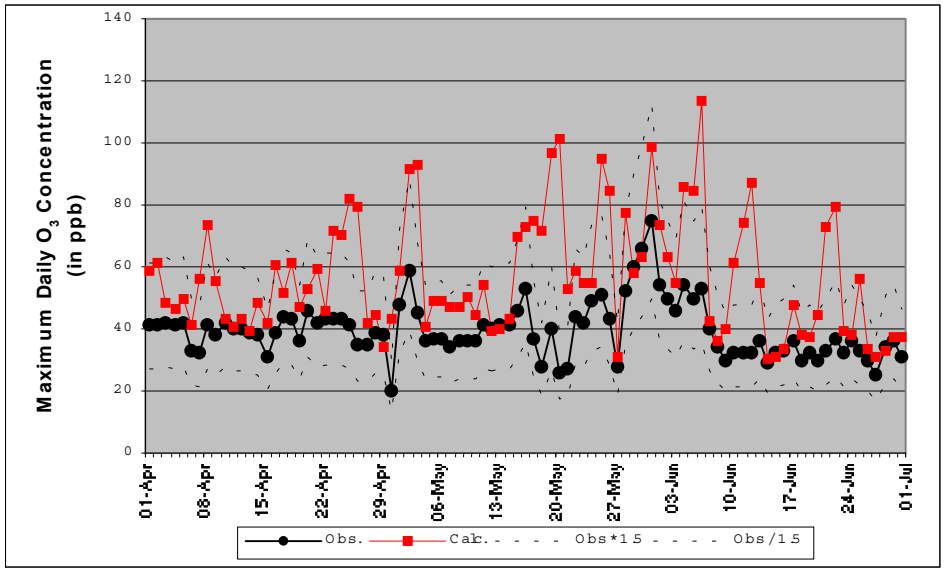
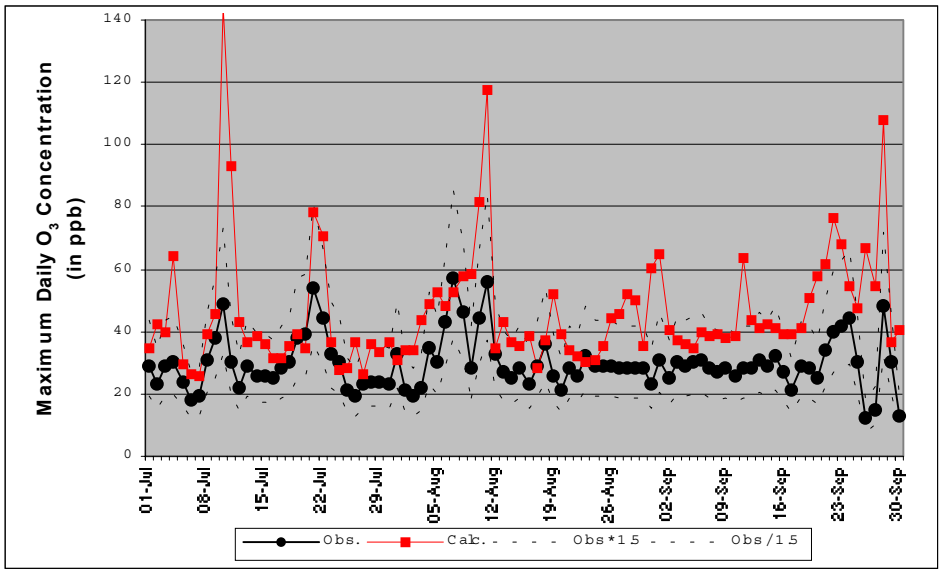
20
40
60
80
100
120
140
01-Jan
08-Jan
15-Jan
22-Jan
29-Jan
05-Feb
12-Feb
19-Feb
26-Feb
05-Mar
12-Mar
19-Mar
26-Mar
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Apr
08-Apr
15-Apr
22-Apr
29-Apr
06-May
13-May
20-May
27-May
03-Jun
10-Jun
17-Jun
24-Jun
01-Jul
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
0
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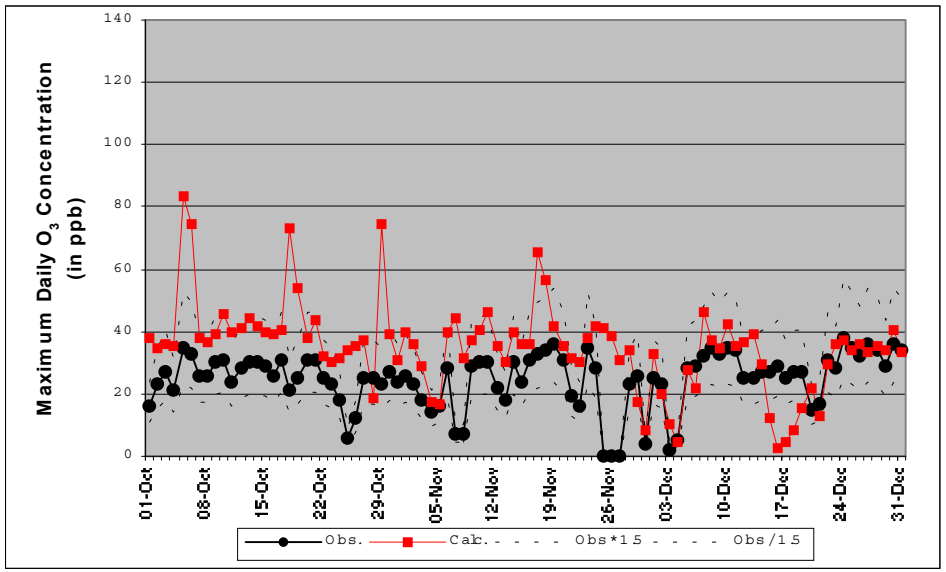
60
80
100
120
140
01-Jul
08-Jul
15-Jul
22-Jul
29-Jul
05-Aug
12-Aug
19-Aug
26-Aug
02-Sep
09-Sep
16-Sep
23-Sep
30-Sep
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
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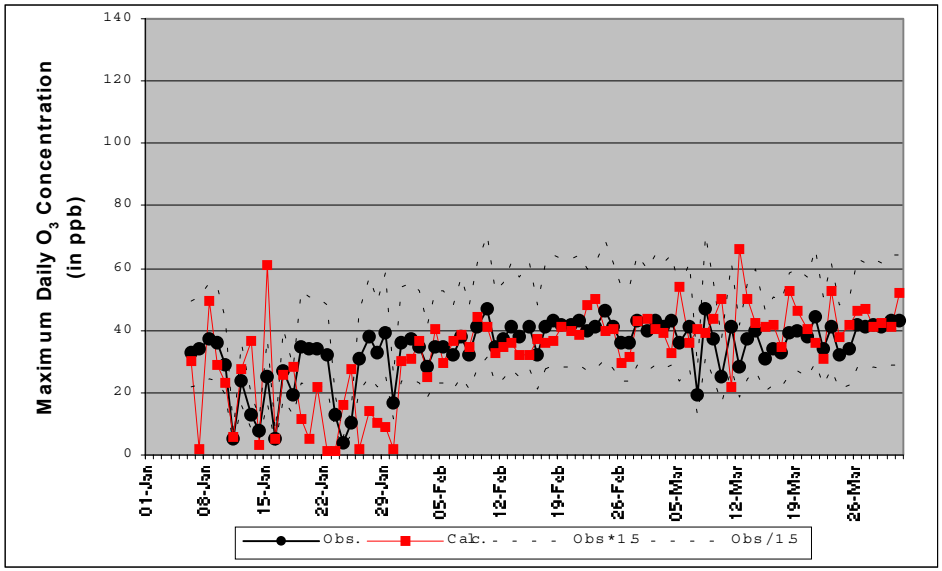
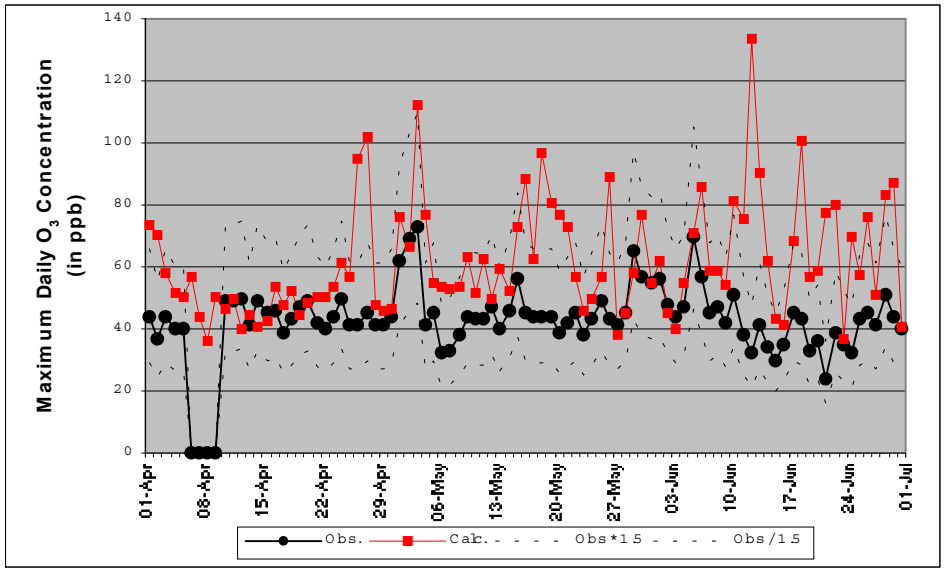
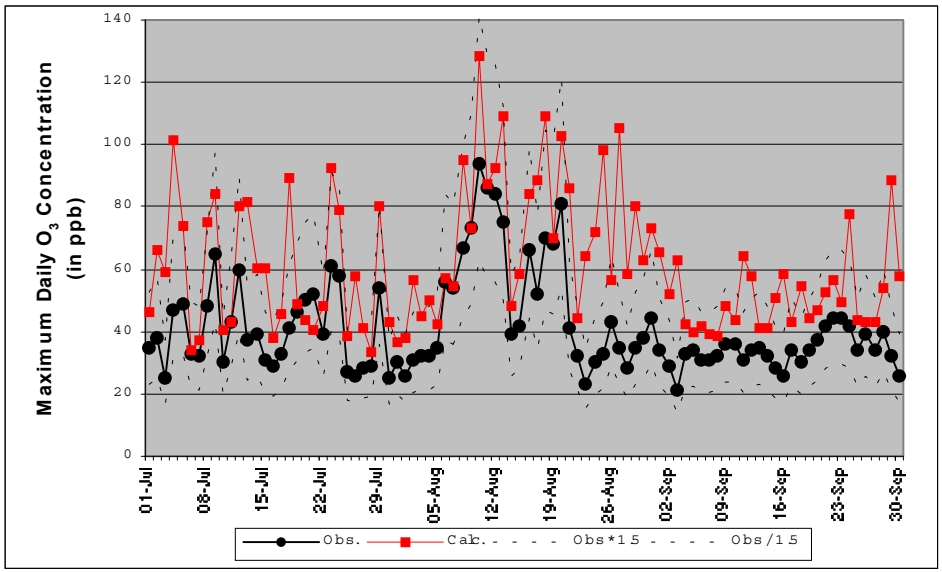
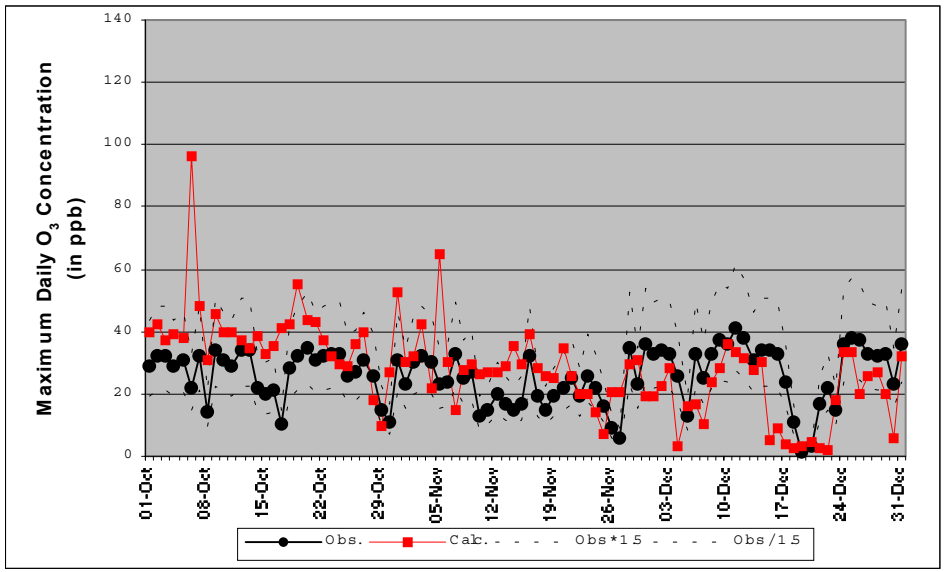
60
80
100
120
140
01-Oct
08-Oct
15-Oct
22-Oct
29-Oct
05-Nov
12-Nov
19-Nov
26-Nov
03-Dec
10-Dec
17-Dec
24-Dec
31-Dec
Obs.
Calc.
Obs*1.5
Obs/1.5

High Muffles

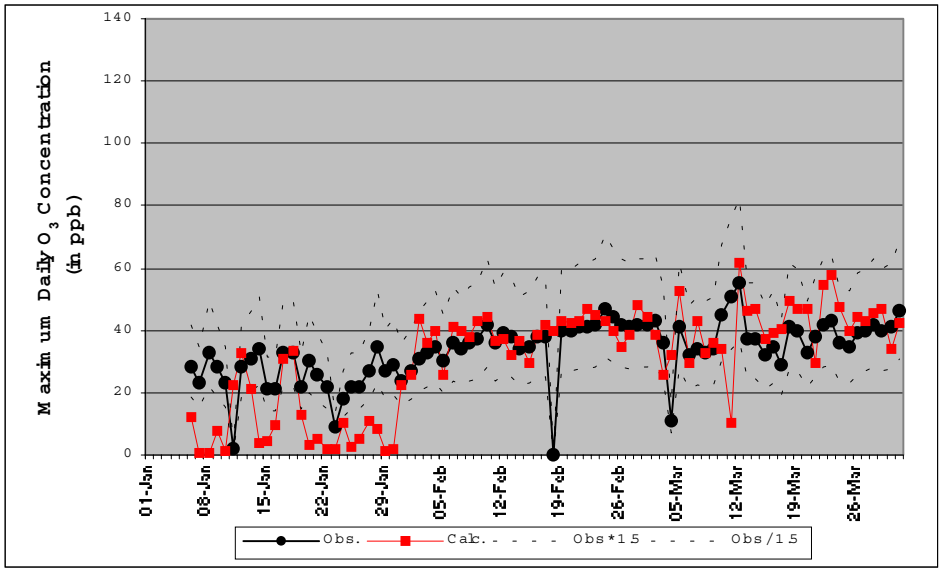


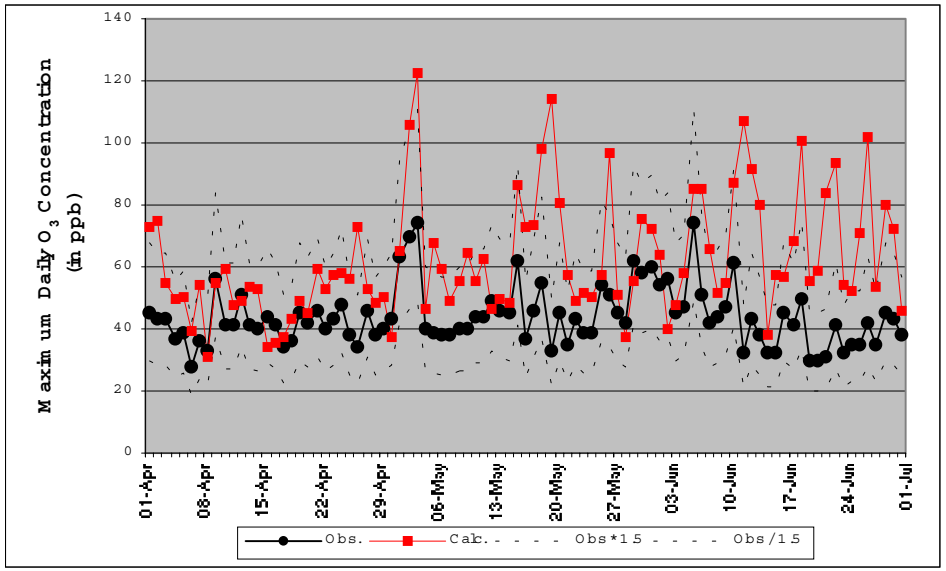


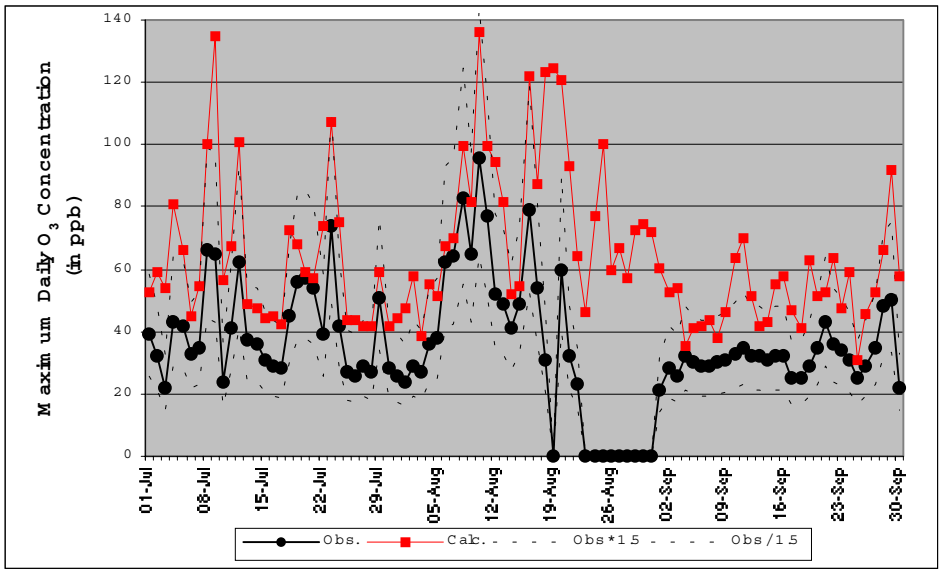


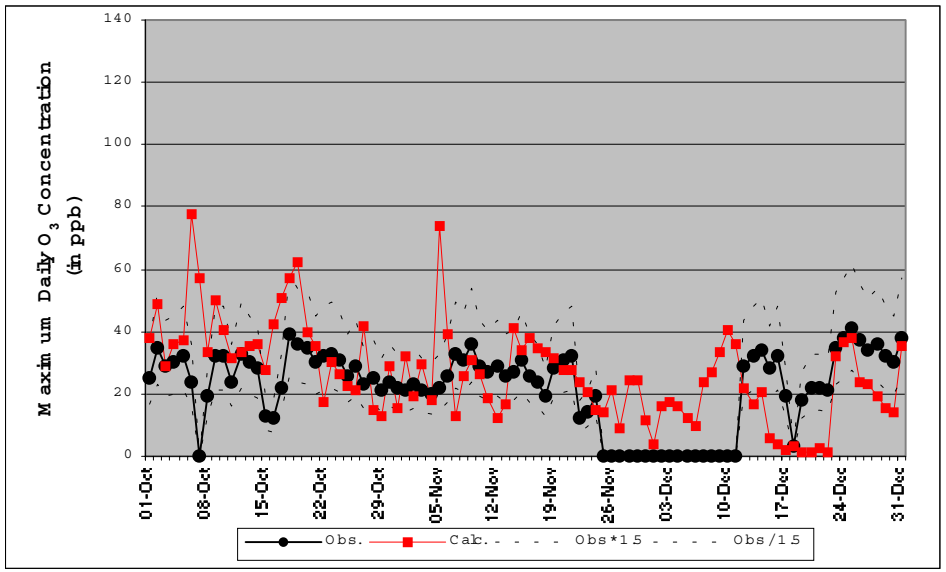


Ladybower

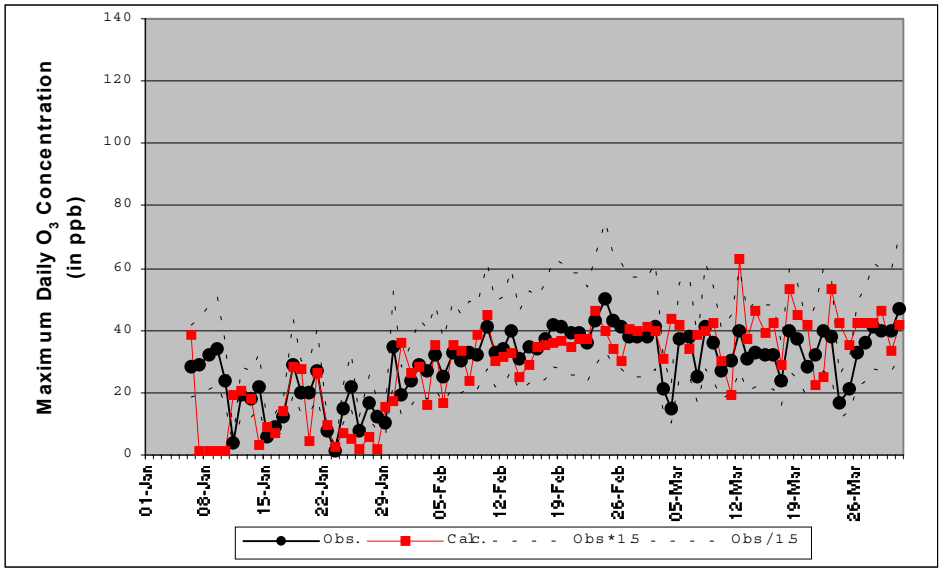

Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Jan
08-Jan
15-Jan
22-Jan
29-Jan
05-Feb
12-Feb
19-Feb
26-Feb
05-Mar
12-Mar
19-Mar
26-Mar
Obs.
Calc.
Obs*1.5
Obs/1.5

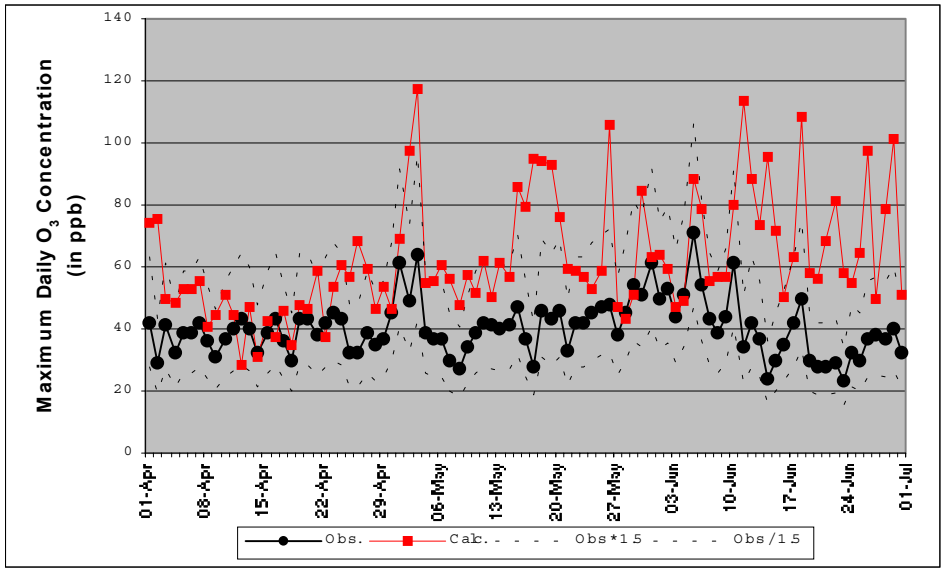

Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Apr
08-Apr
15-Apr
22-Apr
29-Apr
06-May
13-May
20-May
27-May
03-Jun
10-Jun
17-Jun
24-Jun
01-Jul
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Jul
08-Jul
15-Jul
22-Jul
29-Jul
05-Aug
12-Aug
19-Aug
26-Aug
02-Sep
09-Sep
16-Sep
23-Sep
30-Sep
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Oct
08-Oct
15-Oct
22-Oct
29-Oct
05-Nov
12-Nov
19-Nov
26-Nov
03-Dec
10-Dec
17-Dec
24-Dec
31-Dec
Obs.
Calc.
Obs*1.5
Obs/1.5

Bottesford


Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Jan
08-Jan
15-Jan
22-Jan
29-Jan
05-Feb
12-Feb
19-Feb
26-Feb
05-Mar
12-Mar
19-Mar
26-Mar
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
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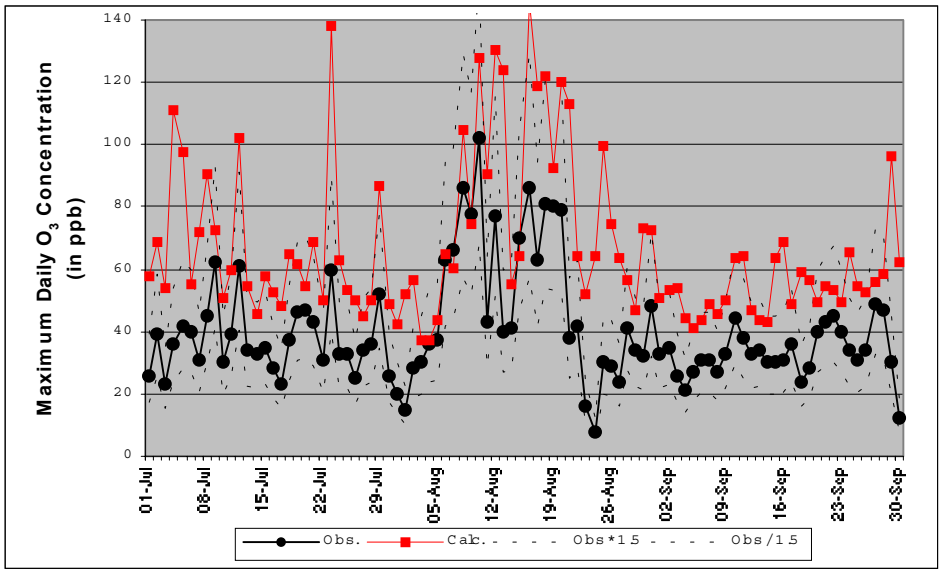
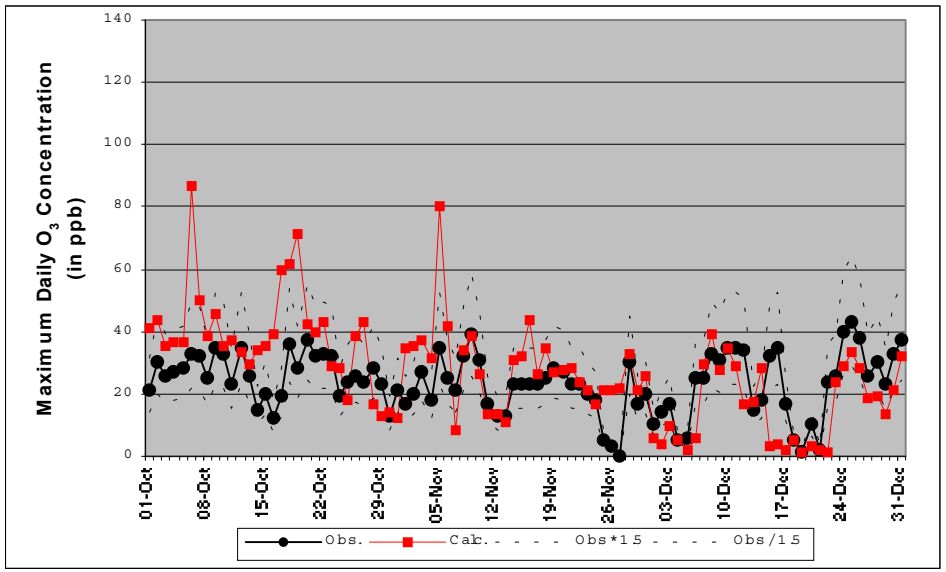
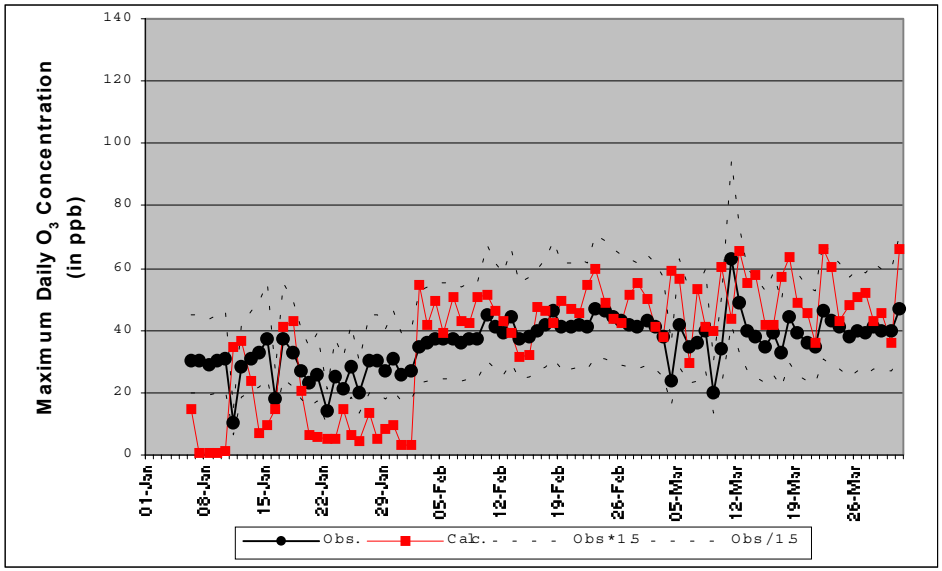
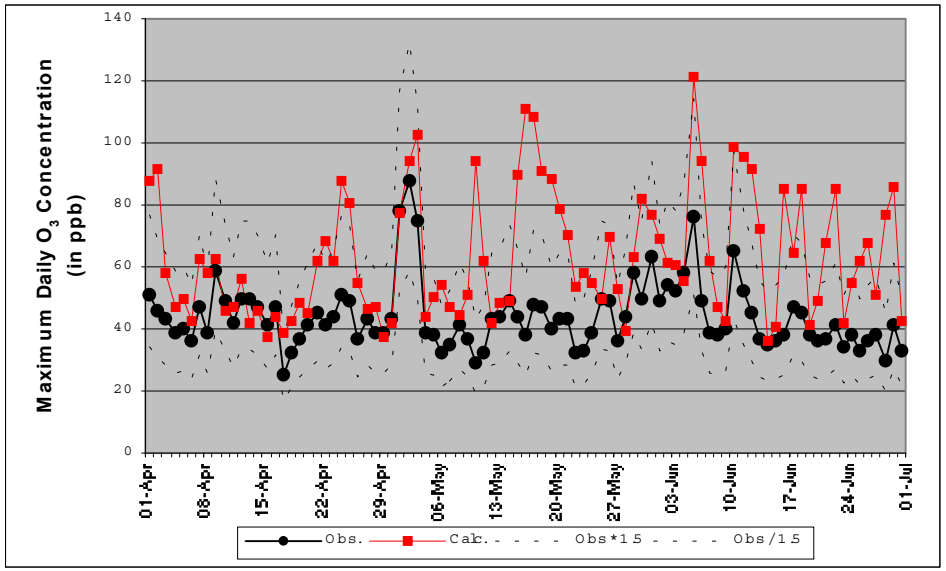
40
60
80
100
120
140
01-Apr
08-Apr
15-Apr
22-Apr
29-Apr
06-May
13-May
20-May
27-May
03-Jun
10-Jun
17-Jun
24-Jun
01-Jul
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Jul
08-Jul
15-Jul
22-Jul
29-Jul
05-Aug
12-Aug
19-Aug
26-Aug
02-Sep
09-Sep
16-Sep
23-Sep
30-Sep
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Oct
08-Oct
15-Oct
22-Oct
29-Oct
05-Nov
12-Nov
19-Nov
26-Nov
03-Dec
10-Dec
17-Dec
24-Dec
31-Dec
Obs.
Calc.
Obs*1.5
Obs/1.5

Aston Hill


Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Jan
08-Jan
15-Jan
22-Jan
29-Jan
05-Feb
12-Feb
19-Feb
26-Feb
05-Mar
12-Mar
19-Mar
26-Mar
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
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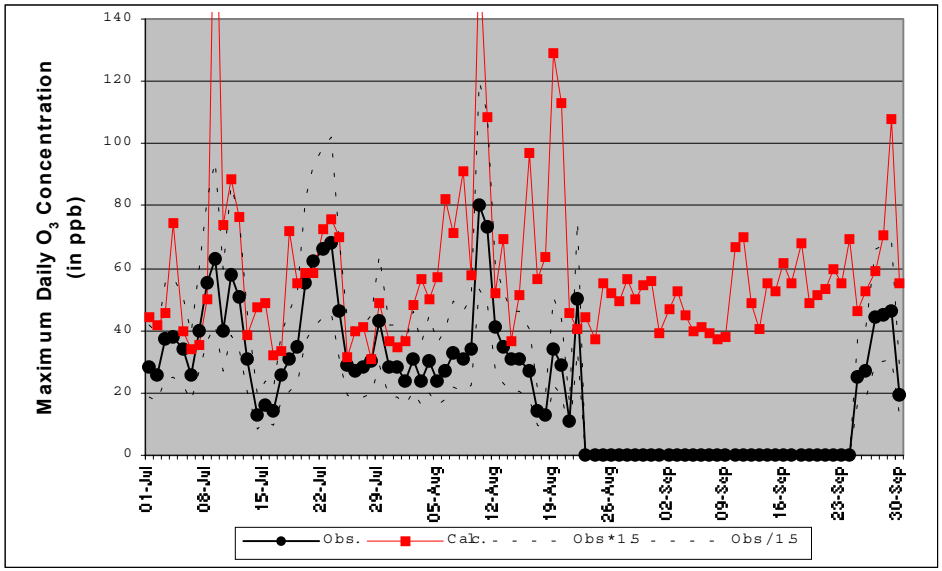
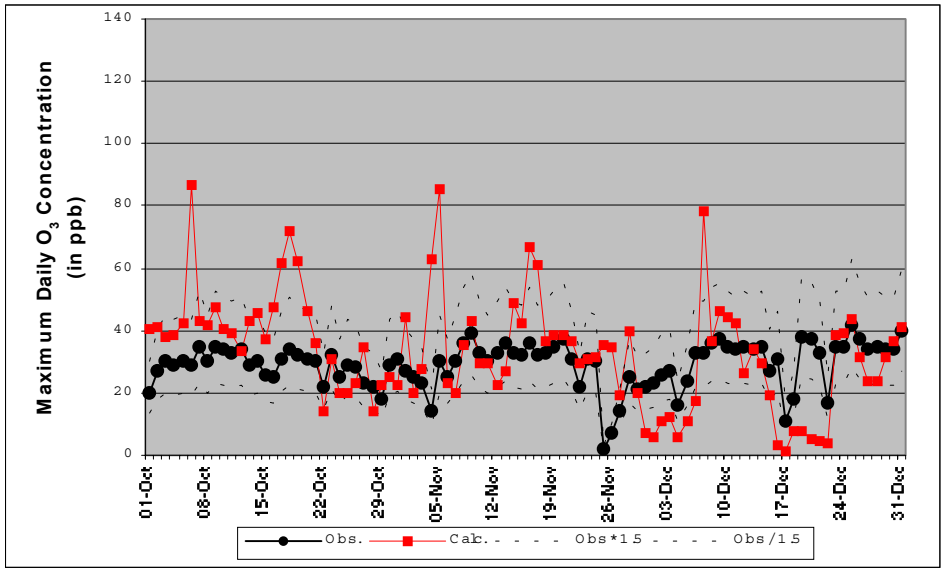
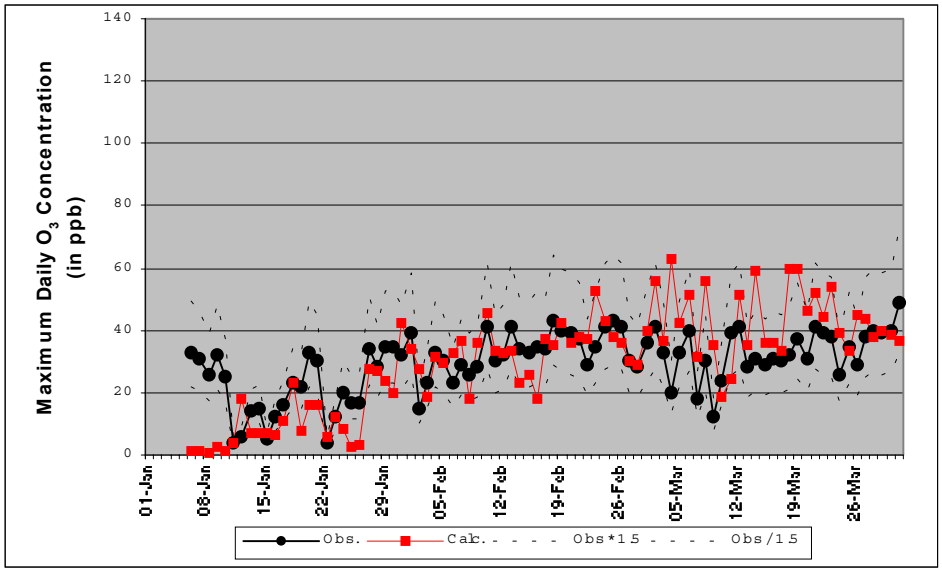
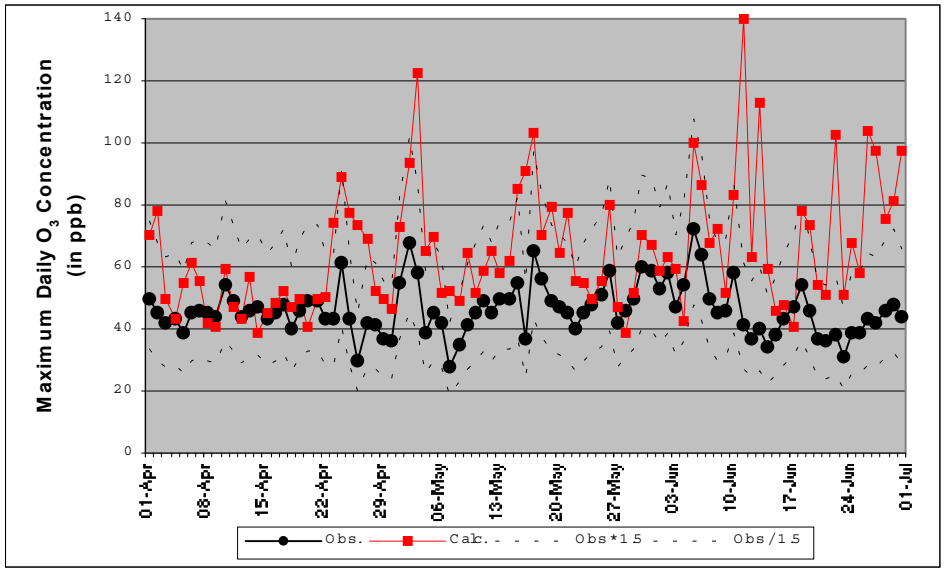
20
40
60
80
100
120
140
01-Apr
08-Apr
15-Apr
22-Apr
29-Apr
06-May
13-May
20-May
27-May
03-Jun
10-Jun
17-Jun
24-Jun
01-Jul
Obs.
Calc.
Obs*1.5
Obs/1.5

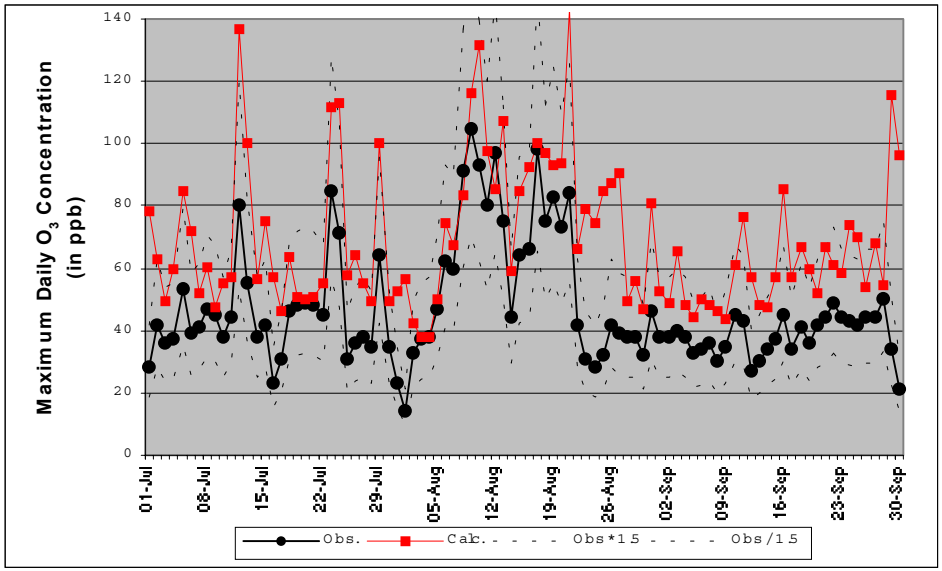

Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Jul
08-Jul
15-Jul
22-Jul
29-Jul
05-Aug
12-Aug
19-Aug
26-Aug
02-Sep
09-Sep
16-Sep
23-Sep
30-Sep
Obs.
Calc.
Obs*1.5
Obs/1.5

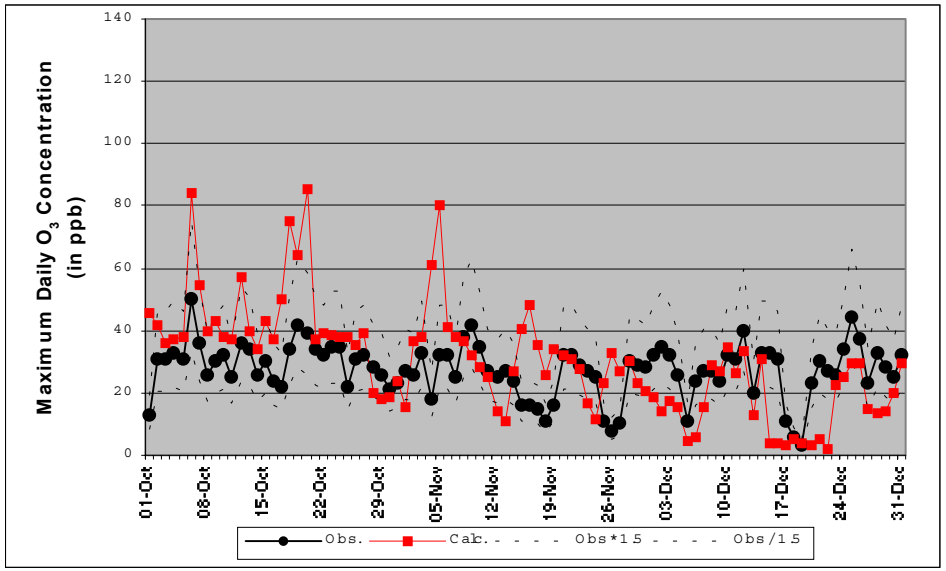

Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Oct
08-Oct
15-Oct
22-Oct
29-Oct
05-Nov
12-Nov
19-Nov
26-Nov
03-Dec
10-Dec
17-Dec
24-Dec
31-Dec
Obs.
Calc.
Obs*1.5
Obs/1.5

Sibton

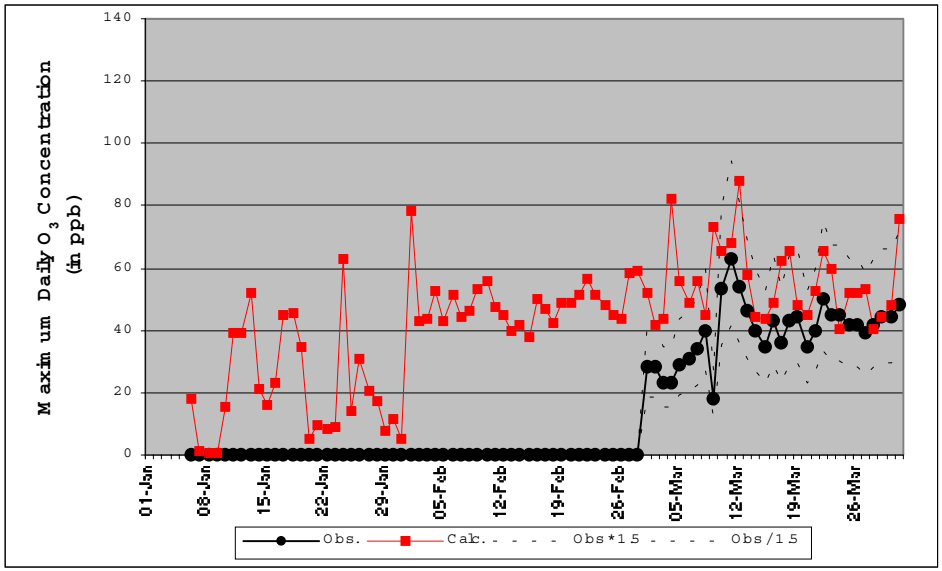

Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Jan
08-Jan
15-Jan
22-Jan
29-Jan
05-Feb
12-Feb
19-Feb
26-Feb
05-Mar
12-Mar
19-Mar
26-Mar
Obs.
Calc.
Obs*1.5
Obs/1.5

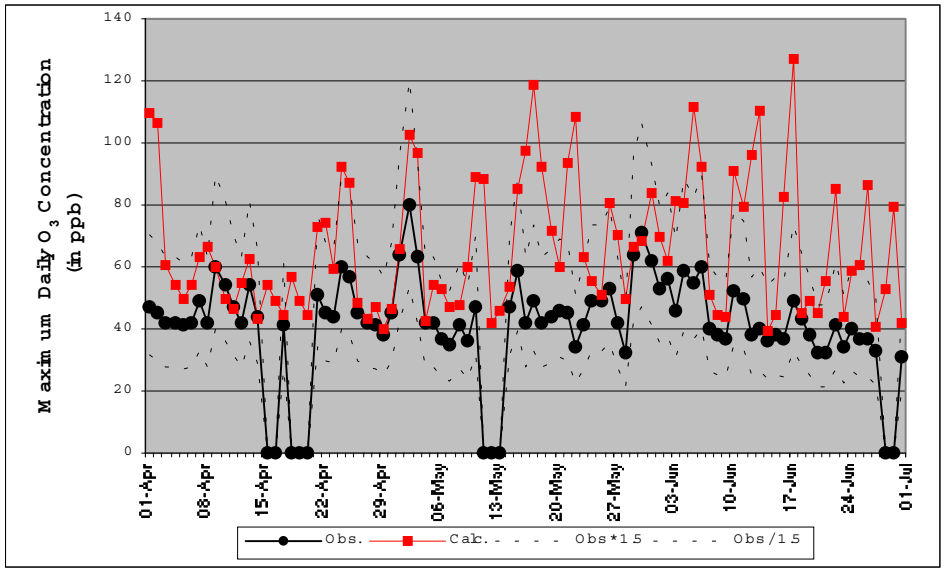

Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Apr
08-Apr
15-Apr
22-Apr
29-Apr
06-May
13-May
20-May
27-May
03-Jun
10-Jun
17-Jun
24-Jun
01-Jul
Obs.
Calc.
Obs*1.5
Obs/1.5

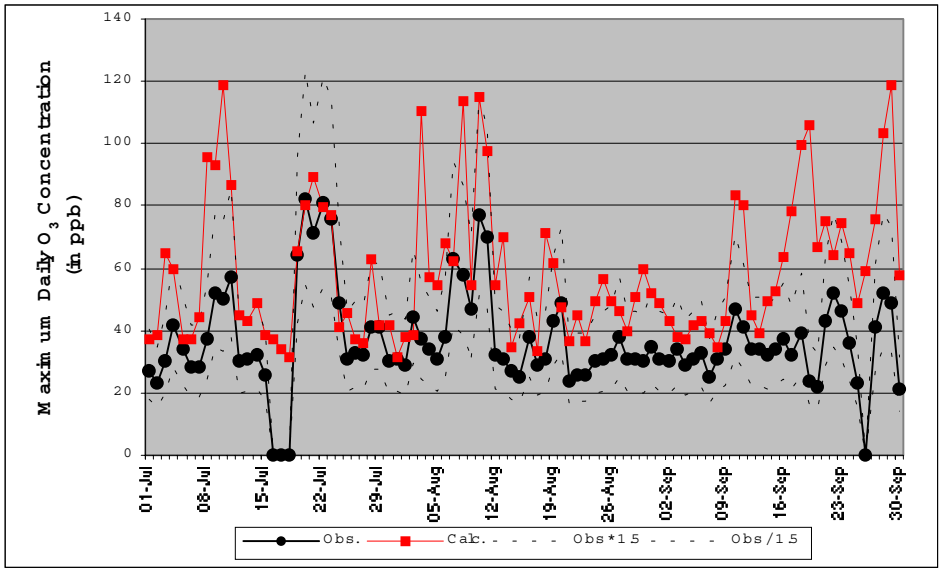

Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Jul
08-Jul
15-Jul
22-Jul
29-Jul
05-Aug
12-Aug
19-Aug
26-Aug
02-Sep
09-Sep
16-Sep
23-Sep
30-Sep
Obs.
Calc.
Obs*1.5
Obs/1.5

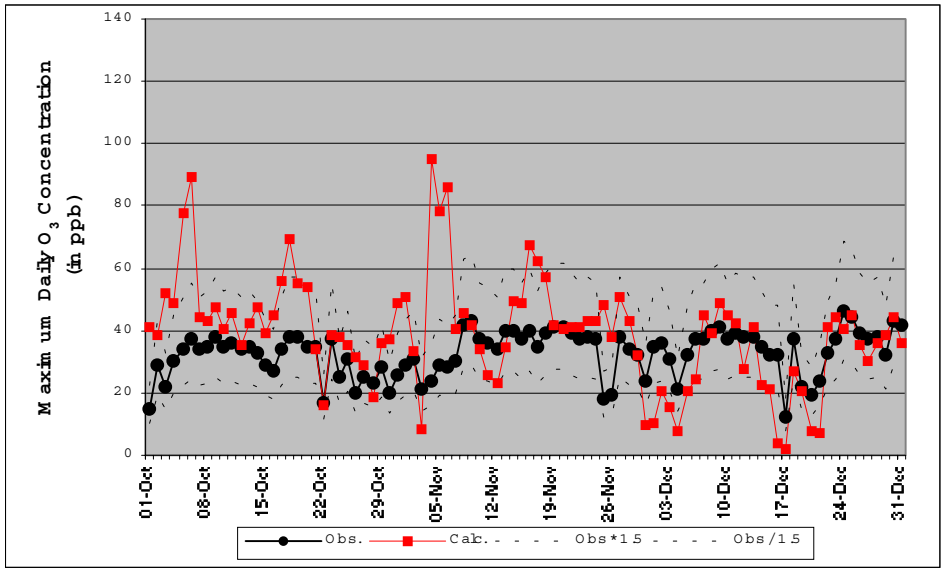

Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Oct
08-Oct
15-Oct
22-Oct
29-Oct
05-Nov
12-Nov
19-Nov
26-Nov
03-Dec
10-Dec
17-Dec
24-Dec
31-Dec
Obs.
Calc.
Obs*1.5
Obs/1.5

Narberth

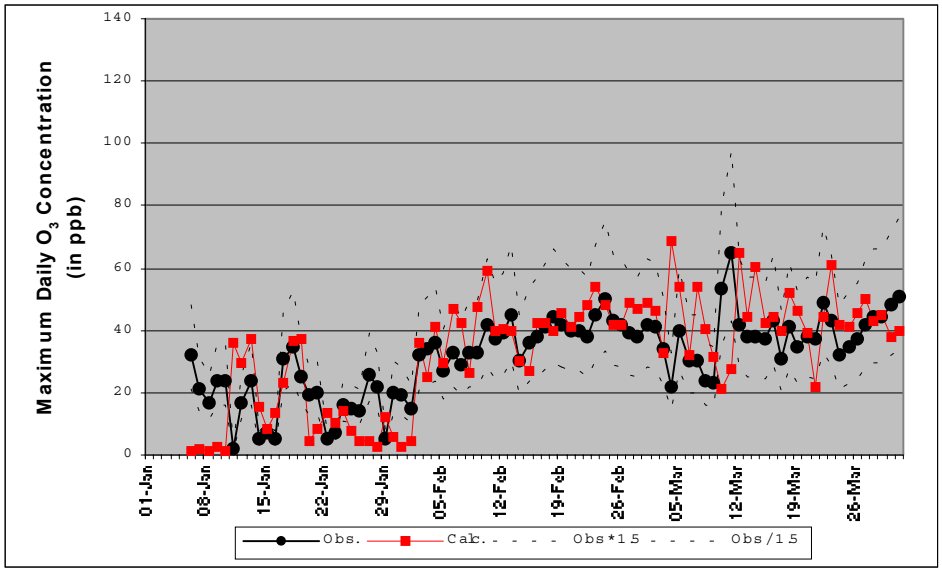

Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Jan
08-Jan
15-Jan
22-Jan
29-Jan
05-Feb
12-Feb
19-Feb
26-Feb
05-Mar
12-Mar
19-Mar
26-Mar
Obs.
Calc.
Obs*1.5
Obs/1.5

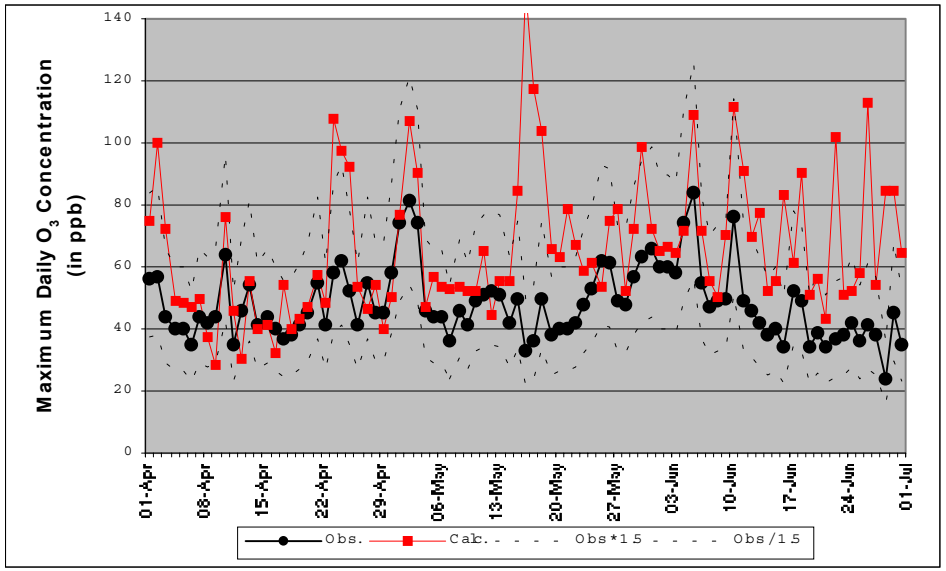

Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Apr
08-Apr
15-Apr
22-Apr
29-Apr
06-May
13-May
20-May
27-May
03-Jun
10-Jun
17-Jun
24-Jun
01-Jul
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Jul
08-Jul
15-Jul
22-Jul
29-Jul
05-Aug
12-Aug
19-Aug
26-Aug
02-Sep
09-Sep
16-Sep
23-Sep
30-Sep
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Oct
08-Oct
15-Oct
22-Oct
29-Oct
05-Nov
12-Nov
19-Nov
26-Nov
03-Dec
10-Dec
17-Dec
24-Dec
31-Dec
Obs.
Calc.
Obs*1.5
Obs/1.5

Harwell


Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Jan
08-Jan
15-Jan
22-Jan
29-Jan
05-Feb
12-Feb
19-Feb
26-Feb
05-Mar
12-Mar
19-Mar
26-Mar
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
0
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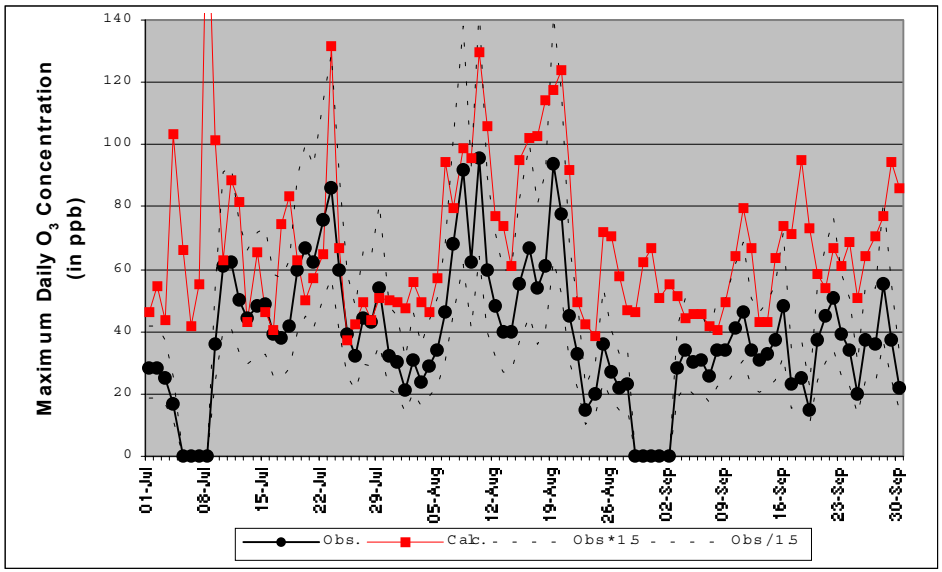
40
60
80
100
120
140
01-Apr
08-Apr
15-Apr
22-Apr
29-Apr
06-May
13-May
20-May
27-May
03-Jun
10-Jun
17-Jun
24-Jun
01-Jul
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
0
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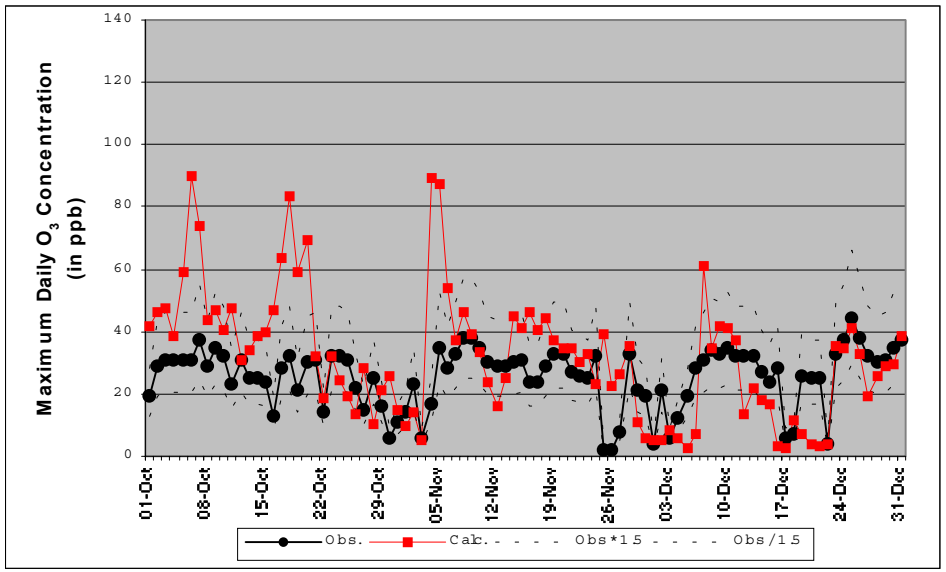
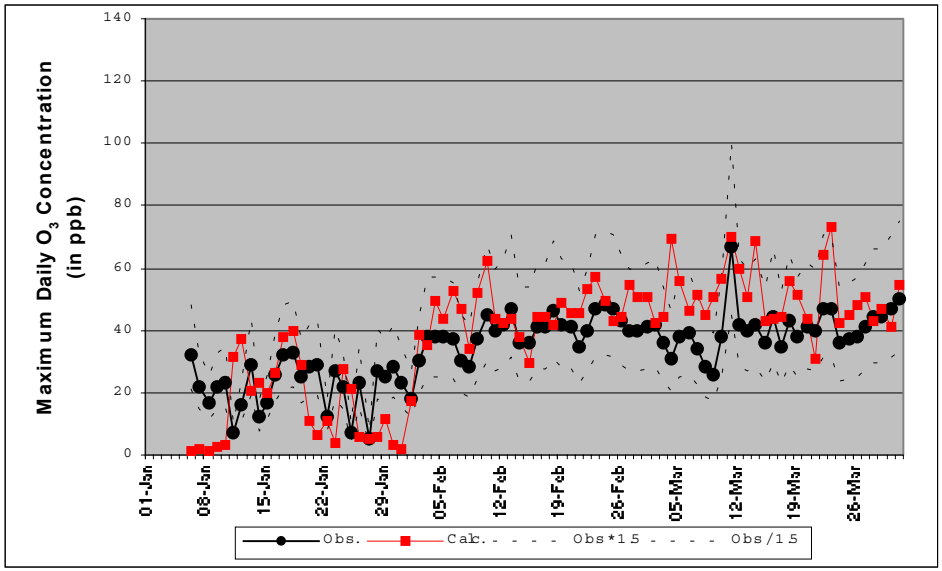
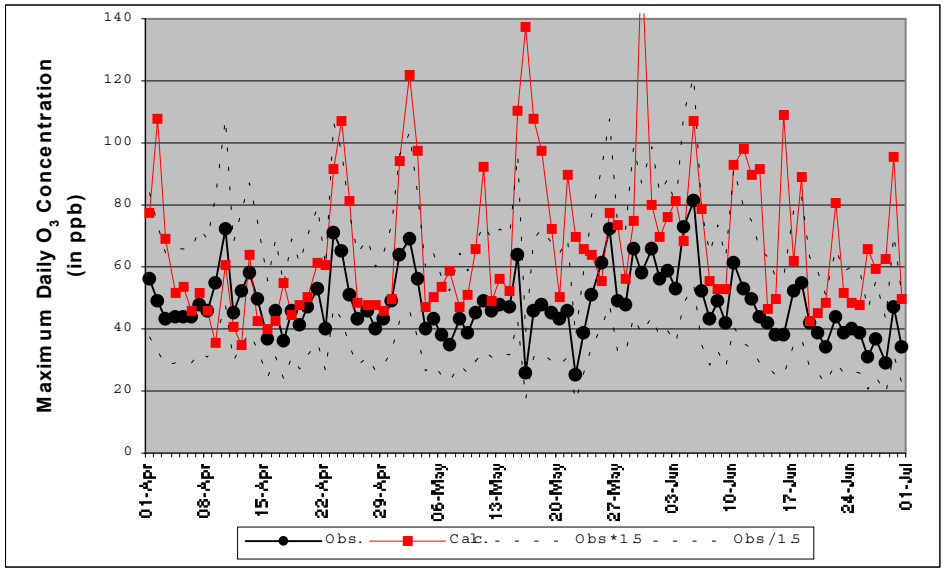
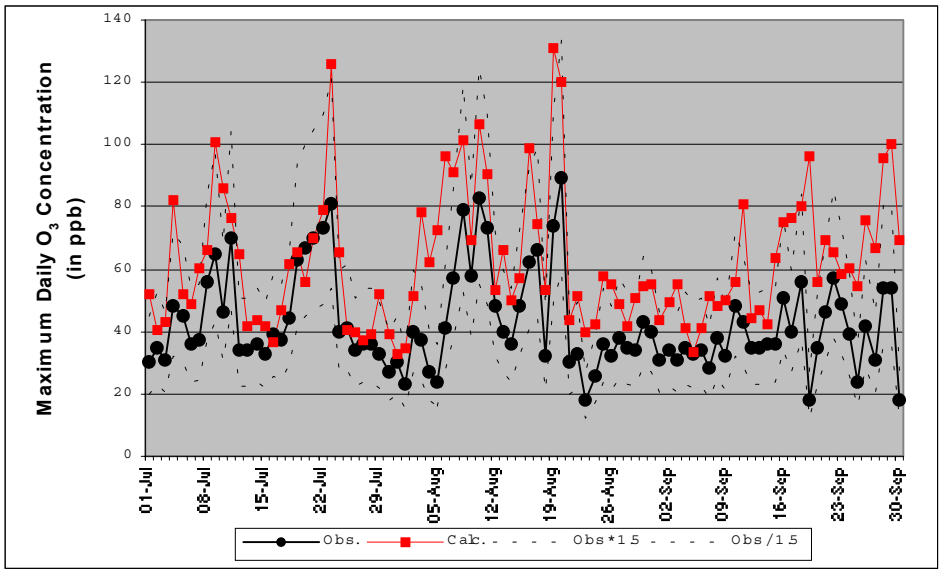
40
60
80
100
120
140
01-Jul
08-Jul
15-Jul
22-Jul
29-Jul
05-Aug
12-Aug
19-Aug
26-Aug
02-Sep
09-Sep
16-Sep
23-Sep
30-Sep
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Oct
08-Oct
15-Oct
22-Oct
29-Oct
05-Nov
12-Nov
19-Nov
26-Nov
03-Dec
10-Dec
17-Dec
24-Dec
31-Dec
Obs.
Calc.
Obs*1.5
Obs/1.5

Somerton


Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Jan
08-Jan
15-Jan
22-Jan
29-Jan
05-Feb
12-Feb
19-Feb
26-Feb
05-Mar
12-Mar
19-Mar
26-Mar
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Apr
08-Apr
15-Apr
22-Apr
29-Apr
06-May
13-May
20-May
27-May
03-Jun
10-Jun
17-Jun
24-Jun
01-Jul
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
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20
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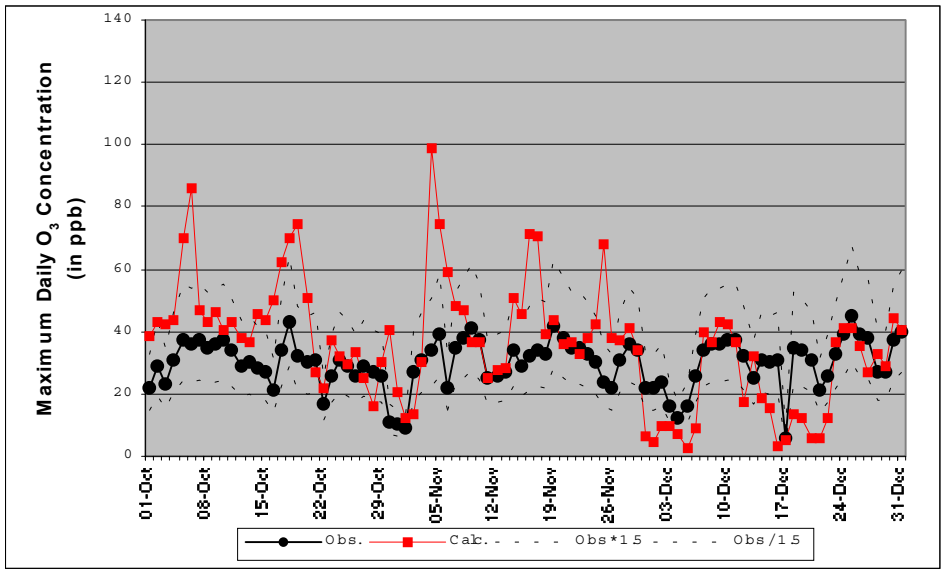
60
80
100
120
140
01-Jul
08-Jul
15-Jul
22-Jul
29-Jul
05-Aug
12-Aug
19-Aug
26-Aug
02-Sep
09-Sep
16-Sep
23-Sep
30-Sep
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
0
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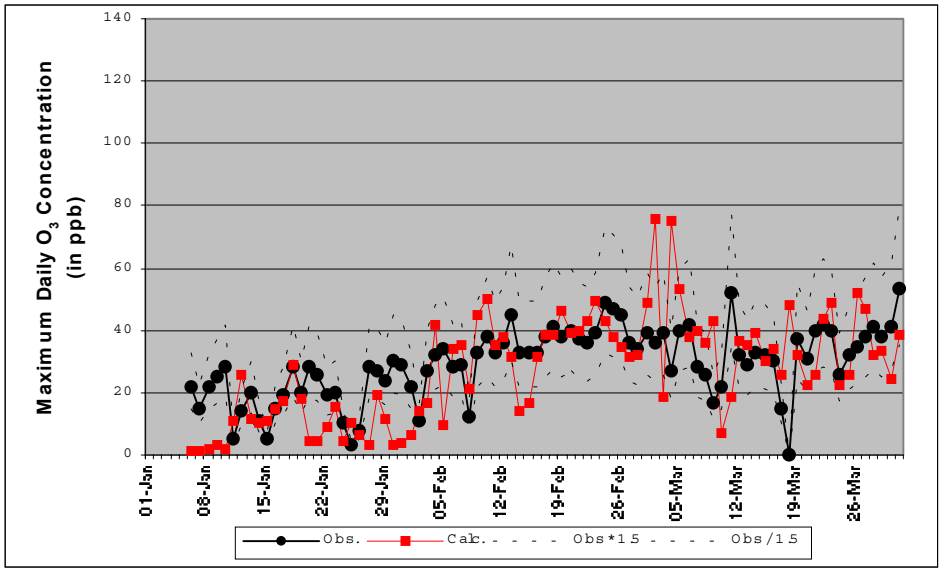
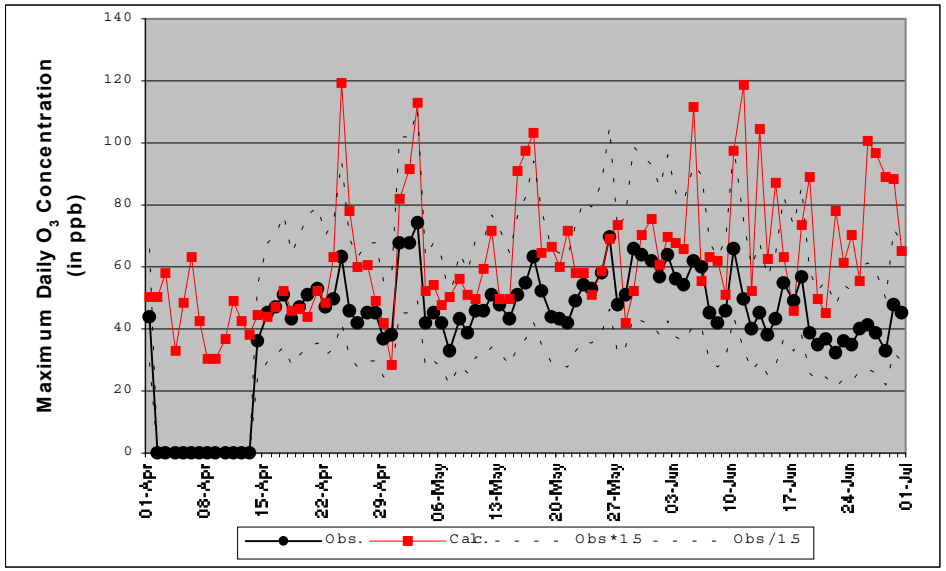
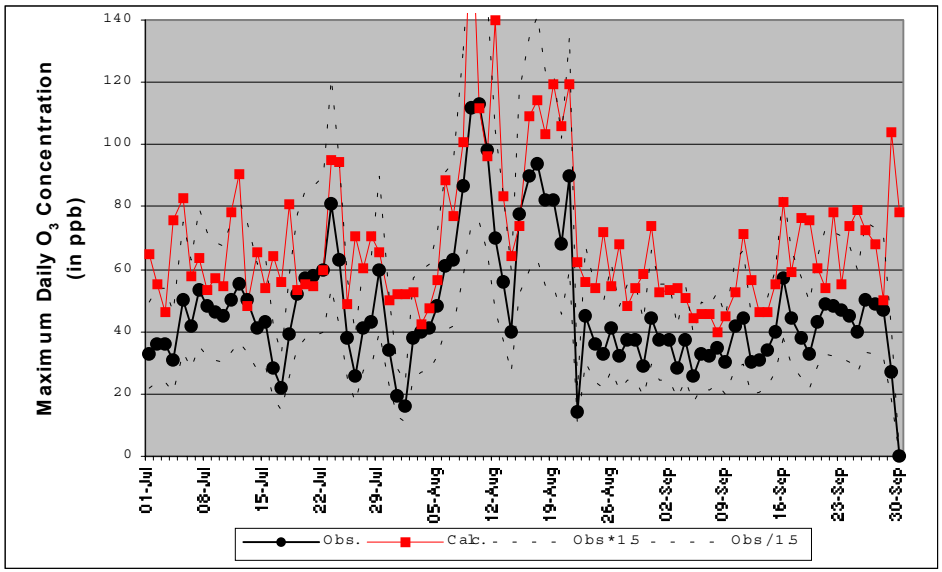
60
80
100
120
140
01-Oct
08-Oct
15-Oct
22-Oct
29-Oct
05-Nov
12-Nov
19-Nov
26-Nov
03-Dec
10-Dec
17-Dec
24-Dec
31-Dec
Obs.
Calc.
Obs*1.5
Obs/1.5

Rochester


Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Jan
08-Jan
15-Jan
22-Jan
29-Jan
05-Feb
12-Feb
19-Feb
26-Feb
05-Mar
12-Mar
19-Mar
26-Mar
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
0
20
40
60
80
100
120
140
01-Apr
08-Apr
15-Apr
22-Apr
29-Apr
06-May
13-May
20-May
27-May
03-Jun
10-Jun
17-Jun
24-Jun
01-Jul
Obs.
Calc.
Obs*1.5
Obs/1.5


Maximum Daily O_3 Concentration (in ppb)
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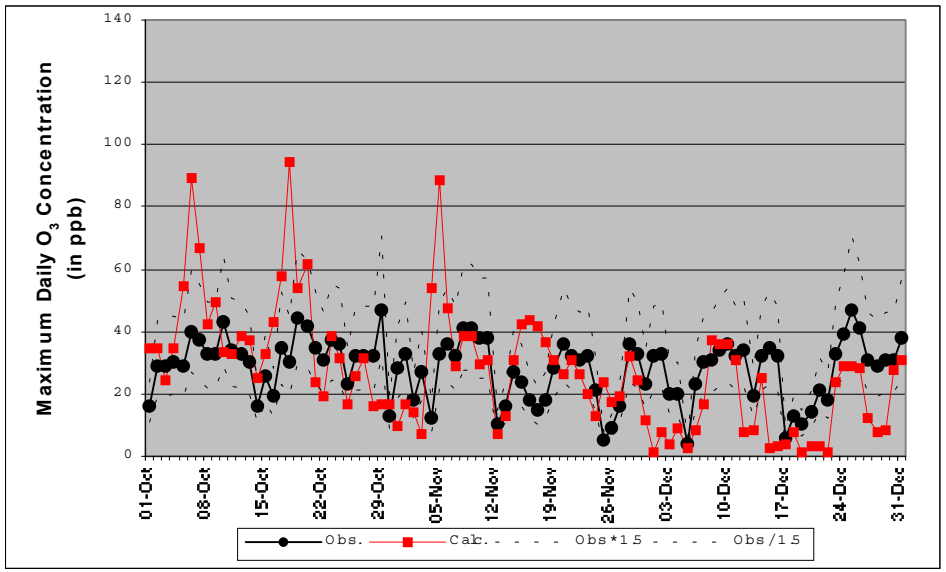
20
40
60
80
100
120
140
01-Jul
08-Jul
15-Jul
22-Jul
29-Jul
05-Aug
12-Aug
19-Aug
26-Aug
02-Sep
09-Sep
16-Sep
23-Sep
30-Sep
Obs.
Calc.
Obs*1.5
Obs/1.5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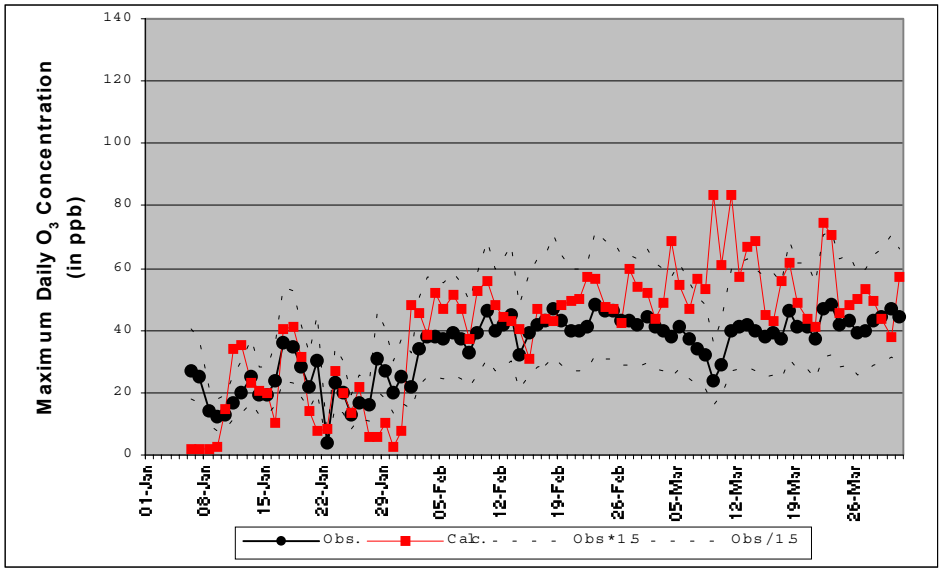
100
120
140
01-Oct
08-Oct
15-Oct
22-Oct
29-Oct
05-Nov
12-Nov
19-Nov
26-Nov
03-Dec
10-Dec
17-Dec
24-Dec
31-Dec
Obs.
Calc.
Obs*1.5
Obs/1.5

Yarner Wood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60
80
100
120
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01-Jan
08-Jan
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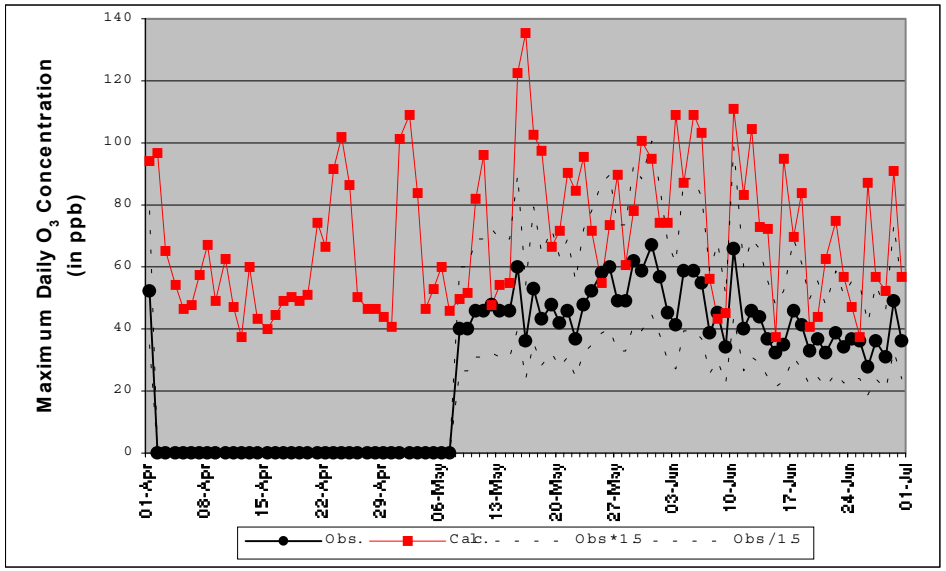
22-Jan
29-Jan
05-Feb
12-Feb
19-Feb
26-Feb
05-Mar
12-Mar
19-Mar
26-Mar
Obs.
Calc.
Obs*1.5
Obs/1.5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120
140
01-Apr
08-Apr
15-Apr
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29-Apr
06-May
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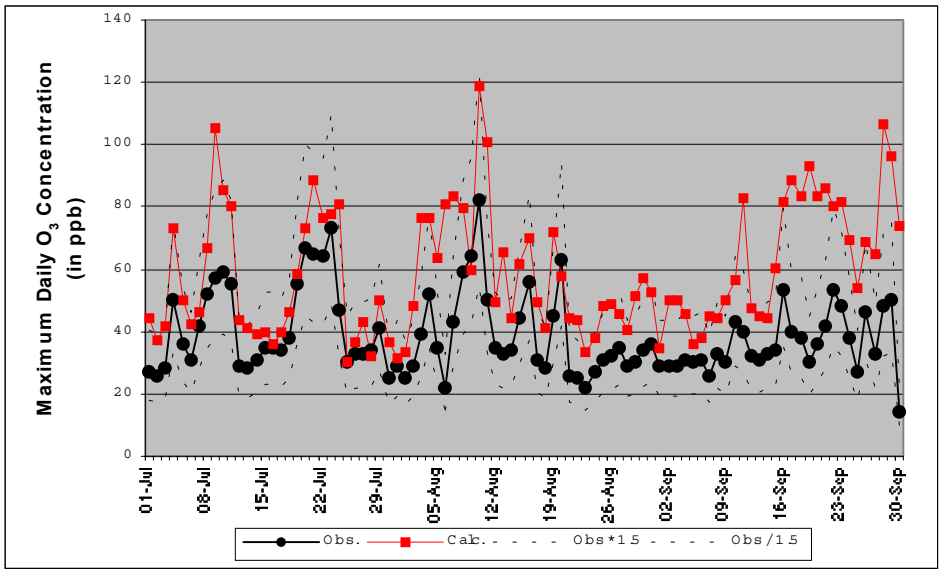
03-Jun
10-Jun
17-Jun
24-Jun
01-Jul
Obs.
Calc.
Obs*1.5
Obs/1.5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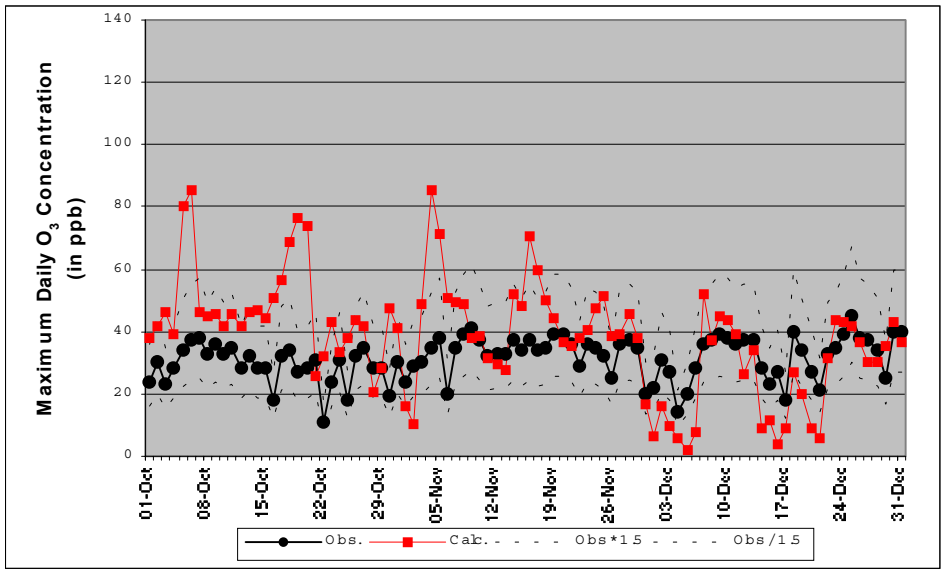
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140
01-Oct
08-Oct
15-Oct
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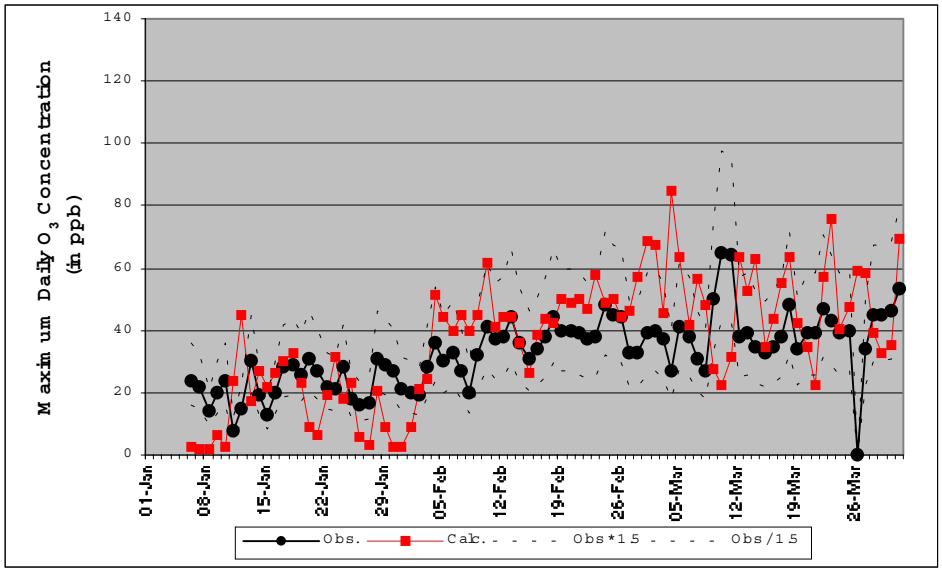
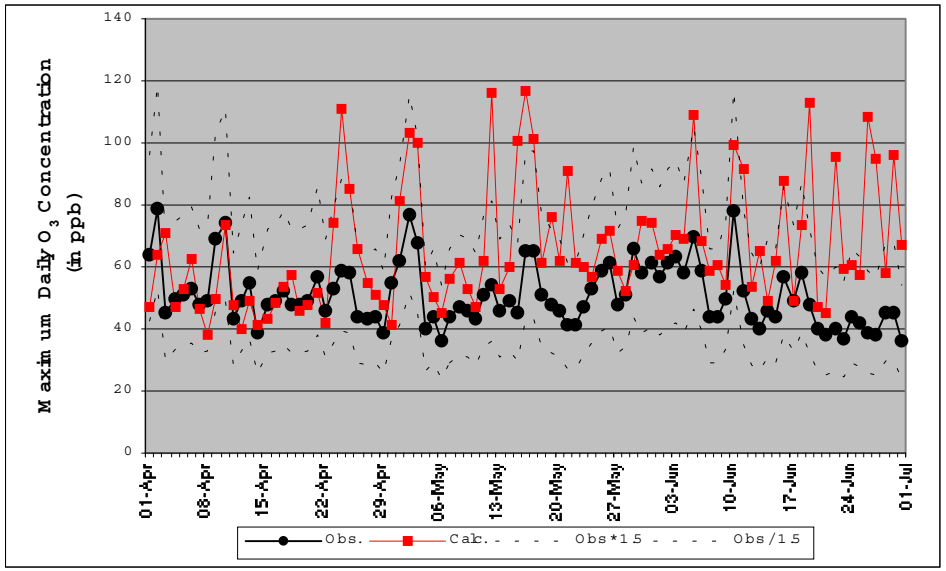
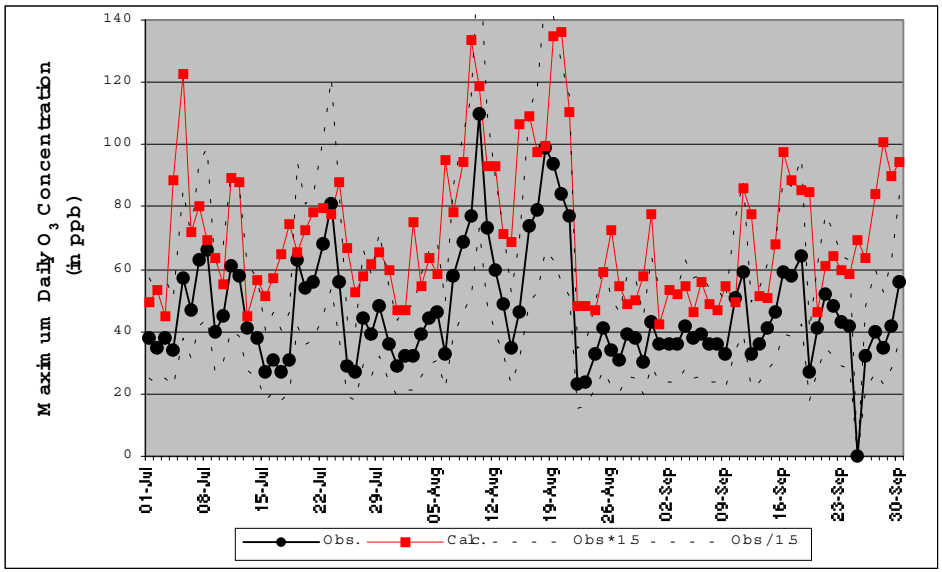
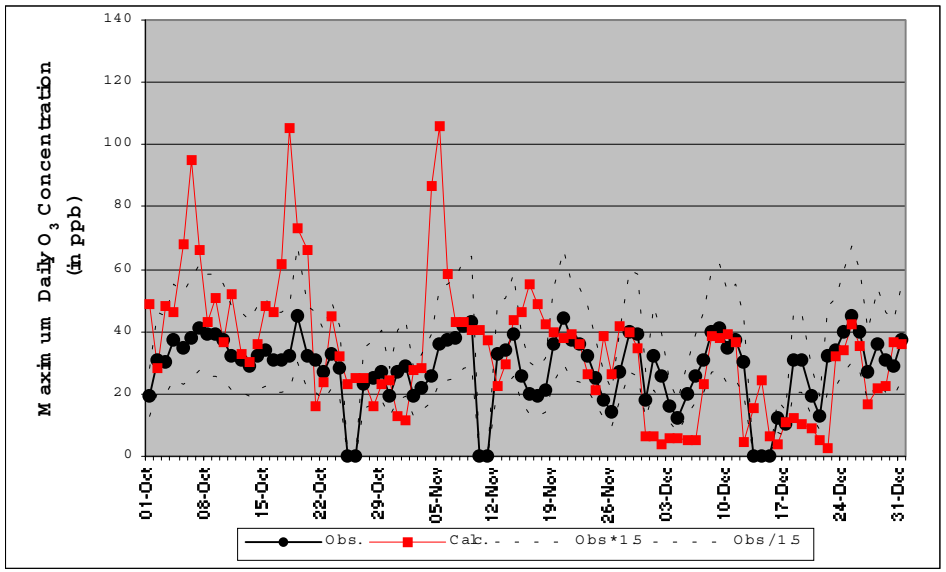
29-Oct
05-Nov
12-Nov
19-Nov
26-Nov
03-Dec
10-Dec
17-Dec
24-Dec
31-Dec
Obs.
Calc.
Obs*1.5
Obs/1.5

Lullington Heath









Appendix 3

The 125 VOC degraded in the Master Chemical Mechanism (MCM 3.0)

CONTENTS

AEA Technology
National Environmental Technology Centre

Alkanes	
• methane	• 2,2 dimethyl butane
• ethane	• 2,3 dimethyl butane
• propane	• cyclohexane
• butane (n-butane)	• heptane (n-heptane)
• 2-methyl propane (i-butane)	• 2-methyl hexane
• pentane (n-pentane)	• 3-methyl hexane
• 2-methyl butane (i-pentane)	• octane (n-octane)
• 2,2-dimethyl propane (neo-pentane)	• nonane (n-nonane)
• hexane (n-hexane)	• decane (n-decane)
• 2-methyl pentane	• hendecane (n-undecane)
• 3-methyl pentane	• dodecane(n-dodecane)
Alkenes	
• ethene (ethylene)	• trans-2-pentene
• propene (propylene)	• 2-methyl 1-butene
• methyl propene (butylene)	• 3-methyl 1-butene
• 1-butene	• 2-methyl 2-butene
• cis-2-butene	• 1-hexene
• trans-2-butene	• cis-2-hexene
• 1-pentene	• trans-2-hexene
• cis-2-pentene	• 2,3-dimethyl-2-butene ⋆
Dialkenes	
• 1,3-butadiene	• 2-methyl 1,3-butadiene (isoprene)
Terpenes	
• α-pinene	• β-pinene ⋆
Alkynes	
• ethyne (acetylene)	
Aromatic hydrocarbons	
• benzene	• 1,2,4-trimethyl benzene (pseudocumene)
• methyl benzene (toluene)	• 1,3,5-trimethyl benzene (mesitilene)
• 1,2-dimethyl benzene (o-xylene)	• 1-ethyl 2-methyl benzene (o-ethyl toluene)
• 1,3-dimethyl benzene (m-xylene)	• 1-ethyl 3-methyl benzene (m-ethyl toluene)
• 1,4-dimethyl benzene (p-xylene)	• 1-ethyl 4-methyl benzene (p-ethyl toluene)
• ethyl benzene	• 1,3-dimethyl 5-ethyl benzene
• n-propyl benzene	• 1,3-diethyl 5-methyl benzene (3,5 diethyl toluene)
• i-propyl benzene (cumene)	• ethenyl benzene (styrene)
• 1,2,3-trimethyl benzene (hemimellitene)	• benzenecarbonal (benzaldehyde)
Aldehydes	
• methanal (formaldehyde)	• butanal (butyraldehyde)
• ethanal (acetaldehyde)	• methyl propanal (i-butyraldehyde)
• propanal (propionaldehyde)	• pentanal (valeraldehyde)

Ketones	
• propanone (acetone)	• 2-hexanone
• 2- butanone (methyl ethyl ketone)	• 3-hexanone
• 2-pentanone	• 2-methyl 4-pentanone (methyl i-butyl ketone)
• 3-pentanone	• 3,3-dimethyl 2-butanone (methyl t-butyl ketone)
• 3-methyl 2-butanone (methyl i-propyl ketone)	• cyclohexanone
Alcohols and Glycols	
• methanol	• 2-methyl 1-butanol
• ethanol	• 2-methyl 2-butanol (t-amyl alcohol)
• 1-propanol (n-propanol)	• 3-methyl 1-butanol (i-amyl alcohol)
• 2-propanol (i-propanol)	• 3-methyl 2-butanol
• 1-butanol (n-butanol)	• cyclohexanol
• 2-butanol (sec-butanol)	• 4-hydroxy 4-methyl 2-pentanone (diacetone alcohol)
• 2-methyl 1-propanol (i-butanol)	• ethane 1,2-diol (ethylene glycol)
• 2-methyl 2-propanol (t-butanol)	• propane 1,2-diol (propylene glycol)
• 3-pentanol	•
Ethers and glycol ethers	
• dimethyl ether	• 2-methoxy ethanol
• diethyl ether	• 1-methoxy 2-propanol (methoxypropanol)
• di-i-propyl ether	• 2-ethoxy ethanol
• methyl t-butyl ether	• 2-butoxy ethanol (butyl glycol)
• ethyl t-butyl ether	• 1-butoxy 2-propanol
Esters	
• methyl methanoate (methyl formate)	• propyl ethanoate (n-propyl acetate)
• methyl ethanoate (methyl acetate)	• n-butyl ethanoate (n-butyl acetate)
• ethyl ethanoate (ethyl acetate)	• sec-butyl ethanoate (sec-butyl acetate)
• n-propyl ethanoate (n-propyl acetate)	• t-butyl ethanoate (t-butyl acetate)
Organic acids	
• methanoic acid (formic acid)	• propanoic acid (propionic acid)
• ethanoic acid (acetic acid)	•
Other oxygenates	
• dimethoxy methane	• dimethyl carbonate
Chloro- and Hydrochlorocarbons	
• chloromethane (methyl chloride)	• trichloroethene
• dichoromethane (methylene chloride)	• tetrachoroethene (perchloroethene)
• trichoromethane (chloroform)	• cis-1,2-dichloroethene
• 1,1,1 trichloroethane (methyl chloroform)	• trans-1,2-dichloroethene
Those VOCs marked ⋆ were not treated in MCM 2.0	

Appendix 4

A poster presented at the 15th Task Force Meeting of the UN/ECE ICP on Vegetation

CONTENTS

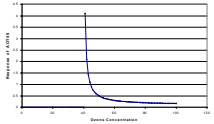
AEA Technology
National Environmental Technology Centre

Review and Application of Current and Suggested Ozone Exposure Metrics

Catherine Brady, Garry Hayman

At present, ozone exposure is quantified by the index AOT-L, where L is a threshold in ppb, commonly 40 ppb or 60 ppb. This index has problems in its response around the threshold area. This is demonstrated in figure 1, where the response of the AOT-40 index to a 10 % increase in ozone concentration is shown.

Figure 1: Response of AOT-40 to a 10 % increase in ozone concentration



The discontinuous jump in response at the threshold level is what makes the AOT-40 index difficult to apply to data. Since it is probable that errors of 10 % will be present in the data, values falling around 40 ppb could easily be incorrectly handled.

The paper

A paper by Sofiev and Tuovinen (Sofiev and Tuovinen, 2001) investigated this problem by looking at the mathematical stability of the AOT-40 index. The paper also mentioned some alternative ozone exposure indices, shown in table 1, and described a modified AOT-40 index devised by Sofiev and Tuovinen, shown in equation 1. This work prompted me to take some of the ozone exposure indices from the paper and apply them to six sites in the UK.

The indices

The indices described by Sofiev and Tuovinen are shown in table 1 and equation 1. ξ is the ozone concentration and Θ is the Heaviside function.

Table 1: Ozone exposure indices and their stability

Index	Description	Filter Function	Stability
SUM-*L*	Sum of concentrations above the threshold, L	$f(\xi)=\xi\Theta(\xi-L)$	Unstable
PER-*n*	*n*th percentile of the concentration distribution	No time integration	N/A
AOT-*L*	As for SUM-*L*, but L is subtracted before summation	$f(\xi)=(\xi-L)\Theta(\xi-L)$	Unstable
NUM-*L*	Number of 1 hour concentrations above L	$f(\xi)=\Theta(\xi-L)$	Unstable
SIG-*M,k*	Sum of concentrations weighted by a sigmoid function with parameters M and k	$f(\xi)=\xi[1+M\exp(-k\xi)]$	Stable
AL-*i,j*	Sum of concentrations weighted by an allometric function with parameters i and j.	$f(\xi)=\xi(\xi/j)^{i}$	Stable

Equation 1: Modified AOT-L index devised by Sofiev and Tuovinen (Sofiev and Tuovinen , 2001)

$$\varphi(\xi)=\exp\left(-0.1\frac{L^2}{(\xi-a)^2}\right)\begin{cases}\left(\varepsilon^{1}\frac{\xi-L}{\varepsilon^{1}\left(\xi-\xi+L\right)^{n_1}}\right)^{n} & \xi\geq\varepsilon^{1}+L\\ \varepsilon^{1}\left(\xi-\xi+L\right)^{n_1} & a\leq\xi<\varepsilon^{1}+L\\ 0 & \xi<a\end{cases}$$

I investigated the AOT-40, SIG-*M,k*, AL-*i,j* and the modified AOT-40 index. I decided not to investigate the SUM-*L* and PER-*n* indices because the filter function for the SUM-*L* index is very similar to that of the AOT-40 index and the PER-*n* index does not rely on time integration and so cannot be classified as stable or unstable.

The sites

I applied the indices to 2000 data from six sites in the UK. The indices were based on hourly data between 8 am and 8 pm. The sites used are shown in figure 2.

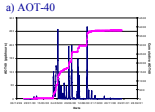
Figure 2: Sites used to investigate the different ozone exposure indices

Results

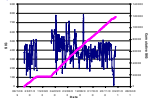
The results presented in figure 3 are for the Yarner Wood site. The results were consistent and comparable across the other sites.

Figure 3: Ozone exposure indices and cumulative indices for Yarner Wood (2000)

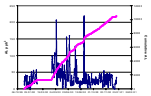
a) AOT-40



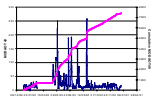
b) SIG-100,500



c) AL-2,120



d) Modified AOT-40
ε=7.5, n=1.5



The modified AOT-40 plot shows good comparison with the AOT-40 index with the more stable properties of the modified AOT-40 index clear to see. The increased stability is evident in the variation in the points around the baseline; for the AOT-40 index, the distinction between the baseline (0 ppb) and the rest of the data is a lot more distinct. The smoother gradient of the cumulative index in the modified AOT-40 is also indicative of a more constant response.

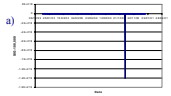
The SIG and AL indices do not compare as well with the AOT-40 index in scale and range of values. However, this is not thought to be a particular problem if they are introduced as the standard ozone exposure index. This is because any change in the index will require thorough implementation, and a different scale should not stand in the way of a more effective index being used. In terms of the stability of the indices, the smooth gradients of the cumulative indices, particularly of the SIG index show that the response of the indices is robust to varying ozone concentration values.

The role of the parameters present in the indices SIG and AL is unclear. Changing the values of *M* and *k* in the SIG index to others recommended in the paper (Sofiev and Tuovinen, 2001) had limited effect on the plot and sensitivity. Changing the values of *i* and *j* in the AL index resulted in substantial changes in the value of the AL index, but it was not clear what these changes implied.

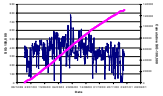
One potential quirk of the SIG index is its response to poor data. This was seen at the Harwell site during the 20/10/00, where a value of -1 ppb was included as part of the data for that day. This poor data point dominated the response of the index for the whole year, as shown in figure 4a. This was confirmed, when the -1 ppb concentration had been replaced with a missing data point, and the plot returned to an expected SIG index plot, as shown in figure 4b.

Figure 4: a) The SIG-100,500 ozone exposure index for Harwell (2000), b) The SIG-100,500 ozone exposure index for Harwell (2000), -1 ppb replaced with missing value.

a)



b)

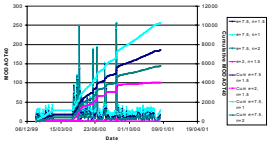


Whilst this response initially seems undesirable, it could act as a useful quality control check on the data (M. Williams, personal communication, 2002) and should not be seen as a reason for the SIG index not being considered as an alternative to the AOT-40 index.

Modified AOT-40 index - potential problems

The value of the modified AOT-40 index is highly dependent on the choice of parameters, ε and n to the extent that an unwise choice of ε and n could result in higher sensitivity of the modified AOT-40 index compared to the standard AOT-40 index. An indication of how changing ε and n can affect the modified AOT-40 index, and the cumulative modified AOT-40 index is shown in figure 5.

Figure 5: Changing response of the modified AOT40 index to different parameters, ε and n, at the Yarner Wood site (2000)



This raises questions as to how areas with different parameters could be compared, and how the parameters should be chosen. If an area requires different parameters for different times in the year, could the results then be compared for the whole year?

Another problem with the modified AOT-40 index, as described by Sofiev and Tuovinen is the choice of filter function, as shown in equation 1. The exponential part of equation 1 is used to fit the data to the standard AOT-40 plot. However, this choice has problems when the ozone concentration values, ξ, are near or equal to the minimum ozone concentration, parameter *a*. When ξ=*a*, the expression is undefined as a result of the division by zero.

Conclusions

- The paper by Sofiev and Tuovinen (2001) presents a number of alternatives to the AOT-40 ozone exposure index.
- SIG-*M,k* and AL-*i,j* are stable indices that represent real alternatives to the AOT-40 index, but require deeper understanding.
- The modified AOT-40 devised by Sofiev and Tuovinen also provides an alternative to the AOT-40 index that is stable, but it still has problems with the filter function and choice of parameters.

Bibliography

Sofiev M., Tuovinen J.-P., 2001. Factors determining the robustness of AOT40 and other ozone exposure indices. Atmospheric Environment 35, 3521-3528

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