

REPORT

Ratification of data produced by the UK Ambient Hydrocarbon Automatic Air Quality Network, 1 January 2003 to 31 March 2003

A report produced for the Department for Environment, Food and Rural Affairs, the Scottish Executive, the Welsh Assembly Government and the Department of the Environment in Northern Ireland

AEAT/ENV/R/1526 Issue 1
July 2003

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1 Introduction

This report contains information on the quality and statistical parameters associated with ratified data from the UK Ambient Hydrocarbon Automatic Air Quality Network (The UK Hydrocarbon Network). The presented information and data cover the period 1 January 2003 to 31 March 2003. The ratified data have been made available on the World Wide Web at http://www.airquality.co.uk/archive/data_and_statistics_home.php

This report contains:

- The definition of a Data Quality Code for each reported hydrocarbon.
- The Data Quality Codes assigned to the data presented on the web.
- A list of periods of data loss, reasons for data loss and descriptions of the most significant causes of data loss.
- Statistical information for each measured hydrocarbon for each individual month.

In this report the unit used for expressing concentrations of gases is micrograms per cubic metre ($\mu\text{g}/\text{m}^3$). This allows comparison to the relevant Air Quality Standards that are now expressed in micrograms per cubic metre ($\mu\text{g}/\text{m}^3$).

2 Hydrocarbon Data Quality

All hydrocarbon data are assigned a quality value. In general ratified hourly data have an uncertainty (at 95% confidence) of $\pm 10\%$ for values above $0.5 \mu\text{g}/\text{m}^3$ and $\pm 0.05 \mu\text{g}/\text{m}^3$ for values below $0.5 \mu\text{g}/\text{m}^3$. These data are termed 'good quality'.

In some cases, because of instrument problems, data cannot be described as 'good' quality, but the data may still be of use to modellers and is therefore included in the archive. This is termed 'acceptable' quality data, and has an uncertainty (at 95% confidence) of $\pm 25\%$ above $0.5 \mu\text{g}/\text{m}^3$ and $\pm 0.1 \mu\text{g}/\text{m}^3$ below $0.5 \mu\text{g}/\text{m}^3$.

Data that do not meet either the 'good' or 'acceptable' criteria do not appear in the archive.

Each month's data are assigned a Data Quality Code for each species as follows:

- A. all 'good' quality data
- B. most ($> 75\%$) data points 'good', remainder 'acceptable' quality
- C. roughly equal numbers of 'good' and 'acceptable' quality data
- D. some ($< 25\%$) data points 'good' quality; remainder 'acceptable' quality
- E. all points 'acceptable' quality

3 Monthly Data Reports

The following sections give details of issues affecting data on a month by month basis. Data quality codes have been assigned for each monthly set of data.

3.1 CARDIFF

3.1.1 January

3.1.1.1 Data Quality Codes

Data quality code A for all data for all of the month.

3.1.1.2 Missing Data – All hydrocarbons

- Calibration 08/01/03 hours 09 to 11.
- Calibration 23/01/03 hours 13 to 14.
- PC/GC communication problem 28/01/03 hours 08 to 10.

3.1.1.3 Missing Data – Specific hydrocarbons

None, except where the integration was unreliable due to very low concentrations.

3.1.2 February

3.1.2.1 Data Quality Codes

Data quality code A for all data for all of the month.

3.1.2.2 Missing Data - All hydrocarbons

- Calibration 06/02/03 hours 10 to 11.
- Calibration 19/02/03 hours 10 to 11.

3.1.2.3 Missing Data - Specific hydrocarbons

None, except where the integration was unreliable due to very low concentrations.

3.1.3 March

3.1.3.1 Data Quality Codes

Data quality code A for all data for all of the month.

3.1.3.2 Missing Data - All hydrocarbons

- Calibration 07/03/03 hours 10 to 12.
- Calibration 19/03/03 hours 12 to 13.

3.1.3.3 Missing Data - Specific hydrocarbons

None, except where the integration was unreliable due to very low concentrations.

3.2 GLASGOW

3.2.1 January

3.2.1.1 Data Quality Codes

Data quality code A for all data for all of the month except:
Data quality code E for 1,3-butadiene for all of the month.
Data quality code B for toluene and (m+p)-xylene for all of the month.

3.2.1.2 Missing Data - All hydrocarbons

- Calibration 14/01/03 hours 12 to 15.
- PC/GC communication problem 24/01/03 hours 06 to 07.
- Calibration 28/01/03 hours 13 to 16.
- QA/QC site audit 29/01/03 hour 17 to 30/01/03 hour 08.
- Calibration 30/01/03 hours 09 to 11.

3.2.1.3 Missing Data - Specific hydrocarbons

None, except where the integration was unreliable due to peak truncation.

3.2.2 February

3.2.2.1 Data Quality Codes

Data quality code A for all data for all of the month except:
Data quality code E for 1,3-butadiene for all of the month.
Data quality code B for toluene and (m+p)-xylene for all of the month.

3.2.2.2 Missing Data - All hydrocarbons

- Calibration 11/02/03 hours 12 to 18.
- Calibration 25/02/03 hours 12 to 16.

3.2.2.3 Missing Data - Specific hydrocarbons

None, except where the integration was unreliable due to peak truncation.

3.2.3 March

3.2.3.1 Data Quality Codes

Data quality code A for all data for all of the month except:
Data quality code E for 1,3-butadiene for all of the month.
Data quality code B for toluene and (m+p)-xylene for all of the month.

3.2.3.2 Missing Data - All hydrocarbons

- Calibration 11/03/03 hours 11 to 21.
- PC/GC communication problem 14/03/03 hours 23 to 24.
- Calibration 25/03/03 hours 13 to 21.

3.2.3.3 Missing Data - Specific hydrocarbons

None, except where the integration was unreliable due to peak truncation.

3.3 HARWELL

3.3.1 January

3.3.1.1 Data Quality Codes

Data quality code A for all data for all of the month.

3.3.1.2 Missing Data - All hydrocarbons

- Calibration 09/01/03 hours 10 to 17.
- PC/GC communication problem 15/01/03 hours 04 to 06.
- Calibration 23/01/03 hours 11 to 12.

3.3.1.3 Missing Data - Specific hydrocarbons

None, except where the integration was unreliable due to very low concentrations.

3.3.2 February

3.3.2.1 Data Quality Codes

Data quality code A for all data for all of the month.

3.3.2.2 Missing Data - All hydrocarbons

- Calibration 05/02/03 hours 10 to 11.
- Calibration 13/02/03 hours 10 to 11.
- Calibration 27/02/03 hours 10 to 11.
- CMCU Service visit 27/02/03 hours 17 to 20.

3.3.2.3 Missing Data - Specific hydrocarbons

None, except where the integration was unreliable due to very low concentrations.

3.3.3 March

3.3.3.1 Data Quality Codes

Data quality code A for all data for all of the month.

3.3.3.2 Missing Data - All hydrocarbons

- PC/GC communication problem 06/03/03 hours 14 to 18.
- Calibration 11/03/03 hours 17 to 18.
- Calibration 28/03/03 hours 10 to 11.

3.3.3.3 Missing Data - Specific hydrocarbons

None, except where the integration was unreliable due to very low concentrations.

3.4 MARYLEBONE ROAD

3.4.1 January

3.4.1.1 Data Quality Codes

Data quality code A for all data for all of the month.

3.4.1.2 Missing Data - All hydrocarbons

- PC/GC communication problem 08/01/03 hours 03 to 15.
- PC/GC communication problem 10/01/03 hours 14 to 16.
- Calibration 14/01/03 hours 19 to 22.
- Calibration 22/01/03 hours 15 to 18.

3.4.1.3 Missing Data - Specific hydrocarbons

None.

3.4.2 February

3.4.2.1 Data Quality Codes

Data quality code A for all data for all of the month.

3.4.2.2 Missing Data - All hydrocarbons

- PC/GC communication problem 03/02/03 hours 15 to 16.
- Compressed air supply fault 04/02/03 hours 02 to 16.
- Calibration 06/02/03 hours 21 to 24.
- Compressed air supply fault 07/02/02 hour 09 to 11/02/03 hour 10.
- Calibration 11/02/03 hours 13 to 16.
- Compressed air supply fault 14/02/03 hour 11 to 18/02/03 hour 12.
- Calibration 18/02/03 hours 15 to 18.

3.4.2.3 Missing Data - Specific hydrocarbons

None.

3.4.3 March

3.4.3.1 Data Quality Codes

Data quality code A for all data for all of the month.

3.4.3.2 Missing Data - All hydrocarbons

- Calibration 05/03/03 hours 06 to 09.
- Calibration 12/03/03 hours 17 to 20.
- Calibration 27/03/03 hours 08 to 11.

3.4.3.3 Missing Data - Specific hydrocarbons

None.

4 Discussion

4.1 THE RATIFIED DATA

Tables 1 to 4, Appendix 1 contain statistical information relating to the ratified data, for each measured hydrocarbon, over the period 1 January 2003 to 31 March 2003. The tables list the percentage data capture, maximum concentration, mean concentration and minimum concentration of each hydrocarbon. The data capture is the number of ratified hourly data values expressed as a percentage of the number of hours in the specified period.

4.1.1 Cardiff

For the Cardiff site the data capture for benzene was 99.21% and for 1,3-butadiene was 99.21%. There have been no significant problems for the period covered by this report.

4.1.2 Glasgow

For the Glasgow site the data capture for benzene was 97.08% and for 1,3-butadiene was 97.08%.

During the process of calculating response factors for the data covered in this report it was observed that the 1,3-butadiene peak had merged with a neighbouring peak, trans-2-Butene, in the chromatograms of the calibration samples. The reported peak areas for 1,3-butadiene in the standards were therefore, overestimated. As a result an accurate response factor for 1,3-butadiene could not be generated as the degree of overestimation could not be accurately quantified.

An alternative approach was used to generate the response factor for 1,3-butadiene. The response factor for cis-2-Butene, a well-resolved peak, was used to derive a response factor for 1,3-butadiene. The relative response factors for 1,3-butadiene and cis-2-Butene are fairly constant over time when both peaks are well resolved. The cis-2-Butene response factor and relative response factor were used to derive a response factor for 1,3-butadiene.

It is likely that this approach generates a relatively accurate response factor for 1,3-butadiene. Due to the increased uncertainty associated with this method, all the 1,3-butadiene data has been assigned data quality code E.

It was observed that during periods of high concentrations, the peaks on the chromatograms were truncated. As a result the concentrations will be underestimated. It is difficult to quantify the magnitude of the truncation therefore, some compounds have been given lower data quality codes.

- 1,3-Butadiene was not affected by this problem but has been given data quality code E for the whole period because of the problem described above.
- Benzene was not affected by this problem and has been given data quality code A for the whole period.
- Toluene has been affected for all three months, 7% of the data for January, 2% of the data for February and 5% of the data for March. Toluene has been assigned data quality code B for the whole period.
- (m+p)-Xylene has been affected for all three months, 1% of the data for January, 1% of the data for February and 2% of the data for March. (m+p)-Xylene has been assigned data quality code B for the whole period.
- Ethylbenzene and o-xylene have not been affected by this problem and have been given data quality code A for the whole period.

There have been no other significant problems for the period covered by this report.

It should be noted that the hydrocarbon instrumentation at the Glasgow site samples air through a separate inlet from that used for the inorganic measurements. The inlet for the inorganic measurements is within one metre from the kerb and hence these are classed as kerbside measurements. The sample inlet for the hydrocarbon measurements is more than one metre from the kerb (but less than five metres) and hence these are classed as roadside measurements.

4.1.3 Harwell

For the Harwell site the data capture for benzene was 98.52% and for 1,3-butadiene was 98.52%. There have been no significant problems for the period covered by this report.

4.1.4 Marylebone Road

For the Marylebone Road site the data capture for benzene was 87.45% and for 1,3-butadiene was 87.73%.

During February a fault developed with part of the system that supplies compressed air to the GC FID. Approximately 200 hours of data was lost before the system was repaired.

There have been no other significant problems for the period covered by this report.

4.2 CONCENTRATION TRENDS

The periods when data for benzene and 1,3-butadiene were available, for all the sites, are plotted graphically in Figures 1 to 8, Appendix 2. The measured concentrations of 1,3-butadiene fell below $0.02 \mu\text{g}/\text{m}^3$ on a number of occasions see figures 2 and 6, Appendix 2. Where concentrations fell below $0.02 \mu\text{g}/\text{m}^3$ the ratified concentrations have been reported as $0.00 \mu\text{g}/\text{m}^3$.

At Cardiff and Harwell the measured concentrations of hydrocarbons were low for most of the period covered by this report. At these urban background and rural sites there tends to be a pattern of seasonal variation with higher levels during the winter when dispersion is generally poorer and photochemical removal is at a minimum.

The Glasgow and Marylebone Road data tend to exhibit higher levels with less seasonal variation than is apparent in data from the other two sites. The measured concentrations and trends are typical of sites close to busy roads where the source of the measured hydrocarbons is close to the monitoring location. The emitted hydrocarbons will have had little time to mix and react in the atmosphere.

There is insufficient information to provide an explanation of the observed difference in the trends from site to site, although spatial variations in meteorological conditions may well be the cause. The time series for reported concentrations of nitrogen oxides (NO_x) exhibited a high degree of similarity to the time series for reported hydrocarbons at each of the sites. The variation in trends from site to site is probably due to variations in atmospheric dispersion.

4.3 COMPARISON WITH AIR QUALITY OBJECTIVES

The Air Quality Strategy for the UK has set Air Quality Objectives for benzene and 1,3-butadiene. The Air Quality Objective for benzene in the UK is $16.25 \mu\text{g}/\text{m}^3$ expressed as a running annual mean to be met by 31 March 2003. In England and Wales there is an additional objective for benzene of $5 \mu\text{g}/\text{m}^3$ expressed as an annual mean to be met by end of 2010. In Scotland an additional objective has been set for benzene of $3.25 \mu\text{g}/\text{m}^3$ to be met by the end of 2010. The Air Quality Objective for 1,3-butadiene is specified as a running annual mean of $2.25 \mu\text{g}/\text{m}^3$ to be met by the end of 2003.

The annual means for benzene and 1,3-butadiene for 2000, 2001 and 2002 together with the quarterly means for the first quarter of 2003 are given in Tables 1 and 2 below. For benzene the annual means for 2000, 2001 and 2002 were well below the respective Air Quality Objective of $16.25 \mu\text{g}/\text{m}^3$ to be met by the end of 2003. The annual means for 2002 were also below the Air Quality Objective to be met by 2010 for the respective region.

The means for both benzene and 1,3-butadiene for quarter 1, 2003 were slightly higher than the annual means for 2002. This is probably due to seasonal variation as higher concentrations tend to be observed during the winter months.

Table 1. Means of measured benzene Concentrations ($\mu\text{g}/\text{m}^3$) at each of the UK Automatic Hydrocarbon Sites.

Monitoring Site	2000 Annual Mean	2001 Annual Mean	2002 Annual Mean	Quarter 1 2003 Mean
Cardiff Centre	\$\$	\$\$	1.22\$	1.36
Glasgow	\$\$\$	\$\$\$	2.33 \$	2.43
Harwell	0.53	0.62	0.60	0.91
Marylebone Road	6.29	4.55	3.91	3.86

\$ Annual means calculated from significantly less than 12 months data

\$\$ The Cardiff Centre site was installed on 5th September 2002.

\$\$\$ The Glasgow site was installed on 1st August 2002.

Table 2. Means of measured 1,3-butadiene Concentrations ($\mu\text{g}/\text{m}^3$) at each of the UK Automatic Hydrocarbon Sites.

Monitoring Site	2000 Annual Mean	2001 Annual Mean	2002 Annual Mean	Quarter 1 2003 Mean
Cardiff Centre	\$\$	\$\$	0.15\$	0.16
Glasgow	\$\$\$	\$\$\$	0.36\$	0.38
Harwell	0.09	0.11	0.04	0.04
Marylebone Road	1.63	1.12	0.95	0.70

\$ Annual means calculated from significantly less than 12 months data

\$\$ The Cardiff Centre site was installed on 5th September 2002.

\$\$\$ The Glasgow site was installed on 1st August 2002.

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Appendix 1

Summary Statistical Information

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- Table 3. Percentage data capture, maximum, mean and minimum values of ratified data from the Harwell site of the UK Hydrocarbon Network, for the period; 1 January 2003 to 31 March 2003
- Table 4. Percentage data capture, maximum, mean and minimum values of ratified data from the Marylebone Road site affiliated to the UK Hydrocarbon Network, for the period; 1 January 2003 to 31 March 2003

Table 1. Percentage data capture, maximum, mean and minimum values of the ratified data from the Cardiff site of the UK Hydrocarbon Network, for the period 1 January 2003 to 31 March 2003

Compound	%Data capture	Maximum concentration ($\mu\text{g}/\text{m}^3$)	Mean concentration ($\mu\text{g}/\text{m}^3$)	Minimum concentration ($\mu\text{g}/\text{m}^3$)
1,3-Butadiene	99.21	4.49	0.16	0.00
Benzene	99.21	8.04	1.36	0.23
Toluene	99.21	33.66	4.32	0.38
Ethylbenzene	89.03	7.40	0.75	0.04
(m+p)-Xylene *	98.66	27.37	2.47	0.09
o-Xylene	88.70	10.58	1.19	0.04

* (m+p)-Xylene data are reported as the sum of the 2 individual components due to the fact that they are not sufficiently well resolved in the chromatogram.

Table 2. Percentage data capture maximum, mean and minimum values of ratified data from the Glasgow site of the UK Hydrocarbon Network, for the period 1 January 2003 to 31 March 2003

Compound	%data capture	Maximum concentration ($\mu\text{g}/\text{m}^3$)	Mean concentration ($\mu\text{g}/\text{m}^3$)	Minimum concentration ($\mu\text{g}/\text{m}^3$)
1,3-Butadiene	97.08	2.72	0.38	0.00
Benzene	97.08	17.03	2.43	0.19
Toluene	97.08	36.84	8.22	0.50
Ethylbenzene	97.04	32.97	1.67	0.04
(m+p)-Xylene *	96.71	35.70	5.77	0.13
o-Xylene	96.99	31.56	2.60	0.04

* (m+p)-Xylene data are reported as the sum of the 2 individual components due to the fact that they are not sufficiently well resolved in the chromatogram.

Table 3. Percentage data capture, maximum, mean and minimum values of ratified data from the Harwell site of the UK Hydrocarbon Network, for the period; 1 January 2003 to 31 March 2003

Compound	%data capture	Maximum concentration ($\mu\text{g}/\text{m}^3$)	Mean concentration ($\mu\text{g}/\text{m}^3$)	Minimum concentration ($\mu\text{g}/\text{m}^3$)
1,3-Butadiene	98.52	0.63	0.04	0.00
Benzene	98.52	4.18	0.91	0.00
Toluene	98.10	15.34	1.68	0.04
Ethylbenzene	62.96	2.64	0.44	0.04
(m+p)-Xylene *	87.92	8.77	1.01	0.04
o-Xylene	65.19	3.92	0.53	0.04

* (m+p)-Xylene data are reported as the sum of the 2 individual components due to the fact that they are not sufficiently well resolved in the chromatogram.

Table 4. Percentage data capture, maximum, mean and minimum values of ratified data from the Marylebone Road site affiliated to the UK Hydrocarbon Network for the period; 1 January 2003 to 31 March 2003

Compound	%data capture	Maximum concentration ($\mu\text{g}/\text{m}^3$)	Mean concentration ($\mu\text{g}/\text{m}^3$)	Minimum concentration ($\mu\text{g}/\text{m}^3$)
Ethane	87.73	83.69	13.63	3.19
Ethene	87.73	29.07	7.42	0.49
Propane	87.73	39.51	7.87	2.31
Propene	87.73	12.92	3.44	0.30
Ethyne	87.73	31.59	5.86	0.71
2-Methylpropane	87.73	39.38	8.17	0.72
n-Butane	87.73	63.06	13.36	1.18
trans-2-Butene	87.73	3.45	0.84	0.19
1-Butene	87.69	8.38	0.84	0.05
cis-2-Butene	87.73	2.77	0.61	0.07
2-Methylbutane	87.73	58.31	12.21	0.87
n-Pentane	87.73	13.59	3.32	0.42
1,3-Butadiene	87.73	2.76	0.70	0.07
trans-2-Pentene	87.73	4.10	0.81	0.03
cis-2-Pentene	87.13	2.24	0.47	0.03
2-Methylpentane	87.73	24.60	4.04	0.32
3-Methylpentane	87.73	12.48	2.47	0.18
Isoprene	87.50	1.27	0.31	0.03
n-Hexane	87.78	6.33	1.39	0.11
n-Heptane	87.78	4.82	0.87	0.00
Benzene	87.45	17.45	3.86	0.16
Toluene	87.78	73.98	14.34	0.54
Ethylbenzene	87.78	12.74	2.73	0.09
(m+p)-Xylene *	84.58	42.88	9.56	0.26
o-Xylene	87.59	15.51	3.26	0.13
1,3,5-Trimethylbenzene	87.78	5.24	1.15	0.00
1,2,4-Trimethylbenzene	87.78	15.12	3.64	0.15

* (m+p)-Xylene are reported as the sum of the 2 individual components due to the fact that they are not sufficiently well resolved in the chromatogram.

Appendix 2

Time Series Plots of Hydrocarbon Concentrations

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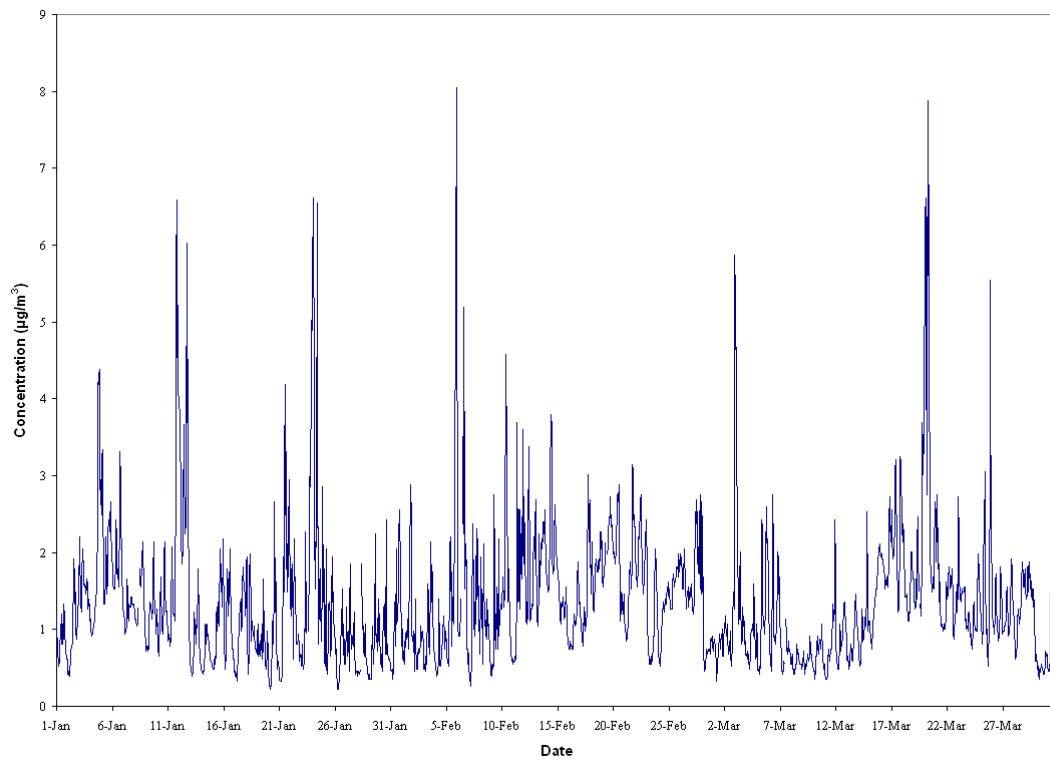


Figure 1. Time series plot of the ratified Benzene data from the Cardiff site of the UK Hydrocarbon Network, for the period; 1 January 2003 to 31 March 2003

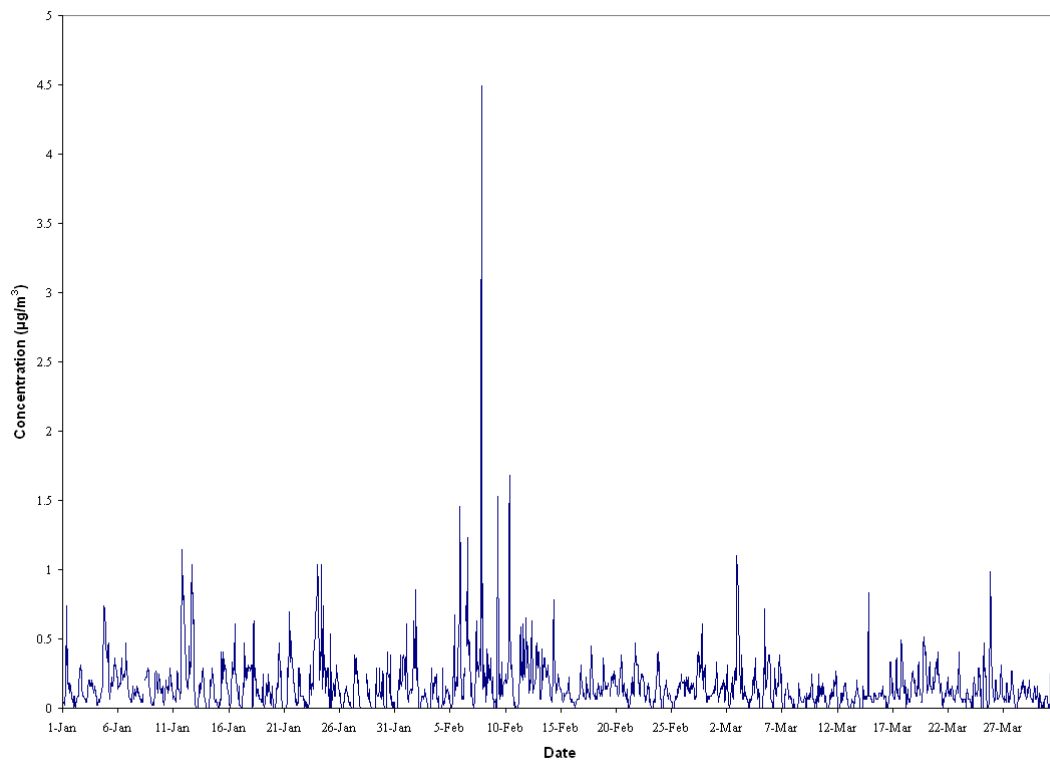


Figure 2. Time series plot of the ratified 1,3-butadiene data from the Cardiff site of the UK Hydrocarbon Network, for the period; 1 January 2003 to 31 March 2003

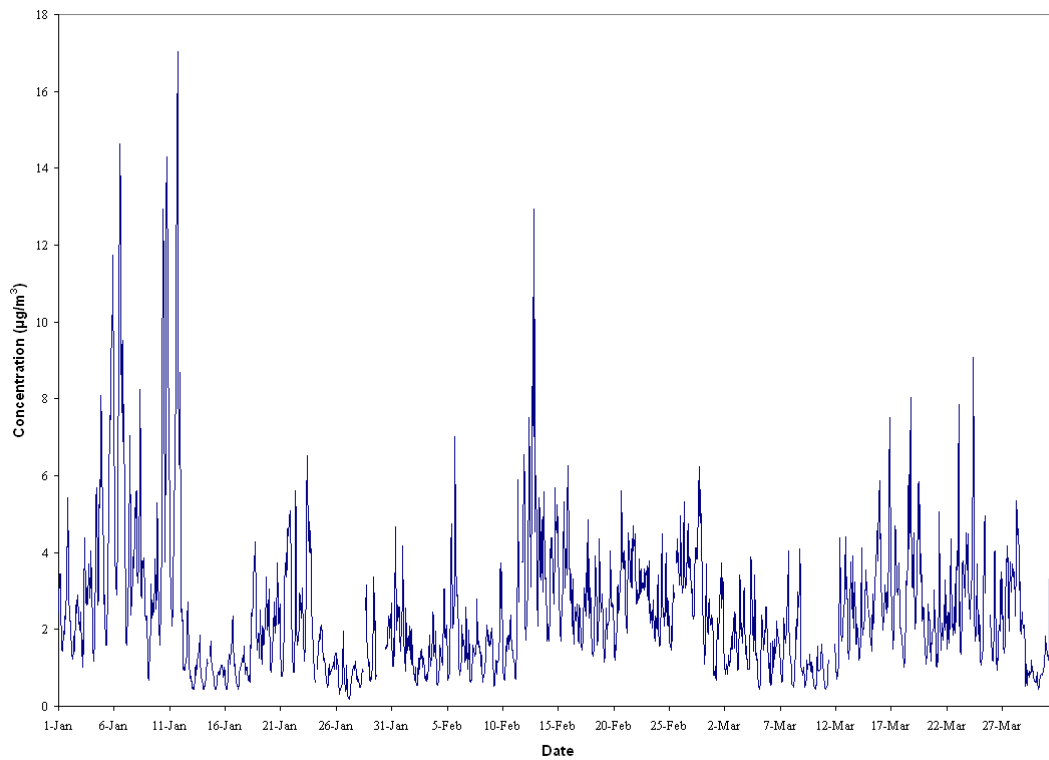


Figure 3. Time series plots for the ratified Benzene data from the Glasgow site of the UK Hydrocarbon Network, for the period; 1 January 2003 to 31 March 2003

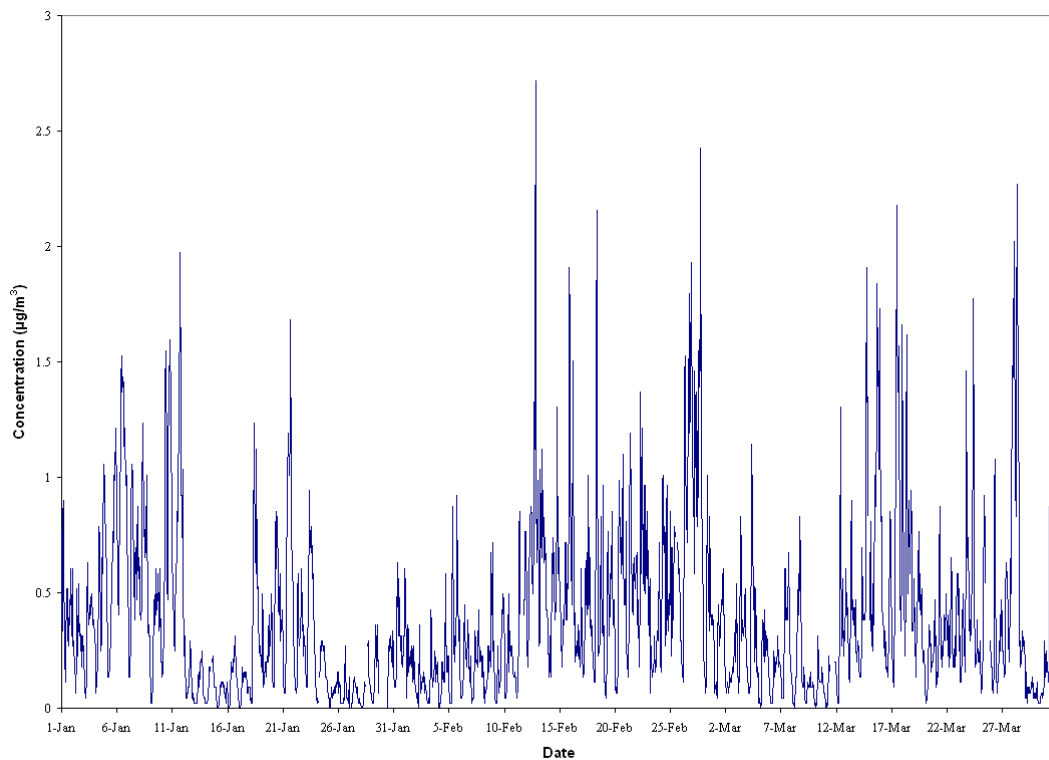


Figure 4. Time series plots for the ratified 1,3-butadiene data from the Glasgow site of the UK Hydrocarbon Network, for the period; 1 January 2003 to 31 March 2003

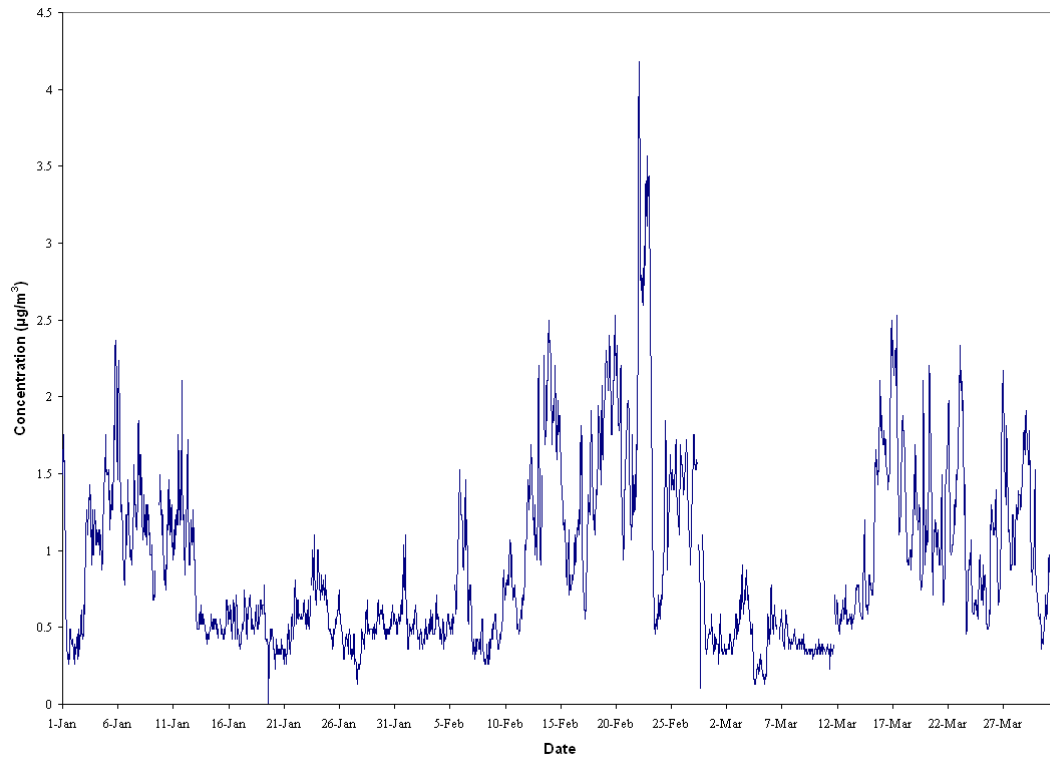


Figure 5. Time series plots for the ratified Benzene data from the Harwell site of the UK Hydrocarbon Network, for the period; 1 January 2003 to 31 March 2003

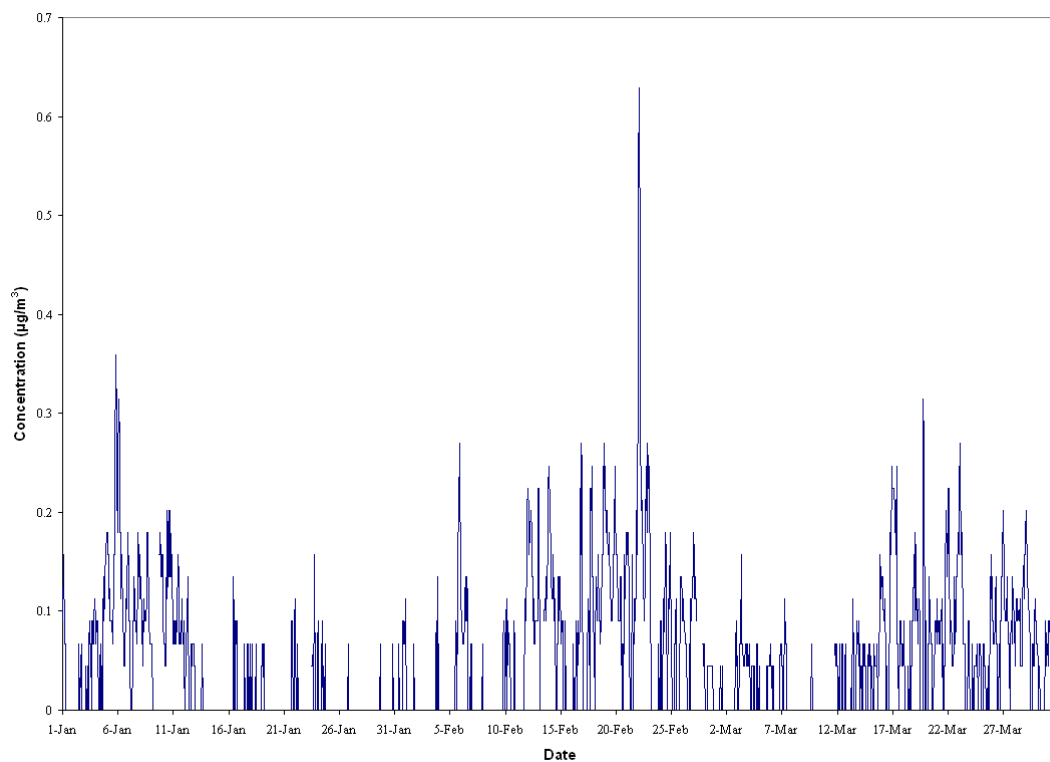


Figure 6. Time series plots for the ratified 1,3-butadiene data from the Harwell site of The UK Hydrocarbon Network, for the period; 1 January 2003 to 31 March 2003

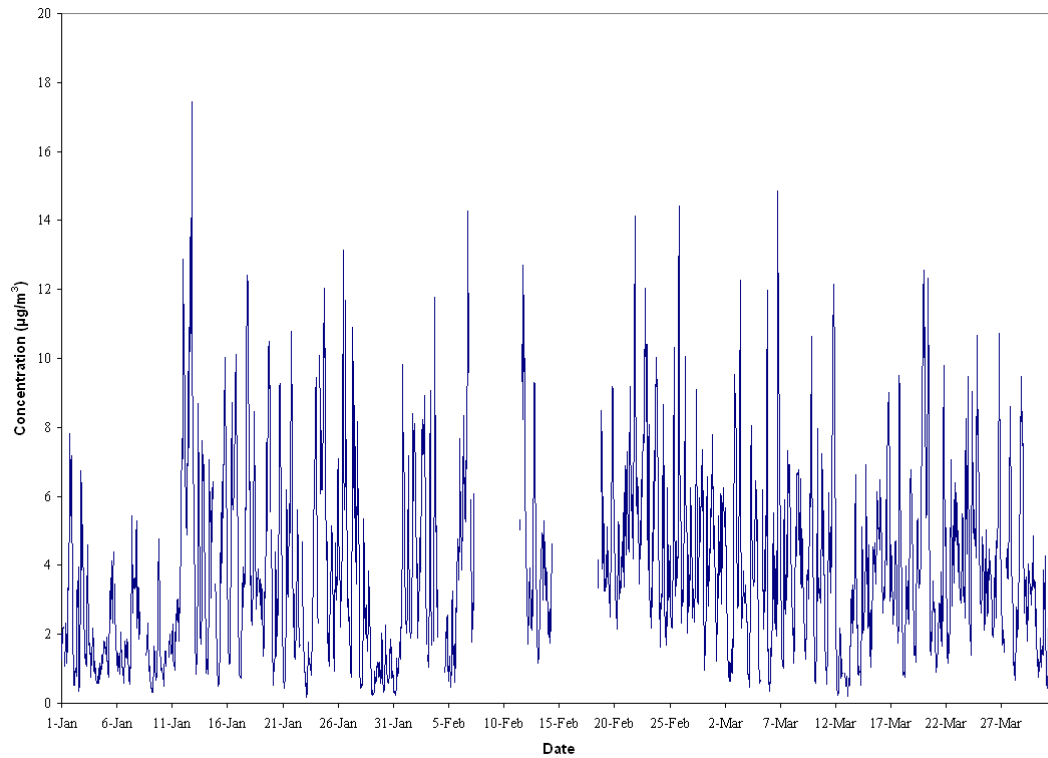


Figure 7. Time series plots for the ratified Benzene data from the Marylebone Road site affiliated to the UK Hydrocarbon Network, for the period; 1 January 2003 to 31 March 2003

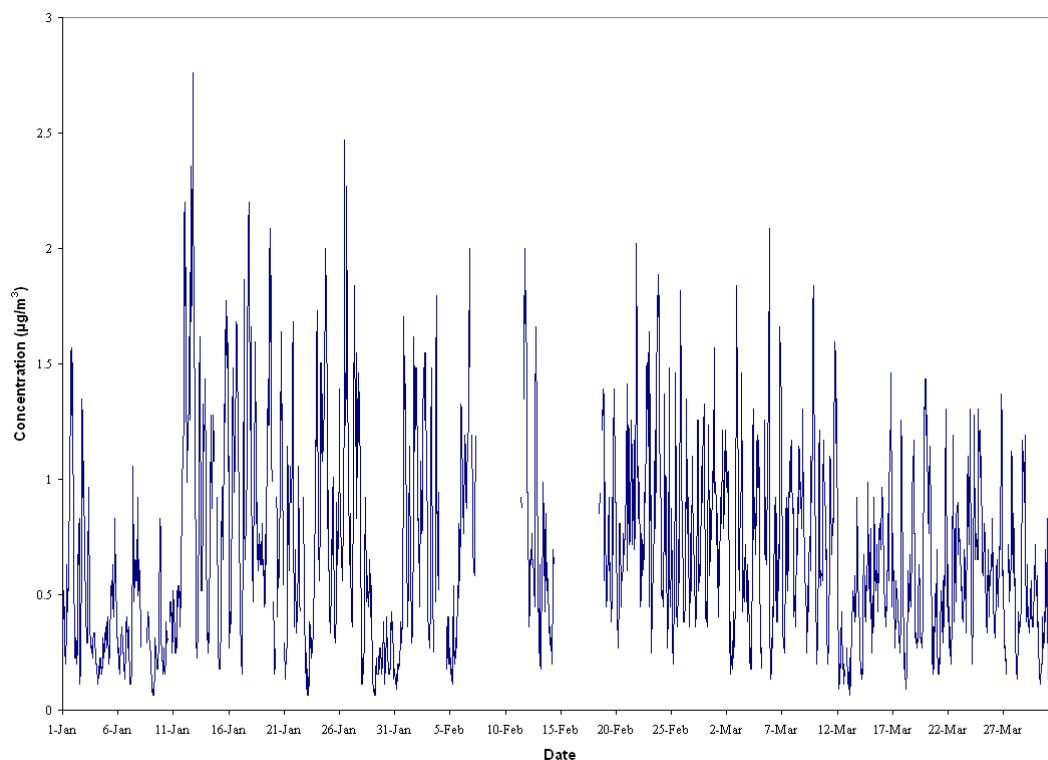


Figure 8. Time series plots for the ratified 1,3-butadiene data from the Marylebone Road site affiliated to the UK Hydrocarbon Network, for the period; 1 January 2003 to 31 March 2003