

Ratification of data produced by the UK Ambient Hydrocarbon Automatic Air Quality Network, 1 January 2001 to 31 March 2001

July 2001

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Contents

1	Introduction	1
2	Hydrocarbon Data Quality	2
3	Monthly Data Reports	3
3.1	CARDIFF	3
3.1.1	January	3
3.1.1.1	Data Quality Codes	3
3.1.1.2	Missing Data – All hydrocarbons	3
3.1.1.3	Missing Data – Specific hydrocarbons	3
3.1.2	February	3
3.1.2.1	Data Quality Codes	3
3.1.2.2	Missing Data - All hydrocarbons	3
3.1.2.3	Missing Data - Specific hydrocarbons	3
3.1.3	March	4
3.1.3.1	Data Quality Codes	4
3.1.3.2	Missing Data - All hydrocarbons	4
3.1.3.3	Missing Data - Specific hydrocarbons	4
3.2	EDINBURGH	5
3.2.1	January	5
3.2.1.1	Data Quality Codes	5
3.2.1.2	Missing Data - All hydrocarbons	5
3.2.1.3	Missing Data - Specific hydrocarbons	5
3.2.2	February	5
3.2.2.1	Data Quality Codes	5
3.2.2.2	Missing Data - All hydrocarbons	5
3.2.2.3	Missing Data - Specific hydrocarbons	5
3.2.3	March	5
3.2.3.1	Data Quality Codes	5
3.2.3.2	Missing Data - All hydrocarbons	6
3.2.3.3	Missing Data - Specific hydrocarbons	6
3.3	HARWELL	7
3.3.1	January	7
3.3.1.1	Data Quality Codes	7
3.3.1.2	Missing Data - All hydrocarbons	7
3.3.1.3	Missing Data - Specific hydrocarbons	7
3.3.2	February	7
3.3.2.1	Data Quality Codes	7
3.3.2.2	Missing Data - All hydrocarbons	7
3.3.2.3	Missing Data - Specific hydrocarbons	7
3.3.3	March	8

3.3.3.1	Data Quality Codes	8
3.3.3.2	Missing Data - All hydrocarbons	8
3.3.3.3	Missing Data - Specific hydrocarbons	8
3.4	MARYLEBONE ROAD	9
3.4.1	January	9
3.4.1.1	Data Quality Codes	9
3.4.1.2	Missing Data - All hydrocarbons	9
3.4.1.3	Missing Data - Specific hydrocarbons	9
3.4.2	February	9
3.4.2.1	Data Quality Codes	9
3.4.2.2	Missing Data - All hydrocarbons	9
3.4.2.3	Missing Data - Specific hydrocarbons	9
3.4.3	March	10
3.4.3.1	Data Quality Codes	10
3.4.3.2	Missing Data - All hydrocarbons	10
3.4.3.3	Missing Data - Specific hydrocarbons	10
4	Discussion	11

Appendices

APPENDIX 1	Summary Statistical Information
APPENDIX 2	Time Series Plots of Hydrocarbon Concentrations

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 2001 to 31 March 2001. The ratified data have been made available on the World Wide Web at www.aeat.co.uk/netcen/airqual.

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.

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 0.1 ppb and ± 0.01 ppb for values below 0.1 ppb. 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 0.2ppb and ± 0.05 ppb below 0.2 ppb.

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 except:
Data quality code E for Ethyne and 2-Methylpropane from 01/01/01 to 12/01/01.
Data quality code E for Ethane, n-Hexane, Isoprene, n-Heptane, Toluene, Ethylbenzene, (m+p)-Xylene and o-Xylene for the whole month.

3.1.1.2 Missing Data – All hydrocarbons

Calibration 19/01/01 hours 12 to 16.
GC Oven Failure 01/01/01 hour 23 to 02/01/01 hour 09.
GC Oven Failure 03/01/01 hours 13 to 15.
GC Oven Failure 03/01/01 hour 20 to 04/01/01 hour 10.
GC Oven Failure 06/01/01 hour 09 to 08/01/01 hour 09.
GC Oven Failure and CMCU maintenance visit 12/01/01 hour 13 to 17/01/01 hour 15.

3.1.1.3 Missing Data – Specific hydrocarbons

Ethyne and 2-Methylpropane coeluted from 17/01/01 to 31/01/01.

3.1.2 February

3.1.2.1 Data Quality Codes

Data quality code A for all data for all of the month except:
Data quality code E for Ethane, n-Hexane, Isoprene, n-Heptane, Toluene, Ethylbenzene, (m+p)-Xylene and o-Xylene for the whole month.

3.1.2.2 Missing Data - All hydrocarbons

Calibration 02/02/01 hours 10 to 13.
Calibration 22/02/01 hours 11 to 14.

3.1.2.3 Missing Data - Specific hydrocarbons

Ethyne and 2-Methylpropane coeluted for the whole month.

3.1.3 March

3.1.3.1 Data Quality Codes

Data quality code A for all data for all of the month except:

Data quality code E for Ethane, n-Hexane, Isoprene, n-Heptane, Toluene, Ethylbenzene, (m+p)-Xylene and o-Xylene for the whole month.

3.1.3.2 Missing Data - All hydrocarbons

Calibration 08/03/01 hours 12 to 15.

Calibration 22/03/01 hours 09 to 12.

3.1.3.3 Missing Data - Specific hydrocarbons

Ethyne and 2-Methylpropane coeluted for the whole month.

3.2 EDINBURGH

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 Ethyne, 2-Methylpropane, n-Hexane, Isoprene, Ethylbenzene, (m+p)-Xylene and o-Xylene for the whole month.

3.2.1.2 Missing Data - All hydrocarbons

Calibration 08/01/01 hours 11 to 15.

Calibration 26/01/01 hours 15 to 18.

PC/GC communication problem 22/01/01 hour 13 to 24/01/01 hour 13

3.2.1.3 Missing Data - Specific hydrocarbons

Isoprene coeluted with an unknown compound for 69% of the month.

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 Ethyne, 2-Methylpropane, n-Hexane, Isoprene, Ethylbenzene, (m+p)-Xylene and o-Xylene for the whole month.

3.2.2.2 Missing Data - All hydrocarbons

Calibration 06/02/01 hours 13 to 16.

Calibration 21/02/01 hours 13 to 16.

PC/GC communication problem 27/02/01 hour 03 to 28/02/01 hour 24.

3.2.2.3 Missing Data - Specific hydrocarbons

Isoprene coeluted with an unknown compound for the whole month.

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 Ethyne, 2-Methylpropane, n-Hexane, Isoprene, Ethylbenzene, (m+p)-Xylene and o-Xylene for the whole month.

3.2.3.2 Missing Data - All hydrocarbons

Calibration 02/03/01 hours 13 to 16.

Calibration 14/03/01 hours 12 to 15.

Calibration 27/03/01 hours 12 to 15.

PC/GC communication problem 01/03/01 hour 01 to 01/03/01 hour 17.

3.2.3.3 Missing Data - Specific hydrocarbons

Isoprene coeluted with an unknown compound for 48% of the month.

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 except:
Data quality code E for n-Hexane, Isoprene, Ethylbenzene, (m+p)-Xylene and o-Xylene for the whole month.

3.3.1.2 Missing Data - All hydrocarbons

Calibration 04/01/01 hours 10 to 13.
Calibration 18/01/01 hours 10 to 13.
No Liquid Nitrogen 01/01/01 hour 01 to 03/01/01 hour 14.
Broken analytical column 14/01/01 hour 06 to 15/01/01 hour 19.

3.3.1.3 Missing Data - Specific hydrocarbons

Ethyne and 2-Methylpropane coeluted for the whole month.
n-Hexane and Isoprene coeluted for 94% of the month.

3.3.2 February

3.3.2.1 Data Quality Codes

Data quality code A for all data for all of the month except:
Data quality code E for n-Hexane, Isoprene, Ethylbenzene, (m+p)-Xylene and o-Xylene for the whole month.

3.3.2.2 Missing Data - All hydrocarbons

Calibration 01/02/01 hours 10 to 13.
Calibration 15/02/01 hours 11 to 14.
Helium supply problem 07/02/01 hour 14 to 08/02/01 hour 20.

3.3.2.3 Missing Data - Specific hydrocarbons

Ethyne and 2-Methylpropane coeluted for the whole month.

3.3.3 March

3.3.3.1 Data Quality Codes

Data quality code A for all data for all of the month except:

Data quality code E for n-Hexane, Isoprene, Ethylbenzene, (m+p)-Xylene and o-Xylene for the whole month.

3.3.3.2 Missing Data - All hydrocarbons

Calibration 02/03/01 hours 10 to 13.

Calibration 14/03/01 hours 12 to 15.

Calibration 28/03/01 hours 09 to 12.

PC communication problem 29/03/01 hour 08 to 30/03/01 hour 14.

3.3.3.3 Missing Data - Specific hydrocarbons

Ethyne and 2-Methylpropane coeluted for the whole month.

3.4 MARYLEBONE ROAD

3.4.1 January

3.4.1.1 Data Quality Codes

Data quality code A for all species and periods.

3.4.1.2 Missing Data - All hydrocarbons

Calibration 11/01/01 hours 07 to 10.

Calibration 17/01/01 hours 16 to 19.

3.4.1.3 Missing Data - Specific hydrocarbons

Isoprene coeluted with an unknown compound for 63% of the month.

3.4.2 February

3.4.2.1 Data Quality Codes

Data quality code A for all species 01/02/01 to 10/02/01.

Data quality code E for all other species and periods.

3.4.2.2 Missing Data - All hydrocarbons

Calibration 01/02/01 hour 07 to 10.

Calibration 07/02/01 hours 19 to 22.

Calibration 27/02/01 hours 09 to 12.

PC problem / no data files 11/02/01 hour 22 to 12/02/01 hour 24.

GC oven failure 28/02/01 hour 14 to 28/02/01 hour 24.

3.4.2.3 Missing Data - Specific hydrocarbons

None.

3.4.3 March

3.4.3.1 Data Quality Codes

Data quality code E for all species and periods.

3.4.3.2 Missing Data - All hydrocarbons

Calibration 21/03/01 hours 19 to 22.

GC oven failure 01/03/01 hour 01 to 20/03/01 hour 06.

GC oven failure 23/03/01 hour 08 to 31/03/01 hour 24.

3.4.3.3 Missing Data - Specific hydrocarbons

None.

4 Discussion

Tables 1 to 4, Appendix 1 contain statistical information relating to the ratified data, for each measured hydrocarbon, over the period 1 January 2001 to 31 March 2001. 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.

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.

For the Edinburgh and Harwell sites the data capture values for benzene and 1,3-butadiene were greater than 90%.

For the Cardiff site, the data capture for benzene was 89.6 % and for 1,3-butadiene was 89.4%. An intermittent fault at the beginning of the ratification period caused the GC to go into a standby mode on a number of occasions. The fault was traced to an electric motor controlling the GC oven door. The electric motor was replaced. No further problems of this type have occurred.

Data capture for the Marylebone Road site is significantly lower for all compounds. The reasons for the much lower data capture were two independent faults that resulted in a significant period of data loss. A fault occurred with the oven fan motor of the Perkin Elmer/ATD400 (PE/ATD400). The oven fan motor was replaced under the terms of the service agreement. Within a number of days a second fault occurred with one of the heater elements. After replacement of the heater elements there appeared there was a fault with the replacement oven fan motor. A second replacement fan motor was not immediately available. The delay in obtaining a second replacement motor resulted in a period of data loss totalling nearly a month.

The response of the PE/ATD400 to the injection of the on-site standard displayed a higher than usual degree of variability for periods prior to and after the fault described above. The degree of variability of the response resulted in a level of uncertainty (at 95% confidence) of greater than 10%. As a result of the greater uncertainty the data has been assigned the Data Quality Code 'E'.

Appendices

CONTENTS

Appendix 1	Summary Statistical Information
Appendix 2	Time Series Plots of Hydrocarbon Concentrations

Appendix 1

Summary Statistical Information

CONTENTS

Table 1.	Percentage data capture, maximum, mean and minimum values of ratified data from the Cardiff site of the UK Hydrocarbon Network, for the period; 1 January 2001 to 31 March 2001
Table 2.	Percentage data capture, maximum, mean and minimum values of ratified data from the Edinburgh site of the UK Hydrocarbon Network, for the period; 1 January 2001 to 31 March 2001
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 2001 to 31 March 2001
Table 4.	Percentage data capture, maximum, mean and minimum values of ratified data from the Marylebone Road site for the period; 1 January 2001 to 31 March 2001

Table 1. Percentage data capture, maximum, mean and minimum values of ratified data from the Cardiff site of the UK Hydrocarbon Network, for the period 1 January 2001 to 31 March 2001

Compound	%data capture	Maximum concentration (ppb)	Mean concentration (ppb)	Minimum concentration (ppb)
Ethane	89.44	45.7	6.94	2.01
Ethene	89.44	35.98	3.7	0.24
Propane	89.54	68.81	3.33	0.56
Propene	89.54	11.01	1.45	0.27
Ethyne	8.06	7.22	1.65	0.73
2-Methylpropane	8.06	5.24	1.35	0.29
n-Butane	89.26	28.88	3.35	0.34
trans-2-Butene	89.26	0.96	0.16	0.05
1-Butene	83.38	1.25	0.14	0.01
cis-2-Butene	85.65	0.89	0.1	0.02
2-Methylbutane	88.89	23.72	2.14	0.16
n-Pentane	89.17	11.37	0.82	0.08
1,3-Butadiene	89.4	2.09	0.14	0
trans-2-Pentene	85	1.2	0.1	0.01
cis-2-Pentene	74.81	0.62	0.05	0.01
(2+3)-Methylpentane *	89.49	15.84	0.81	0.03
Isoprene	86.81	5.59	0.12	0.01
n-Hexane	89.58	5.55	0.26	0.04
n-Heptane	88.38	8.45	0.15	0.01
Benzene	89.58	6.41	0.75	0.11
Toluene	87.69	16.67	1.84	0.03
Ethylbenzene	68.7	3.19	0.38	0.02
(m+p)-Xylene *	73.7	11.28	1.19	0.04
o-Xylene	39.49	4.67	0.55	0.05

* (2+3)-Methylpentane and (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.

Table 2. Percentage data capture, maximum, mean and minimum values of ratified data from the Edinburgh site of the UK Hydrocarbon Network, for the period 1 January 2001 to 31 March 2001

Compound	%data capture	Maximum concentration (ppb)	Mean concentration (ppb)	Minimum concentration (ppb)
Ethane	93.38	98.33	7.16	1.98
Ethene	93.38	38.17	2.51	0.23
Propane	93.38	291.3	5.17	0.57
Propene	93.38	9.54	1.2	0.41
Ethyne	93.33	28.52	2.04	0.32
2-Methylpropane	93.38	85.57	1.64	0.17
n-Butane	93.38	213.8	3.32	0.3
trans-2-Butene	93.38	2.02	0.31	0.11
1-Butene	92.31	2.47	0.13	0.01
cis-2-Butene	93.38	1.45	0.12	0.02
2-Methylbutane	93.43	54.5	1.39	0.1
n-Pentane	93.43	60.87	0.89	0.07
1,3-Butadiene	93.1	1.76	0.11	0
trans-2-Pentene	89.26	2.12	0.08	0.01
cis-2-Pentene	73.43	1.01	0.04	0.01
(2+3)-Methylpentane *	93.38	17.29	0.52	0.03
Isoprene	27.5	0.51	0.05	0.01
n-Hexane	93.38	14.49	0.27	0.02
n-Heptane	92.22	3.04	0.1	0
Benzene	93.43	7.11	0.56	0.14
Toluene	92.69	33.7	1.55	0.04
Ethylbenzene	80.37	5.68	0.26	0.01
(m+p)-Xylene *	83.19	20.32	0.77	0.01
o-Xylene	72.27	6.84	0.29	0.01

* (2+3)-Methylpentane and (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.

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 2001 to 31 March 2001

Compound	%data capture	Maximum concentration (ppb)	Mean concentration (ppb)	Minimum concentration (ppb)
Ethane	90.88	8.66	2.41	0.74
Ethene	90.65	5.3	0.87	0.04
Propane	90.97	5.53	1.54	0.22
Propene	91.02	2.69	0.39	0.05
Ethyne	0	-	-	-
2-Methylpropane	0	-	-	-
n-Butane	90.88	12.87	0.94	0.05
trans-2-Butene	41.53	0.26	0.04	0.01
1-Butene	53.24	0.38	0.06	0.01
cis-2-Butene	17.55	0.24	0.05	0.01
2-Methylbutane	90.97	6.92	0.45	0.02
n-Pentane	90.14	1.84	0.19	0.01
1,3-Butadiene	91.02	0.49	0.06	0.01
trans-2-Pentene	22.04	0.6	0.02	0
cis-2-Pentene	8.33	0.27	0.02	0
(2+3)-Methylpentane *	86.57	1.77	0.2	0
Isoprene	30.93	0.34	0.02	0
n-Hexane	58.01	0.47	0.06	0
n-Heptane	68.33	0.36	0.05	0
Benzene	91.02	1.53	0.31	0.05
Toluene	82.31	7.99	0.56	0.02
Ethylbenzene	54.91	0.78	0.12	0.01
(m+p)-Xylene *	62.73	2.56	0.32	0.02
o-Xylene	39.35	0.98	0.15	0

* (2+3)-Methylpentane and (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.

Table 4. Percentage data capture, maximum, mean and minimum values of ratified data from the Marylebone Road site for the period; 1 January 2001 to 31 March 2001

Compound	%data capture	Maximum concentration (ppb)	Mean concentration (ppb)	Minimum concentration (ppb)
Ethane	65.23	78.74	10.65	3.11
Ethene	65.19	66.92	10.86	0.7
Propane	63.1	28.2	4.05	0.84
Propene	64.35	17.35	3.38	0.06
Ethyne	64.95	35.6	7.37	0.78
2-Methylpropane	65.42	24.6	3.95	0.47
n-Butane	65.56	46.71	7.73	0.02
trans-2-Butene	65.69	2.59	0.5	0.02
1-Butene	65.74	2.43	0.55	0.03
cis-2-Butene	65.79	1.96	0.4	0.02
2-Methylbutane	65.88	28.67	5.76	0.41
n-Pentane	65.93	8.19	1.53	0.22
1,3-Butadiene	65.93	3.44	0.5	0.03
trans-2-Pentene	65.93	1.68	0.4	0.01
cis-2-Pentene	65.93	0.92	0.22	0.01
2-Methylpentane	65.88	16.79	1.74	0.14
3-Methylpentane	65.79	5.8	0.98	0.06
Isoprene	43.94	1.49	0.2	0.02
n-Hexane	65.97	2.64	0.49	0.03
n-Heptane	62.59	2.29	0.27	0.02
Benzene	66.16	8.81	1.64	0.09
Toluene	66.16	33.25	6.08	0.21
Ethylbenzene	66.16	5.6	0.98	0.04
(m+p)-Xylene *	66.16	18.51	3.38	0.07
o-Xylene	66.16	6.8	1.21	0.06
1,3,5-Trimethylbenzene	65.97	3.66	0.37	0.02
1,2,4-Trimethylbenzene	66.16	13.46	1.11	0.06

* (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

CONTENTS

- Figure 1. Time series plot of the ratified Benzene data from the Cardiff site of the UK Hydrocarbon Network, for the period; 1 January 2001 to 31 March 2001
- 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 2001 to 31 March 2001
- Figure 3. Time series plots for the ratified Benzene data from the Edinburgh site of the UK Hydrocarbon Network, for the period; 1 January 2001 to 31 March 2001
- Figure 4. Time series plots for the ratified 1,3-Butadiene data from the Edinburgh site of the UK Hydrocarbon Network, for the period; 1 January 2001 to 31 March 2001
- Figure 5. Time series plots for the ratified Benzene data from the Harwell site of the UK Hydrocarbon Network, for the period; 1 January 2001 to 31 March 2001
- 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 2001 to 31 March 2001
- 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 2001 to 31 March 2001
- 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 2001 to 31 March 2001



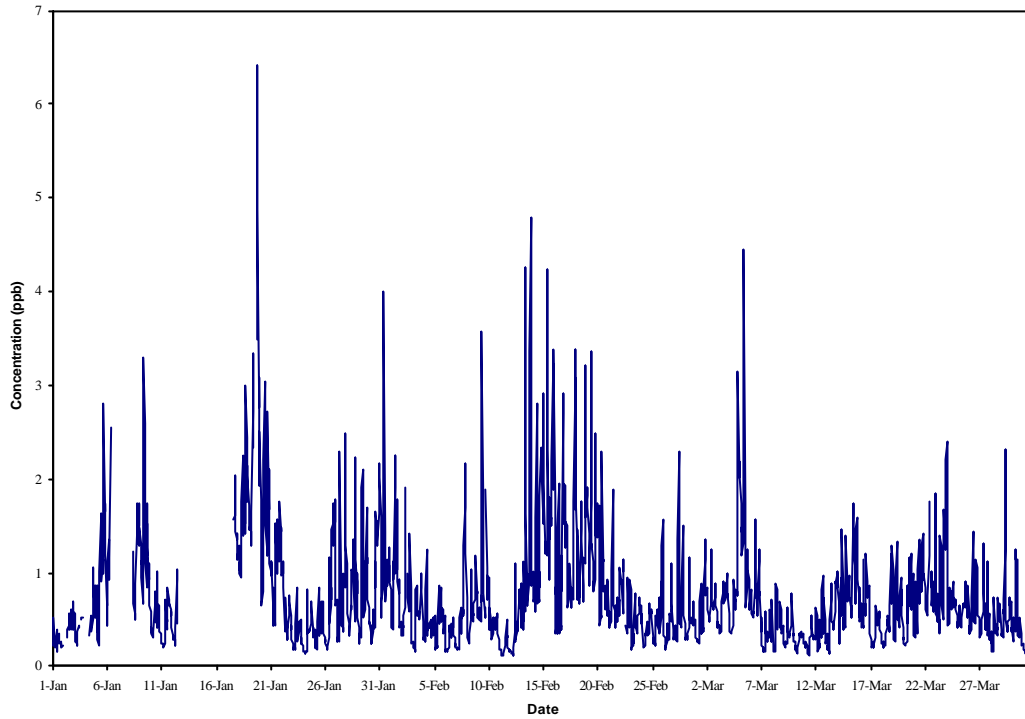


Figure 1. Time series plot of the ratified Benzene data from the Cardiff site of the UK Hydrocarbon Network, for the period; 1 January 2001 to 31 March 2001

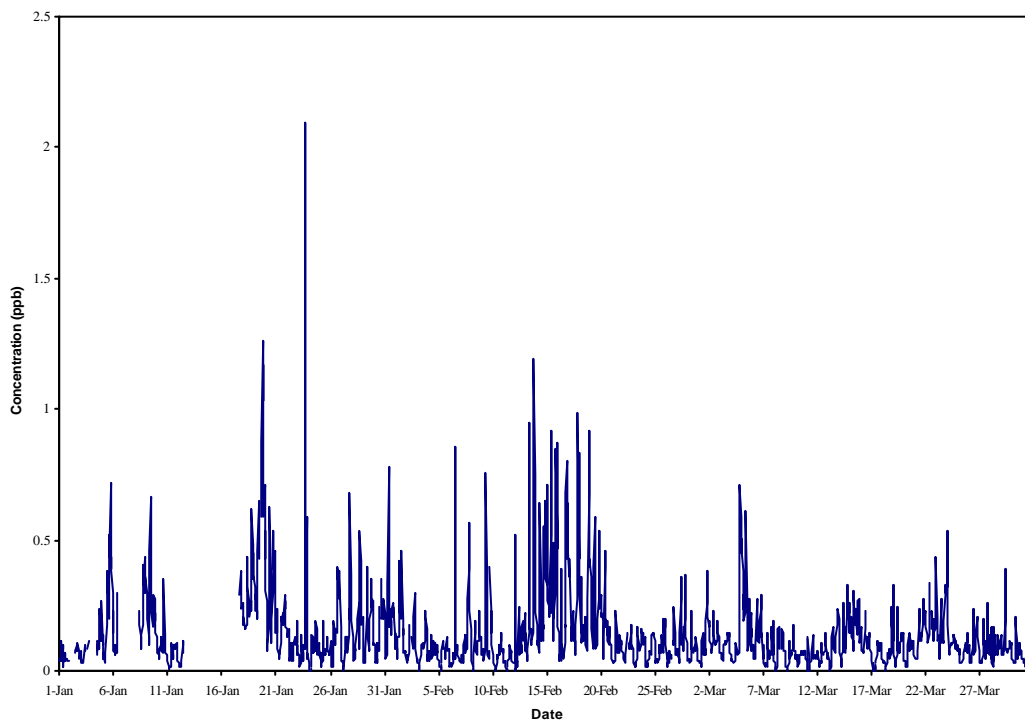


Figure 2. Time series plot of the ratified 1,3-Butadiene data from the Cardiff site of the UK Hydrocarbon Network, for the period; 1 January 2001 to 31 March 2001

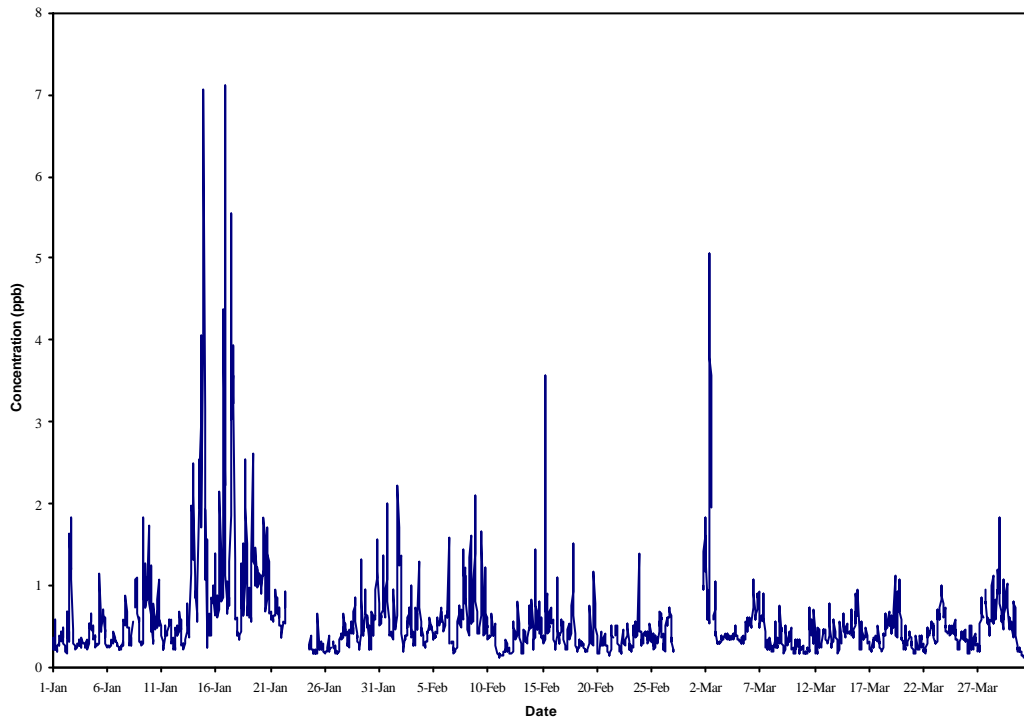


Figure 3. Time series plots for the ratified Benzene data from the Edinburgh site of the UK Hydrocarbon Network, for the period; 1 January 2001 to 31 March 2001

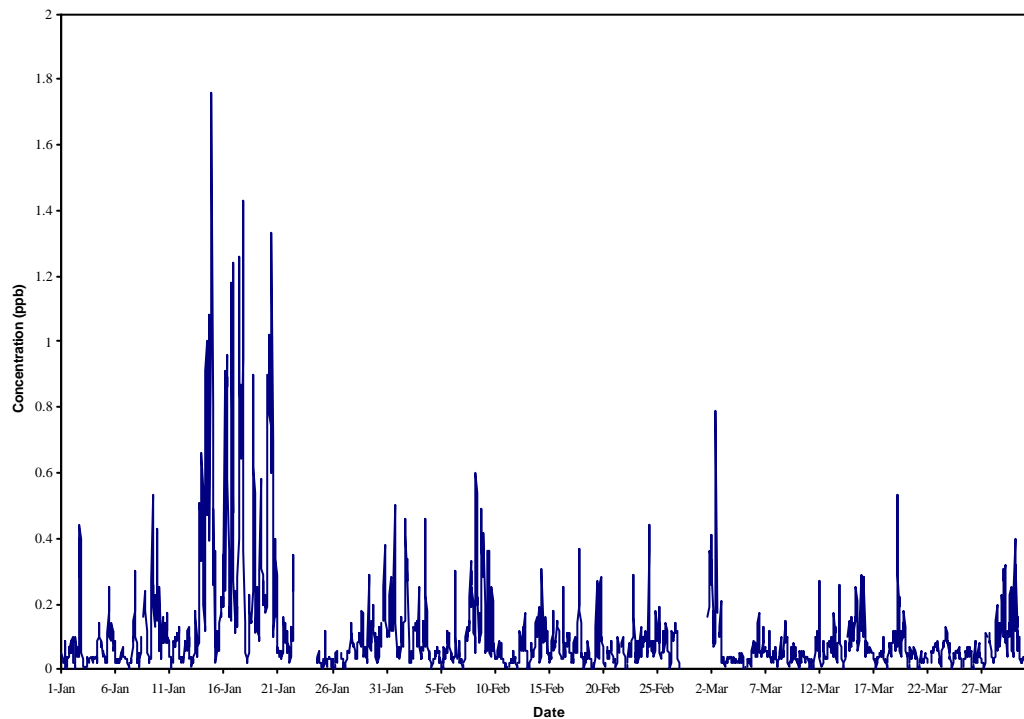


Figure 4. Time series plots for the ratified 1,3-Butadiene data from the Edinburgh site of the UK Hydrocarbon Network, for the period; 1 January 2001 to 31 March 2001

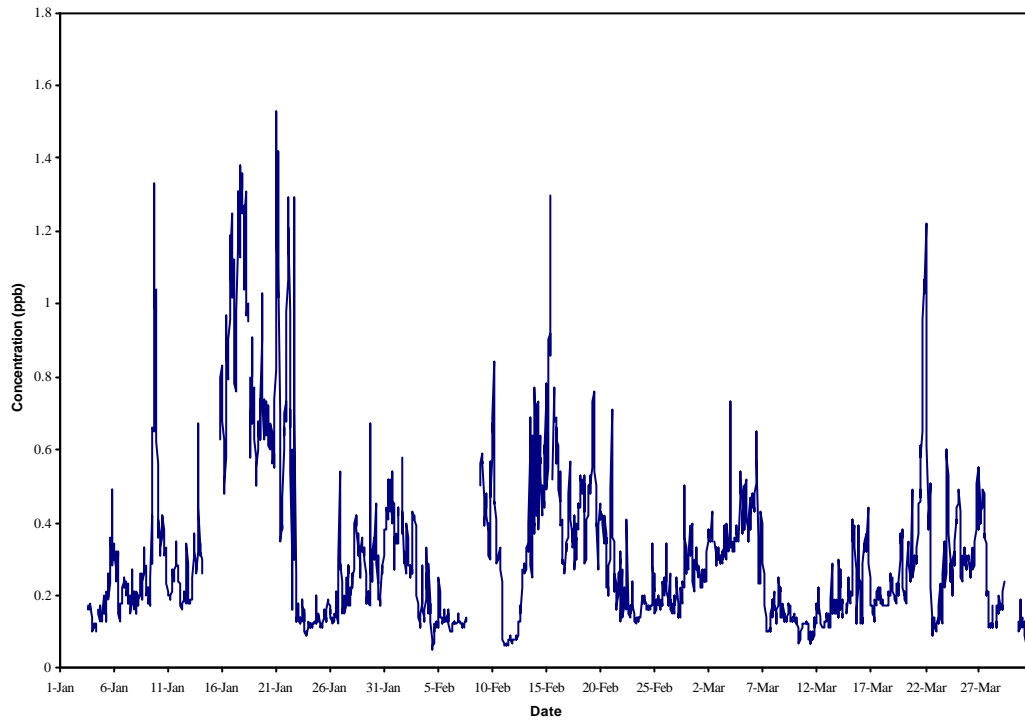


Figure 5. Time series plots for the ratified Benzene data from the Harwell site of the UK Hydrocarbon Network, for the period; 1 January 2001 to 31 March 2001

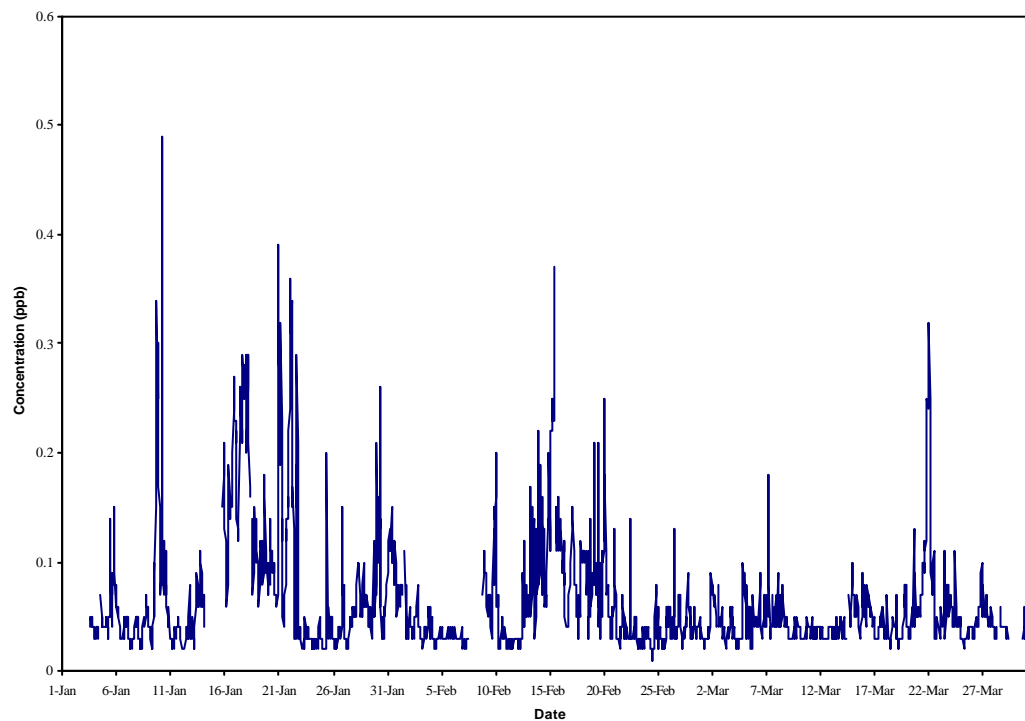


Figure 6. Time series plots for the ratified 1,3-Butadiene data from the Harwell site of the UK Hydrocarbon Network, for the period; 1 January 2001 to 31 March 2001

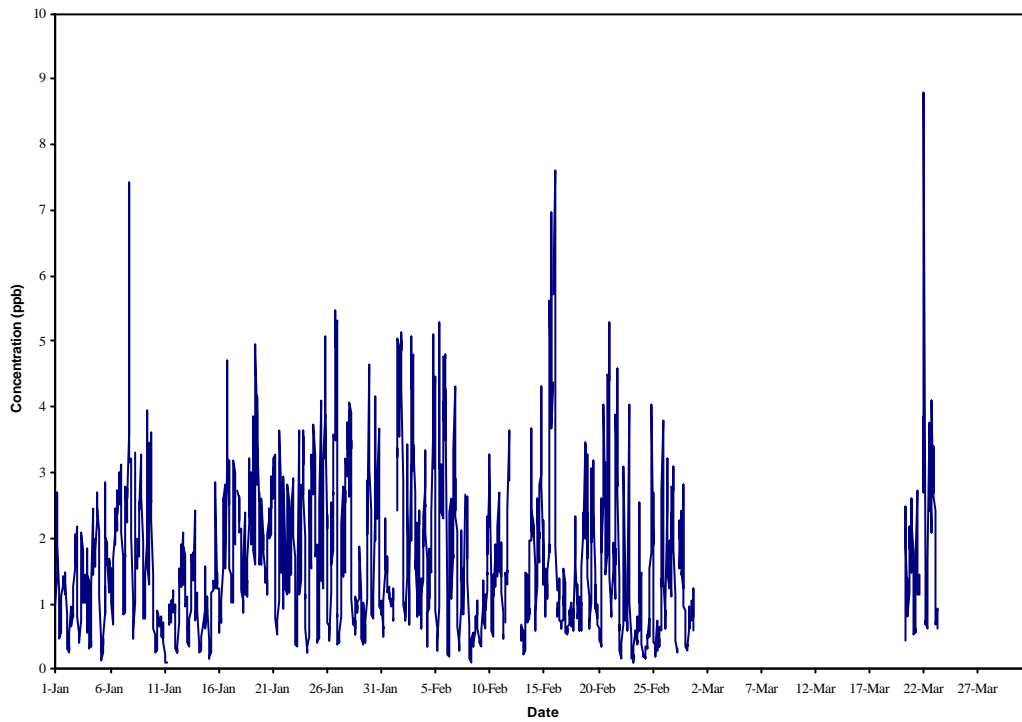


Figure 7. Time series plots for the ratified Benzene data from the Marylebone Road site affiliated to the UK Hydrocarbon Network, for the period; 1 January 2001 to 31 March 2001

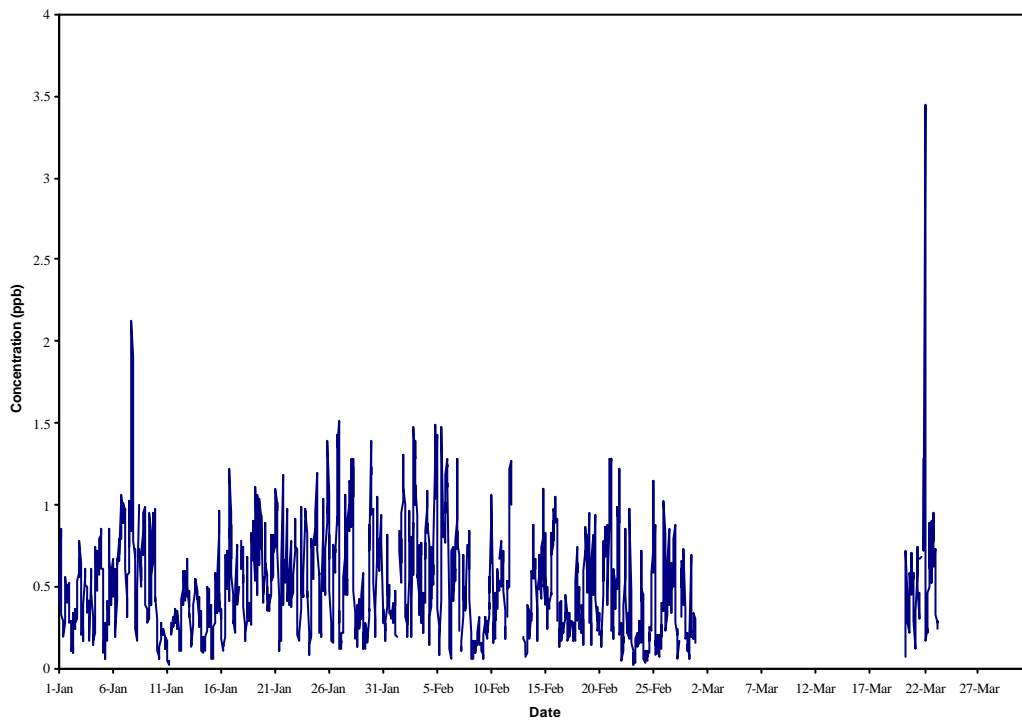


Figure 8. Time series plots for the ratified 1,3-Butadiene data from the Marylebone Road site affiliated to the UK Hydrocarbon Network, for the period; 1 January 2001 to 31 March 2001