NAME III Document
MD13/8(version 1)
23/03/07

Testing the NAME III chemistry scheme – updated comparisons with NAME II predictions for the PUMA summer campaign

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1 Introduction

The Pollution of the Urban Midlands Atmosphere (PUMA) project was an intensive study to investigate air quality in the West Midlands urban area, conducted as part of the NERC URGENT (Urban Regeneration and the Environment) programme of research. Earlier modelling of the PUMA summer campaign by NAME II and NAME III has been reported in some detail in the previous version of this document. The aim of that earlier report was simply to show a direct comparison of the NAME II and NAME III chemistry predictions as a basic test of the integrity of the chemistry code developed for NAME III. Details of the PUMA study are not repeated again here. Instead, the present report focuses on the follow-up activities that have been carried out to understand the differences observed in the earlier report and to provide reassurance on the chemistry modelling in NAME III prior to using NAME III in chemistry and air quality applications. These activites have included further NAME III simulations designed to test the operation of its chemistry scheme.

2 Version of NAME III used for updated modelling work

The previous modelling exercise used version 2.0 of NAME III, and results were compared against those obtained using version 8.12 of NAME II. The updated modelling uses a modified form of version 4.1 of NAME III that includes all changes up to and including 23/11/2006 (see Changes file for details). Also note that the two-thirds correction factor appropriate for the STOCHEM values of background ozone was not applied when resetting ozone in the absence of particles within a grid box. This is intended to be consistent with the error in version 8.12 of NAME II.

Obviously there have been a large number of model changes in the development of NAME III between version 2.0 and version 4.1. However it is believed that the most significant changes, in terms of likely impact on the chemistry calculations, have been the correction of a dry deposition bug (which erroneously caused particles above the boundary layer to be deposited), and the calculation of output from chemistry fields on unstructured horizontal grids (this was not properly supported previously).

NAME III can model ozone by one of two methods, either by representing ozone on a static 3-d grid or by carrying ozone on particles. Ozone is modelled on a grid in this study.

3 Results of the comparison study

Since the underlying chemistry scheme is the same in both models, then we should expect there to be reasonable agreement in the chemistry evolutions. In particular, any gross errors in the implementation of the NAME III chemistry scheme should be revealed by this type of comparative study. At the same time, differences in the formulation of the dispersion models mean that we should not expect precise agreement in the time series, although we have tried to minimize such differences by setting up the NAME II and NAME III model runs to be as consistent as possible.

One significant difference between the two models, however, is the manner in which particles are released from each source. NAME III tends to be more 'economical' with particles by using a release interval calculated from the particle mass limit and source strength (as well as imposing a minimum particle release rate for each source). This release interval is carried forward from one model time step to the next, so that the release of particles is independent of the model synchronisation step. The approach in NAME II is slightly different in that the release 'clock' is reset at the start of each model time step. As a consequence, the NAME III run is expected to produce slightly fewer particles in total than the NAME II simulation. In an attempt to assess the impact of this difference, a second NAME III simulation was also considered (using an enhanced minimum release rate of at least 8 particles per hour from each source, as against 4 particles per hour in the standard run). This allowed us to bracket the NAME II simulation between two NAME III runs. Time series of total particle numbers in the NAME II and NAME III simulations are plotted in Figure 1. Results from the second NAME III run are not shown elsewhere in this report, but it is noted that differences between the two NAME III simulations are typically smaller than the differences between NAME III and NAME II. This suggests that particle numbers are sufficient to ensure that results are not being adversely affected by statistical noise.

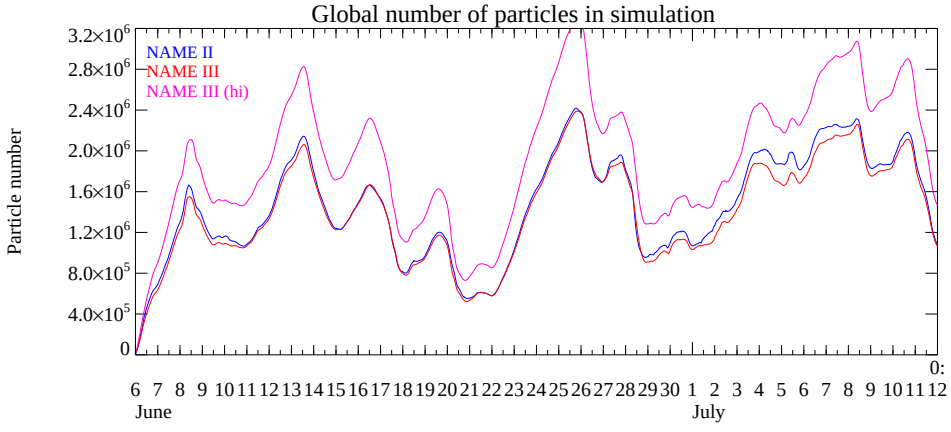

Figure 1: A comparison of the total number of particles in the model domain between the NAME II and NAME III simulations. Note that two NAME III simulations are considered with different minimum particle release rates. The NAME II run lies between these two scenarios.

A comprehensive set of plots in Appendix A provides a speciated comparison of the chemistry evolution in the two models during the PUMA summer campaign. Here we consider all the main species represented in the NAME chemistry scheme that can be requested as output (that is, the species carried on particles and the chemistry fields) at the Birmingham location. Figures 4 – 27 show species that are carried on particles (both as a 0 – 50 m concentration and as a boundary-layer average concentration), whereas Figures 28 – 38 compare the evolution of the chemistry fields in the lowest chemistry layer (effectively, a 0 – 50 m concentration). Tables 1 and 2 provide a statistical analysis of these time series.

We observe that there is generally very good temporal agreement between the predictions of NAME III and those of NAME II for most species. However the agreement is perhaps a little less strong for a few species, notably ammonia and sulphate aerosol (particles carrying ammonia are relatively sparse and this is a likely reason for the poorer agreement seen for these species). The relative magnitudes of the chemistry species in the two simulations (see column 'III/II' for mean concentrations in Tables 1 and 2) are generally in good agreement, as are the correlation values; see Figure 2 for 0 – 50 m data shown graphically.

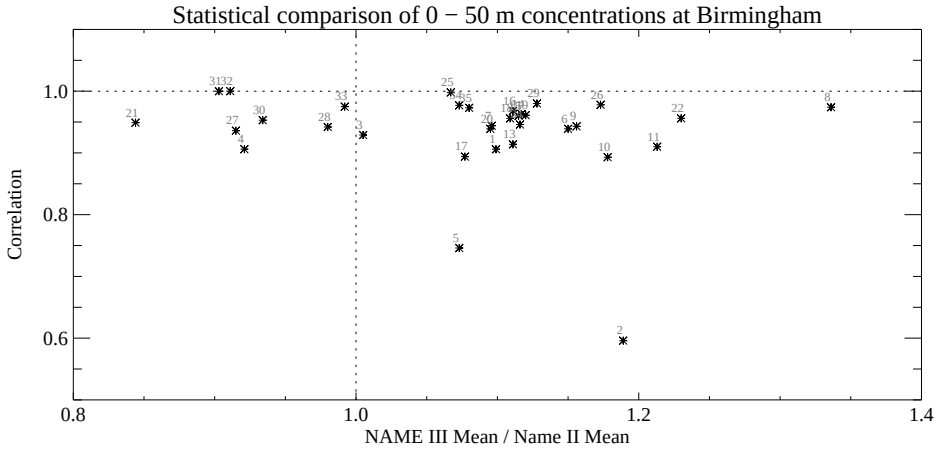

Figure 2: Comparison of the NAME II and NAME III predictions of the 0 – 50 m concentrations at Birmingham (residual versus correlation). Numbers indicate species in the order shown in Table 1 (1 – 24 for particle species; 25 – 35 for chemistry fields). Data are shown in Table 1.

It is noted that the Birmingham location is well resolved in the modelling domain (in the sense that surrounding regional sources are well represented and so there are always particles within that region). At locations nearer to the periphery of the domain, general particle numbers per grid box are typically fewer and there are often times when there are no particles in a grid box (causing the chemistry to reset in that grid box). In these instances, the NAME II and NAME III simulations also generally demonstrate good agreement. Results for such locations are not shown explicitly here, with the exception of the ozone field at Yarner Wood, shown in Figure 3, which illustrates the behaviour of the ozone field resetting to the STOCHEM background in the absence of

	Mean concentration			Standard deviation			Correlation
Species	NAME III	NAME II	III/II	NAME III	NAME II	III/II	
SO2	1.085E+01	9.871E+00	1.099	1.473E+01	1.400E+01	1.052	0.906
AMMONIA	4.422E+00	3.719E+00	1.189	3.653E+00	2.997E+00	1.219	0.596
NO	8.936E+00	8.891E+00	1.005	7.266E+00	6.603E+00	1.100	0.929
NH42SO4	2.674E+00	2.903E+00	0.921	3.889E+00	4.226E+00	0.920	0.906
SULPHATE	5.215E-01	4.860E-01	1.073	8.355E-01	6.971E-01	1.199	0.746
NO2	1.547E+01	1.345E+01	1.150	1.219E+01	9.398E+00	1.297	0.939
NO3	3.329E-07	3.037E-07	1.096	7.448E-07	6.158E-07	1.209	0.944
N2O5	1.556E-05	1.165E-05	1.336	5.709E-05	4.069E-05	1.403	0.974
HNO3	2.025E+00	1.752E+00	1.156	3.128E+00	2.487E+00	1.258	0.943
NAER	2.314E-01	1.965E-01	1.178	3.695E-01	3.245E-01	1.139	0.893
NH4NO3	1.198E+00	9.876E-01	1.213	1.975E+00	1.593E+00	1.239	0.910
O3_PART†	0.000E+00	1.239E-02	—	0.000E+00	1.476E-02	—	—
CO	1.520E+02	1.369E+02	1.111	1.005E+02	8.571E+01	1.173	0.914
HCHO	9.144E+00	8.186E+00	1.117	7.579E+00	5.962E+00	1.271	0.963
C2H4	1.278E+01	1.147E+01	1.115	9.443E+00	7.402E+00	1.276	0.960
C3H6	5.053E+00	4.547E+00	1.111	5.466E+00	4.426E+00	1.235	0.968
C5H8	4.370E-02	4.059E-02	1.077	3.483E-02	2.935E-02	1.187	0.894
OXYL	3.780E+00	3.408E+00	1.109	2.722E+00	2.142E+00	1.270	0.956
TOLUEN	2.239E+01	1.999E+01	1.120	1.688E+01	1.321E+01	1.278	0.961
BD	7.847E-01	7.168E-01	1.095	5.973E-01	4.729E-01	1.263	0.939
CH3CHO	2.266E-01	2.686E-01	0.844	2.561E-01	2.925E-01	0.876	0.949
PAN	1.209E+00	9.833E-01	1.230	2.172E+00	1.591E+00	1.365	0.956
HONO	0.000E+00	0.000E+00	—	0.000E+00	0.000E+00	—	—
PM10	4.936E+00	4.421E+00	1.116	3.237E+00	2.618E+00	1.236	0.946
H2O2	1.738E-01	1.629E-01	1.067	1.971E-01	1.988E-01	0.991	0.998
O3	1.453E+01	1.239E+01	1.173	1.789E+01	1.476E+01	1.211	0.978
OH	6.639E-05	7.258E-05	0.915	7.774E-05	7.967E-05	0.976	0.936
HO2	6.803E-04	6.941E-04	0.980	8.892E-04	8.408E-04	1.058	0.942
CH3OOH	4.244E-03	3.763E-03	1.128	1.709E-03	1.416E-03	1.207	0.980
MVK	6.011E-02	6.435E-02	0.934	1.821E-02	1.905E-02	0.956	0.953
ISOPOOH	4.169E-03	4.619E-03	0.903	2.612E-03	2.944E-03	0.887	1.000
MVKOOH	4.076E-03	4.476E-03	0.911	2.563E-03	2.855E-03	0.898	1.000
MGLYOX	8.606E-01	8.675E-01	0.992	6.217E-01	5.362E-01	1.160	0.975
GLYOX	5.574E+00	5.194E+00	1.073	2.152E+00	1.845E+00	1.167	0.977
MEMALD	6.352E-01	5.883E-01	1.080	3.413E-01	2.845E-01	1.199	0.973

Table 1: A comparison of the 0-50 m air concentration predictions at Birmingham (all species). Concentration units are $\mu g/m^3$ for species carried on particles ($SO_2 \rightarrow PM_{10}$), and ppbv for species on chemistry fields ($H_2O_2 \rightarrow$ MEMALD).
†O_3 is modelled on a static field in this test case. The $O_{3_{part}}$ species in NAME II carries a local production term on the particles; this particle species is not used in NAME III.

	Mean concentration			Standard deviation			Correlation
Species	NAME III	NAME II	III/II	NAME III	NAME II	III/II	
SO2	1.064E+01	9.945E+00	1.070	1.493E+01	1.421E+01	1.051	0.942
AMMONIA	3.443E+00	3.110E+00	1.107	2.736E+00	2.458E+00	1.113	0.733
NO	5.863E+00	5.768E+00	1.016	5.992E+00	5.598E+00	1.070	0.972
NH42SO4	2.749E+00	3.108E+00	0.885	3.981E+00	4.497E+00	0.885	0.959
SULPHATE	5.065E-01	4.967E-01	1.020	8.086E-01	6.687E-01	1.209	0.826
NO2	1.291E+01	1.153E+01	1.120	1.091E+01	9.109E+00	1.198	0.973
NO3	2.933E-07	2.662E-07	1.102	6.873E-07	6.245E-07	1.101	0.973
N2O5	1.686E-05	1.405E-05	1.200	7.221E-05	6.252E-05	1.155	0.983
HNO3	1.836E+00	1.615E+00	1.137	3.001E+00	2.551E+00	1.176	0.970
NAER	2.297E-01	2.059E-01	1.116	3.592E-01	3.299E-01	1.089	0.932
NH4NO3	1.196E+00	1.043E+00	1.147	1.920E+00	1.632E+00	1.176	0.940
O3_PART†	0.000E+00	1.239E-02	—	0.000E+00	1.476E-02	—	—
CO	1.190E+02	1.065E+02	1.117	9.277E+01	7.926E+01	1.170	0.966
HCHO	6.476E+00	5.798E+00	1.117	6.861E+00	5.629E+00	1.219	0.980
C2H4	9.265E+00	8.347E+00	1.110	8.474E+00	6.955E+00	1.218	0.977
C3H6	3.280E+00	3.044E+00	1.078	4.381E+00	3.753E+00	1.168	0.974
C5H8	2.825E-02	2.586E-02	1.092	2.483E-02	2.211E-02	1.123	0.945
OXYL	2.718E+00	2.454E+00	1.108	2.432E+00	2.004E+00	1.214	0.976
TOLUEN	1.639E+01	1.473E+01	1.113	1.520E+01	1.245E+01	1.221	0.978
BD	5.288E-01	4.821E-01	1.097	4.902E-01	4.141E-01	1.184	0.967
CH3CHO	1.903E-01	2.135E-01	0.891	2.377E-01	2.547E-01	0.933	0.972
PAN	1.117E+00	9.381E-01	1.191	2.138E+00	1.729E+00	1.236	0.985
HONO	0.000E+00	0.000E+00	—	0.000E+00	0.000E+00	—	—
PM10	3.805E+00	3.428E+00	1.110	2.970E+00	2.483E+00	1.196	0.971

Table 2: A comparison of the boundary-layer average concentration predictions (for species held on particles only). Concentration units are μg/m^3.

grid box particles. This behaviour is qualitatively similar in the NAME II and NAME III runs, and offers support that the chemistry scheme is functioning similarly in the two models. The figure also demonstrates that, with an increased number of particles in the second NAME III simulation (pink curve), the resetting of ozone to background occurs less frequently (as should be expected).

4 Remarks and conclusions

The report has compared predictions of the NAME III chemistry scheme with those of NAME II chemistry for the PUMA summer campaign. The primary aim of this work has been to understand differences observed in the earlier comparison and to provide reassurance on the chemistry modelling in NAME III prior to using NAME III in chemistry and air quality applications.

The NAME II and NAME III model runs were set up to be as consistent as possible, although small differences in the particle numbers did occur in the two simulations as a consequence of the different method used in the two models to release particles from the sources (as well as other model differences). The NAME II and NAME III predictions demonstrate a good level of mutual agreement, with the temporal evolution of chemistry species at the Birmingham location being strongly correlated between the two runs. In summary, we have concluded that we believe the chemistry scheme in NAME III is functioning correctly.

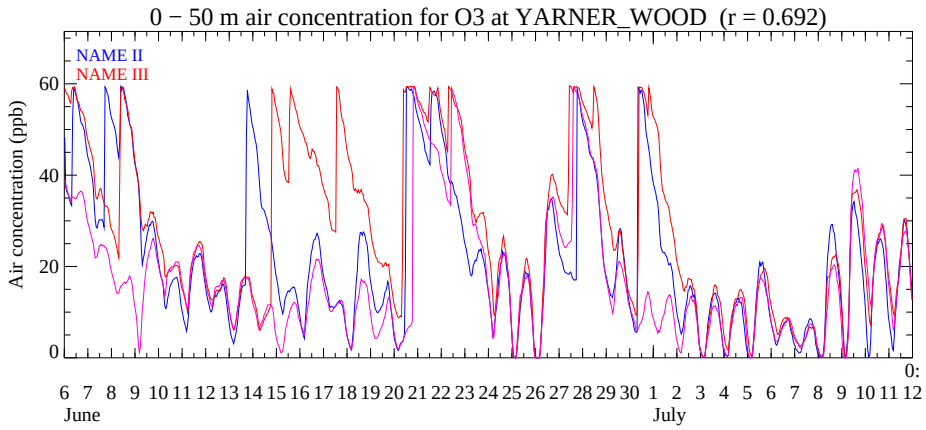

Figure 3: Comparison of the NAME II and NAME III predictions of the 0 – 50 m ozone concentrations at Yarner Wood. Ozone is reset to the background STOCHEM value when there are no particles in the chemistry grid box.

References

[1] Jones, A.R. (2005). Testing the NAME III chemistry scheme by a comparison of the NAME II and NAME III model predictions for the PUMA summer campaign, NAME III Document MD13/7(version 1).

[2] Redington, A.L., Derwent, R.G., Ryall, D.B., Matthew, S. and Manning, A.J. (2001). Pollution of the Urban Midlands Atmosphere: Development of an 'urban airshed' model for the West Midlands, Hadley Centre Technical Note 31, Met Office.

Appendix A: Comparison of the temporal evolutions of each species

Chemistry species stored on particles

Figure 4: SULPHUR DIOXIDE (SO_2)
Figure 5: AMMONIA (NH_3)
Figure 6: NITRIC OXIDE (NO)
Figure 7: AMMONIUM SULPHATE ($(NH_4)_2SO_4$)
Figure 8: SULPHATE AEROSOL (SULPHATE)
Figure 9: NITROGEN DIOXIDE (NO_2)
Figure 10: NITRATE (NO_3)
Figure 11: DI-NITROGEN PENTOXIDE (N_2O_5)
Figure 12: NITRIC ACID (HNO_3)
Figure 13: NITRATE AEROSOL (NAER)
Figure 14: AMMONIUM NITRATE (NH_4NO_3)
Figure 15: OZONE ON PARTICLES ($O_{3_{PART}}$)
Figure 16: CARBON MONOXIDE (CO)
Figure 17: FORMALDEHYDE (HCHO)
Figure 18: ETHYLENE (C_2H_4)
Figure 19: PROPYLENE (C_3H_6)
Figure 20: ISOPRENE (C_5H_8)
Figure 21: O-XYLENE (OXYL)
Figure 22: TOLUENE (TOLUEN)
Figure 23: 1,3-BUTADIENE (BD)
Figure 24: ACETALDEHYDE (CH_3CHO)
Figure 25: PEROXYACETYL NITRATE (PAN)
Figure 26: NITROUS ACID (HONO)
Figure 27: PM10

Chemistry species stored on fields

Figure 28: HYDROGEN PEROXIDE (H_2O_2)
Figure 29: OZONE ON FIELD ($O_{3_{FIELD}}$)
Figure 30: HYDROXYL (OH)
Figure 31: HYDROPEROXY (HO_2)
Figure 32: CH3OOH
Figure 33: MVK
Figure 34: ISOPOOH
Figure 35: MVKOOH
Figure 36: MGLYOX
Figure 37: GLYOX
Figure 38: MEMALD

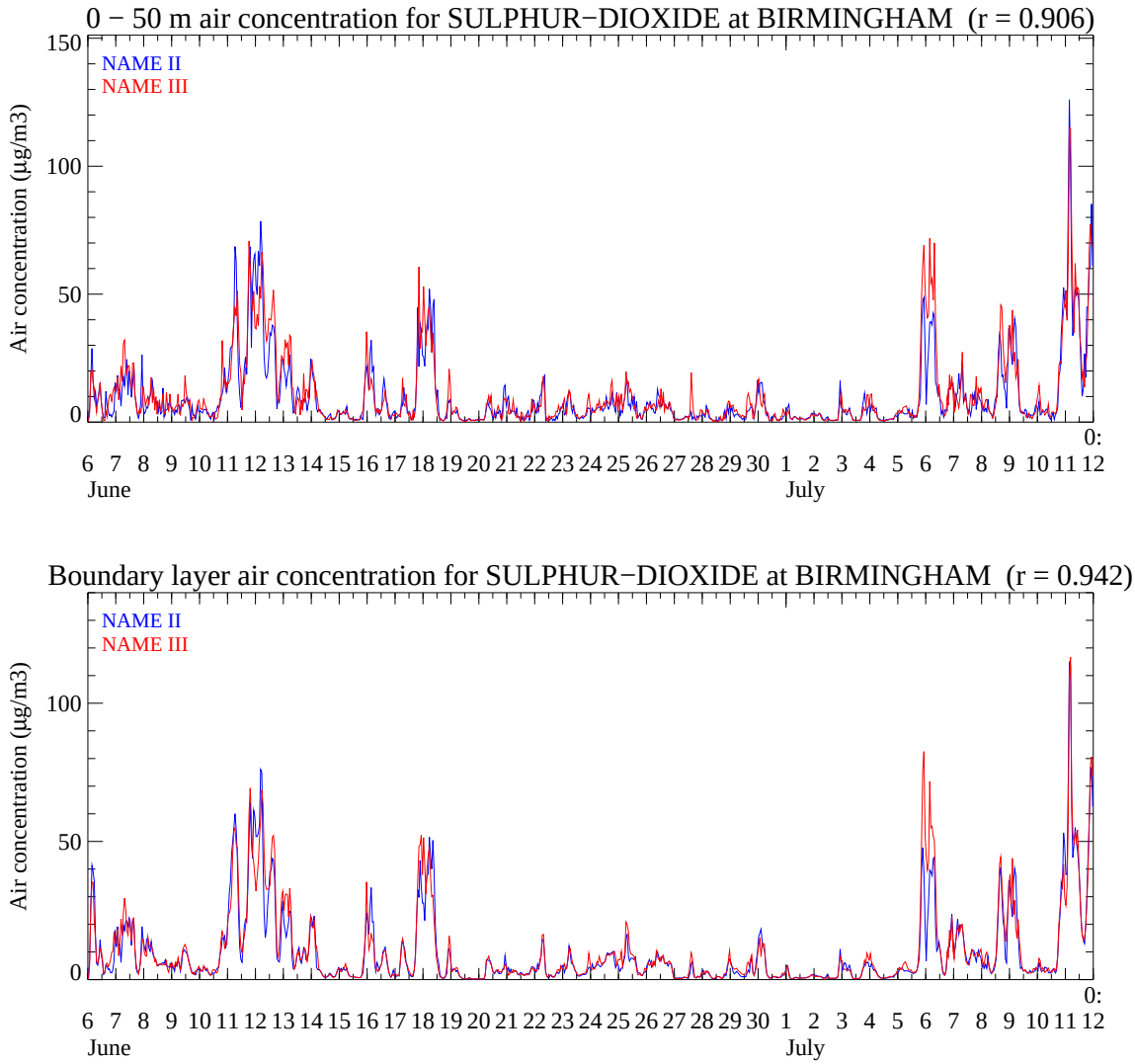

Figure 4: (a) 0-50 m and (b) boundary-layer average concentrations of sulphur dioxide

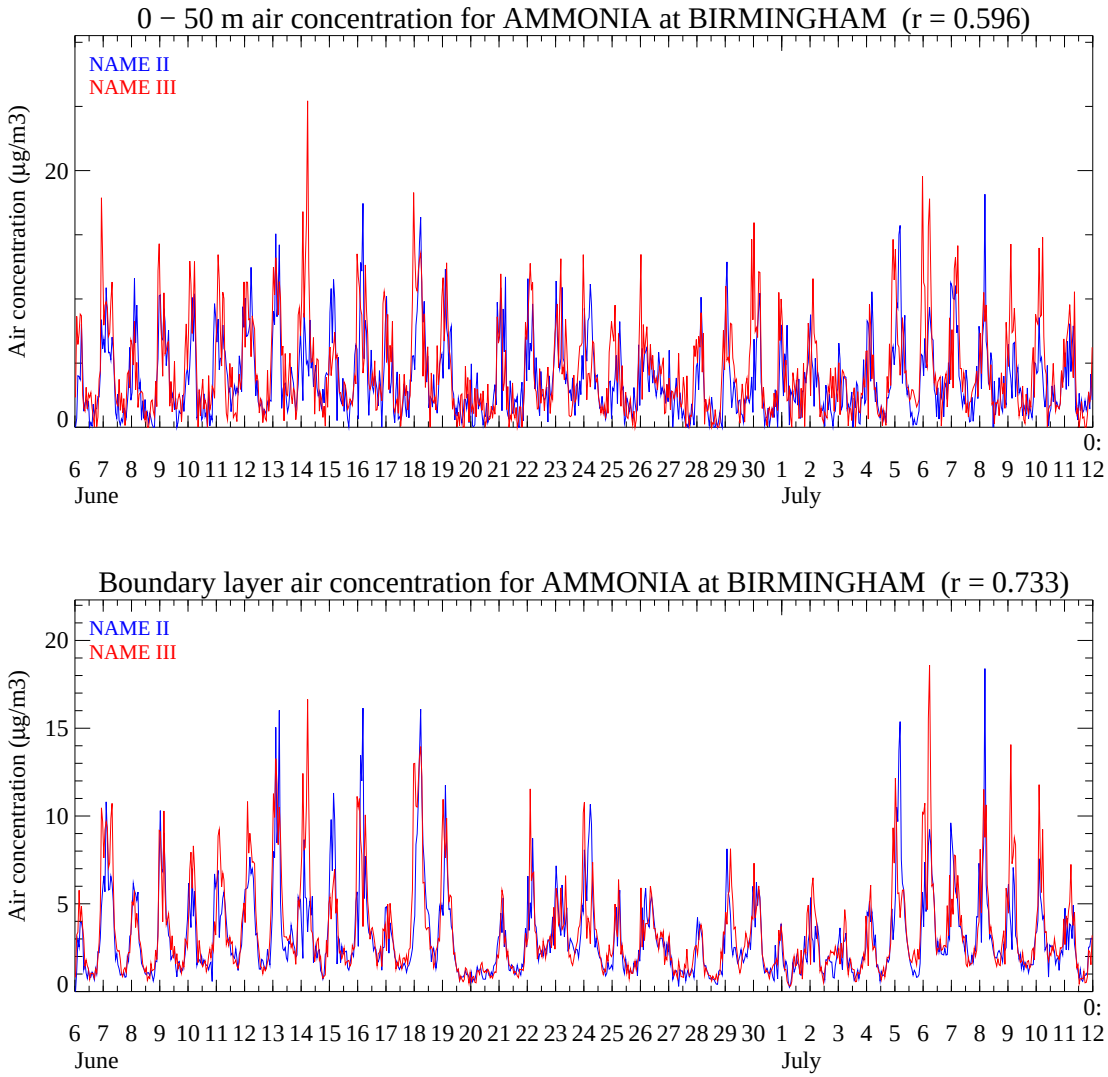

Figure 5: (a) 0-50 m and (b) boundary-layer average concentrations of ammonia

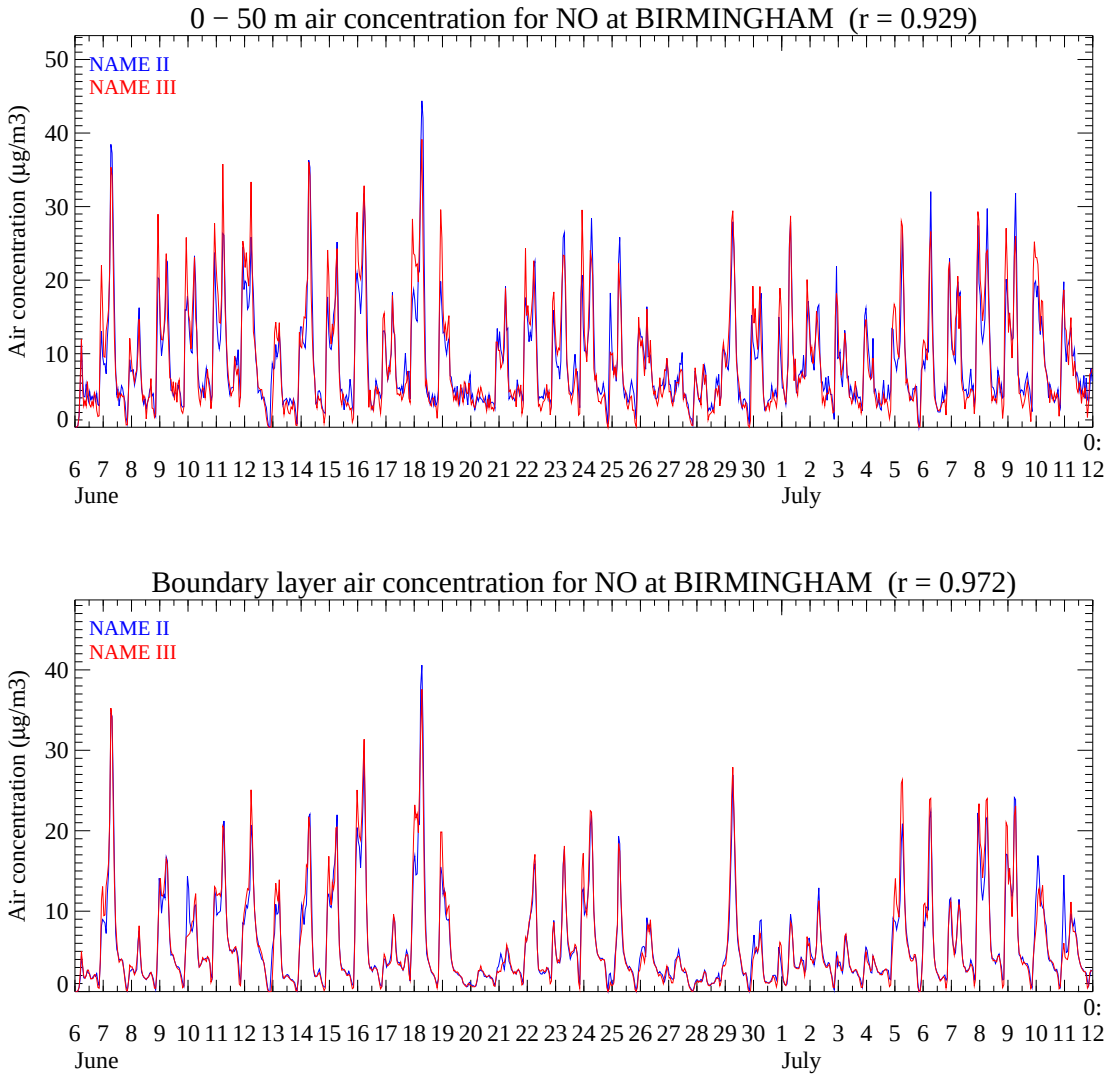

Figure 6: (a) 0-50 m and (b) boundary-layer average concentrations of nitric oxide

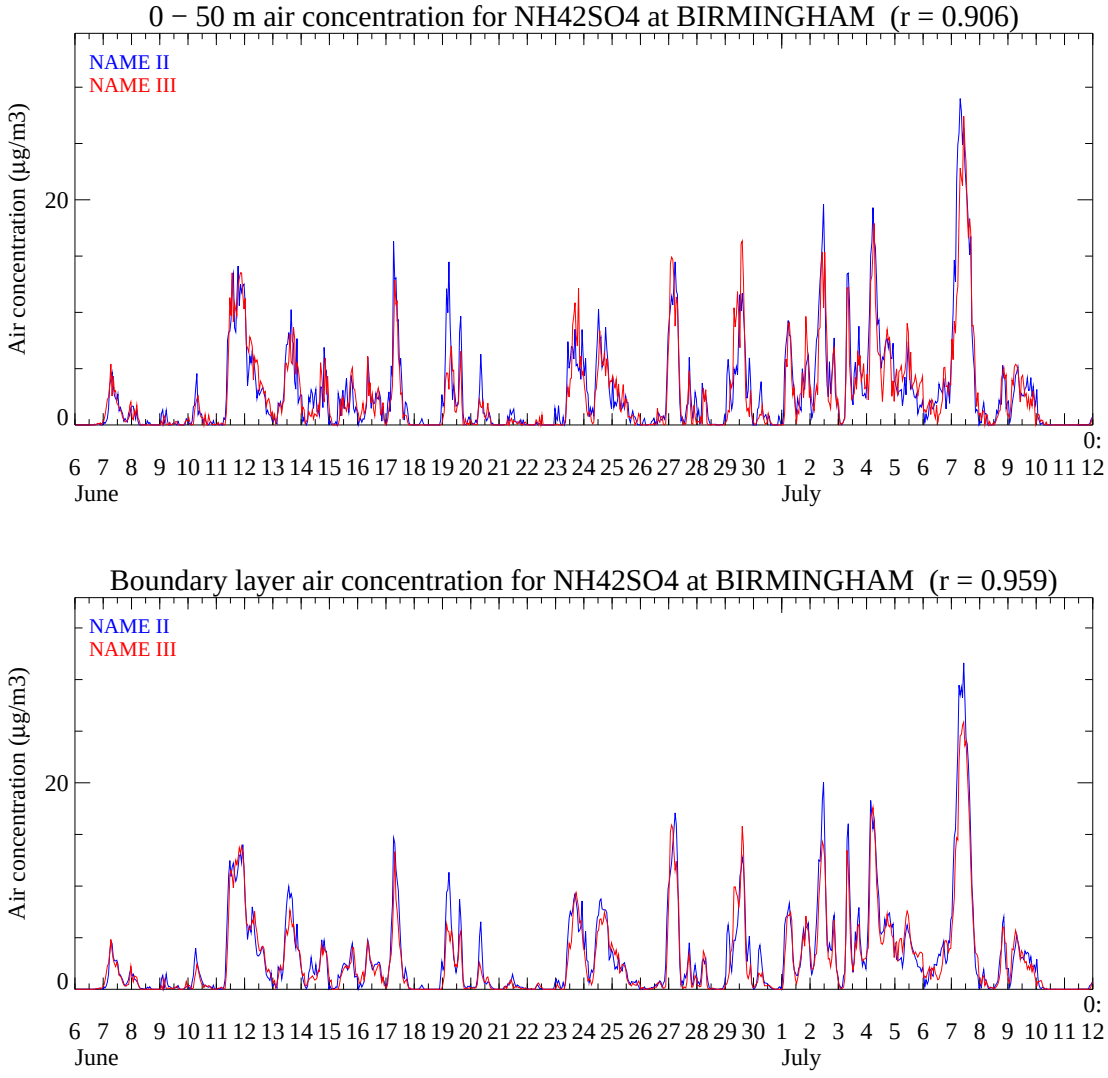

Figure 7: (a) 0-50 m and (b) boundary-layer average concentrations of ammonium sulphate

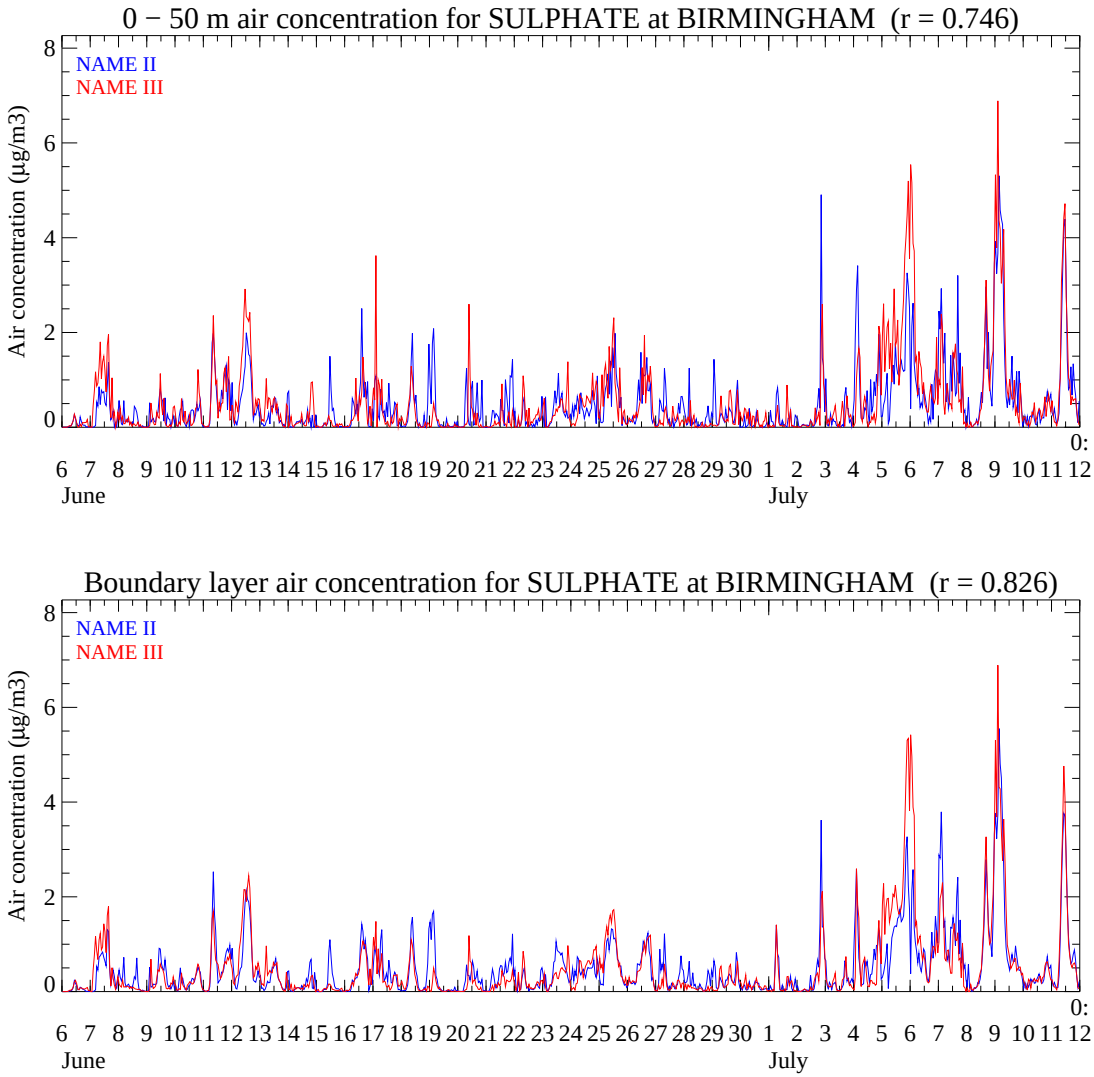

Figure 8: (a) 0-50 m and (b) boundary-layer average concentrations of sulphate aerosol

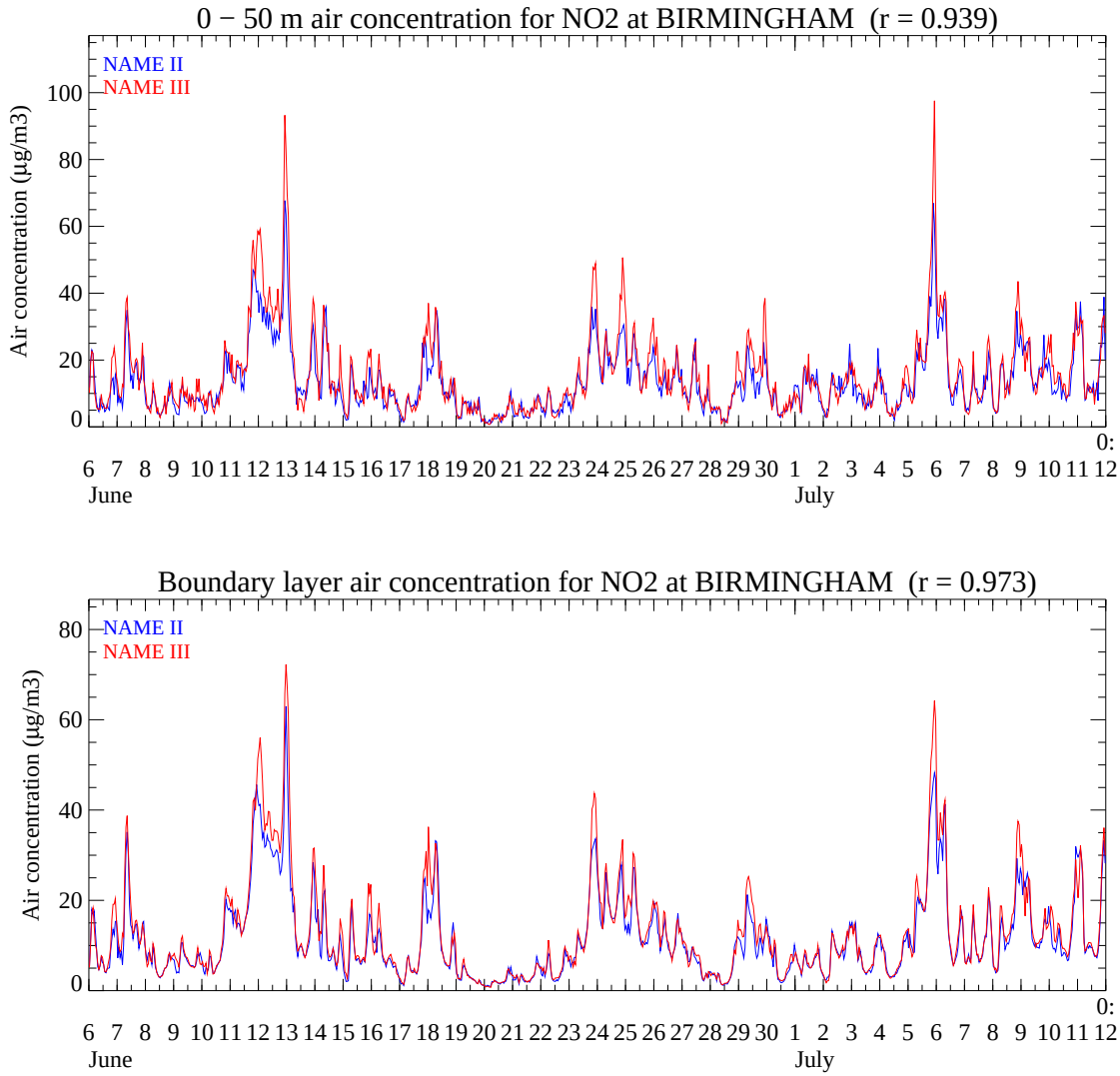

Figure 9: (a) 0-50 m and (b) boundary-layer average concentrations of nitrogen dioxide

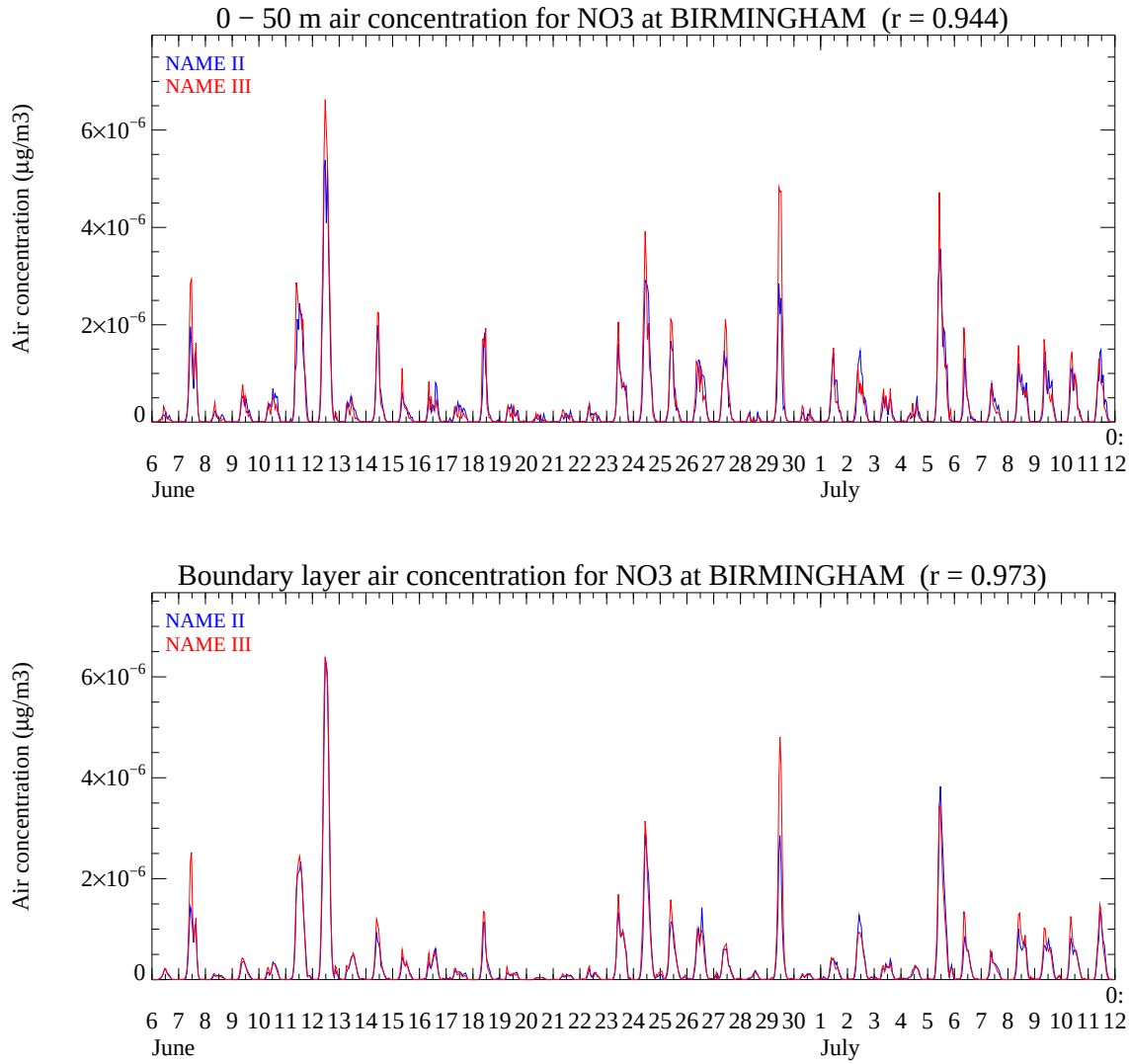

Figure 10: (a) 0-50 m and (b) boundary-layer average concentrations of nitrate

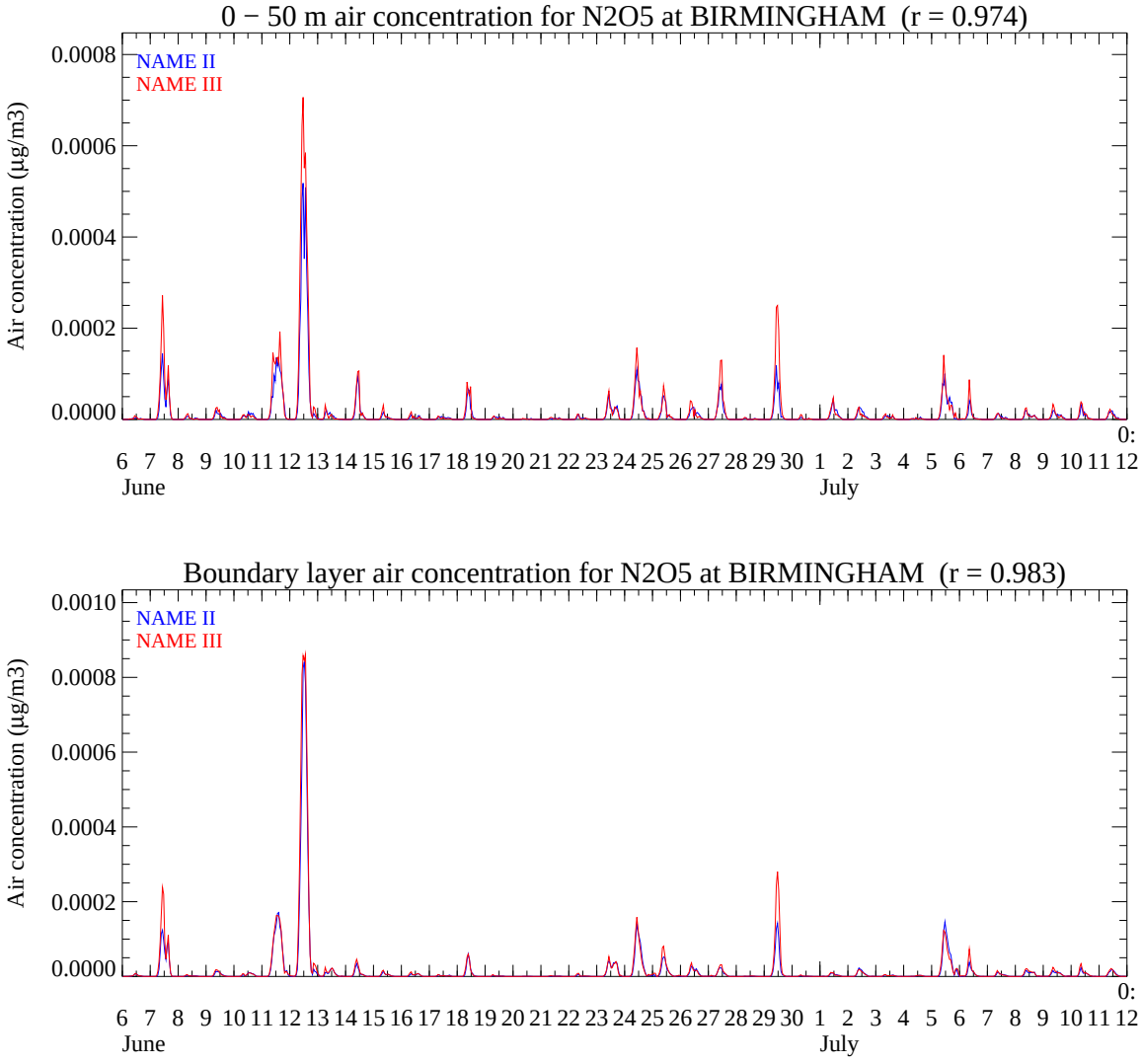

Figure 11: (a) 0-50 m and (b) boundary-layer average concentrations of di-nitrogen pentoxide

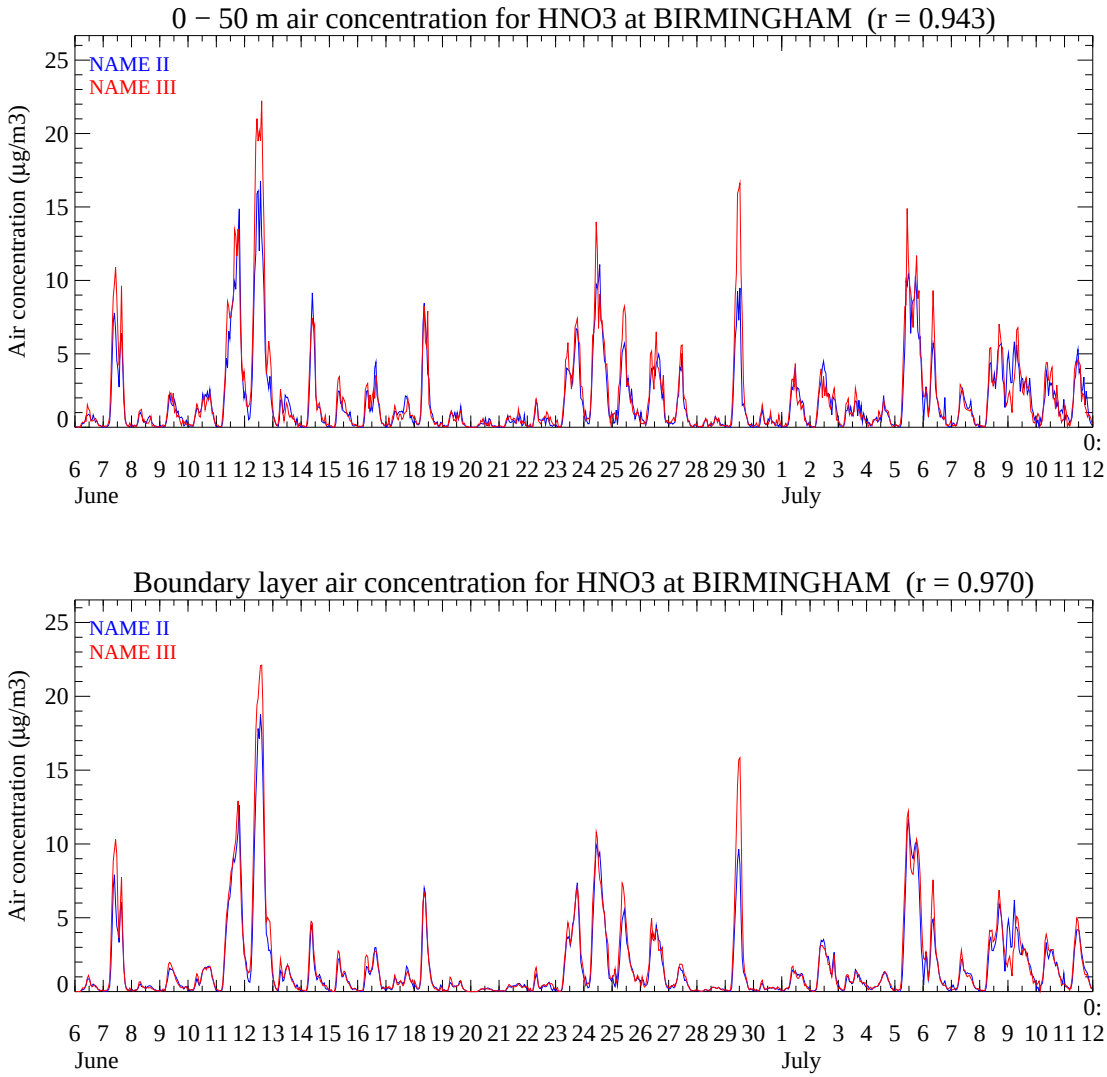

Figure 12: (a) 0-50 m and (b) boundary-layer average concentrations of nitric acid

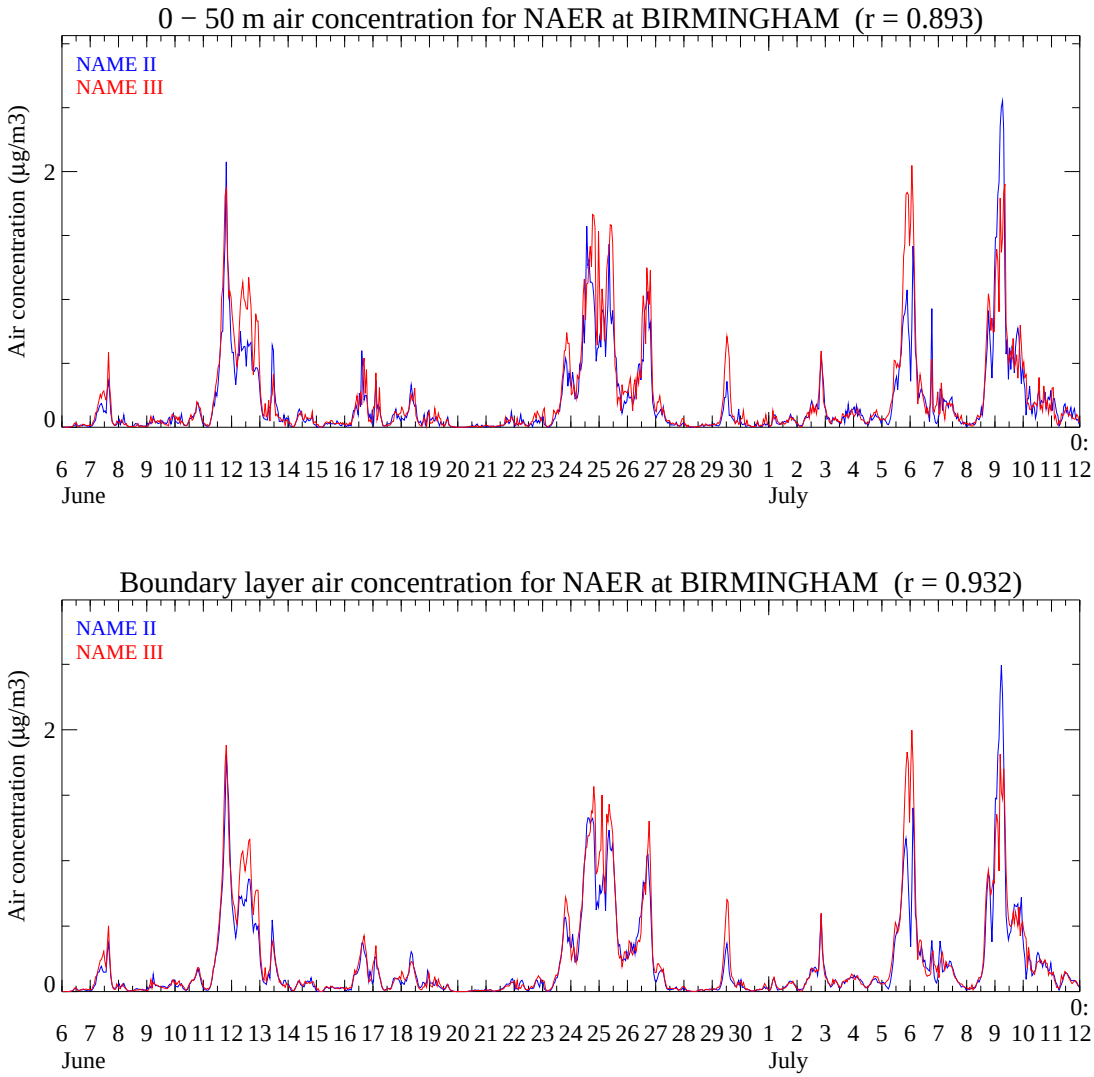

Figure 13: (a) 0-50 m and (b) boundary-layer average concentrations of nitrate aerosol

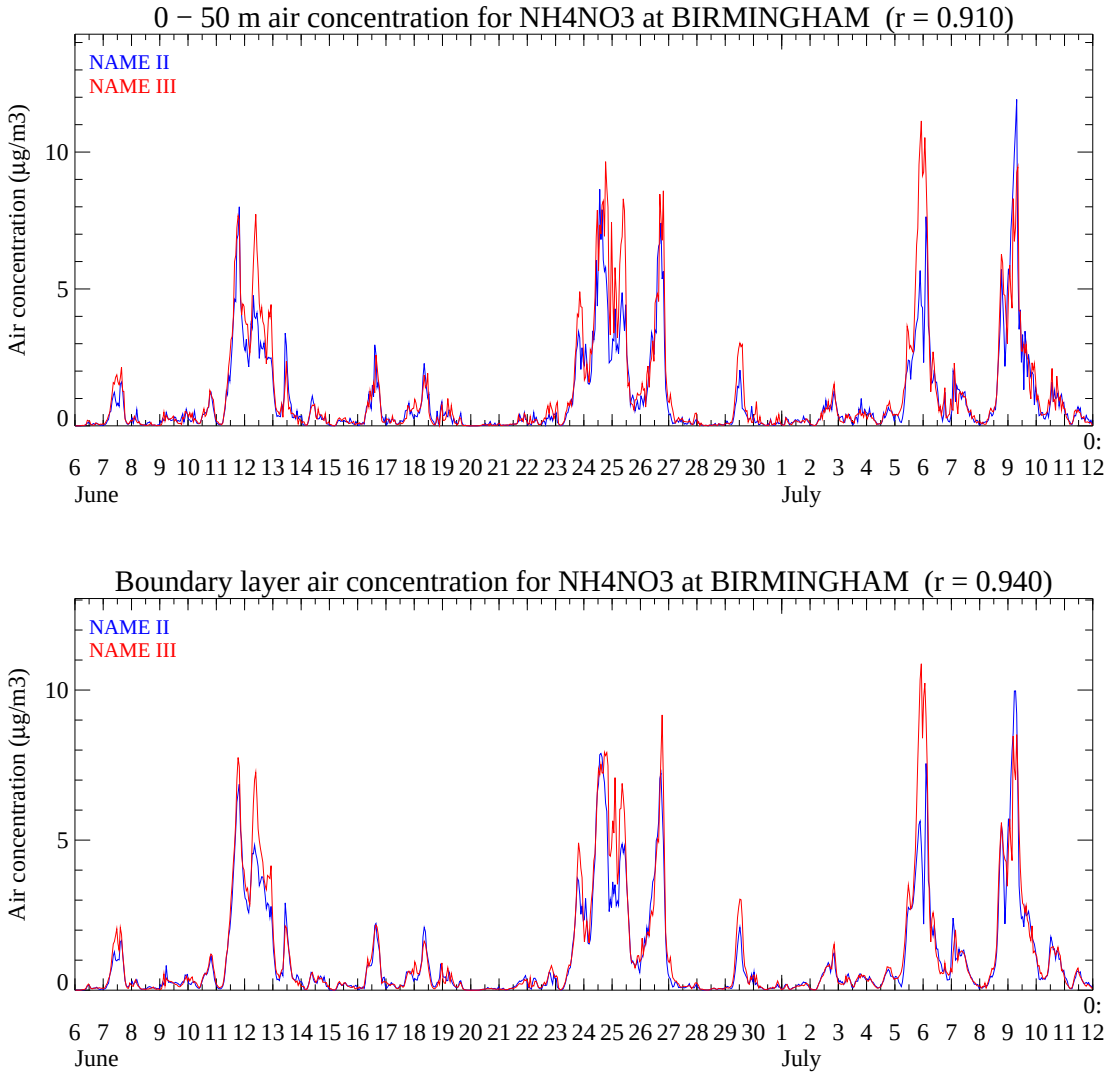

Figure 14: (a) 0-50 m and (b) boundary-layer average concentrations of ammonium nitrate

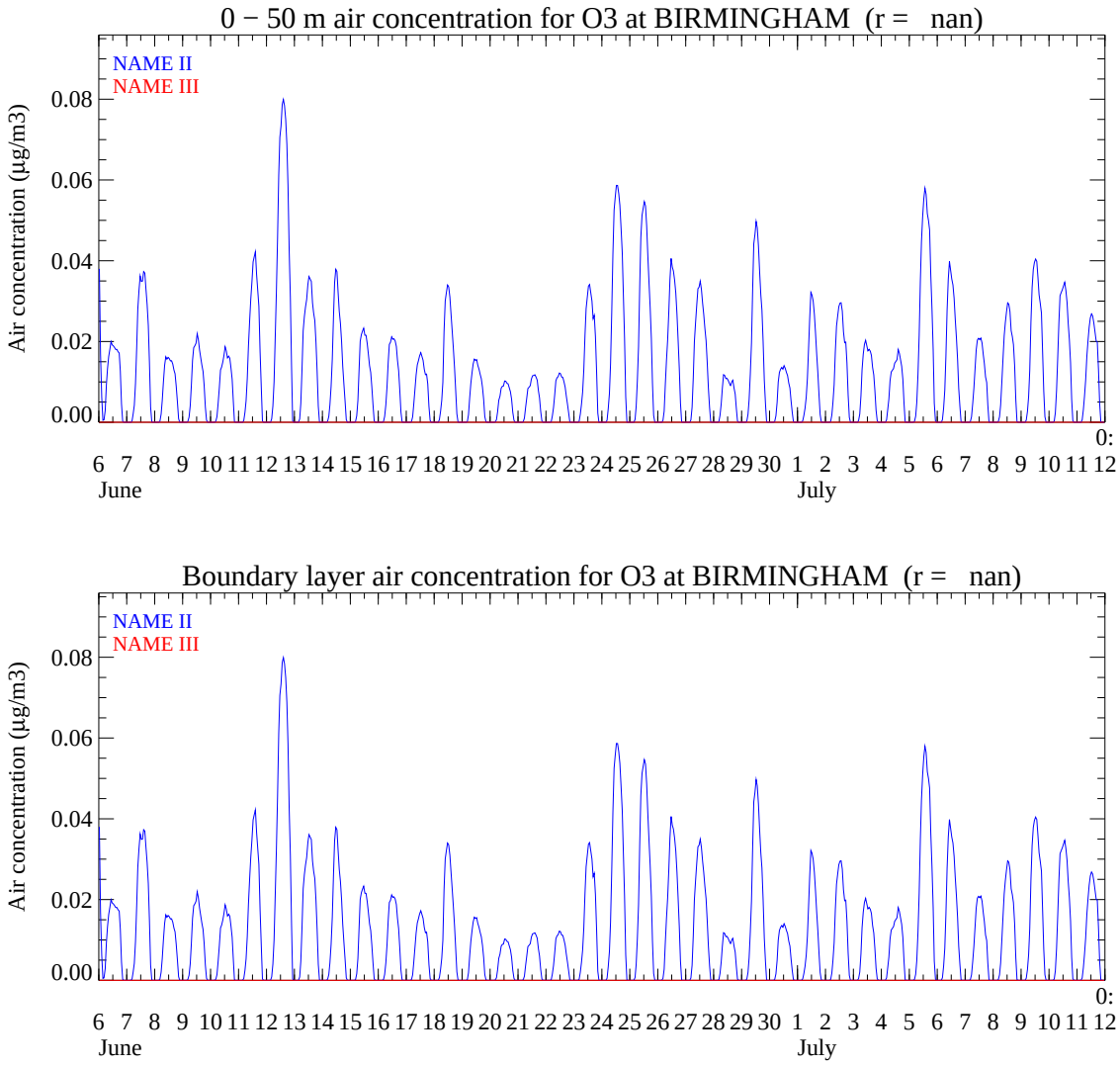

Figure 15: (a) 0-50 m and (b) boundary-layer average concentrations of ozone (on particles)

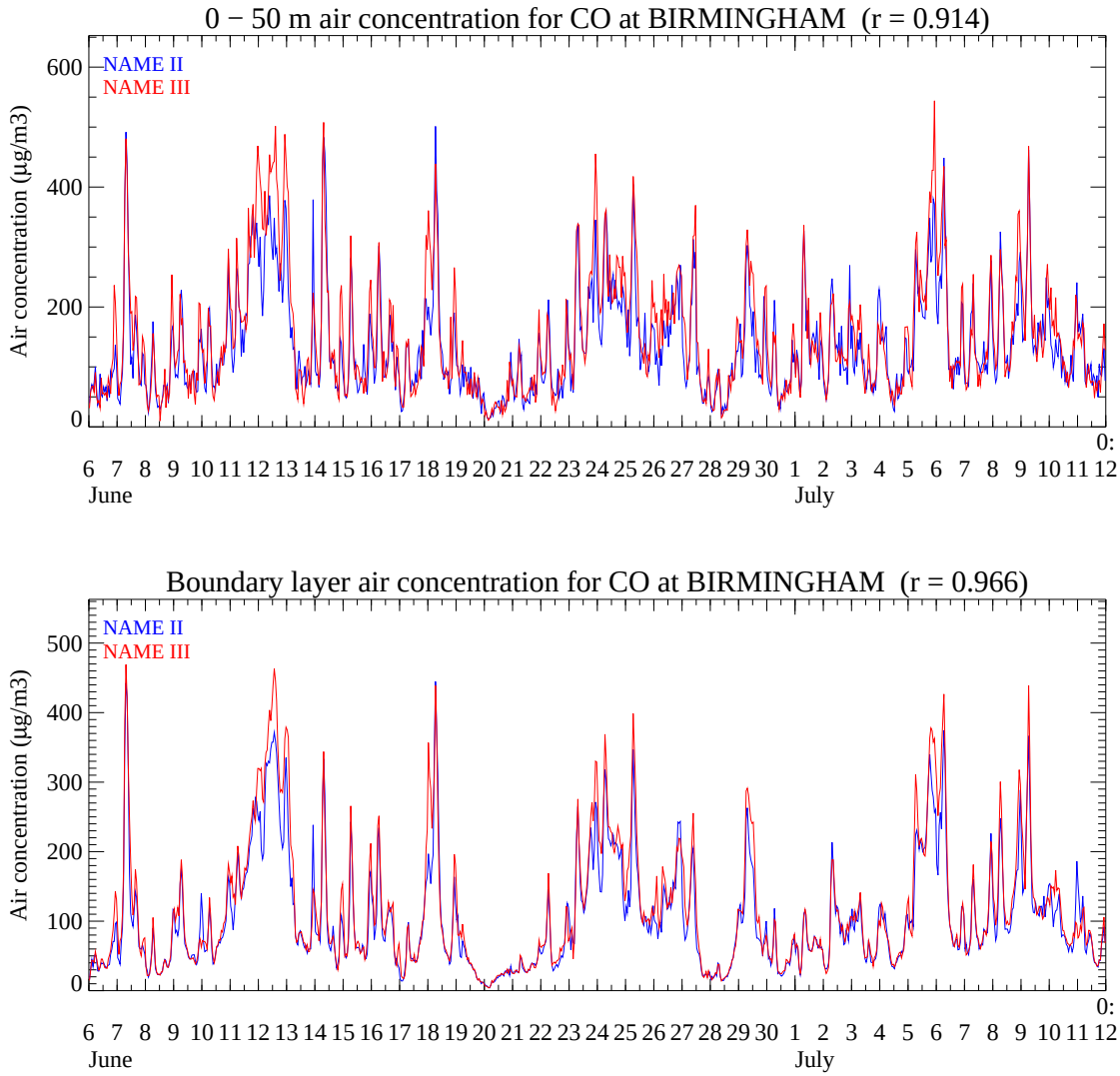

Figure 16: (a) 0-50 m and (b) boundary-layer average concentrations of carbon monoxide

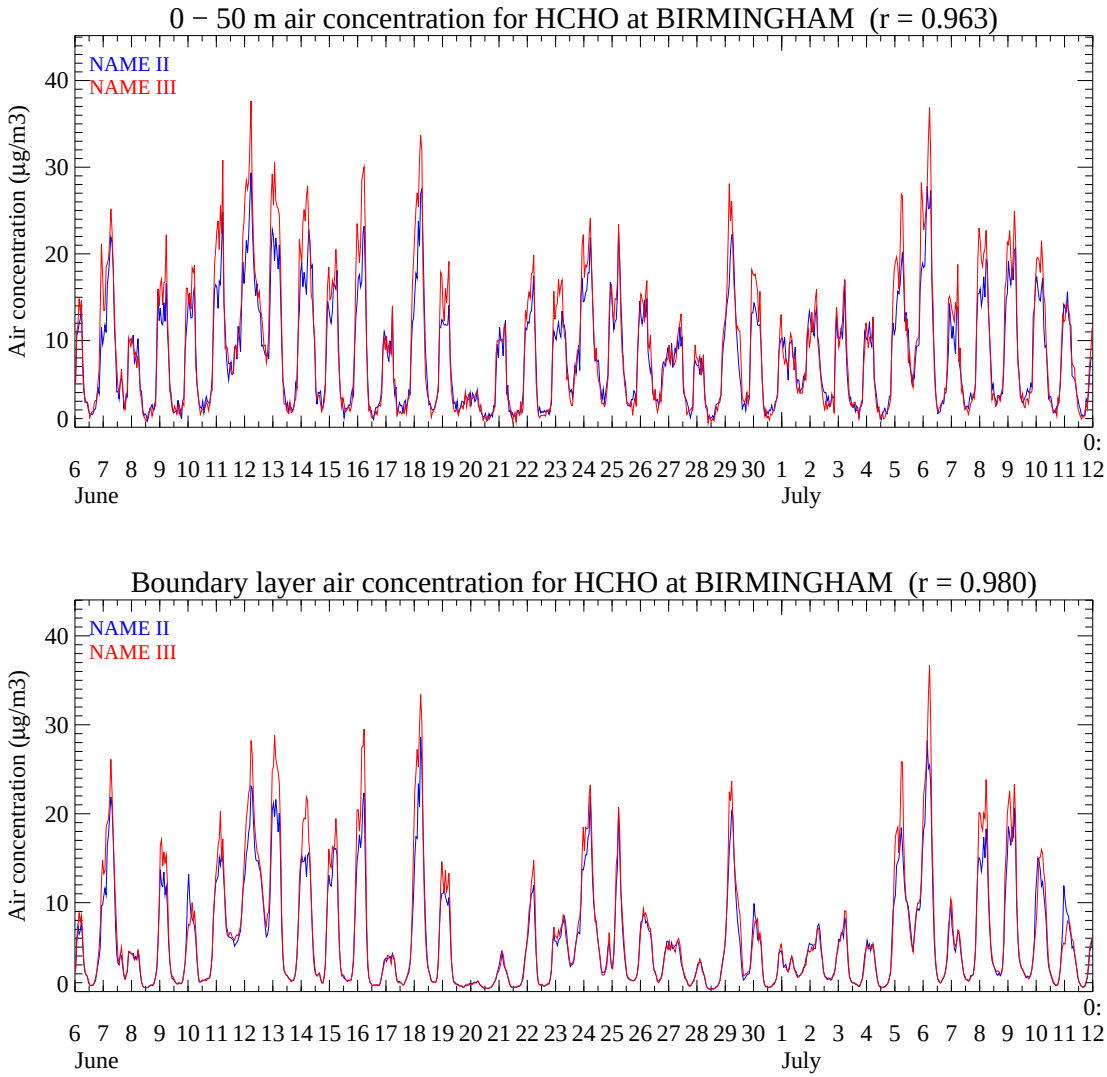

Figure 17: (a) 0-50 m and (b) boundary-layer average concentrations of formaldehyde

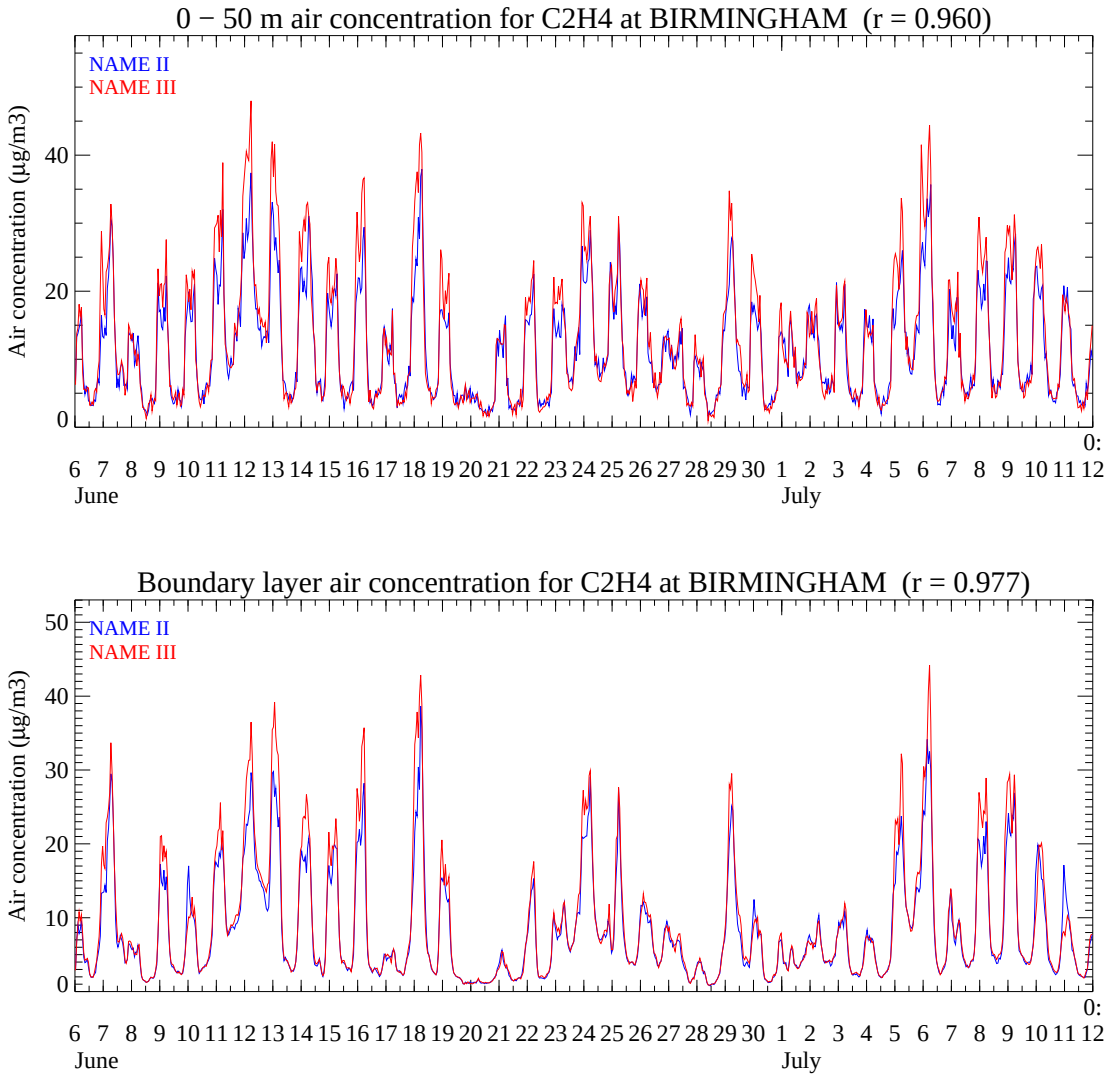

Figure 18: (a) 0-50 m and (b) boundary-layer average concentrations of ethylene

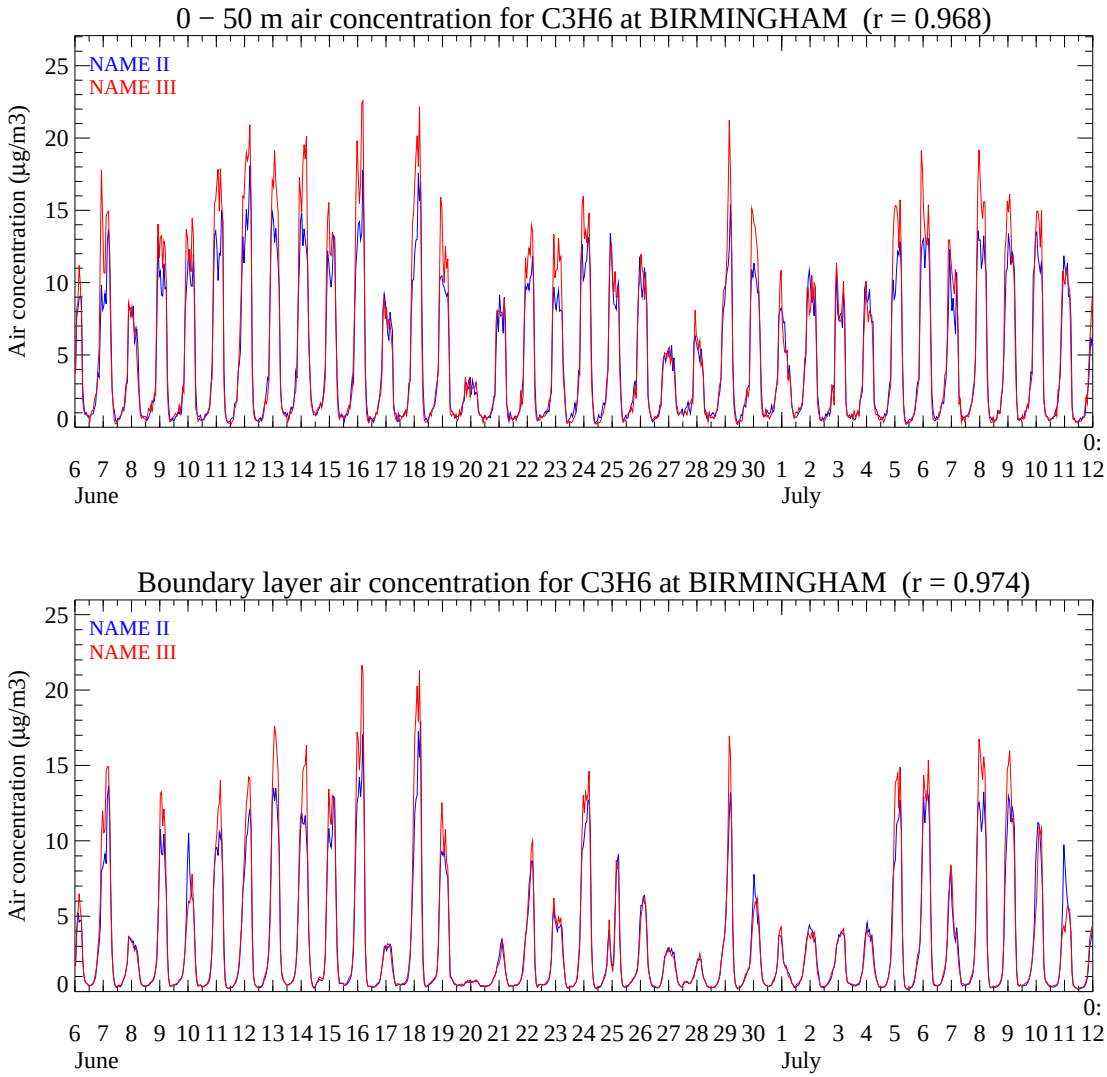

Figure 19: (a) 0-50 m and (b) boundary-layer average concentrations of propylene

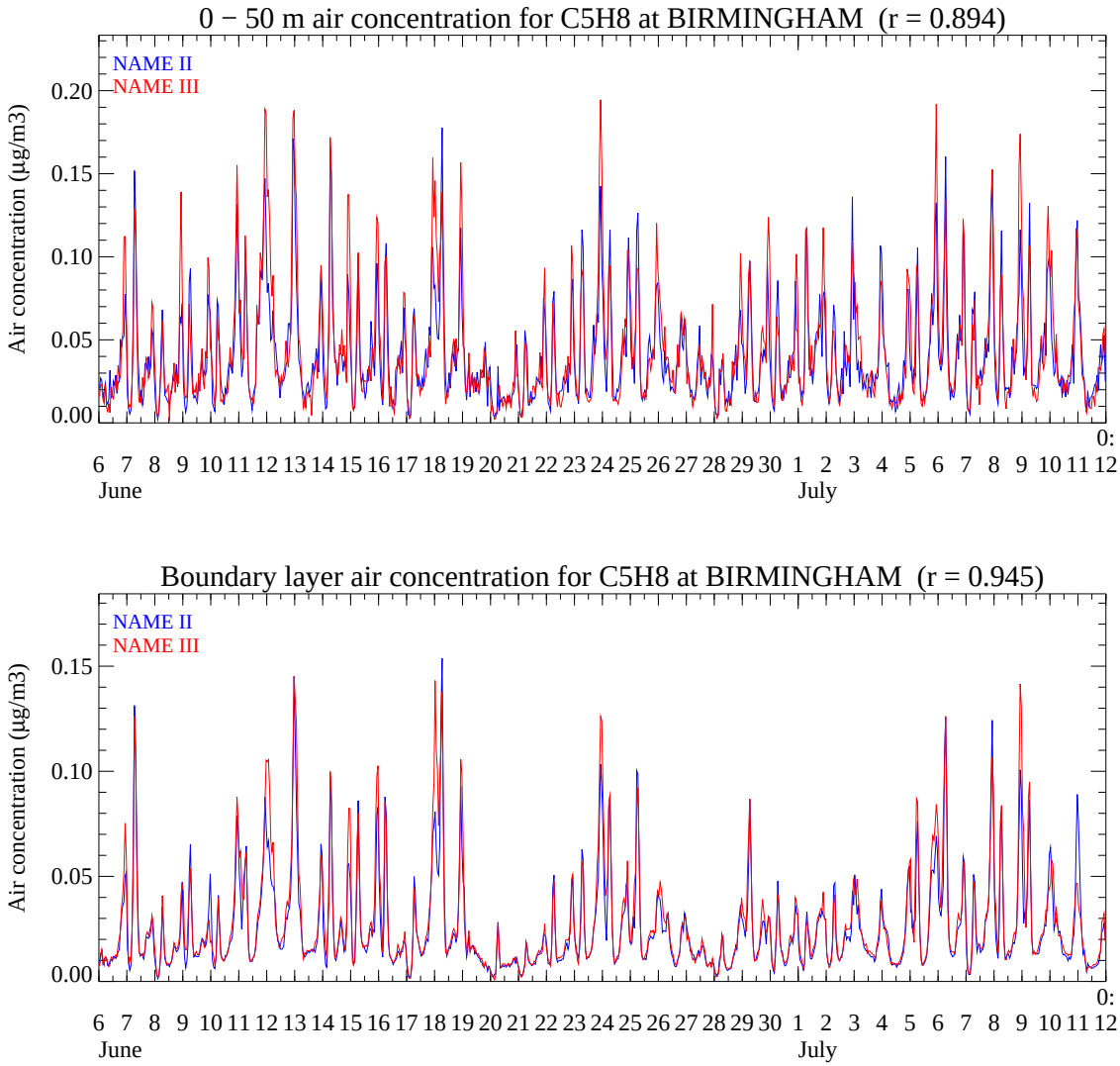

Figure 20: (a) 0-50 m and (b) boundary-layer average concentrations of isoprene

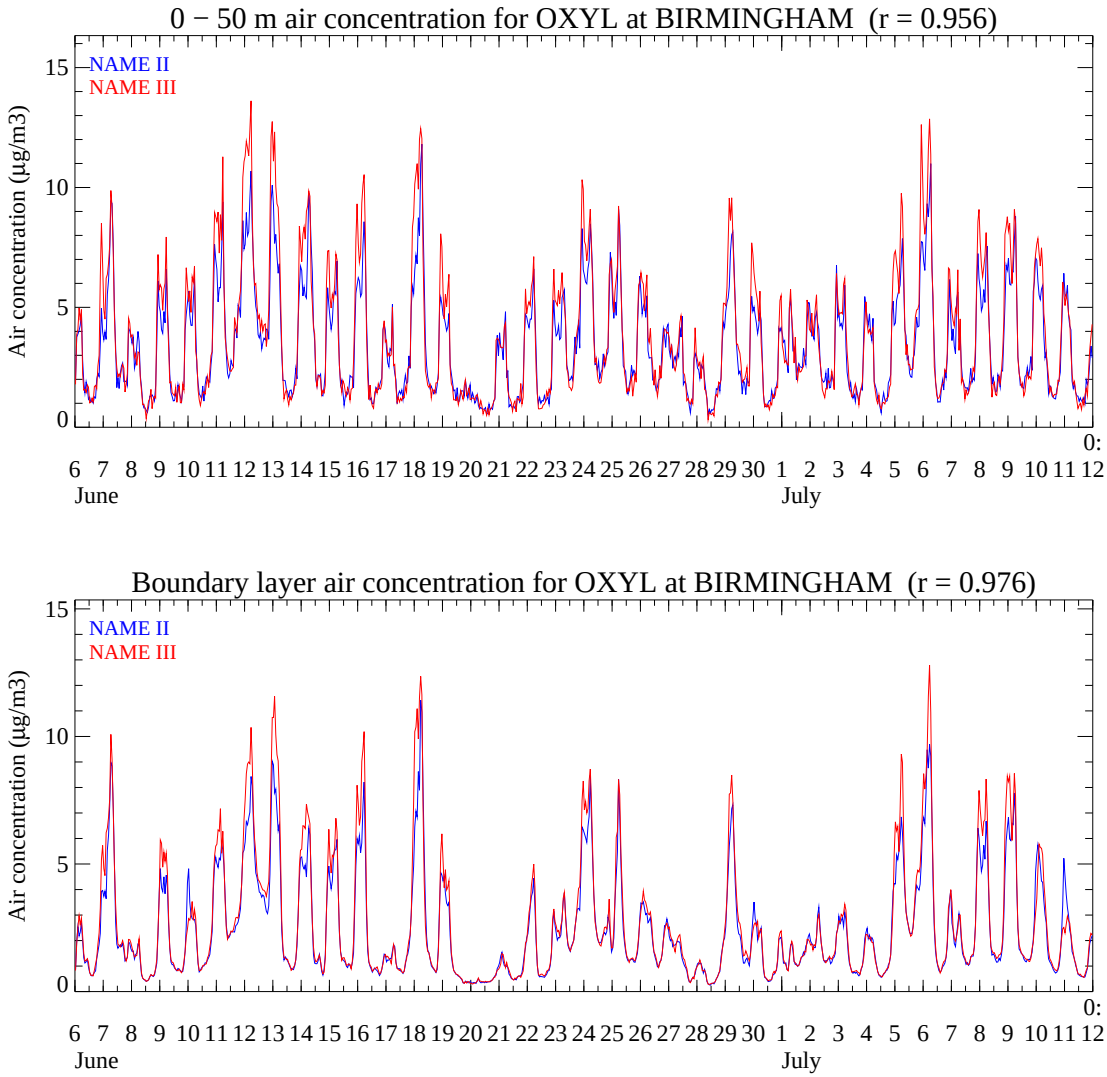

Figure 21: (a) 0-50 m and (b) boundary-layer average concentrations of o-xylene

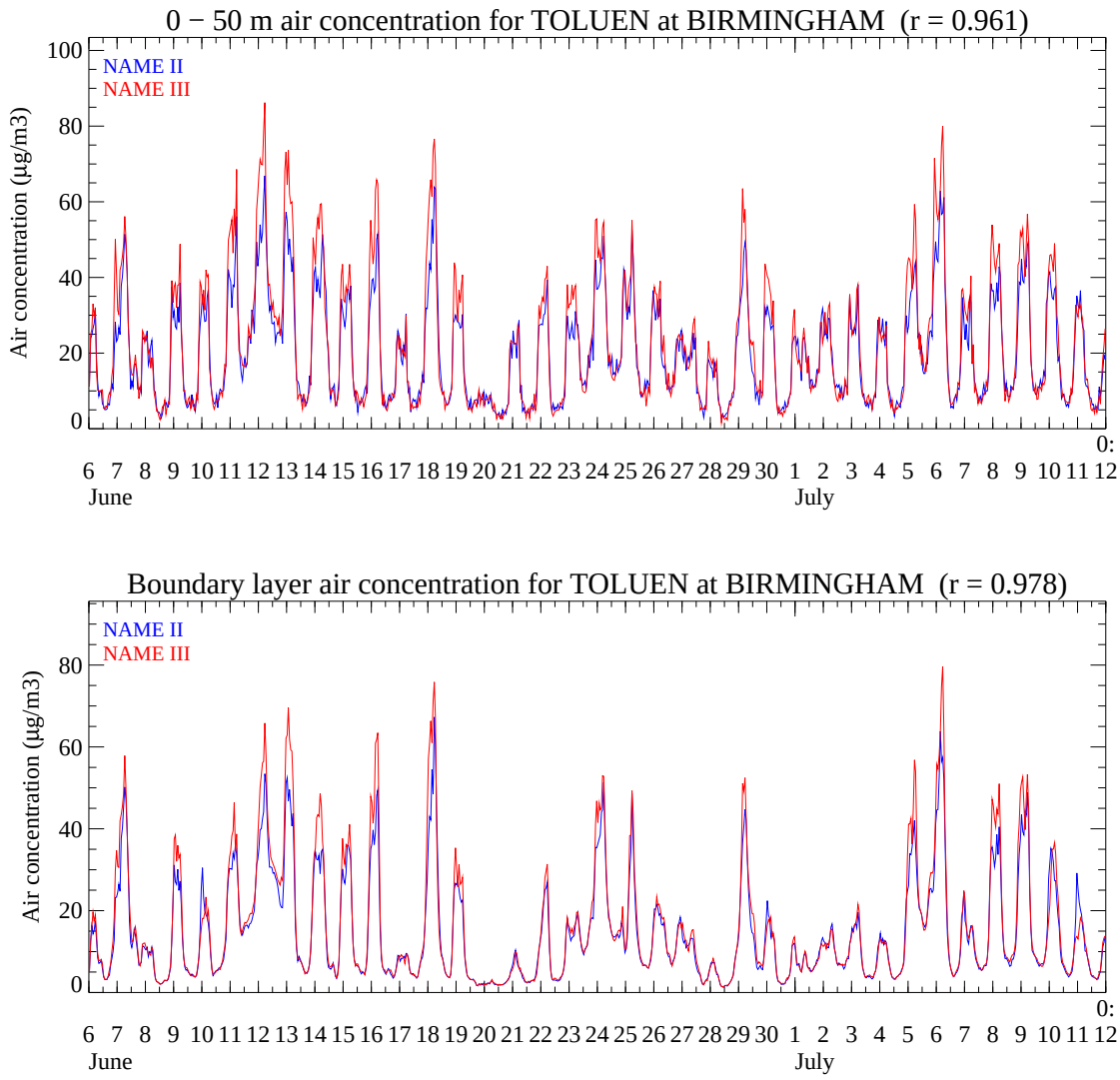

Figure 22: (a) 0-50 m and (b) boundary-layer average concentrations of toluene

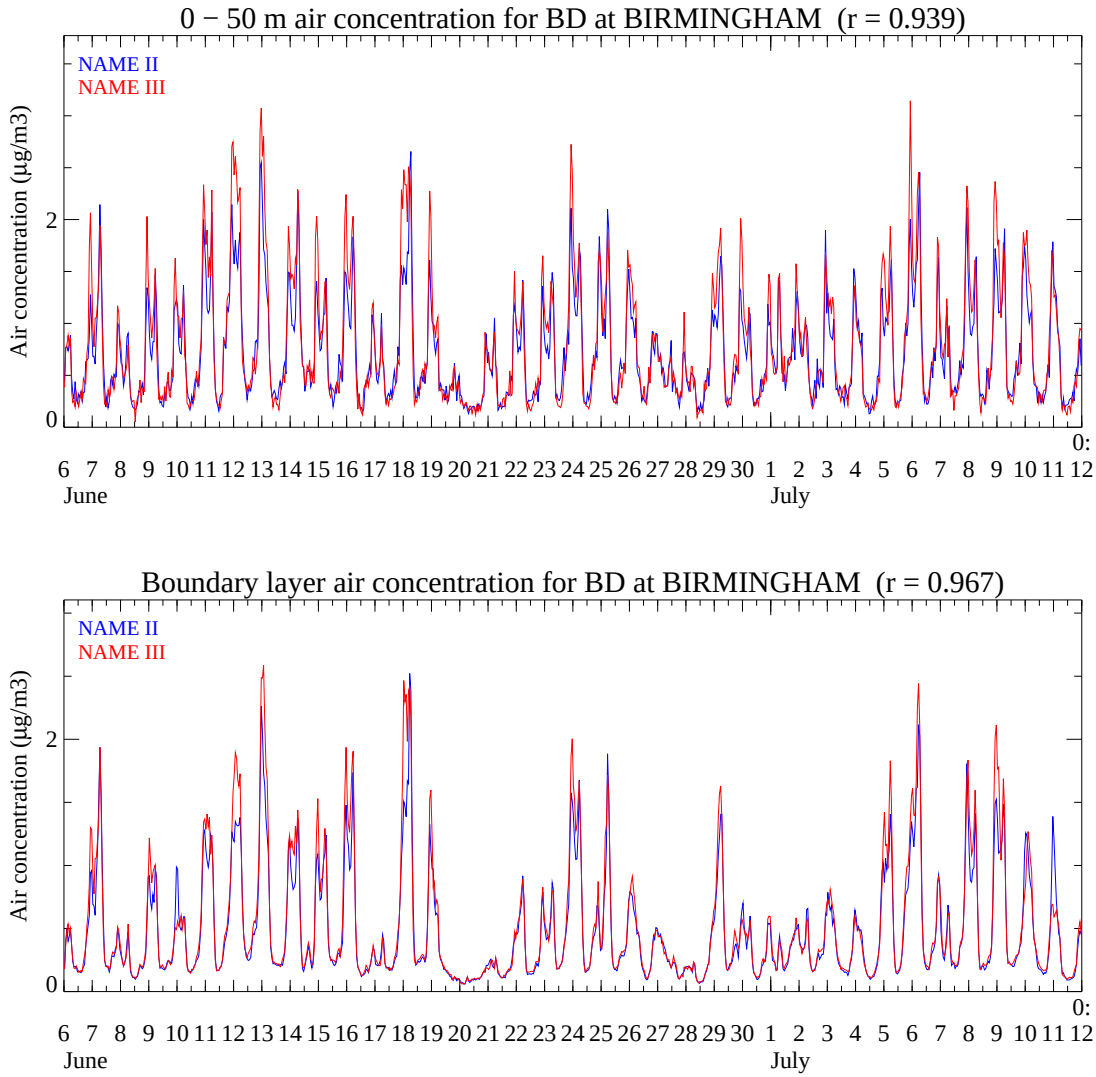

Figure 23: (a) 0-50 m and (b) boundary-layer average concentrations of 1,3-butadiene

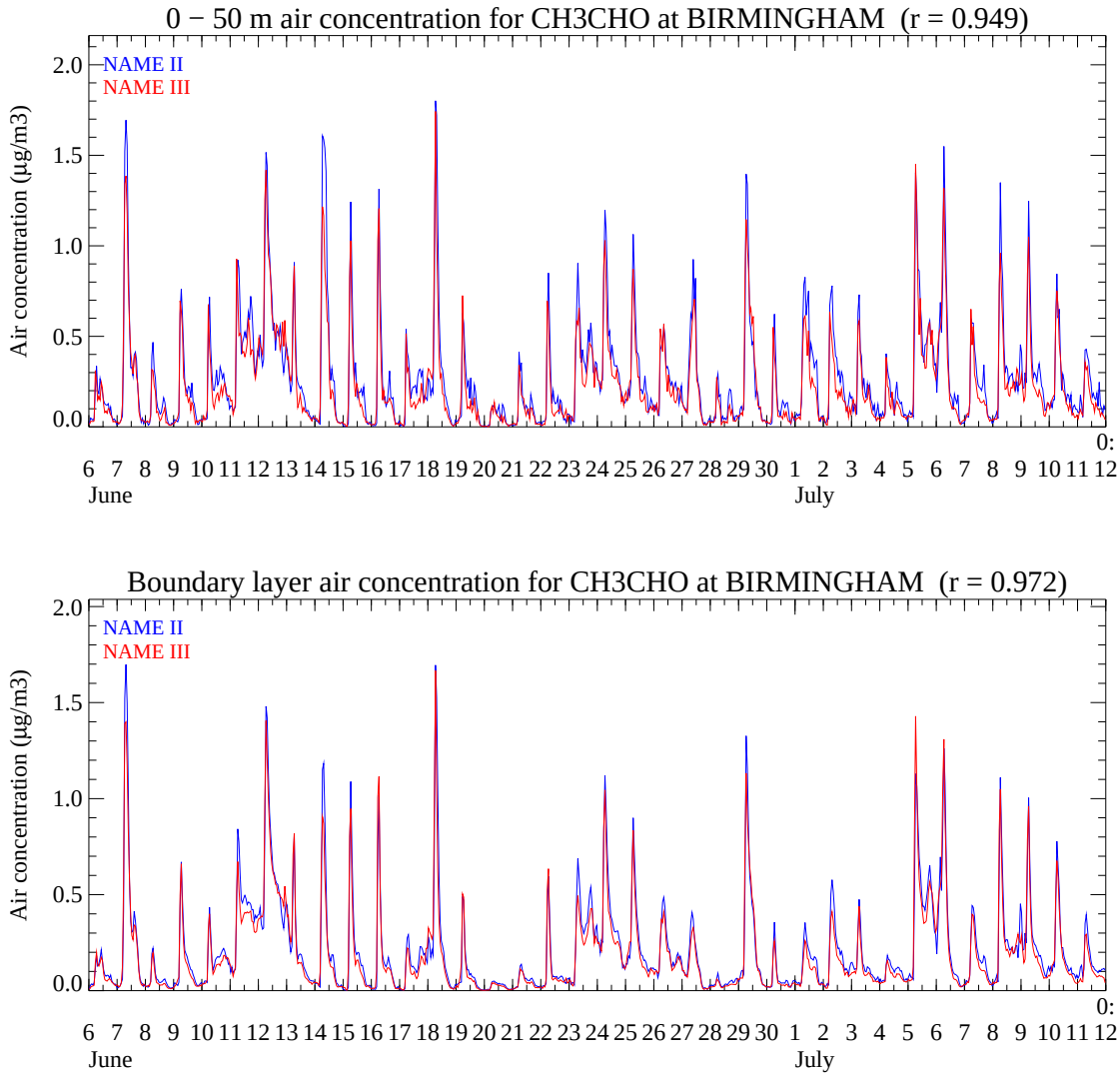

Figure 24: (a) 0-50 m and (b) boundary-layer average concentrations of acetaldehyde

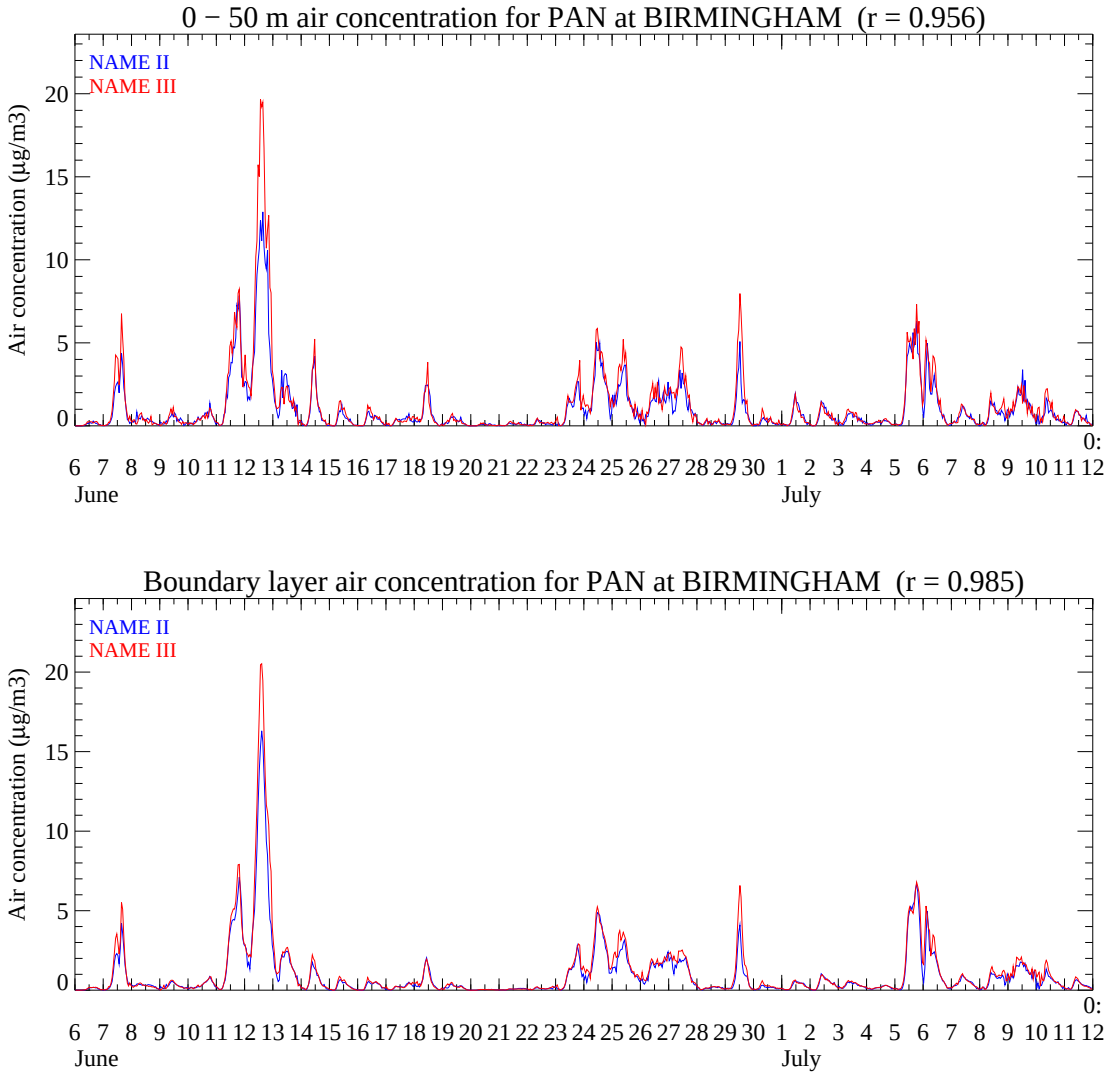

Figure 25: (a) 0-50 m and (b) boundary-layer average concentrations of peroxyacetyl nitrate

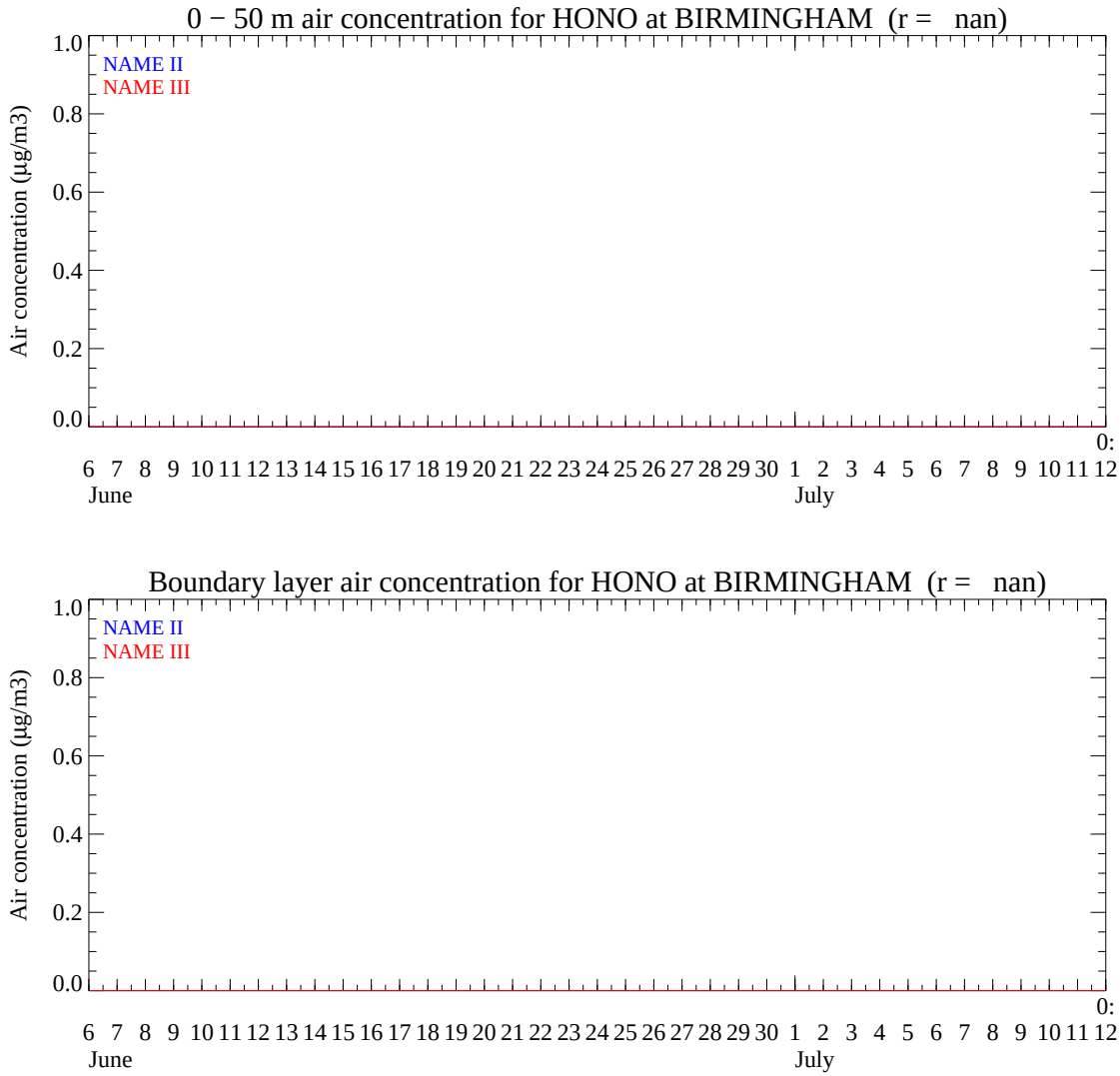

Figure 26: (a) 0-50 m and (b) boundary-layer average concentrations of nitrous acid

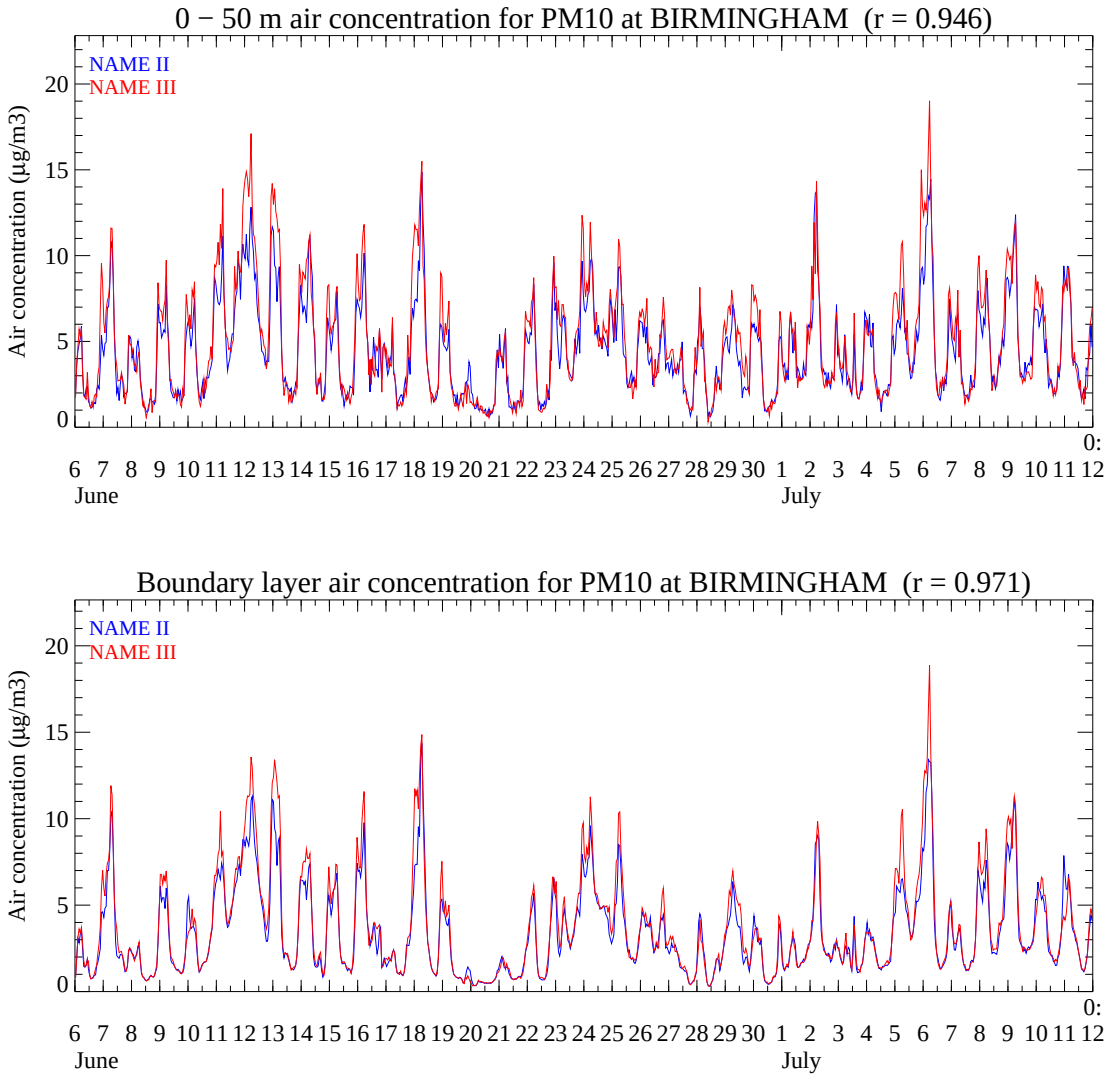

Figure 27: (a) 0-50 m and (b) boundary-layer average concentrations of PM_{10}

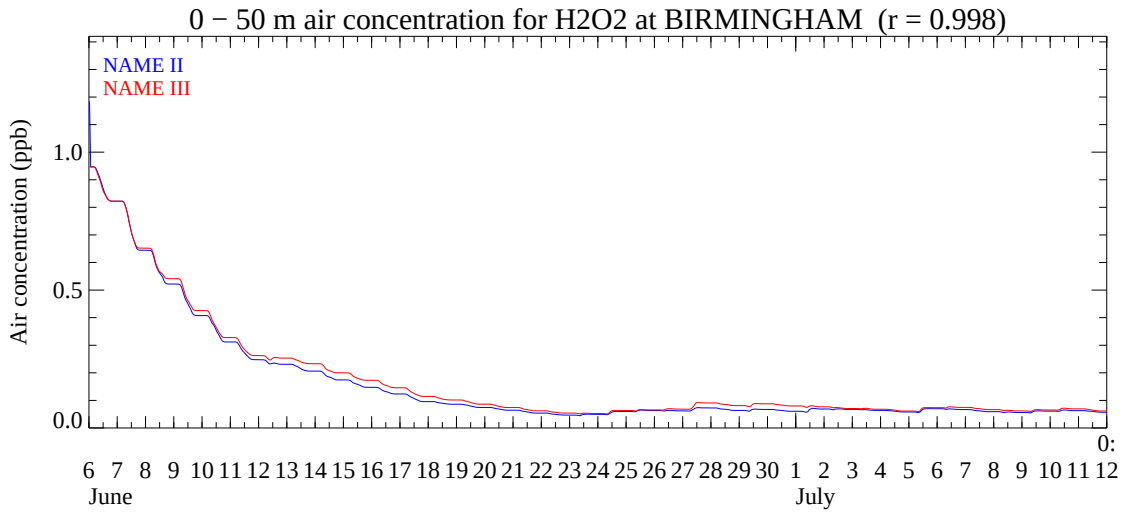

Figure 28: 0-50 m air concentration of hydrogen peroxide

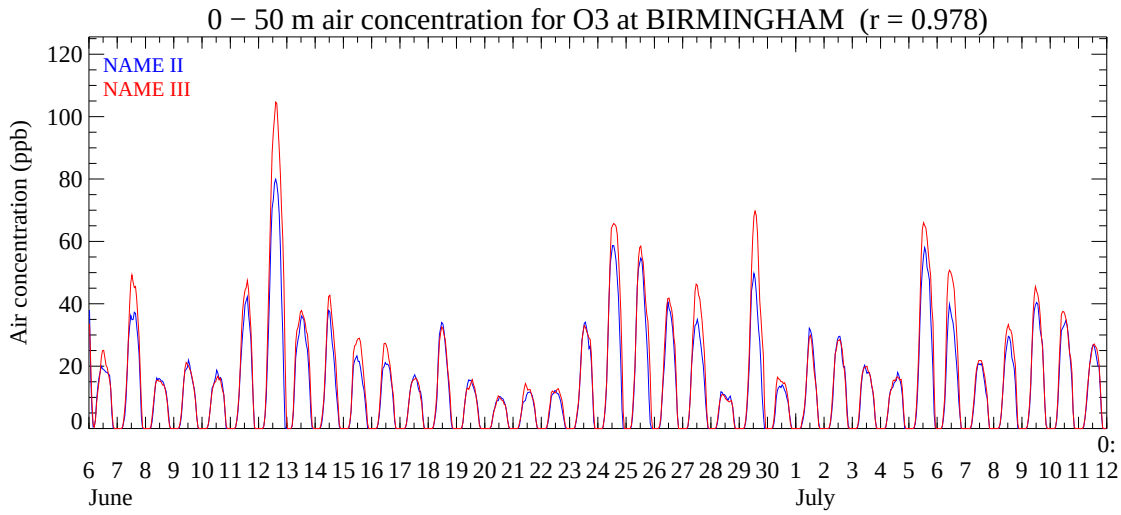

Figure 29: 0-50 m air concentration of ozone (on field)

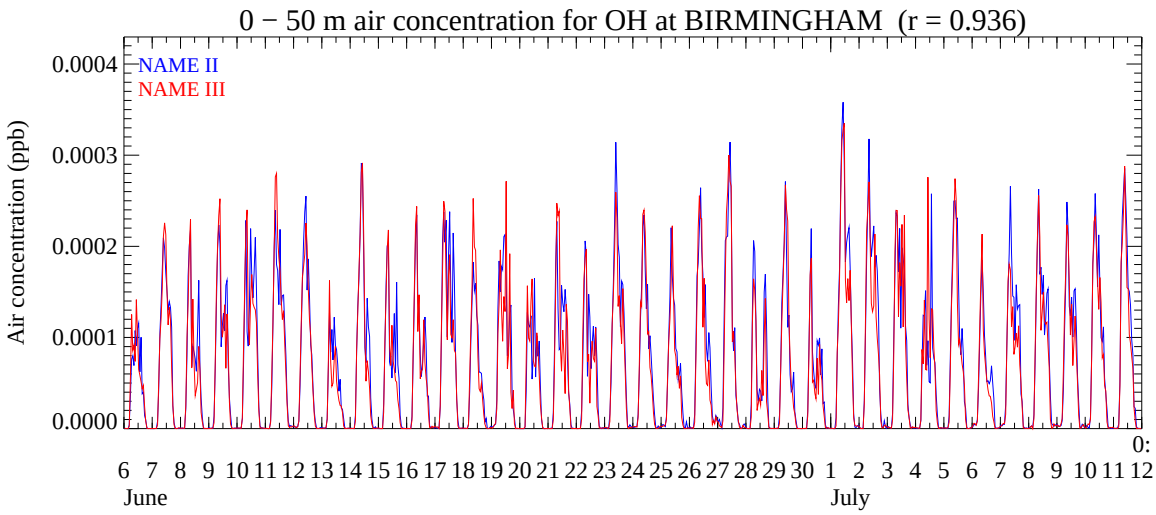

Figure 30: 0-50 m air concentration of hydroxyl

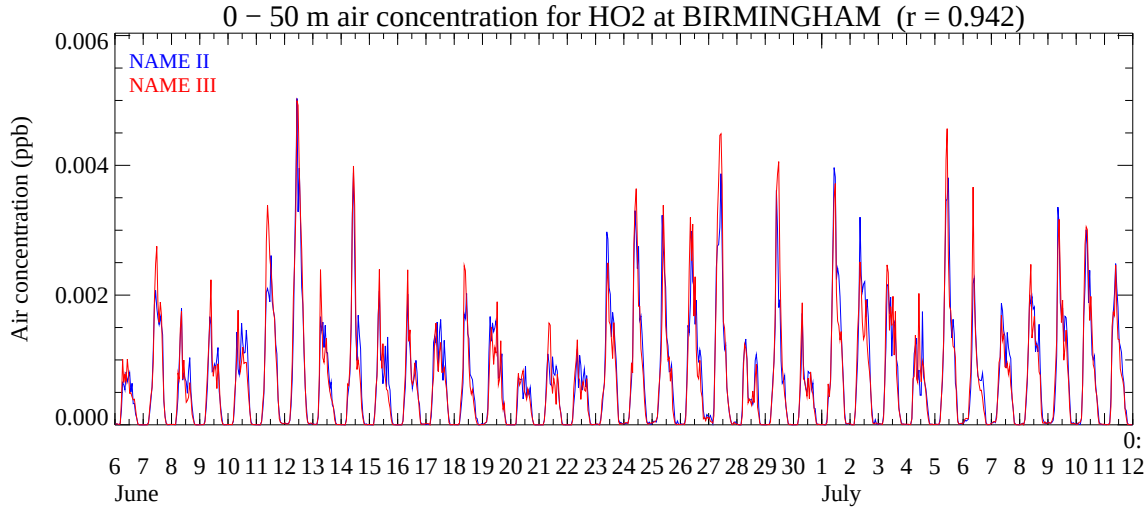

Figure 31: 0-50 m air concentration of hydroperoxy

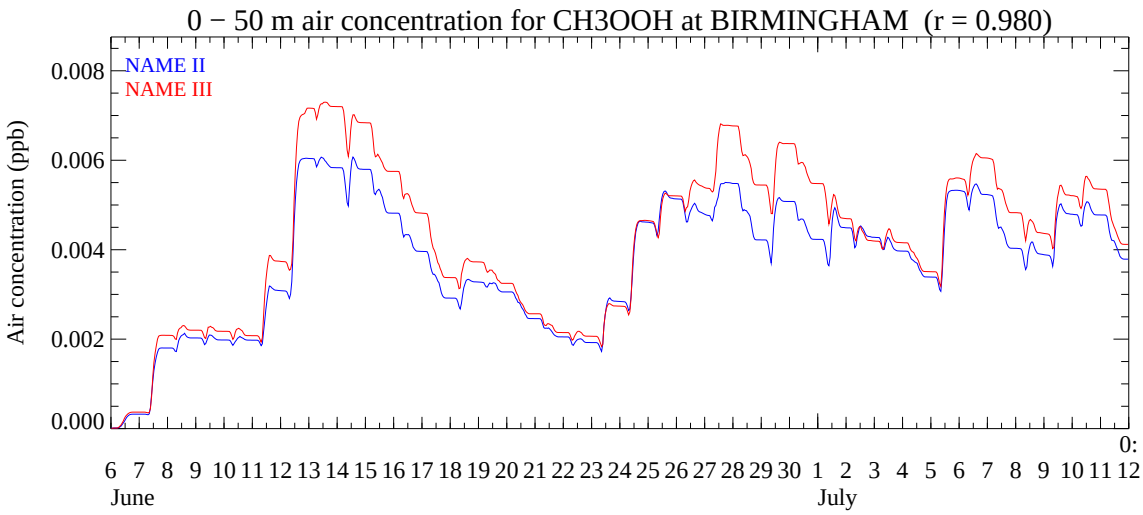

Figure 32: 0-50 m air concentration of CH3OOH

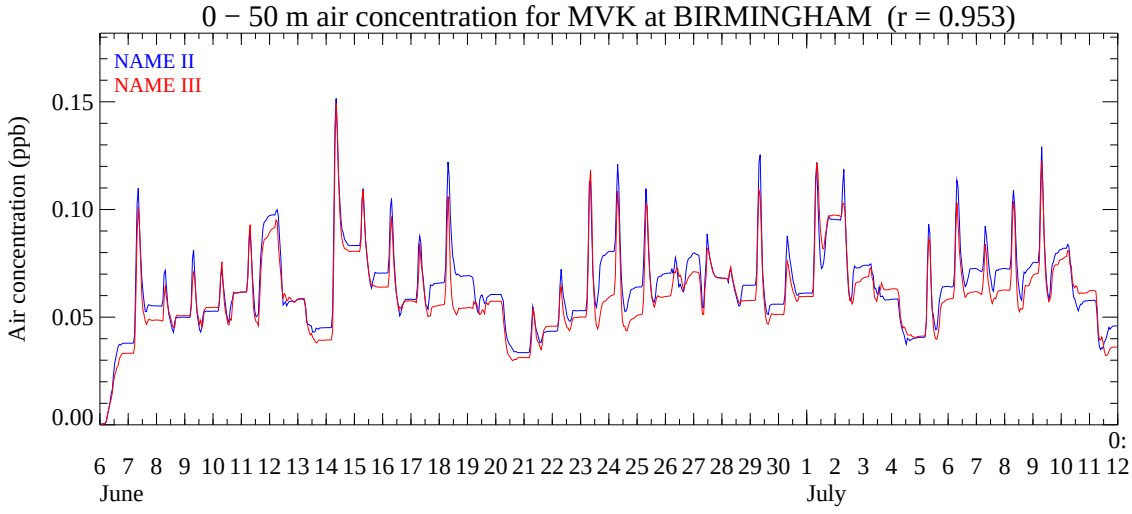

Figure 33: 0-50 m air concentration of MVK

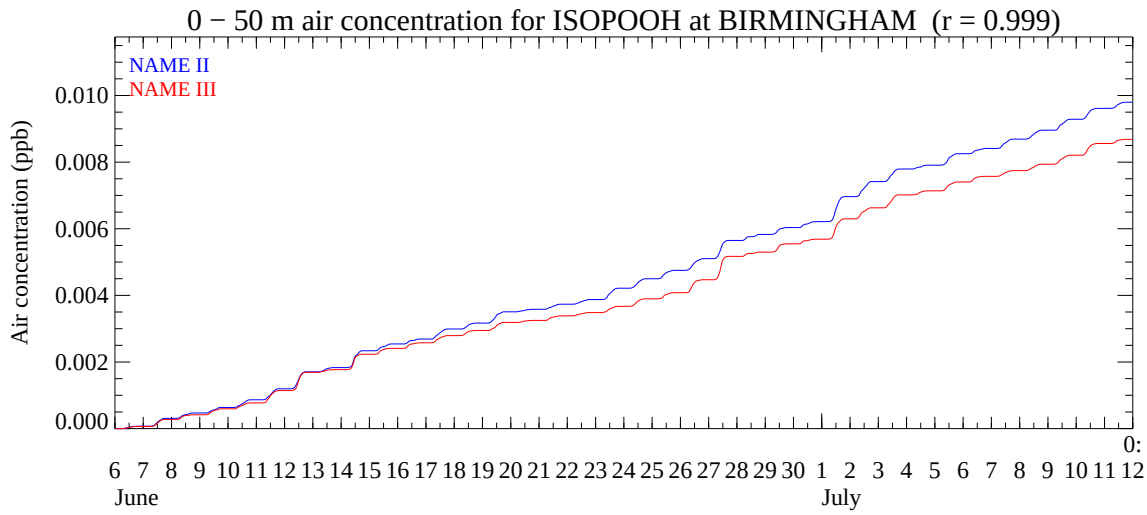

Figure 34: 0-50 m air concentration of ISOPOOH

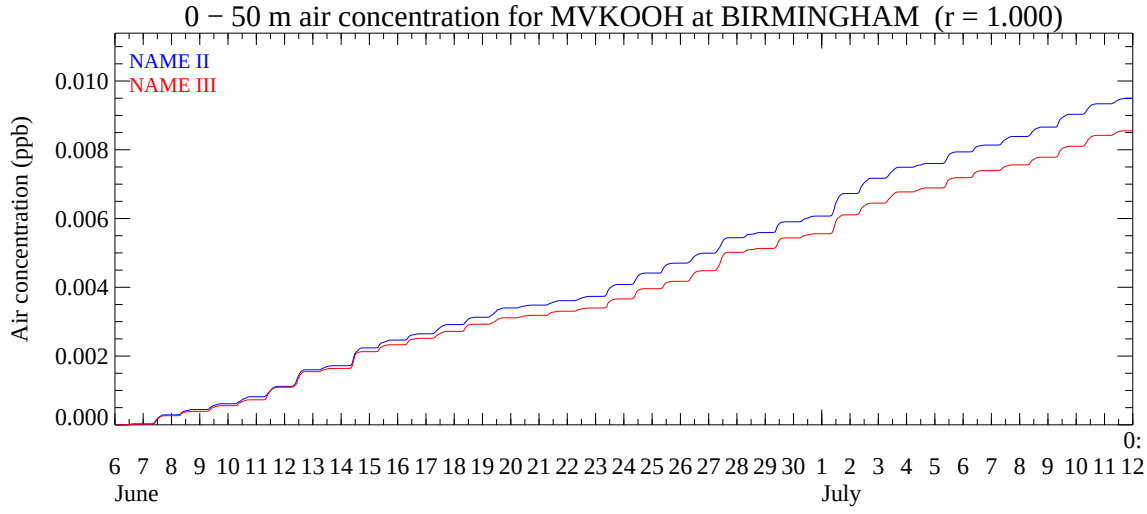

Figure 35: 0-50 m air concentration of MVKOOH

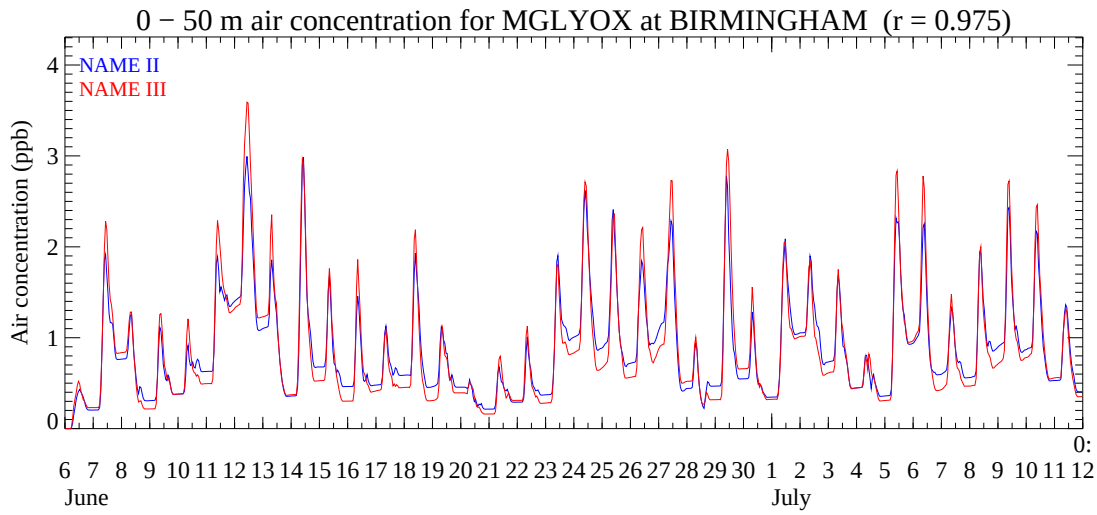

Figure 36: 0-50 m air concentration of MGLYOX

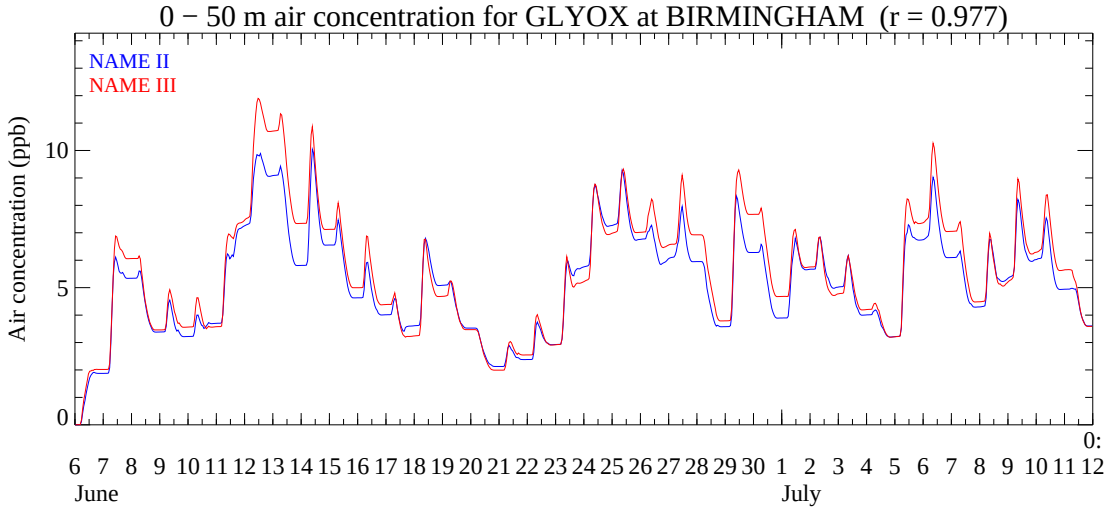

Figure 37: 0-50 m air concentration of GLYOX

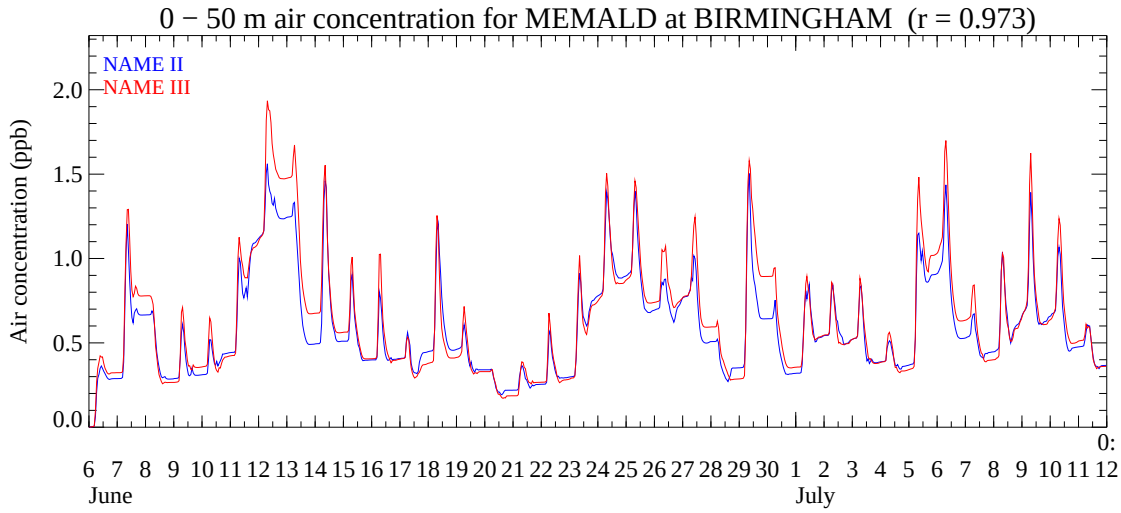

Figure 38: 0-50 m air concentration of MEMALD