Testing the NAME III chemistry scheme by a comparison of the NAME II and NAME III model predictions for the PUMA summer campaign

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1 Overview of the PUMA summer campaign

The Pollution of the Urban Midlands Atmosphere (PUMA) project was a 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. One aim of the PUMA project was the development of an 'urban airshed' model [1] capable of producing urban background concentrations of key atmospheric pollutants at hourly time scales and at resolutions of 2 km or less. Another aspect of PUMA was the collection of extensive measurement data from a variety of observational sources for two campaign periods, a summer campaign (12 June – 12 July, 1999) and a winter campaign (17 January – 17 February, 2000), allowing model output to be compared with observational measurement data. A modelling exercise based on the PUMA summer campaign is presented in the current report.

2 The NAME III model set up

The modelling exercise used version 2.0 of NAME III, and our results were compared against those obtained using version 8.12 of NAME II. The main NAME III input files for the PUMA summer modelling exercise, included in Appendix A, provide full details on the model set up used in the study. Some of the main features of this set up (including settings for the chemistry scheme) are now discussed further.

Two 'standard' input files were used by NAME III in the model run, namely Met-DefnUMHR.txt (the met definition file for running with hi-res UM4 regional met data) and STOCHEMGridDefn.txt (the STOCHEM grid definition for the background chemistry fields). The sources file PUMAsources_NAMEIII.dat contains information on the emission sources (UK emissions are defined in terms of National Grid 100 m coordinates, whereas European sources use the EMEP 50 km coordinate grid), with the NAME III sources file being obtained simply by reformatting the sources file used by NAME II.

¹NAME II with its chemistry scheme (including sulphur, nitrogen and hydrocarbon chemistry) was used for the PUMA modelling study. It was driven by meteorological fields from the mesoscale version of the Met Office's Unified Model UM4 (12 km resolution), and also higher resolution (down to 2 km) meteorological fields generated by the non-hydrostatic mesoscale RAMS model (itself forced using boundary conditions from the Met Office mesoscale model). Emission information was extracted from the National Atmospheric Emissions Inventory for 1998 (compiled by NETCEN) and EMEP database.

Species	Particle Mass Limit (g)	Species	Particle Mass Limit (g)
SULPHUR-DIOXIDE*	60000.0	CO*	140000.0
AMMONIA*	35000.0	HCHO*	5000.0
NO*	35000.0	C2H4*	7000.0
NH42SO4		C3H6*	6000.0
SULPHATE		C5H8*	800.0
NO2*	3500.0	$OXYL^*$	2800.0
NO3		$TOLUEN^*$	11200.0
N2O5		BD^*	840.0
HNO3		CH3CHO	
NAER		PAN	
NH4NO3		HONO	
O3	80000.0	PM10*	18000.0

Table 1: The particle mass limits of species carried on particles (blank entries indicate there is no limit on that species). Asterisks highlight the species for which there are primary source emissions.

For this study, the dispersion is modelled using particles (because the NAME III chemistry scheme cannot be used with puffs). The model run starts at 00Z on 06/06/1999 and finishes at 00Z on 12/07/1999, giving a run duration of 36 days. Results are output hourly (commencing at 01Z on 06/06/1999) with a total of 864 hours of data. These results are hourly-averaged values based on four contributions during each hour (i.e. the hourly average is calculated as the mean of the four instantaneous values at T-00:45, T-00:30, T-00:15, and T-00:00). This is consistent with the 15-minute synchronisation interval (main advection time step) used for the model run. The cheap random-walk scheme is applied (i.e. homogeneous turbulence with no velocity memory). We model dry and wet deposition, and both turbulence and meander. However, the effect of deep convection is not considered here (because it was not modelled in the NAME II run).

Chemistry is modelled using a 91×92 longitude-latitude grid with grid spacing $(dx, dy) = (0.22^{\circ}, 0.13^{\circ})$ extending over the domain (12W - 8E, 48N - 60N). This is equivalent to an approximate spatial resolution of 15 km. The vertical levels of the chemistry grid are defined with the grid box boundaries occurring at 0 m, 50 m, 100 m, 200 m, 500 m, 1000 m, 5000 m, 10000 m and 20000 m (also air concentrations are calculated on layer 1 (0 - 50 m) consistent with the lowest chemistry layer). The NAME III chemistry scheme represents 24 species on the particles and a further 11 species stored on static three-dimensional fields. There are limits on the mass carried by a single particle for some of the species (see Table 1) to avoid problems with lots of mass being released on a few large particles. Primary pollutants (i.e. species that are, at least in part, emitted from sources – although, of course, there may also be some additional production by the chemistry) are indicated by an asterisk in this table; other species are purely secondary being produced by the chemistry alone.

Hourly time series of air concentrations in the lowest model layer (0 - 50 m) and boundary-layer average concentrations were requested at fifteen locations: Birmingham, Birmingham East, Pritchatts Rd, Ladybower, Bottesford, Harwell, London, Rochester, Lullington, Yarner Wood, Narberth, Coventry, Leicester, Aston Hill and Leamington Spa. However only the time series at the Birmingham location are considered in this report (although the other data are available should any further study be performed).

For species held on particles, concentration is calculated as an average over a box centred on the output location (and of size $(dx, dy) = (0.22^{\circ}, 0.13^{\circ})$ consistent with the chemistry grid). For species stored as chemistry fields, the concentrations are output directly from the chemistry grid box covering that location. Hourly output of the 'particle numbers' field on the chemistry grid (i.e. the number of particles in each chemistry grid box) for the lowest model layer were also generated. This field is not plotted here, but we note that particle numbers were typically in the range 10-100 over the Midlands region during this modelling run.

3 Results of the comparison study

It is not our intention here to present a detailed scientific discussion on modelling of the PUMA summer campaign. Instead, the aim of this report is 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. 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 new implementation of the NAME chemistry scheme should be revealed by this type of comparative study.

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. For instance, we aim to have a similar number of particles at any instant in the two simulations (although, of course, the instantaneous number of particles will vary through time in each simulation as the meteorology changes). A comparable number of particles ensures that the concentration predictions in each model run will have similar levels of noise. Figure 1 shows the time evolution of the number of particles in the two simulations. It is observed that these two time series are strongly correlated, although the NAME II simulation typically has a greater number of particles than the NAME III run. This comment is supported by a comparison of the mean particle number over the full 36-day modelling period (1.46 million in NAME II against 1.28 million in NAME III). It is quite likely that the difference here is explained by the different approaches to releasing particles in the two models: NAME II tends to release more particles from a source (each having sub-optimal mass) whereas NAME III is 'economical' with its particles, releasing only particles with the optimal mass.²

Time series of total NO_x concentration, and its constituents NO and NO_2 , are plotted in Figure 2. These show the NAME II and NAME III predictions of 0-50 m air concentration at Birmingham, together with the observed urban-background concentrations from the Birmingham measurement site.

²In broad terms, NAME II releases a fixed number of particles from a (steady) source in every model time step. This number is determined by dividing the total mass to be released in the time step by the 'particle mass' parameter, and then rounding up to the nearest whole number (this essentially reduces the actual mass carried on these particles to less than the 'particle mass' value). In particular, at least one particle is always released per time step. In contrast, NAME III calculates a particle release interval (again determined by the mass to be released and the 'particle mass' parameter) which carries over from one time step to the next and thus allows the full mass to be carried on every particle.

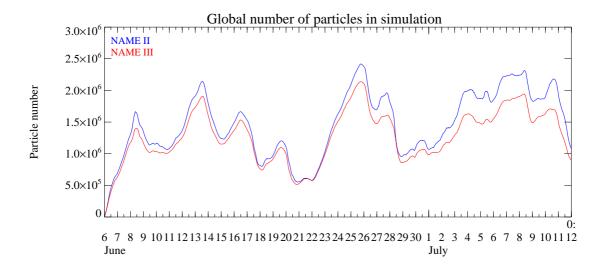


Figure 1: A comparison of the instantaneous number of particles in the two model runs

A comprehensive set of plots in Appendix B provide 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 which can be requested as output (that is, the species carried on particles and the chemistry fields). Figures 3-26 show species that are carried on particles (both as a 0-50 m concentration and as a boundary-layer average concentration), whereas Figures 27-37 compare the evolution of the chemistry fields in the lowest chemistry layer (effectively, a 0-50 m concentration). Tables 2 and 3 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 less strong for a few species, notably ammonia and the secondary 'aerosol' species (ammonium sulphate/nitrate and sulphate/nitrate aerosol). As for the magnitude of the predictions, there is some evidence here that the NAME III chemistry scheme is less 'energetic' than NAME II in the sense that primary species generally see higher concentrations in NAME III whereas secondary species see lower concentrations (see column 'III/II' for mean concentrations in Tables 2 and 3). The reasons for these differences are unclear, but could possibly be related to the particle numbers issue raised earlier.

4 Remarks and conclusions

The report discusses an empirical test of the NAME III chemistry scheme based on a comparison with NAME II chemistry calculations for the PUMA summer campaign. The primary aim of this work was to check the integrity of the NAME III model in an application involving chemistry (using NAME II as our reference model). In other words, rather than a formal analysis of the PUMA experiment, our focus here was to test the operation of the chemistry scheme (input/output, passing between particles for the transport (Lagrangian setting) and grid boxes for running chemistry (Eulerian

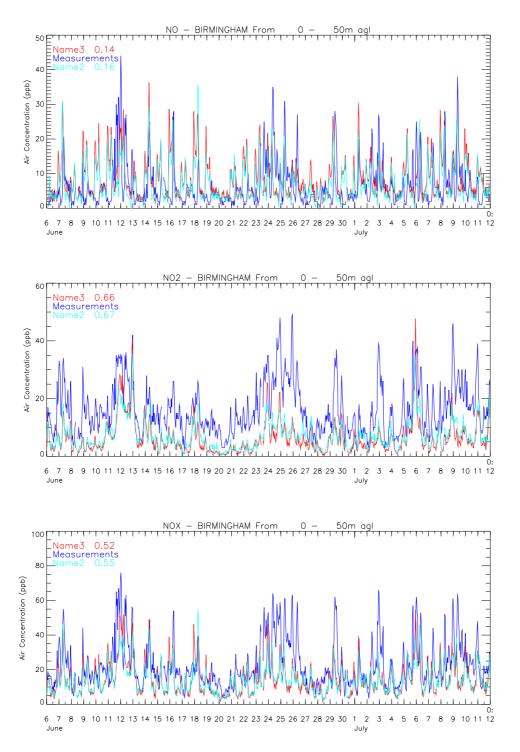


Figure 2: A comparison of the NO, NO_2 and total NO_x predictions of NAME II and NAME III against measurement data for the Birmingham site

	Mean concentration		Stand	Standard deviation			
Species	NAME III	NAME II	III/II	NAME III	NAME II	III/II	
SO2	8.989E+00	9.871E+00	0.911	1.302E+01	1.400E+01	0.930	0.892
AMMONIA	4.212E+00	3.719E+00	1.133	3.735E+00	2.997E+00	1.246	0.592
NO	1.053E+01	8.891E+00	1.184	7.272E+00	6.603E+00	1.101	0.923
NH42SO4	1.710E+00	2.903E+00	0.589	2.640E+00	4.226E+00	0.625	0.804
SULPHATE	3.234E-01	4.860E-01	0.665	5.963E-01	6.971E-01	0.855	0.669
NO2	1.197E+01	1.345E+01	0.890	1.068E + 01	9.398E+00	1.136	0.911
NO3	2.312E-07	3.037E-07	0.761	5.814E-07	6.158E-07	0.944	0.925
N2O5	1.215E-05	1.165E-05	1.043	5.408E-05	4.069E-05	1.329	0.961
HNO3	1.342E+00	1.752E+00	0.766	2.372E+00	2.487E + 00	0.954	0.915
NAER	9.962E-02	1.965E-01	0.507	1.984E-01	3.245E-01	0.612	0.623
NH4NO3	5.941E-01	9.876E-01	0.602	1.196E+00	1.593E+00	0.751	0.646
O3_PART	8.560E + 00	1.004E+01	0.853	1.129E+01	1.013E+01	1.114	0.819
CO	1.513E + 02	1.369E + 02	1.105	1.040E + 02	8.571E + 01	1.213	0.916
HCHO	9.067E + 00	8.186E + 00	1.108	7.632E+00	5.962E+00	1.280	0.961
C2H4	1.301E+01	1.147E + 01	1.135	9.569E + 00	7.402E+00	1.293	0.961
C3H6	5.753E+00	4.547E + 00	1.265	5.470E + 00	4.426E+00	1.236	0.967
C5H8	4.979E-02	4.059E-02	1.227	3.669E-02	2.935E-02	1.250	0.910
OXYL	3.865E + 00	3.408E+00	1.134	2.758E+00	2.142E+00	1.287	0.959
TOLUEN	2.268E+01	1.999E+01	1.134	1.709E+01	1.321E + 01	1.293	0.962
BD	8.492 E-01	7.168E-01	1.185	6.013E-01	4.729E-01	1.272	0.948
СНЗСНО	2.382E-01	2.686E-01	0.887	2.964E-01	2.925E-01	1.013	0.932
PAN	9.422E-01	9.833E-01	0.958	1.964E+00	1.591E+00	1.234	0.944
HONO	0.000E+00	0.000E+00	_	0.000E+00	0.000E+00	_	_
PM10	4.789E+00	4.421E+00	1.083	3.210E+00	2.618E + 00	1.226	0.933
H2O2	1.846E-01	1.629E-01	1.133	2.000E-01	1.988E-01	1.006	0.996
O3	1.343E+01	1.239E+01	1.084	1.665E + 01	1.476E + 01	1.128	0.981
OH	7.110E-05	7.258E-05	0.980	8.872E-05	7.967E-05	1.114	0.852
HO2	7.396E-04	6.941E-04	1.066	1.000E-03	8.408E-04	1.190	0.871
CH3OOH	4.641E-03	3.763E-03	1.233	1.850E-03	1.416E-03	1.307	0.974
MVK	6.335E-02	6.435E-02	0.985	1.873E-02	1.905E-02	0.983	0.941
ISOPOOH	4.484E-03	4.619E-03	0.971	2.765E-03	2.944E-03	0.939	0.999
MVKOOH	4.423E-03	4.476E-03	0.988	2.732E-03	2.855E-03	0.957	1.000
MGLYOX	9.361E-01	8.675E-01	1.079	6.414E-01	5.362E-01	1.196	0.968
GLYOX	5.779E + 00	5.194E+00	1.113	2.242E+00	1.845E + 00	1.215	0.979
MEMALD	6.509E-01	5.883E-01	1.106	3.531E-01	2.845E-01	1.241	0.973

Table 2: A comparison of the 0-50 m air concentration predictions (all species). Concentration units are $\mu g/m^3$ for species carried on particles (SO₂ \rightarrow PM₁₀), and ppbv for species on chemistry fields (H₂O₂ \rightarrow MEMALD).

	Mean concentration			Stand	Standard deviation		
Species	NAME III	NAME II	III/II	NAME III	NAME II	III/II	
SO2	8.832E+00	9.945E+00	0.888	1.294E+01	1.421E+01	0.911	0.917
AMMONIA	3.224E+00	3.110E+00	1.037	2.714E+00	2.458E+00	1.104	0.700
NO	6.680E+00	5.768E+00	1.158	5.958E + 00	5.598E+00	1.064	0.964
NH42SO4	1.718E+00	3.108E+00	0.553	2.566E+00	4.497E+00	0.571	0.843
SULPHATE	3.247E-01	4.967E-01	0.654	5.832E-01	6.687E-01	0.872	0.701
NO2	1.059E+01	1.153E+01	0.919	9.736E + 00	9.109E+00	1.069	0.950
NO3	2.251E-07	2.662E-07	0.846	5.671E-07	6.245 E-07	0.908	0.956
N2O5	1.181E-05	1.405E-05	0.841	5.348E-05	6.252 E-05	0.855	0.971
HNO3	1.273E+00	1.615E+00	0.789	2.277E + 00	2.551E+00	0.893	0.945
NAER	9.763E-02	2.059E-01	0.474	1.926E-01	3.299E-01	0.584	0.658
NH4NO3	5.839E-01	1.043E+00	0.560	1.168E + 00	1.632E+00	0.716	0.673
O3_PART	8.358E + 00	9.961E+00	0.839	1.088E + 01	1.039E + 01	1.047	0.883
CO	1.188E + 02	1.065E + 02	1.115	9.492E + 01	7.926E + 01	1.198	0.963
HCHO	6.538E+00	5.798E+00	1.128	6.925E+00	5.629E+00	1.230	0.978
C2H4	9.470E + 00	8.347E + 00	1.135	8.640E + 00	6.955E+00	1.242	0.978
C3H6	3.700E+00	3.044E+00	1.216	4.537E + 00	3.753E + 00	1.209	0.974
C5H8	3.214E-02	2.586E-02	1.243	2.651E-02	2.211E-02	1.199	0.952
OXYL	2.792E+00	2.454E+00	1.138	2.481E+00	2.004E+00	1.238	0.977
TOLUEN	1.664E + 01	1.473E + 01	1.130	1.546E + 01	1.245E + 01	1.242	0.978
BD	5.707E-01	4.821E-01	1.184	5.024E-01	4.141E-01	1.213	0.970
CH3CHO	2.196E-01	2.135E-01	1.028	2.851E-01	2.547E-01	1.119	0.972
PAN	9.154E-01	9.381E-01	0.976	1.943E+00	1.729E+00	1.123	0.974
HONO	0.000E+00	0.000E+00	_	0.000E+00	0.000E+00	_	_
PM10	3.677E+00	3.428E+00	1.073	2.885E+00	2.483E+00	1.162	0.962

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

framework), chemistry calculations, etc.).

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. The NAME II and NAME III predictions of NO_x species demonstrated a good level of mutual agreement, although correlations with measurements were rather poor in both models (possibly due to local influences not being captured). The temporal evolution of other species represented in the NAME chemistry scheme were also strongly correlated between the NAME II and NAME III runs, although there is perhaps some evidence that the production of secondary species is less in NAME III. However, in summary, we can conclude that this modelling exercise provides evidence to suggest that the implementation of the chemistry scheme in NAME III is functioning correctly.

We finish by giving some suggestions that might be worth exploring further in the future. In this report, we have limited our focus to considering time series at a specific location (Birmingham) but we could investigate other sites as well as looking at the full two-dimensional air concentration fields. It may also be of interest to compare the NAME II and NAME III predictions with measurement data for other species. Finally, we could repeat the modelling exercise for the PUMA winter campaign.

References

[1] 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: Main input files for the modelling exercise

[Note that this is an edited version of the actual input file. The '--->' notation denotes where long input blocks have been split across multiple lines to improve readability.]

```
NAME III PUMA SUMMER RUN (ARJ, 10/12/2004) - for comparison with NAME II PUMA SUMMER RUN
                                  "PUMASpecies.txt", "PUMAGridDefn.txt" and "STOCHEMGridDefn.txt".
Chemistry scheme set-up:
Sources and time-dependencies: "PUMAsources_NAMEIII.dat", "TrafficTimeDep.txt"
Met definition for hi-res reg: "MetDefnUMHR.txt".
Main Options:
Absolute or relative time?, Fixed met?, Time of fixed met, Flat Earth?,
                                                                         No, PUMA SUMMER,
                   absolute,
                                       No.
---> Restart Case Interval, Restart Interval, Random Seed
Multiple Case Options:
Multiple Cases?, Multiple Sets of Dispersion Options?
Output Options:
/data/local2/aprj/ChemistryTests/PUMAsummer/
Input Files:
File names
/home/hc1400/aprj/NameIII/Code/NameIII/Resources/Defns/MetDefnUMHR.txt
../Resources/Defns/PUMAGridDefn.txt
../Resources/Defns/PUMASpecies.txt
../Resources/Defns/STOCHEMGridDefn.txt
../Resources/Defns/TrafficTimeDep.txt
../Resources/PUMAsources_NAMEIII.dat
Horizontal Coordinate Systems:
Lat-Long
UK National Grid (100m)
EMEP 50km Grid
Vertical Coordinate Systems:
Name
m agl
Locations: TimeSeries Locations
                  H-Coord,
                                     Χ,
BIRMINGHAM,
                 Lat-Long, -1.9056, 52.4771
BIRMINGHAM_EAST, Lat-Long, -1.8287, 52.4958
PRITCHATTS_RD, Lat-Long, -1.9990, 52.4560
LADYBOWER, Lat-Long, -1.7528, 53.3973
                Lat-Long, -0.8142, 52.9294
Lat-Long, -1.3167, 51.5833
Lat-Long, -0.1333, 51.5000
BOTTESFORD,
HARWELL,
T.ONDON.
ROCHESTER,
                 Lat-Long, 0.6415, 51.4532
                Lat-Long, 0.1872, 50.7918
Lat-Long, -3.7156, 50.5967
Lat-Long, -4.6941, 51.7802
LULLINGTON,
YARNER WOOD.
NARBERTH,
                 Lat-Long, -1.5196, 52.4114
Lat-Long, -1.1333, 52.6333
COVENTRY,
LEICESTER.
                 Lat-Long, -3.0367, 52.5022
ASTON HILL.
LEAMINGTON_SPA, Lat-Long, -1.5312, 52.2865
```

```
Horizontal Grids:
                  H-Coord,
Name,
                               Set of Locations, Location of Centre, nx, ny, dx,
                    , TimeSeries Locations,
                                                                              , 0.22, 0.13
All Locations.
Birmingham,
                  Lat-Long, TimeSeries Locations,
                                                          BIRMINGHAM,
                                                                              1, 0.22, 0.13
                                                     BIRMINGHAM_EAST, 1, 1, 0.22, 0.13
Birmingham_East, Lat-Long, TimeSeries Locations,
Birmingham_East, Lat-Long, TimeSeries Locations, PRITCHATTS_RD, 1, 1, 0.22, 0.13
Ladybower, Lat-Long, TimeSeries Locations, LADYBOWER, 1, 1, 0.22, 0.13
Bottesford, Lat-Long, TimeSeries Locations, BOTTESFORD, 1, 1, 0.22, 0.13
              Lat-Long, TimeSeries Locations,
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Harwell,
                Lat-Long, TimeSeries Locations,
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                Lat-Long, TimeSeries Locations,
Lat-Long, TimeSeries Locations,
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1, 0.22, 0.13
London,
Rochester.
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                Lat-Long, TimeSeries Locations,
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Lullington,
                                                          YARNER_WOOD, 1,
NARBERTH, 1,
                Lat-Long, TimeSeries Locations,
Lat-Long, TimeSeries Locations,
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1, 0.22, 0.13
Yarner_Wood,
Narberth.
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Coventry,
                 Lat-Long, TimeSeries Locations,
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ASTON_HILL, 1, 1, 0.22, 0.13
Leicester.
                Lat-Long, TimeSeries Locations,
Aston_Hill,
Leamington_Spa, Lat-Long, TimeSeries Locations,
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Temporal Grids:
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Hrly,
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SixHrly, 144, 06:00:00, 6/6/1999 06:00:00
Daily,
          36, 24:00:00, 7/6/1999 00:00:00
Minute, 180, 00:01:00, 6/6/1999 00:01:00
Output Requirements - Fields:
Quantity, Species, Source, H-Grid, Z-Grid, T-Grid, BL Average, Air Concentration, SULPHUR-DIOXIDE, , All Locations, Layer1, Hrly, No, Air Concentration, SULPHUR-DIOXIDE, , All Locations, , Hrly, Yes,
                                        , All Locations, Layer1,
Chemistry Field, H202,
                                            , All Locations, Layer1,
                                                                        Hrly,
                                                                                      No.
(etc. for other chemistry species on particles and fields)
---> T Av Or Int, Av Time, # Av Times, Sync?, Graph?, Screen?, Disk?, Stat?, Across,
              Av, 01:00, 4, No,
Av, 01:00, 4, No,
                                                           No, Yes,
No, Yes,
--->
                                                  No,
                                                                          No,
                                                  No.
                                                                          No,
--->
              Αv,
                  01:00,
                                    4,
                                          No,
                                                  No,
                                                           No, Yes,
                                                                          No,
---> Separate File, Output Format, Output Group
---> XY, AZ, TimeSeries_OTo50m
                               AZ, TimeSeries_BLAv
                XΥ,
                               AZ, TimeSeries_OTo50m
--->
                XY.
Output Requirements - Fields:
Quantity,
                                 Species, Source,
                                                                                    H-Grid,
                                     , , NAME Chemistry Scheme - horizontal grid,
# Particles,
---> Z-Grid, T-Grid, T Av Or Int, Av Time, # Av Times, Sync?, Graph?, Screen?, Disk?, Stat?,
---> Layer1, Hrly, Av, 01:00, 4, No, No, Yes, No,
---> Across, Separate File, Output Format, Output Group
                                IA, Fields_ParticleNumbers
                Т.
Output Requirements - Fields:
Quantity, Species, Source, H-Grid, Z-Grid, T-Grid, T Av Or Int, Sync?, Graph?,
No,
---> Screen?, Disk?, Stat?, Output Format, Output Group
---> No, Yes, No, A, BulkStats
---> No, Yes, No, A, BulkStats
```

```
Sets of Dispersion Options:
Skew Time, Velocity Memory Time, Inhomogeneous Time, DeltaOpt, Puff Time, Sync Time,
                00:00, 00:00, 1, 00:00, 00:15:00,
---> Computational Domain, Puff Interval, Deep Convection?, Radioactive Decay?, Agent Decay?,
---> NAME Chemistry Domain, 00:15:00,
---> Dry Deposition?, Wet Deposition?, Turbulence?, Meander?, Chemistry?
               Yes,
                               Yes, Yes, Yes, Yes
NWP Met Module Instances:
Name, Min B L Depth, Max B L Depth, Use NWP BL Depth?, Restore Met Script, Delete Met?,
Regional,
                  50.0.
                               4000.0.
                                                     No.
                                         Met Folder.
---> /data/local2/aprj/ChemistryTests/met/PUMAsummer/,
                                          Topography Folder, Met Definition Name
---> /home/hc1400/aprj/NameIII/Code/NameIII/Resources/Topog/,
NWP Flow Module Instances:
Name, Met Module, Met, Domain
Regional, NWP Met, Regional, UMHH2001R Whole
Flow Order: Update
Flow Module, Flow
NWP Flow, Regional
Flow Order: Convert
Flow Module, Flow
NWP Flow, Regional
Flow Order: Flow
Flow Module, Flow
NWP Flow,
          Regional
Flow Order: Cloud
Flow Module, Flow
NWP Flow, Regional
Flow Order: Rain
Flow Module, Flow
NWP Flow, Regional
Flow Attributes:
Name, Flow Order
Update, Update
Convert, Convert
Flow, Flow Cloud, Cloud
       Cloud
Rain,
        Rain
[PUMAGridDefn.txt]
** PUMA Chemistry Grid and Domain Definitions **
```

11

The 'interface levels' define the bottom and top of each slab (following the NAME II approach). The 'grid levels' are taken as the centre of each slab, and should be defined at slab midpoints

consistent with these interface heights (c.f. treatment of NWP met data).

Array: InterfaceLevelsForChemistry

Array Values

```
0.0
  50.0
  100.0
  200.0
 500.0
 1000.0
 5000.0
10000.0
20000.0
Array: GridLevelsForChemistry
Array Values
  25.0
  75.0
 150.0
  350.0
 750.0
 3000.0
 7500.0
15000.0
Horizontal Coordinate Systems:
Lat-Long
Vertical Coordinate Systems:
Name
m agl
Horizontal Grids:
Name, H-Coord, nX, nY, dX, dY, X0, Y0 NAME Chemistry Scheme - horizontal grid, Lat-Long, 91, 92, 0.22, 0.13, -11.89, 48.065
Vertical Grids:
                                           Z-Coord, nZ, dZ, ZO, Z-Array
Name.
NAME Chemistry Scheme - interface levels, m agl, , , InterfaceLevelsForChemistry NAME Chemistry Scheme - vertical grid, m agl, , , GridLevelsForChemistry
Domains:
                       H-Coord, X Min, X Max, Y Min, Y Max, H Unbounded?, Z-Coord, Z Max,
Name.
NAME Chemistry Domain, Lat-Long, -12.0, 8.02, 48.0, 59.96, No, m agl, 20000.0,
                        Start Time,
---> Z Unbounded?,
                                               End Time, Max Travel Time
         No, 6/6/1999 00:00:00, 12/7/1999 00:00:00,
[PUMASpecies.txt]
** Listing of species carried on particles for PUMA summer campaign **
Species:
                                         Half Life, UV Loss Rate, Surface Resistance,
Name,
                  Category,
                                          Stable, 0.00E+00, 1.00E+02,
SULPHUR-DIOXIDE, CHEMISTRY-SPECIES,
AMMONIA,
                  CHEMISTRY-SPECIES,
                                            Stable,
                                                       0.00E+00,
                                                                           1.00E+02,
                                          Stable, 0.00E+00,
NO,
                  CHEMISTRY-SPECIES,
                                                                           1.00E+02,
                                                                          1.00E+03,
               CHEMISTRY-SPECIES,
CHEMISTRY-SPECIES,
                                                      0.00E+00,
NH42SO4,
                                           Stable,
SULPHATE,
                                            Stable,
                                                       0.00E+00,
                 CHEMISTRY-SPECIES,
NO2,
                                           Stable,
                                                       0.00E+00,
                                                                          1.00E+02,
                                           Stable,
                                                                          1.00E+02,
NO3,
                 CHEMISTRY-SPECIES,
                                                      0.00E+00,
                                           Stable,
N205,
                  CHEMISTRY-SPECIES,
                                                       0.00E+00,
                                                                           1.00E+02,
                  CHEMISTRY-SPECIES,
                                                                           1.00E+02,
HNO3,
                                                      0.00E+00,
                                           Stable,
                                                      0.00E+00,
                                                                          1.00E+02,
NAER,
                 CHEMISTRY-SPECIES,
                                           Stable,
                                                      0.00E+00,
NH4NO3,
                  CHEMISTRY-SPECIES,
                                                                           1.00E+02,
```

Stable,

0.00E+00,

CHEMISTRY-SPECIES,

03,

5.00E+01,

```
CO,
                 CHEMISTRY-SPECIES,
                                          Stable,
                                                     0.00E+00,
                  CHEMISTRY-SPECIES,
                                          Stable,
                                                     0.00E+00,
C2H4.
                  CHEMISTRY-SPECIES.
                                           Stable.
                                                     0.00E+00.
C3H6,
                  CHEMISTRY-SPECIES,
                                           Stable,
                                                      0.00E+00,
                  CHEMISTRY-SPECIES,
                                                     0.00E+00,
C5H8.
                                           Stable.
OXYL.
                  CHEMISTRY-SPECIES.
                                           Stable,
                                                     0.00E+00.
                  CHEMISTRY-SPECIES,
TOLUEN,
                                           Stable,
                                                      0.00E+00.
                  CHEMISTRY-SPECIES.
BD.
                                           Stable.
                                                     0.00E+00.
CH3CHO,
                  CHEMISTRY-SPECIES,
                                           Stable,
                                                     0.00E+00,
PAN,
                  CHEMISTRY-SPECIES,
                                           Stable,
                                                      0.00E+00,
HONO.
                  CHEMISTRY-SPECIES.
                                                                         1.00E+02.
                                           Stable.
                                                      0.00E+00.
                  CHEMISTRY-SPECIES,
                                           Stable,
                                                      0.00E+00,
                                                                         1.00E+03,
PM10,
---> Deposition Velocity, Wet Type, Molecular Weight, Particle Mass, Material Unit
--->
                                2,
                                              64.00,
                                                          60000.0,
--->
                                             17.00,
                                                          35000.0,
                                1.
--->
                                Ο,
                                             30.00,
                                                          35000.0,
                                                                               g
--->
                                           132.00,
                               1,
                                                                               g
                               1,
--->
                                             96.00,
--->
                                Ο,
                                             46.00,
                                                           3500.0,
                                                                               g
--->
                                Ο,
                                             62.00,
                                                                               g
--->
                               Ο,
                                            108.00,
                                                                               g
--->
                                1,
                                             63.00.
                                                                               g
--->
                                             62.00.
                               1,
                                                                               g
--->
                               1,
                                            80.00,
                                                                               g
--->
                                Ο,
                                             48.00,
                                                          80000.0,
                                                                               g
                   0.0,
                                             28.00,
--->
                                                          140000.0.
                                Ο,
                    0.0,
--->
                                            30.00,
                                                           5000.0,
                                Ο,
                                                                               g
--->
                    0.0,
                                Ο,
                                             28.00,
                                                           7000.0,
                                                                               g
                                             42.00,
--->
                    0.0,
                               Ο,
                                                           6000.0.
                                                                               g
--->
                                             68.00,
                    0.0,
                                Ο,
                                                                               g
--->
                    0.0,
                               Ο,
                                            106.00,
                                                           2800.0.
--->
                    0.0,
                               Ο,
                                             92.00,
                                                          11200.0,
                                                                               g
                               Ο,
                                            54.00,
--->
                    0.0,
                                                           840.0,
                                                                               g
--->
                                             44.00.
                    0.0.
                               Ο,
--->
                    0.0,
                                Ο,
                                            121.00,
                                                                               g
                               1,
                                             47.00,
                     ,
                                                                               g
--->
                               1.
                                            100.00,
                                                          18000.0.
```

[TrafficTimeDep.txt]

** Weekly UK traffic-cycle time dependency used for the traffic sources **

```
Source Time Dependency: Traffic cycle
               To 1 ,
                              From 2 ,
  From 1 ,
                                                   To 2 , Factor
Mon 00:00 , Mon 01:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.0324
Mon 01:00 , Mon 02:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.0065
Mon 02:00 , Mon 03:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.0113
Mon 03:00 , Mon 04:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.032
Mon 04:00 , Mon 05:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.1921
Mon 05:00 , Mon 06:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.4916
Mon 06:00 , Mon 07:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.3022
Mon 07:00 , Mon 08:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.2983
Mon 08:00 , Mon 09:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.4332
Mon 09:00 , Mon 10:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.1893
Mon 10:00 , Mon 11:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.125
Mon 11:00 , Mon 12:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.2764
Mon 12:00 , Mon 13:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.3905
Mon 13:00 , Mon 14:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.3823
Mon 14:00 , Mon 15:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.5744
Mon 15:00 , Mon 16:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.2844
Mon 16:00 , Mon 17:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.2073 Mon 17:00 , Mon 18:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.7071
```

```
Mon 18:00 , Mon 19:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.0152
Mon 19:00 , Mon 20:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.6937
Mon 20:00 , Mon 21:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.6115
Mon 21:00 , Mon 22:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.4588
Mon 22:00 , Mon 23:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.3194
Mon 23:00 , Tue 00:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.1246
Tue 00:00 , Tue 01:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.0566
Tue 01:00 , Tue 02:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.023
Tue 02:00 , Tue 03:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.0142
Tue 03:00 , Tue 04:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.0452
Tue 04:00 , Tue 05:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.1908
Tue 05:00 , Tue 06:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.5645
Tue 06:00 , Tue 07:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.4632
Tue 07:00 , Tue 08:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.2573
Tue 08:00 , Tue 09:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.4327
Tue 09:00 , Tue 10:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.2918
Tue 10:00 , Tue 11:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.1927
Tue 11:00 , Tue 12:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.3458
Tue 12:00 , Tue 13:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.3364
Tue 13:00 , Tue 14:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.4611
Tue 14:00 , Tue 15:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.6845
Tue 15:00 , Tue 16:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.354
Tue 16:00 , Tue 17:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.5186
Tue 17:00 , Tue 18:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.7223
Tue 18:00 , Tue 19:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.1017
Tue 19:00 , Tue 20:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.763
Tue 20:00 , Tue 21:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.5772
Tue 21:00 , Tue 22:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.5294
Tue 22:00 , Tue 23:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.4307
Tue 23:00 , Wed 00:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.1133
Wed 00:00 , Wed 01:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.0502
Wed 01:00 , Wed 02:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.0178
Wed 02:00 , Wed 03:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.0343
Wed 03:00 , Wed 04:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.032
Wed 04:00 , Wed 05:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.1985
Wed 05:00 , Wed 06:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.5914
Wed 06:00 , Wed 07:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.3963
Wed 07:00 , Wed 08:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.4855
Wed 08:00 , Wed 09:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.4961
Wed 09:00 , Wed 10:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.2683
Wed 10:00 , Wed 11:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.4015
Wed 11:00 , Wed 12:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.3565
Wed 12:00 , Wed 13:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.3638
Wed 13:00 , Wed 14:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.6184
Wed 14:00 , Wed 15:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.7531
Wed 15:00 , Wed 16:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.3252
Wed 16:00 , Wed 17:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.6208
Wed 17:00 , Wed 18:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.5721
Wed 18:00 , Wed 19:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.2053
Wed 19:00 , Wed 20:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.7814
Wed 20:00 , Wed 21:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.7254
Wed 21:00 , Wed 22:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.5161
Wed 22:00 , Wed 23:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.375
Wed 23:00 , Thu 00:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.1489
Thu 00:00 , Thu 01:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.0275
Thu 01:00 , Thu 02:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.0421
Thu 02:00 , Thu 03:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.0132
Thu 03:00 , Thu 04:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.0333
Thu 04:00 , Thu 05:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.1833
Thu 05:00 , Thu 06:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.599
Thu 06:00 , Thu 07:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.4314
Thu 07:00 , Thu 08:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.2979
Thu 08:00 , Thu 09:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.3732
Thu 09:00 , Thu 10:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.2432 Thu 10:00 , Thu 11:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.2466
```

```
Thu 11:00 , Thu 12:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.3459
Thu 12:00 , Thu 13:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.563
Thu 13:00 , Thu 14:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.5092
Thu 14:00 , Thu 15:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.8887
Thu 15:00 , Thu 16:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.2672
Thu 16:00 , Thu 17:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.4515
Thu 17:00 , Thu 18:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.7456
Thu 18:00 , Thu 19:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.1964
Thu 19:00 , Thu 20:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.8679
Thu 20:00 , Thu 21:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.7148
Thu 21:00 , Thu 22:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.5116
Thu 22:00 , Thu 23:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.4226
Thu 23:00 , Fri 00:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.1527
Fri 00:00 , Fri 01:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.0764
Fri 01:00 , Fri 02:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.077
Fri 02:00 , Fri 03:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.0491
Fri 03:00 , Fri 04:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.0523
Fri 04:00 , Fri 05:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.1917
Fri 05:00 , Fri 06:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.6226
Fri 06:00 , Fri 07:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.3506
Fri 07:00 , Fri 08:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.312
Fri 08:00 , Fri 09:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.3007
Fri 09:00 , Fri 10:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.3434
Fri 10:00 , Fri 11:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.2868
Fri 11:00 , Fri 12:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.3977
Fri 12:00 , Fri 13:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.5255
Fri 13:00 , Fri 14:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.5682
Fri 14:00 , Fri 15:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.0217
Fri 15:00 , Fri 16:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.5095
Fri 16:00 , Fri 17:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.3327
Fri 17:00 , Fri 18:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.6644
Fri 18:00 , Fri 19:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.257
Fri 19:00 , Fri 20:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.0081
Fri 20:00 , Fri 21:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.6562
Fri 21:00 , Fri 22:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.5627
Fri 22:00 , Fri 23:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.5459
Fri 23:00 , Sat 00:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.1961
Sat 00:00 , Sat 01:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.243
Sat 01:00 , Sat 02:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.1783
Sat 02:00 , Sat 03:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.0534
Sat 03:00 , Sat 04:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.0358
Sat 04:00 , Sat 05:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.1503
Sat 05:00 , Sat 06:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.293
Sat 06:00 , Sat 07:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.5787
Sat 07:00 , Sat 08:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.1177
Sat 08:00 , Sat 09:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.301
Sat 09:00 , Sat 10:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.6785
Sat 10:00 , Sat 11:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.9304
Sat 11:00 , Sat 12:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.9081
Sat 12:00 , Sat 13:00 , 01/03/* 00:00 , 01/09/* 00:00 , 2.1466
Sat 13:00 , Sat 14:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.9456
Sat 14:00 , Sat 15:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.7336
Sat 15:00 , Sat 16:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.6927
Sat 16:00 , Sat 17:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.6222
Sat 17:00 , Sat 18:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.0771
Sat 18:00 , Sat 19:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.8998
Sat 19:00 , Sat 20:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.9354
Sat 20:00 , Sat 21:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.5384
Sat 21:00 , Sat 22:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.4385
Sat 22:00 , Sat 23:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.5931
Sat 23:00 , Sun 00:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.4181
Sun 00:00 , Sun 01:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.1686
Sun 01:00 , Sun 02:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.1831
Sun 02:00 , Sun 03:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.0828
Sun 03:00 , Sun 04:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.0362
```

```
Sun 04:00 , Sun 05:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.0737
Sun 05:00 , Sun 06:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.1171
Sun 06:00 , Sun 07:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.2724
Sun 07:00 , Sun 08:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.3348
Sun 08:00 , Sun 09:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.6321
Sun 09:00 , Sun 10:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.905
Sun 10:00 , Sun 11:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.2111
Sun 11:00 , Sun 12:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.3118
Sun 12:00 , Sun 13:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.3917
Sun 13:00 , Sun 14:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.4173
Sun 14:00 , Sun 15:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.3733
Sun 15:00 , Sun 16:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.2767
Sun 16:00 , Sun 17:00 , 01/03/* 00:00 , 01/09/* 00:00 , 1.0896
Sun 17:00 , Sun 18:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.8688
Sun 18:00 , Sun 19:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.7636
Sun 19:00 , Sun 20:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.6689
Sun 20:00 , Sun 21:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.5608
Sun 21:00 , Sun 22:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.3533
Sun 22:00 , Sun 23:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.2929
Sun 23:00 , Mon 00:00 , 01/03/* 00:00 , 01/09/* 00:00 , 0.1068
Mon 00:00 , Mon 01:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.1068
Mon 01:00 , Mon 02:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.0324
Mon 02:00 , Mon 03:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.0065
Mon 03:00 , Mon 04:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.0113
Mon 04:00 , Mon 05:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.032
Mon 05:00 , Mon 06:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.1921
Mon 06:00 , Mon 07:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.4916
Mon 07:00 , Mon 08:00 , 01/09/* 00:00 , 01/03/* 00:00 , 2.3022
Mon 08:00 , Mon 09:00 , 01/09/* 00:00 , 01/03/* 00:00 , 2.2983
Mon 09:00 , Mon 10:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.4332
Mon 10:00 , Mon 11:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.1893
Mon 11:00 , Mon 12:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.125
Mon 12:00 , Mon 13:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.2764
Mon 13:00 , Mon 14:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.3905
Mon 14:00 , Mon 15:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.3823
Mon 15:00 , Mon 16:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.5744
Mon 16:00 , Mon 17:00 , 01/09/* 00:00 , 01/03/* 00:00 , 2.2844
Mon 17:00 , Mon 18:00 , 01/09/* 00:00 , 01/03/* 00:00 , 2.2073
Mon 18:00 , Mon 19:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.7071
Mon 19:00 , Mon 20:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.0152
Mon 20:00 , Mon 21:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.6937
Mon 21:00 , Mon 22:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.6115
Mon 22:00 , Mon 23:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.4588
Mon 23:00 , Tue 00:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.3194
Tue 00:00 , Tue 01:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.1246
Tue 01:00 , Tue 02:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.0566
Tue 02:00 , Tue 03:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.023
Tue 03:00 , Tue 04:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.0142
Tue 04:00 , Tue 05:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.0452
Tue 05:00 , Tue 06:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.1908
Tue 06:00 , Tue 07:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.5645
Tue 07:00 , Tue 08:00 , 01/09/* 00:00 , 01/03/* 00:00 , 2.4632
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Tue 09:00 , Tue 10:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.4327
Tue 10:00 , Tue 11:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.2918
Tue 11:00 , Tue 12:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.1927
Tue 12:00 , Tue 13:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.3458
Tue 13:00 , Tue 14:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.3364
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Tue 15:00 , Tue 16:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.6845
Tue 16:00 , Tue 17:00 , 01/09/* 00:00 , 01/03/* 00:00 , 2.354
Tue 17:00 , Tue 18:00 , 01/09/* 00:00 , 01/03/* 00:00 , 2.5186
Tue 18:00 , Tue 19:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.7223
Tue 19:00 , Tue 20:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.1017 Tue 20:00 , Tue 21:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.763
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Tue 22:00 , Tue 23:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.5294
Tue 23:00 , Wed 00:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.4307
Wed 00:00 , Wed 01:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.1133
Wed 01:00 , Wed 02:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.0502
Wed 02:00 , Wed 03:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.0178
Wed 03:00 , Wed 04:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.0343
Wed 04:00 , Wed 05:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.032
Wed 05:00 , Wed 06:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.1985
Wed 06:00 , Wed 07:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.5914
Wed 07:00 , Wed 08:00 , 01/09/* 00:00 , 01/03/* 00:00 , 2.3963
Wed 08:00 , Wed 09:00 , 01/09/* 00:00 , 01/03/* 00:00 , 2.4855
Wed 09:00 , Wed 10:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.4961
Wed 10:00 , Wed 11:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.2683
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Wed 22:00 , Wed 23:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.5161
Wed 23:00 , Thu 00:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.375
Thu 00:00 , Thu 01:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.1489
Thu 01:00 , Thu 02:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.0275
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Thu 03:00 , Thu 04:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.0132
Thu 04:00 , Thu 05:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.0333
Thu 05:00 , Thu 06:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.1833
Thu 06:00 , Thu 07:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.599
Thu 07:00 , Thu 08:00 , 01/09/* 00:00 , 01/03/* 00:00 , 2.4314
Thu 08:00 , Thu 09:00 , 01/09/* 00:00 , 01/03/* 00:00 , 2.2979
Thu 09:00 , Thu 10:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.3732
Thu 10:00 , Thu 11:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.2432
Thu 11:00 , Thu 12:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.2466
Thu 12:00 , Thu 13:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.3459
Thu 13:00 , Thu 14:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.563
Thu 14:00 , Thu 15:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.5092
Thu 15:00 , Thu 16:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.8887
Thu 16:00 , Thu 17:00 , 01/09/* 00:00 , 01/03/* 00:00 , 2.2672
Thu 17:00 , Thu 18:00 , 01/09/* 00:00 , 01/03/* 00:00 , 2.4515
Thu 18:00 , Thu 19:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.7456
Thu 19:00 , Thu 20:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.1964
Thu 20:00 , Thu 21:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.8679
Thu 21:00 , Thu 22:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.7148
Thu 22:00 , Thu 23:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.5116
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Fri 00:00 , Fri 01:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.1527
Fri 01:00 , Fri 02:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.0764
Fri 02:00 , Fri 03:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.077
Fri 03:00 , Fri 04:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.0491
Fri 04:00 , Fri 05:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.0523
Fri 05:00 , Fri 06:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.1917
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Fri 10:00 , Fri 11:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.3434
Fri 11:00 , Fri 12:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.2868
Fri 12:00 , Fri 13:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.3977
Fri 13:00 , Fri 14:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.5255
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Fri 15:00 , Fri 16:00 , 01/09/* 00:00 , 01/03/* 00:00 , 2.0217
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Fri 22:00 , Fri 23:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.5627
Fri 23:00 , Sat 00:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.5459
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Sat 01:00 , Sat 02:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.243
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Sat 14:00 , Sat 15:00 , 01/09/* 00:00 , 01/03/* 00:00 , 1.9456
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Sun 21:00 , Sun 22:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.5608
Sun 22:00 , Sun 23:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.3533
Sun 23:00 , Mon 00:00 , 01/09/* 00:00 , 01/03/* 00:00 , 0.2929
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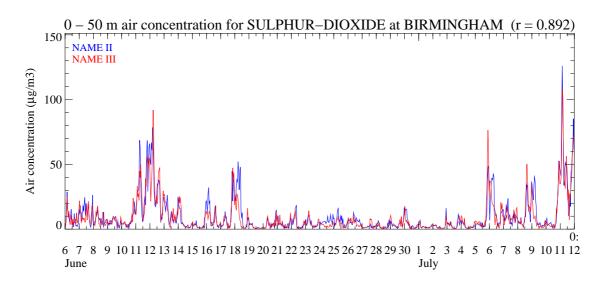
Appendix B: Comparison of the temporal evolutions of each individual species in the NAME chemistry scheme

Chemistry species stored on particles

- Figure 3: SULPHUR DIOXIDE (SO₂)
- Figure 4: AMMONIA (NH₃)
- Figure 5: NITRIC OXIDE (NO)
- Figure 6: AMMONIUM SULPHATE $((NH_4)_2SO_4)$
- Figure 7: SULPHATE AEROSOL (SULPHATE)
- Figure 8: NITROGEN DIOXIDE (NO₂)
- Figure 9: NITRATE (NO₃)
- Figure 10: DI-NITROGEN PENTOXIDE (N₂O₅)
- Figure 11: NITRIC ACID (HNO₃)
- Figure 12: NITRATE AEROSOL (NAER)
- Figure 13: AMMONIUM NITRATE (NH₄NO₃)
- Figure 14: OZONE ON PARTICLES $(O_{3_{PART}})$
- Figure 15: CARBON MONOXIDE (CO)
- Figure 16: FORMALDEHYDE (HCHO)
- Figure 17: ETHYLENE (C_2H_4)
- Figure 18: PROPYLENE (C₃H₆)
- Figure 19: ISOPRENE (C_5H_8)
- Figure 20: O-XYLENE (OXYL)
- Figure 21: TOLUENE (TOLUEN)
- Figure 22: 1,3-BUTADIENE (BD)
- Figure 23: ACETALDEHYDE (CH₃CHO)
- Figure 24: PEROXYACETYL NITRATE (PAN)
- Figure 25: NITROUS ACID (HONO)
- Figure 26: PM10

Chemistry species stored on fields

- Figure 27: HYDROGEN PEROXIDE (H₂O₂)
- Figure 28: OZONE ON FIELD $(O_{3_{FIELD}})$
- Figure 29: HYDROXYL (OH)
- Figure 30: HYDROPEROXY (HO₂)
- Figure 31: CH3OOH
- Figure 32: MVK
- Figure 33: ISOPOOH
- Figure 34: MVKOOH
- Figure 35: MGLYOX
- Figure 36: GLYOX
- Figure 37: MEMALD



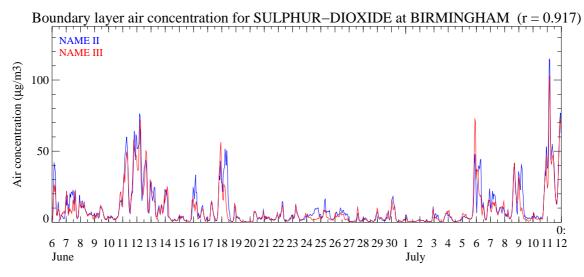
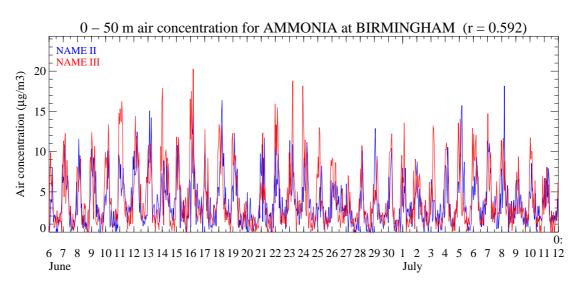


Figure 3: (a) 0-50 m and (b) boundary-layer average concentrations of sulphur dioxide



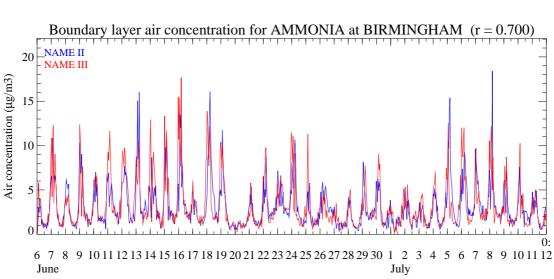
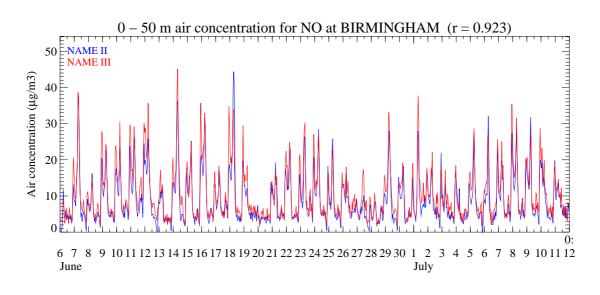


Figure 4: (a) 0-50 m and (b) boundary-layer average concentrations of ammonia



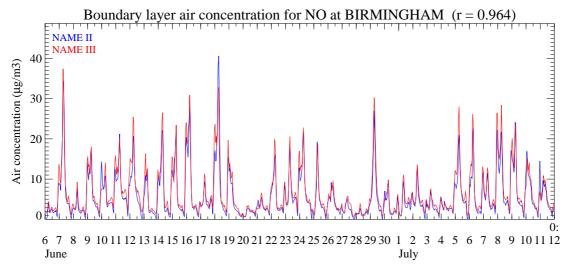


Figure 5: (a) 0-50 m and (b) boundary-layer average concentrations of nitric oxide

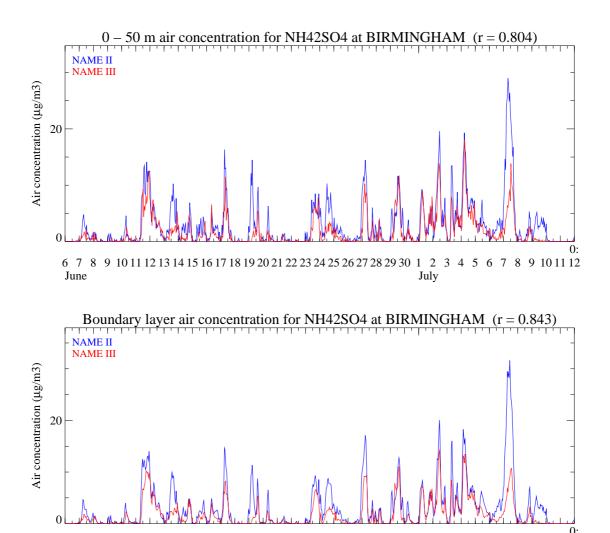


Figure 6: (a) 0-50 m and (b) boundary-layer average concentrations of ammonium sulphate

6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 1 2 3 4 5 6 7 8 9 10 11 12 June

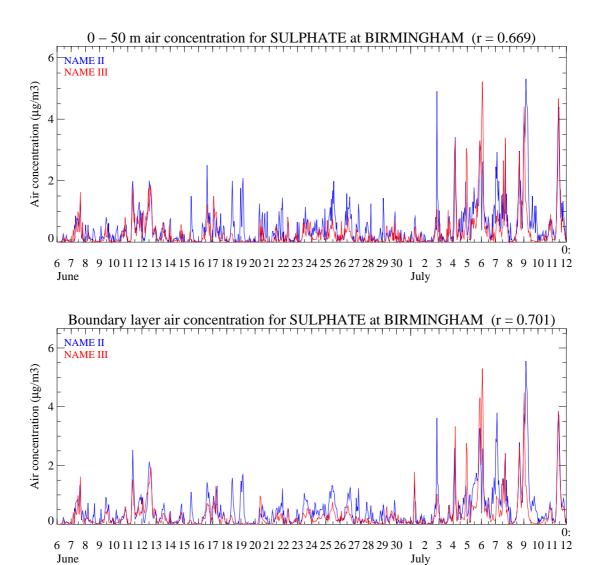
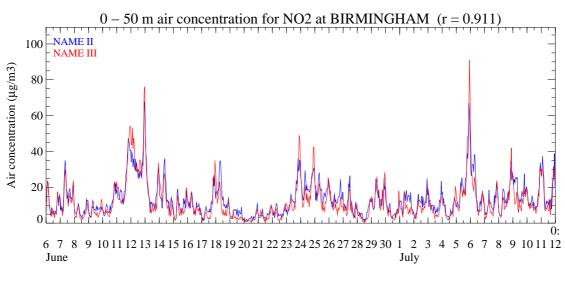


Figure 7: (a) 0-50 m and (b) boundary-layer average concentrations of sulphate aerosol



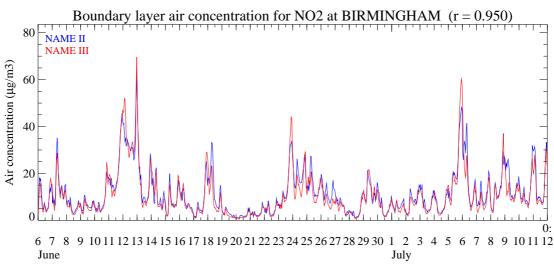


Figure 8: (a) 0-50 m and (b) boundary-layer average concentrations of nitrogen dioxide

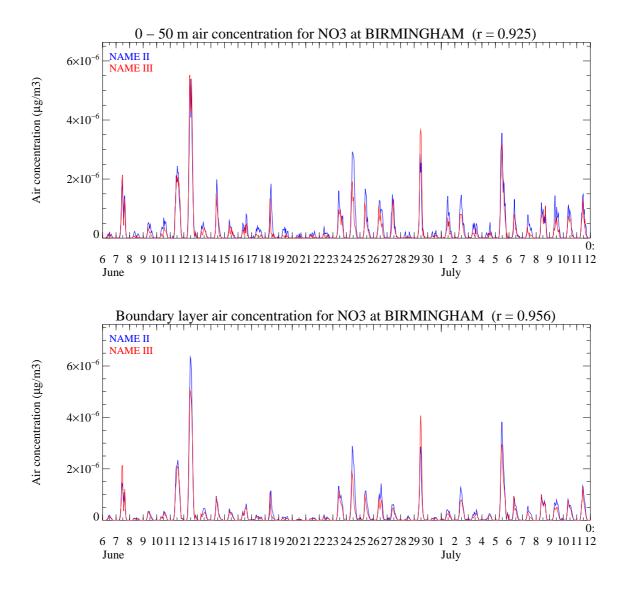
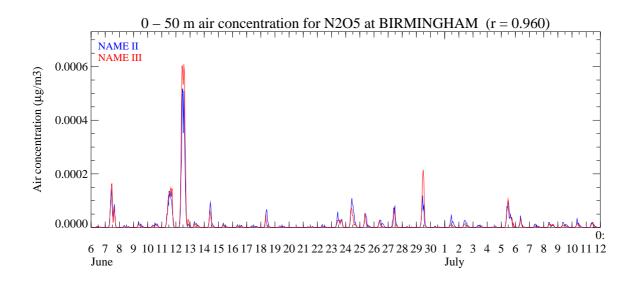


Figure 9: (a) 0-50 m and (b) boundary-layer average concentrations of nitrate



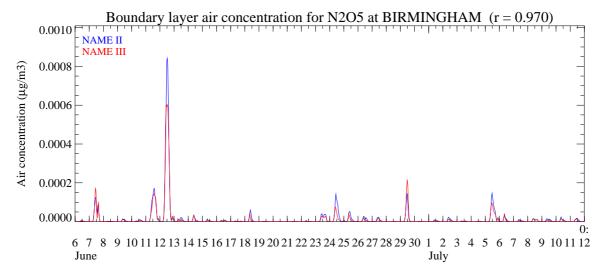


Figure 10: (a) 0-50 m and (b) boundary-layer average concentrations of di-nitrogen pentoxide

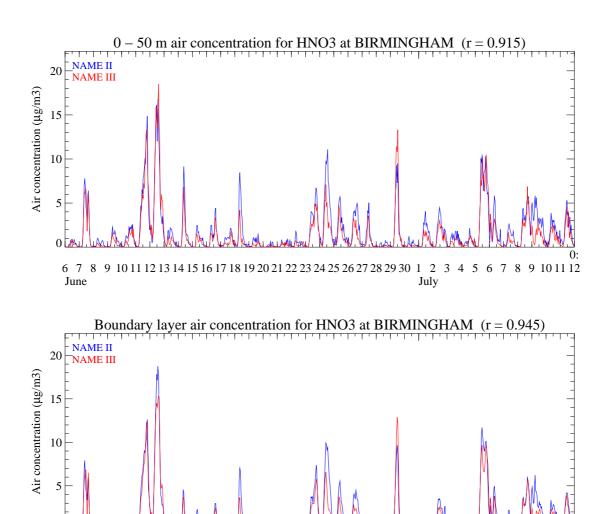
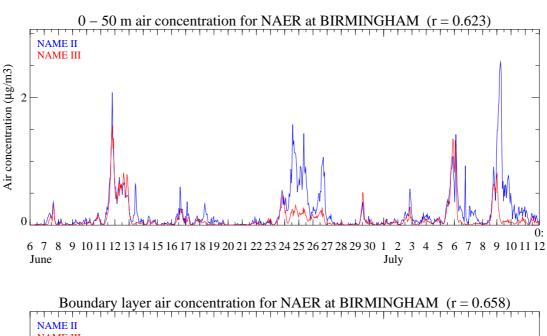


Figure 11: (a) 0-50 m and (b) boundary-layer average concentrations of nitric acid

 $6\ 7\ 8\ 9\ 10\ 11\ 12\ 13\ 14\ 15\ 16\ 17\ 18\ 19\ 20\ 21\ 22\ 23\ 24\ 25\ 26\ 27\ 28\ 29\ 30\ 1\ 2\ 3\ 4\ 5\ 6\ 7\ 8\ 9\ 10\ 11\ 12$

0 🔼

June



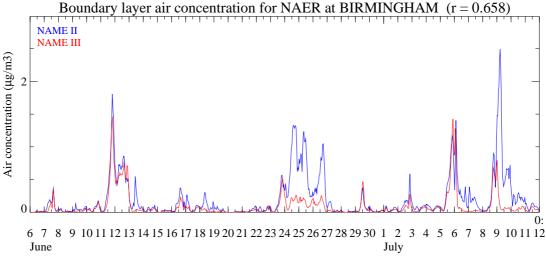
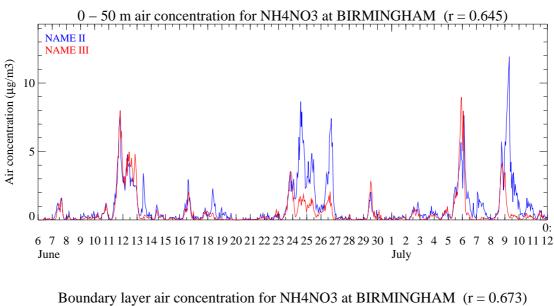


Figure 12: (a) 0-50 m and (b) boundary-layer average concentrations of nitrate aerosol



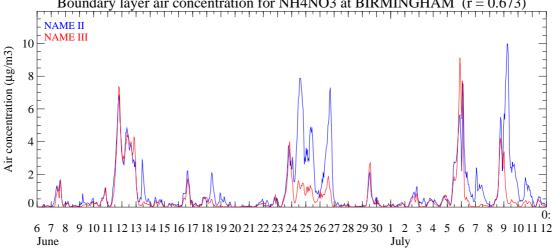
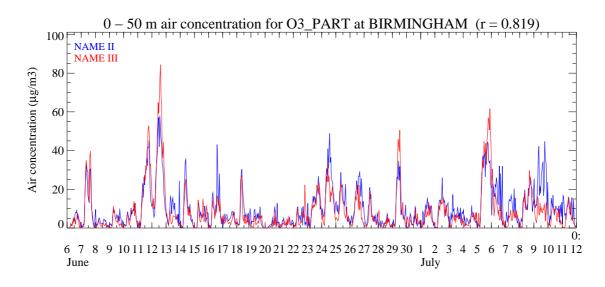


Figure 13: (a) 0-50 m and (b) boundary-layer average concentrations of ammonium nitrate



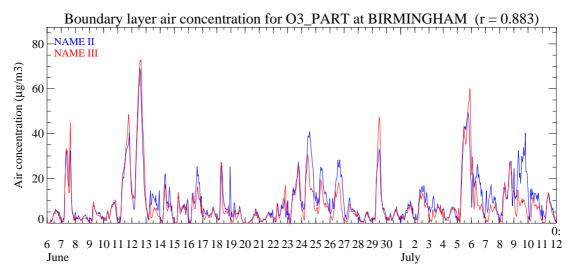
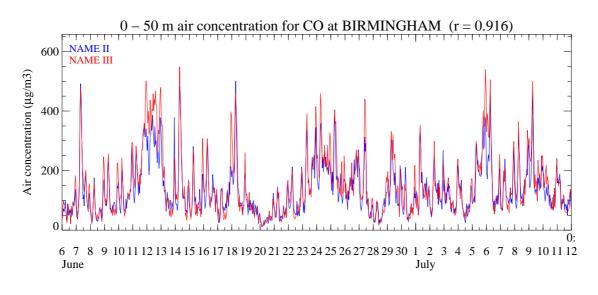


Figure 14: (a) 0-50 m and (b) boundary-layer average concentrations of ozone (on particles)



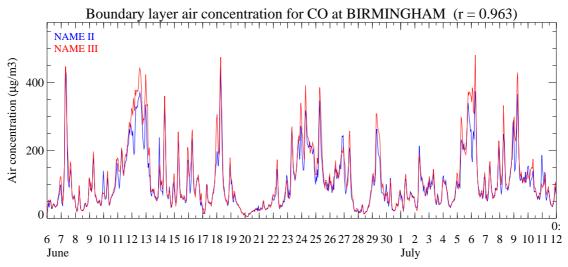
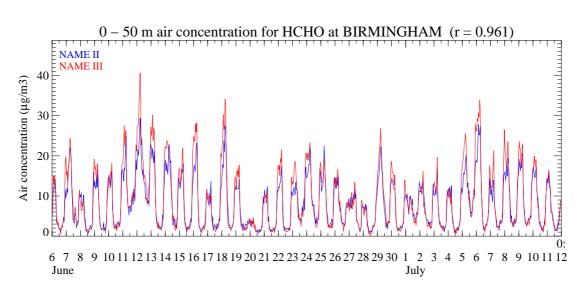


Figure 15: (a) 0-50 m and (b) boundary-layer average concentrations of carbon monoxide



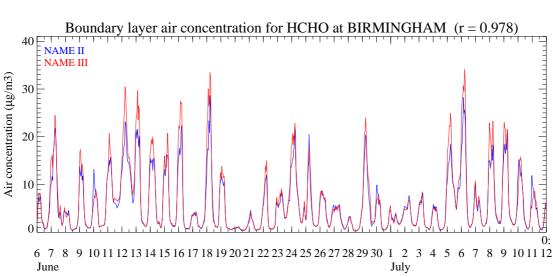
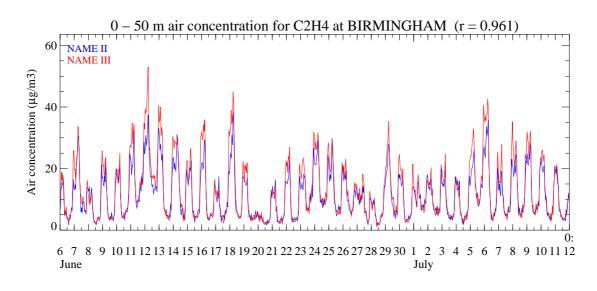


Figure 16: (a) 0-50 m and (b) boundary-layer average concentrations of formaldehyde



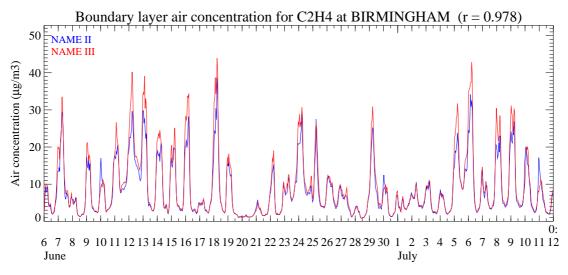
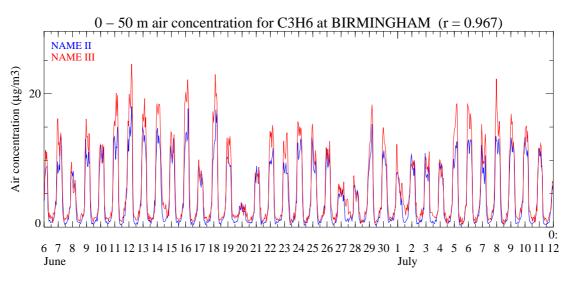


Figure 17: (a) 0-50 m and (b) boundary-layer average concentrations of ethylene



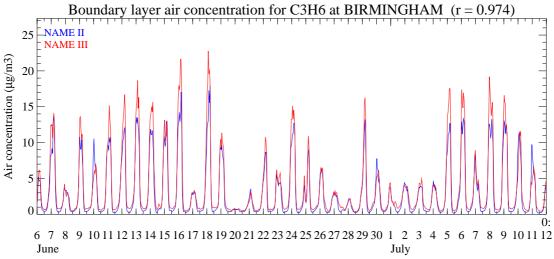
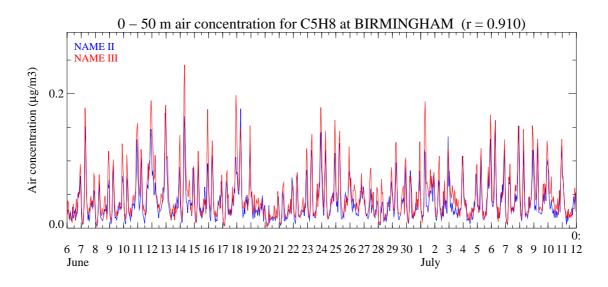


Figure 18: (a) 0-50 m and (b) boundary-layer average concentrations of propylene



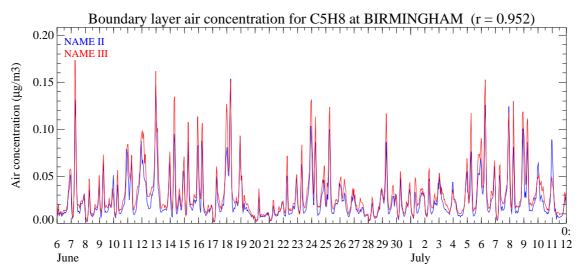
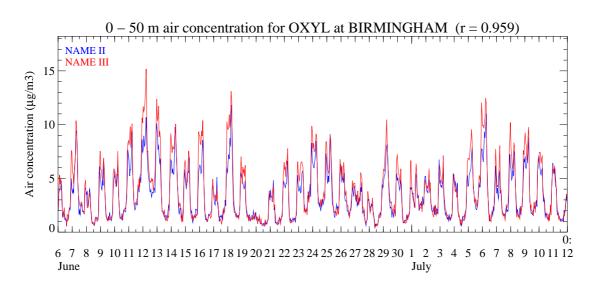


Figure 19: (a) 0-50 m and (b) boundary-layer average concentrations of isoprene



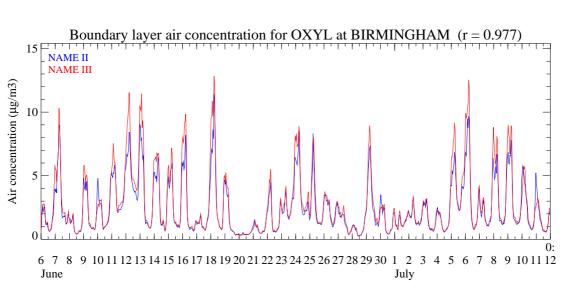
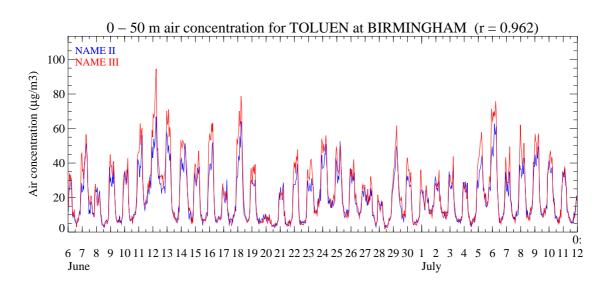


Figure 20: (a) 0-50 m and (b) boundary-layer average concentrations of o-xylene



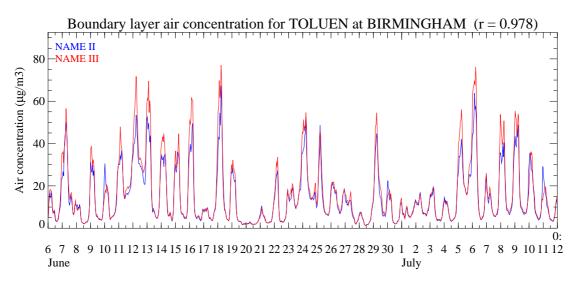
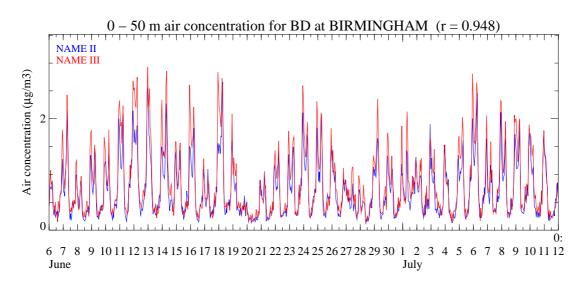


Figure 21: (a) 0-50 m and (b) boundary-layer average concentrations of toluene



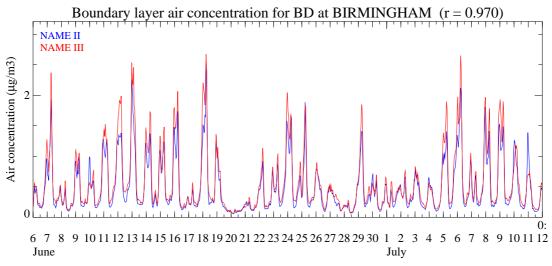


Figure 22: (a) 0-50 m and (b) boundary-layer average concentrations of 1,3-butadiene

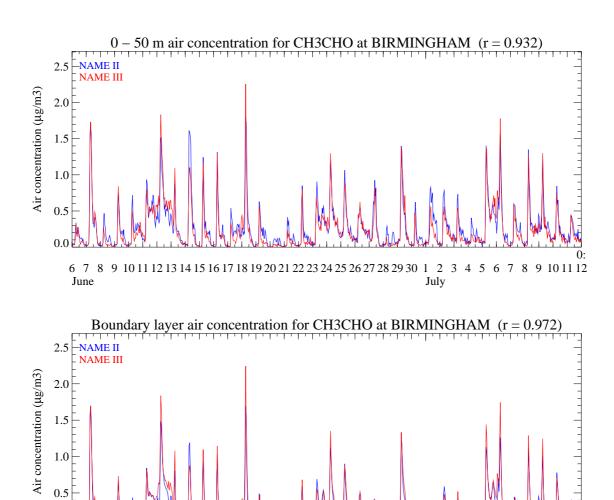
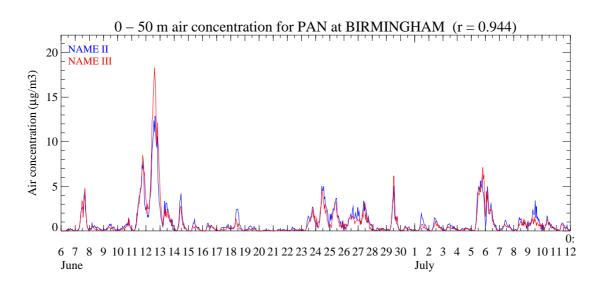


Figure 23: (a) 0-50 m and (b) boundary-layer average concentrations of acetaldehyde

 $6\ 7\ 8\ 9\ 10\ 11\ 12\ 13\ 14\ 15\ 16\ 17\ 18\ 19\ 20\ 21\ 22\ 23\ 24\ 25\ 26\ 27\ 28\ 29\ 30\ 1\ 2\ 3\ 4\ 5\ 6\ 7\ 8\ 9\ 10\ 11\ 12$

0.0

June



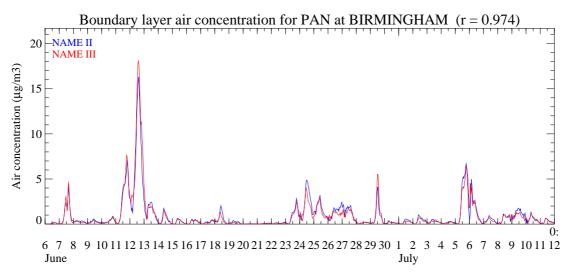


Figure 24: (a) 0-50 m and (b) boundary-layer average concentrations of peroxyacetyl nitrate

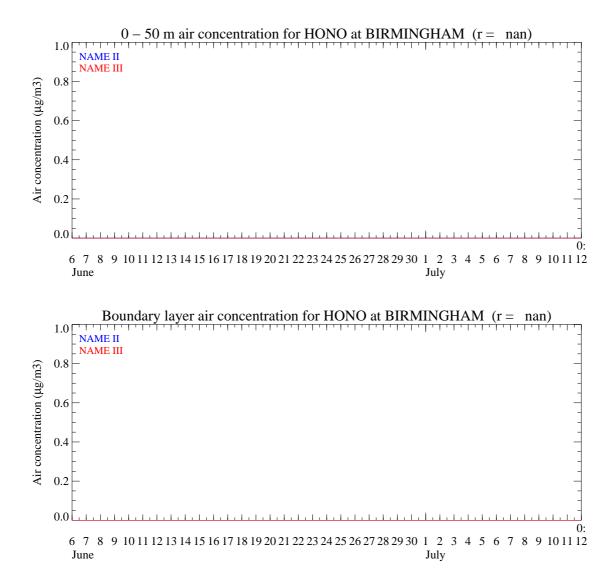
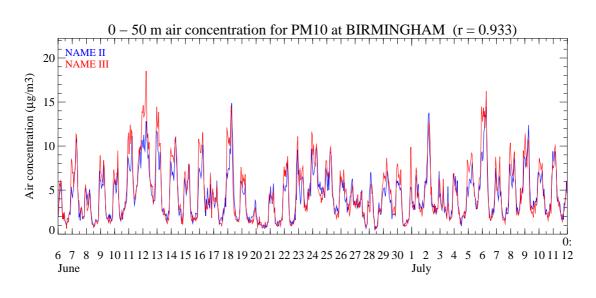


Figure 25: (a) 0-50 m and (b) boundary-layer average concentrations of nitrous acid



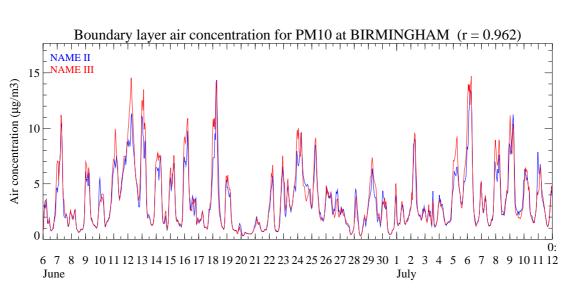


Figure 26: (a) 0-50 m and (b) boundary-layer average concentrations of PM_{10}

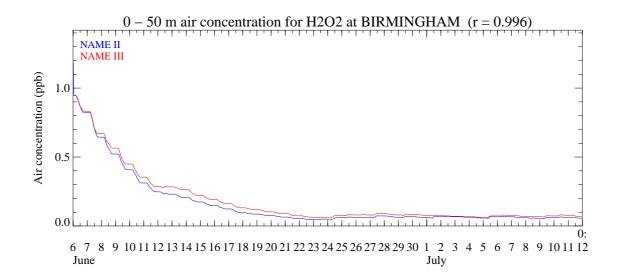


Figure 27: 0-50 m air concentration of hydrogen peroxide

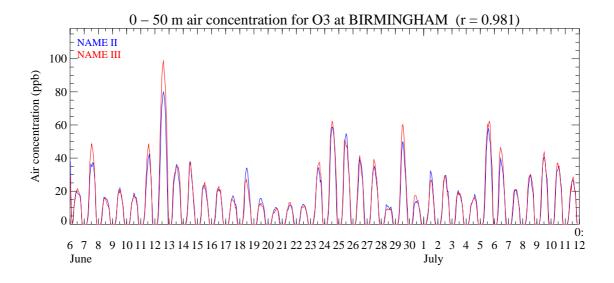


Figure 28: 0-50 m air concentration of ozone (on field)

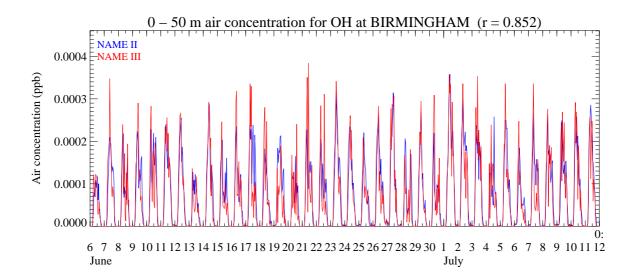


Figure 29: 0-50 m air concentration of hydroxyl

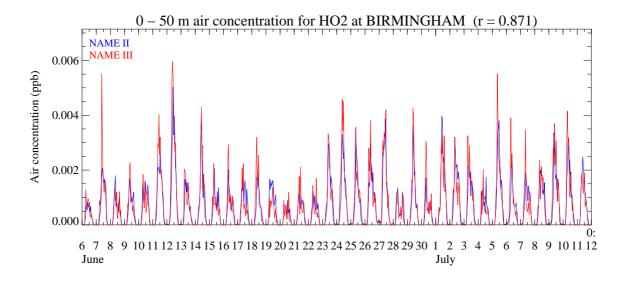


Figure 30: 0-50 m air concentration of hydroperoxy

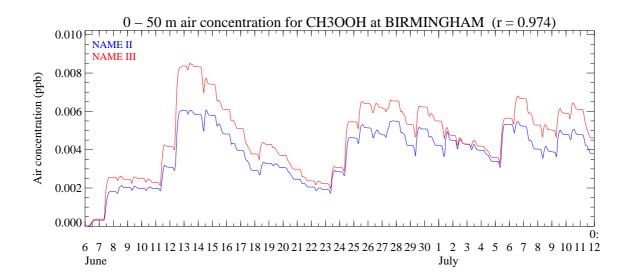


Figure 31: 0-50 m air concentration of CH3OOH

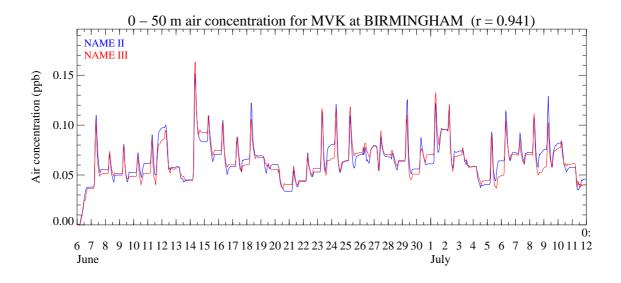


Figure 32: 0-50 m air concentration of MVK

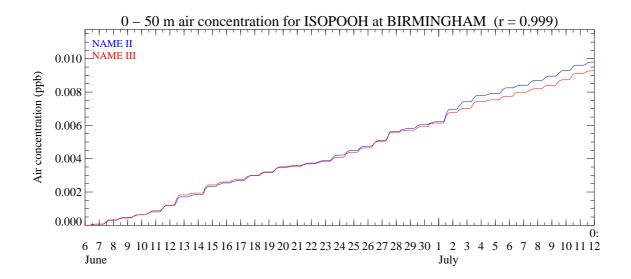


Figure 33: 0-50 m air concentration of ISOPOOH

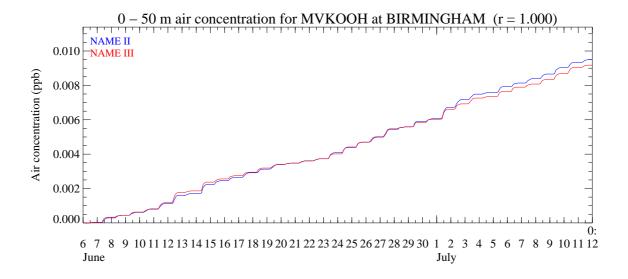


Figure 34: 0-50 m air concentration of MVKOOH

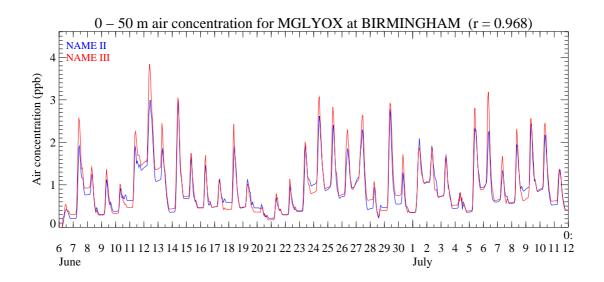


Figure 35: 0-50 m air concentration of MGLYOX

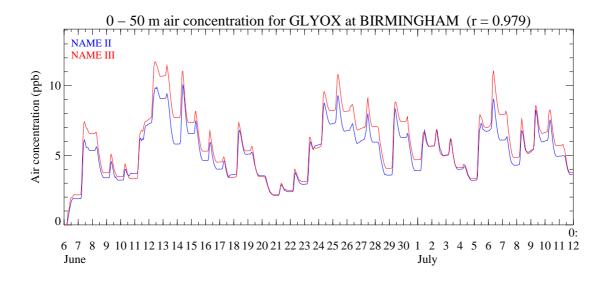


Figure 36: 0-50 m air concentration of GLYOX

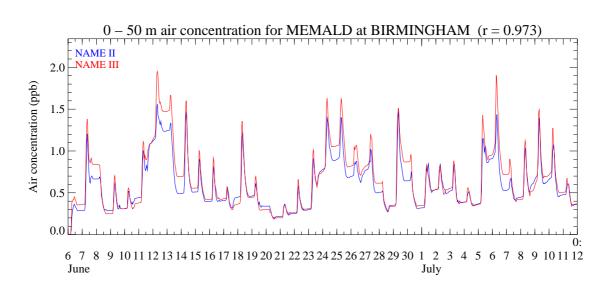


Figure 37: 0-50 m air concentration of MEMALD