Lower Hunter Particle Characterisation Study

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Appendices to the final report to the NSW Environment Protection Authority

April 2016

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Appendix A – Speciation of $PM_{2.5}$ and $PM_{2.5\text{-}10}$

The following figures and tables show the statistics of the species concentrations measured in the year of filter samples as box and whisker plots for the $PM_{2.5}$ and $PM_{2.5\text{-}10}$ samples from each site.

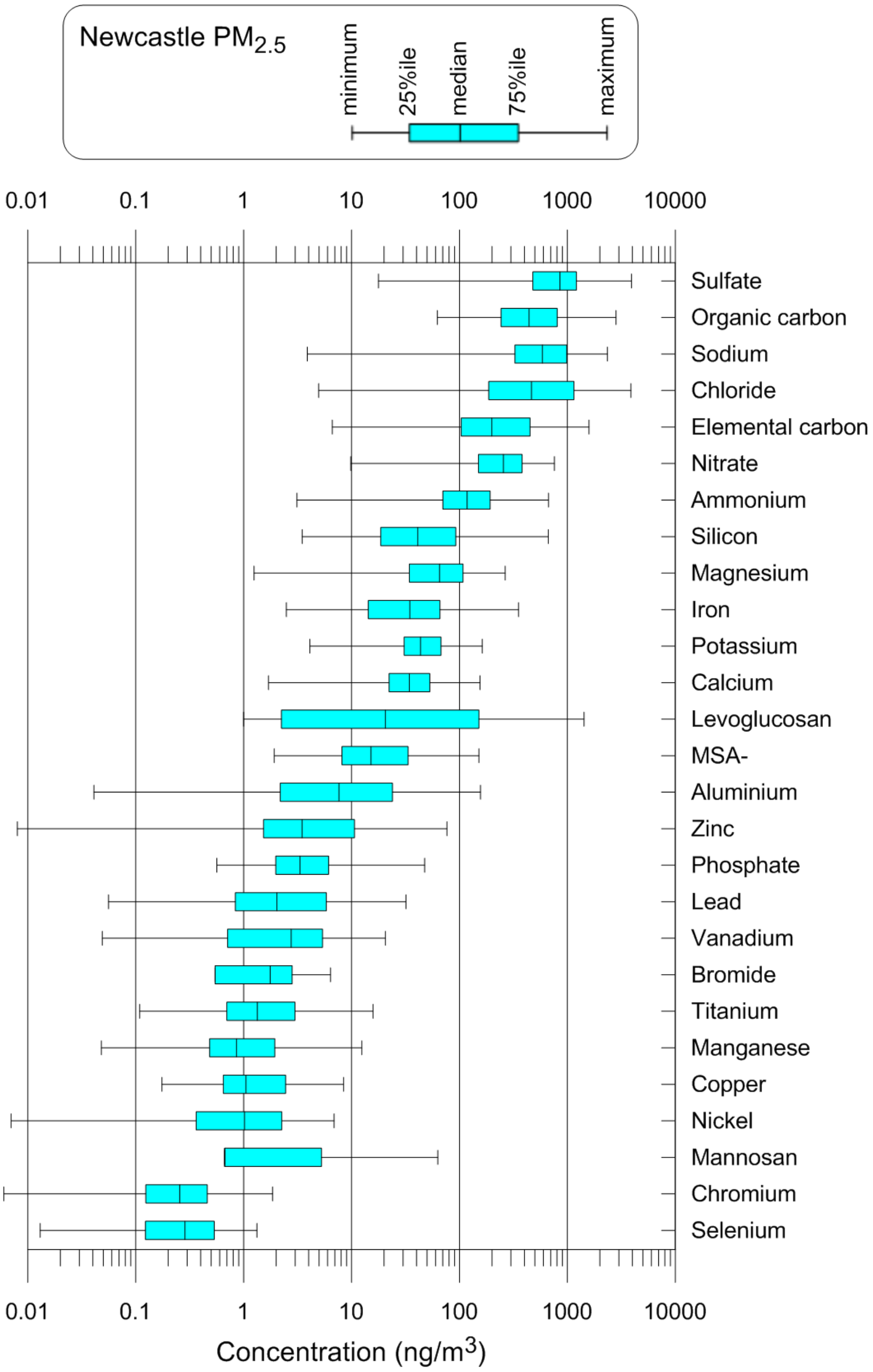

Figure 122: Box and whisker plot of the $PM_{2.5}$ species concentrations measured in the year of filter samples from Newcastle

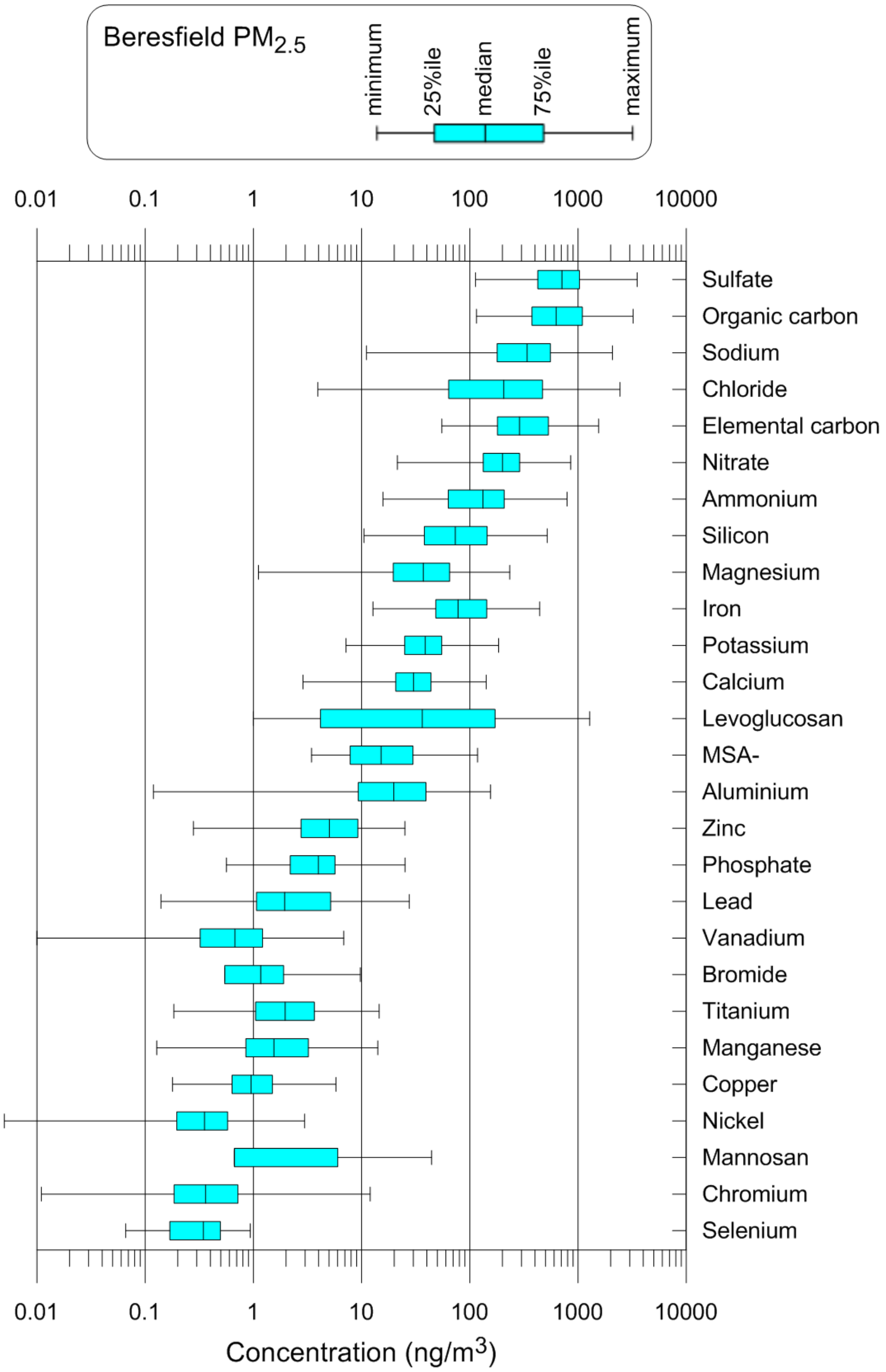

Figure 123: Box and whisker plot of the $PM_{2.5}$ species concentrations measured in the year of filter samples from Beresfield

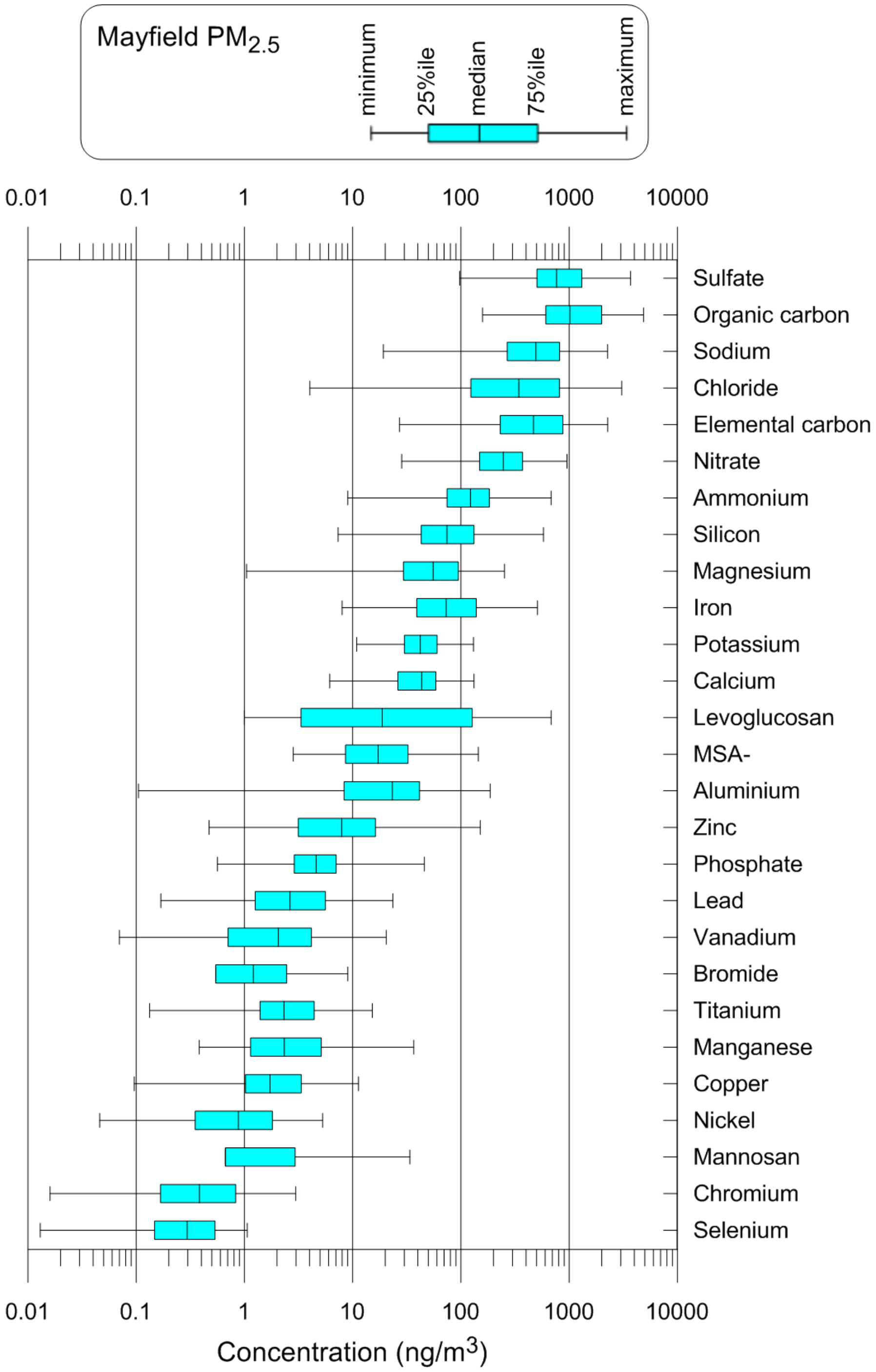

Figure 124: Box and whisker plot of the $PM_{2.5}$ species concentrations measured in the year of filter samples from Mayfield

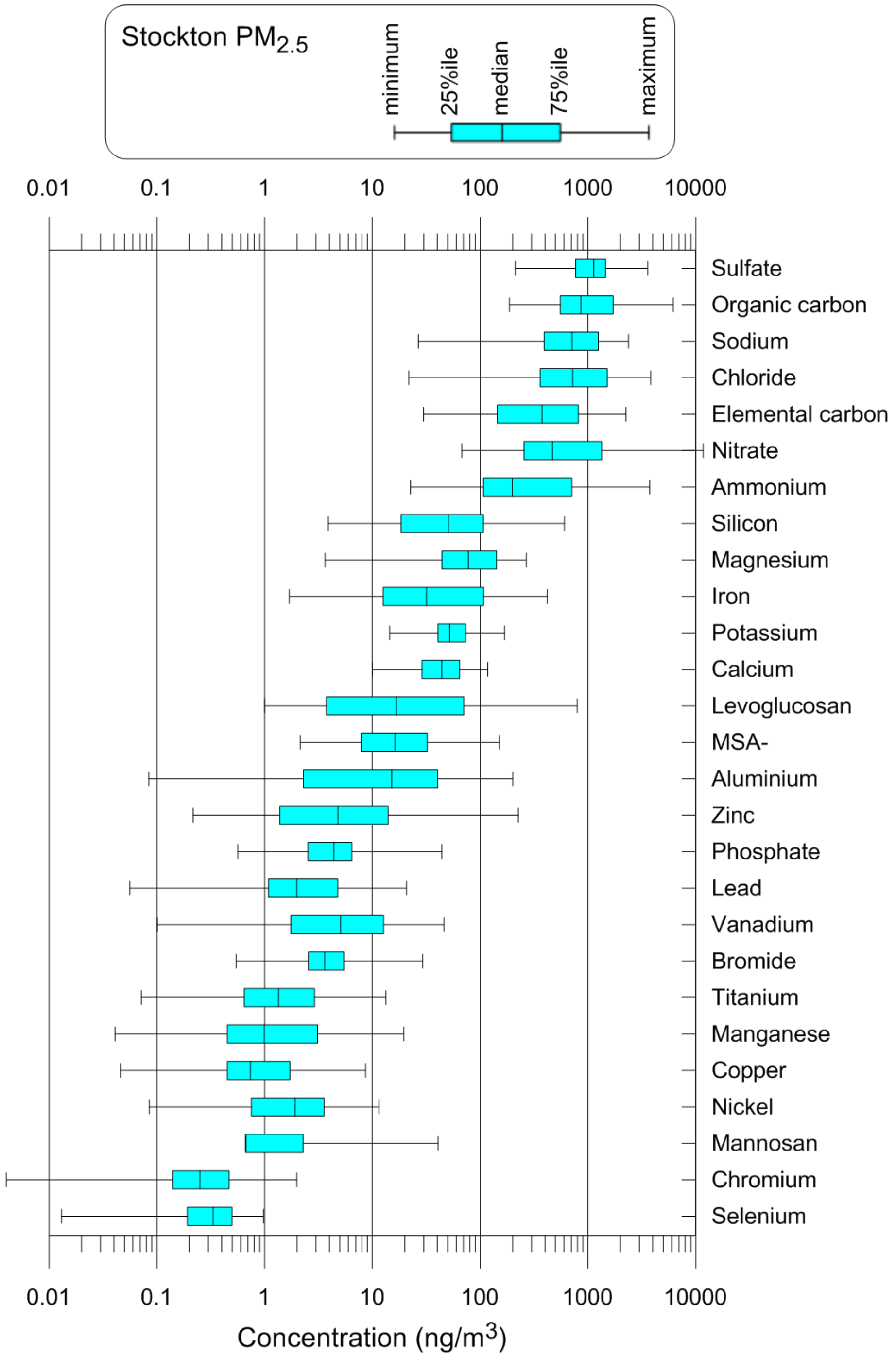

Figure 125: Box and whisker plot of the $PM_{2.5}$ species concentrations measured in the year of filter samples from Stockton

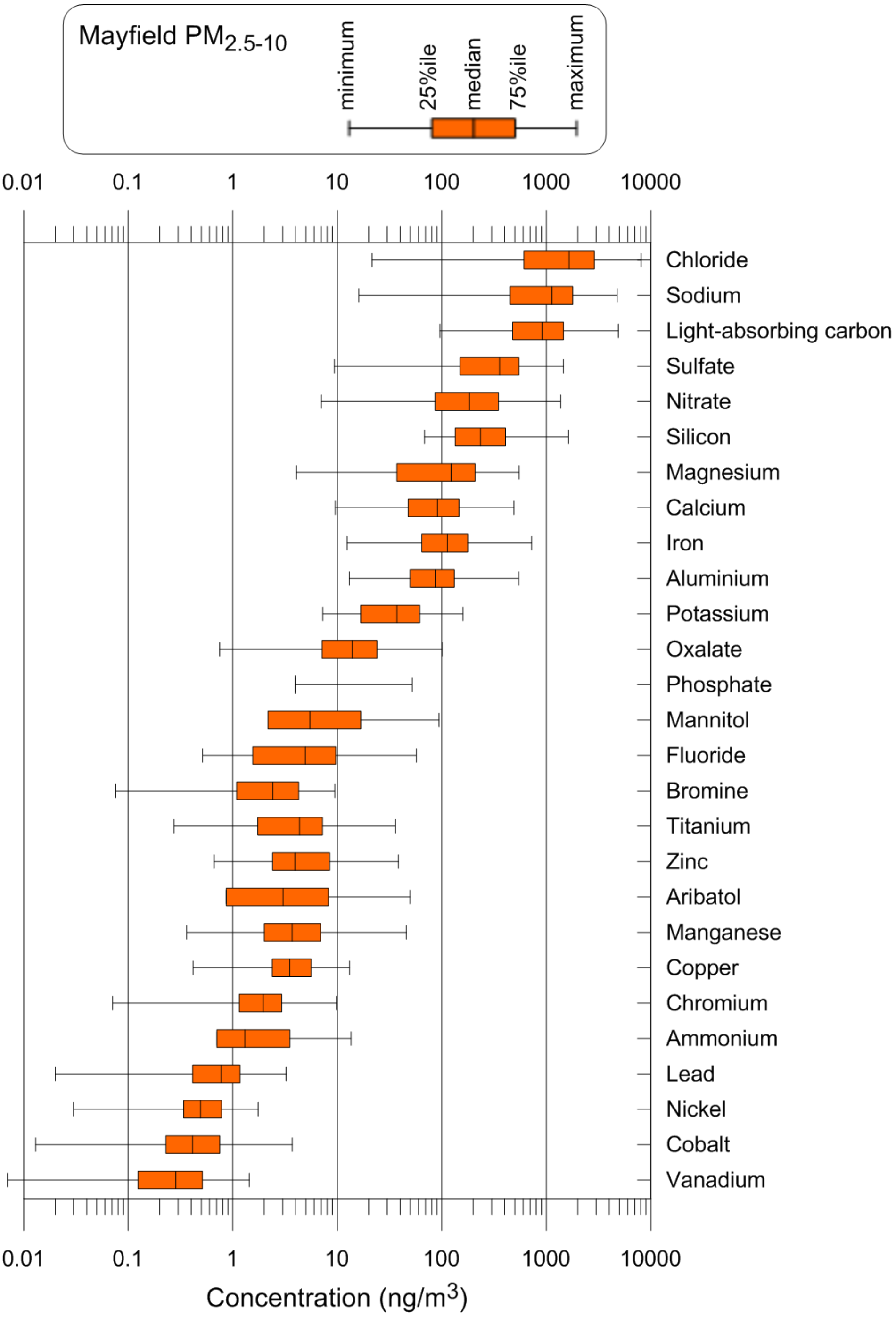

Figure 126: Box and whisker plot of the $PM_{2.5-10}$ species concentrations measured in the year of filter samples from Mayfield

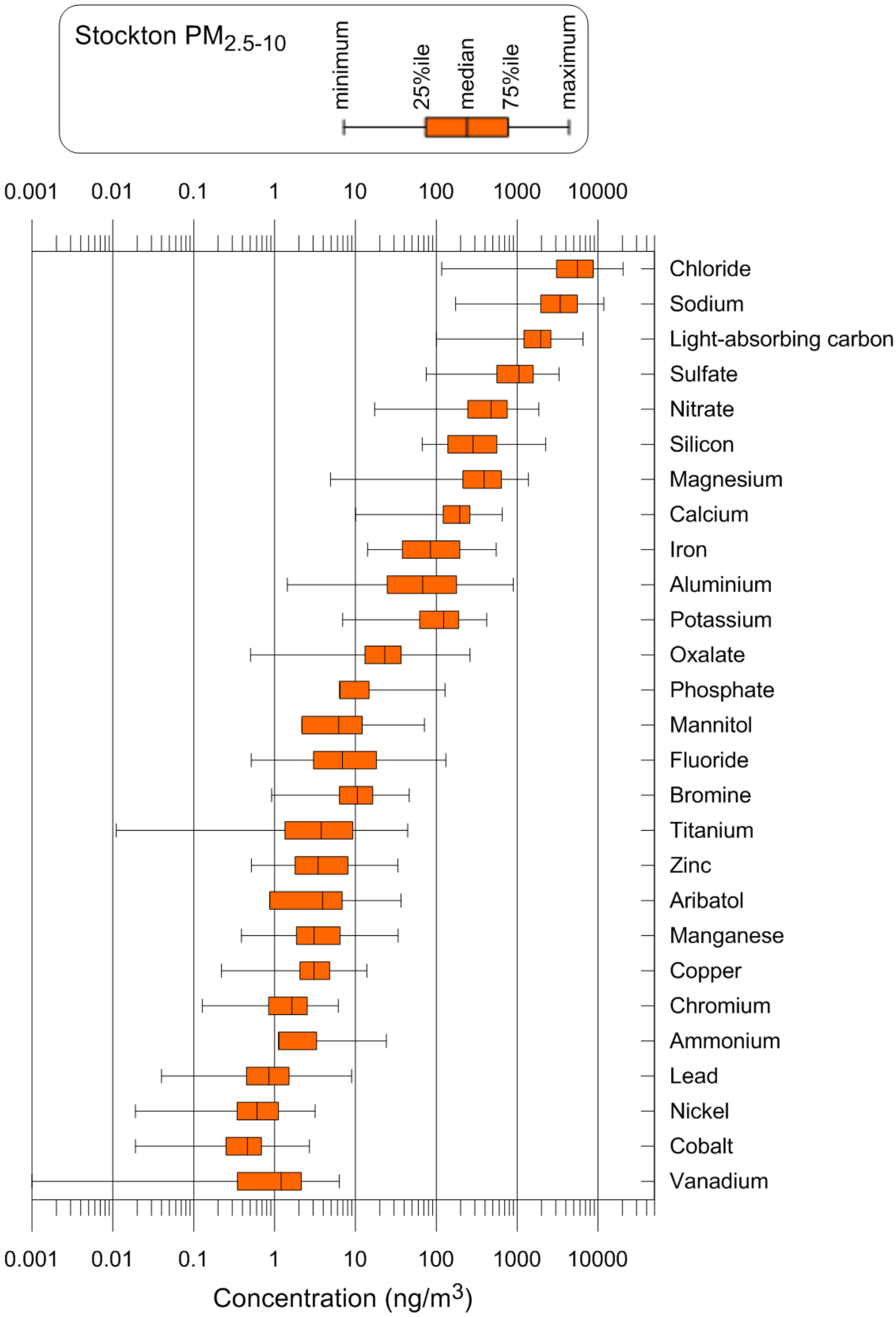

Figure 127: Box and whisker plot of the $PM_{2.5-10}$ species concentrations measured in the year of filter samples from Stockton

Table 22: Concentrations of measured species in the PM$_{2.5}$ samples

Values listed (in ng m^{-3}) of average (c_{avg}), standard deviation (σ), and maximum (c_{max}) at each site. Site with highest average highlighted in yellow.

Species (ng m^{-3})	**Newcastle PM$_{2.5}$**		**Beresfield PM$_{2.5}$**		**Mayfield PM$_{2.5}$**		**Stockton PM$_{2.5}$**	
	c_{avg} ± σ	**c_{max}**	**c_{avg} ± σ**	**c_{max}**	**c_{avg} ± σ**	**c_{max}**	**c_{avg} ± σ**	**c_{max}**
Sulfate	966 ± 660	3924	871 ± 646	3516	953 ± 647	3696	**1197 ± 613**	3599
Organic carbon	642 ± 631	2815	864 ± 688	3226	**1338 ± 1054**	4878	1219 ± 1003	6190
Sodium	717 ± 514	2346	448 ± 380	2079	614 ± 476	2263	**862 ± 586**	2383
Chloride	730 ± 717	3882	374 ± 481	2442	584 ± 643	3060	**1003 ± 883**	3821
Elemental carbon	320 ± 328	1586	414 ± 337	1548	615 ± 535	2268	**518 ± 466**	2250
Nitrate	271 ± 154	758	230 ± 149	856	274 ± 178	954	**1393 ± 2166**	11777
Ammonium	143 ± 114	669	164 ± 141	793	151 ± 117	681	**545 ± 753**	3742
Silicon	66 ± 83	666	**107 ± 98**	519	99 ± 89	580	85 ± 98	605
Magnesium	79 ± 57	265	50 ± 42	234	70 ± 54	253	**96 ± 65**	268
Iron	55 ± 66	352	**100 ± 72**	442	**100 ± 86**	511	66 ± 77	421
Potassium	51 ± 30	163	44 ± 30	184	47 ± 26	131	**60 ± 28**	169
Calcium	40 ± 25	155	35 ± 24	142	46 ± 27	132	**49 ± 24**	118
Levoglucosan	130 ± 250	1424	**181 ± 304**	1279	81 ± 129	681	63 ± 108	795
MSA-	26 ± 26	151	23 ± 21	118	25 ± 23	145	25 ± 24	150
Aluminium	18 ± 25	157	30 ± 32	155	30 ± 30	186	**32 ± 45**	200
Zinc	8.9 ± 13	77	7.2 ± 6.4	25	**18 ± 30**	151	12 ± 24	226
Phosphate	4.7 ± 5.3	47	4.6 ± 3.6	25	**5.9 ± 5.3**	46	5.2 ± 4.9	44
Lead	**4.7 ± 6.8**	32	3.9 ± 4.7	28	4.3 ± 4.7	23	3.8 ± 4.5	21
Vanadium	4.0 ± 4.4	21	0.9 ± 0.9	6.8	3.4 ± 3.8	20	**8.7 ± 9.3**	46
Bromide	2.0 ± 1.3	6.4	1.4 ± 1.3	10	1.7 ± 1.4	9.0	**5.0 ± 4.6**	29
Titanium	2.3 ± 2.4	16	2.9 ± 2.7	15	**3.0 ± 2.4**	15	2.1 ± 2.3	13
Manganese	1.8 ± 2.3	12	2.3 ± 2.2	14	**4.0 ± 5.9**	38	1.9 ± 2.4	20
Copper	1.9 ± 2	8.4	1.2 ± 1.0	5.8	**2.5 ± 1.9**	11	1.2 ± 1.3	8.6
Nickel	1.5 ± 1.4	6.9	0.54 ± 0.6	3.0	1.2 ± 1.1	5.3	**2.8 ± 2.7**	12
Mannosan	4.6 ± 9.6	63	**5.9 ± 10**	44	3.0 ± 5.1	34	2.5 ± 4.8	41
Chromium	0.36 ± 0.4	1.9	**0.88 ± 1.6**	12	0.59 ± 0.6	3.0	0.40 ± 0.4	2.0
Selenium	0.35 ± 0.3	1.3	0.36 ± 0.2	0.94	0.35 ± 0.2	1.1	0.37 ± 0.2	1.0

Table 23: Concentrations of measured species in the $PM_{2.5\text{-}10}$ samples

Values listed (in ng m^{-3}) of average (c_{avg}), standard deviation (σ), and maximum (c_{max}) at each site. Site with highest average highlighted in yellow.

Species (ng m^{-3})	**Stockton $PM_{2.5\text{-}10}$**		**Mayfield $PM_{2.5\text{-}10}$**	
	c_{avg} ± σ	**c_{max}**	**c_{avg} ± σ**	**c_{max}**
Chloride	**6945 ± 4985**	20406	1943 ± 1565	8074
Sodium	**4200 ± 2795**	11782	1246 ± 952	4769
Light-absorbing carbon	**2278 ± 1388**	6532	1101 ± 916	4892
Sulfate	**1197 ± 771**	3299	382 ± 281	1463
Nitrate	**543 ± 390**	1856	269 ± 277	1369
Silicon	**404 ± 398**	2252	320 ± 265	1631
Magnesium	**481 ± 339**	1382	137 ± 110	550
Calcium	**228 ± 139**	653	110 ± 92	489
Iron	125 ± 121	550	**134 ± 108**	724
Aluminium	**119 ± 150**	897	103 ± 82	543
Potassium	**148 ± 102**	420	43 ± 31	159
Oxalate	**29 ± 29**	261	18 ± 16	101
Phosphate	**13 ± 15**	128	7.5 ± 8.6	52
Mannitol	10 ± 11	71	**12 ± 17**	94
Fluoride	**18 ± 29**	132	7.2 ± 9.5	57
Bromine	**14 ± 10**	46	3 ± 2.3	9
Titanium	**6.7 ± 8.6**	44	5.8 ± 6.4	36
Zinc	6.1 ± 6.5	34	**6.6 ± 7.1**	39
Arabitol	5.7 ± 6.5	37	**6.7 ± 8.8**	50
Manganese	4.6 ± 4.5	34	**6 ± 6.8**	46
Copper	3.4 ± 2.4	14	**4.2 ± 2.5**	13
Chromium	2.0 ± 1.7	10	**2.3 ± 1.7**	10
Ammonium	**3.0 ± 3.9**	24	2.3 ± 2.3	14
Lead	**1.13 ± 1.2**	9.0	0.92 ± 0.7	3.2
Nickel	**0.83 ± 0.6**	3.2	0.59 ± 0.4	1.8
Cobalt	0.54 ± 0.4	2.7	**0.57 ± 0.5**	3.7
Vanadium	**1.50 ± 1.5**	6.3	0.39 ± 0.4	1.4

Appendix B – Data quality

NATA accreditation

The wet chemistry laboratory at CSIRO Aspendale has National Association of Testing Authority (NATA) accreditation, No. 245, for IC analysis. As part of the NATA accreditation a check standard is analysed in each analysis run after the seven calibration standards and then every 20 samples. The samples are reanalysed if:

- two or more of the control or replicate standards exceed the 'warning' limit, which means the measured value is greater than two standard deviations from the true value
- one or more control or replicate standards exceed the 'recal' limit, which means the measured value is greater than three standard deviations from the true value.

Blank filters

Blank filters were analysed throughout the study. The average of the blank concentration is subtracted from each measurement. The blanks are also used to calculate the method detection limit (MDL). We followed the Standards Australia procedures which are those of the International Standard *ISO 6879:1995 Air quality – Performance characteristics and related concepts for air quality measuring methods*. Section 5.2.7 of the Standard states that a zero sample has a 5% probability of causing a measured concentration above the detection limit, so that:

$$MDL = t_{0.95} \times s_{c(0)} \qquad (1)$$

where:

$S_{c(0)}$ is the standard deviation of the blanks, and

$t_{0.95}$ is value of the 1-tailed t distribution for P<0.05 (i.e. the 95 % confidence limit).

Ion balance

The ion balance (IB) gives an indication of the aerosol chemistry data quality in that the total cation equivalents (positive charged ions) should equal the total anion equivalents (negative charged ions). The Global Atmospheric Watch Program (GAW) which is part of the World Meteorological Organisation (WMO) gives the IB equation and criteria for assessing valid data results in its technical report 160, *Manual for the GAW Precipitation Chemistry Programme*.

Note that a poor IB does not always indicate bad data quality. For example pH is not measured in this project and samples with high pH levels might have a poor IB due to high levels of bicarbonate; these samples usually also have high levels of calcium. Similarly, samples with low pH may have excess anions. Samples that have been flagged as invalid have been reanalysed. The IB plot for all sites is shown in Figure 128 and shows excellent quality.

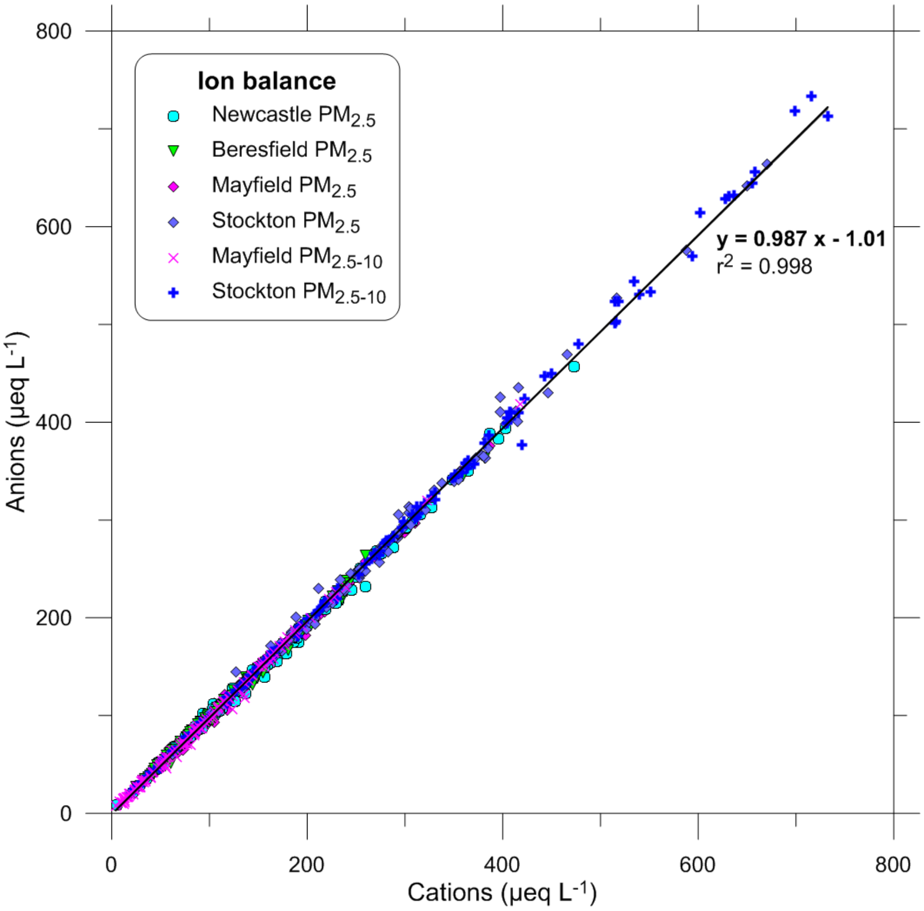

Figure 128: Ion balance for the ion chromatography measurements with the anions and cations listed in Section 3.1.3.

(Anions: Cl^-, NO_3^-, SO_4^{2-}, $C_2O_4^-$, $HCOO^-$, CH_3COO^-, PO_4^{3-}, MSA^-; Cations: Na^+, NH_4^+, Mg^{2+}, Ca^{2+}, K^+)

Comparison of species from IC and IBA analysis

The IC (ion chromatography) and IBA (ion beam analysis) techniques analysed for some common species, but it is important to note they measure slightly different things: IC measures soluble species concentrations whereas IBA measures total species concentrations. Thus we expect that the IC concentrations should not be greater than the IBA concentrations. However, both techniques have an uncertainty of approximately ±5%.

The results are compared in Figure 129 to Figure 135 for sodium, chloride, sulfur, calcium, and potassium, as well as EC and BC, and organic carbon by two techniques. The sulfur concentrations from IBA analysis are multiplied by 3 to account for the difference in molecular weight of sulfate.

The two analysis methods generally show very good agreement in mass concentrations for the species shown. However this is not the case for the $PM_{2.5-10}$ data from Stockton where the IBA concentrations show a negative bias compared to the soluble ion concentrations. This is possibly due to self-absorption of the emitted x-rays as it only occurs for the very high filter loadings at Stockton.

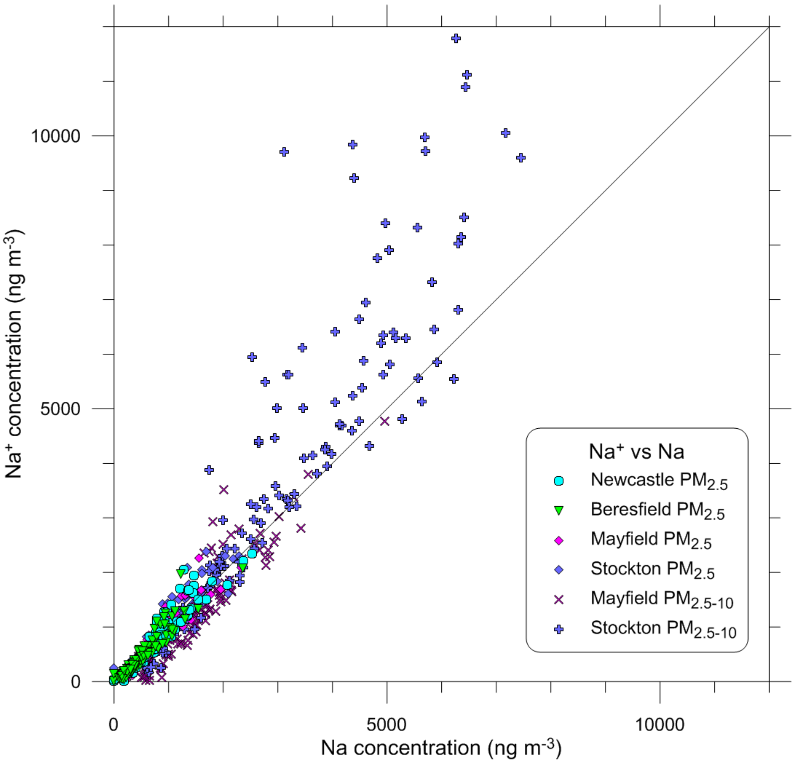

Figure 129: Comparison of sodium ion (Na^+) concentrations determined by ion chromatography and elemental sodium (Na) concentrations determined by ion beam analysis

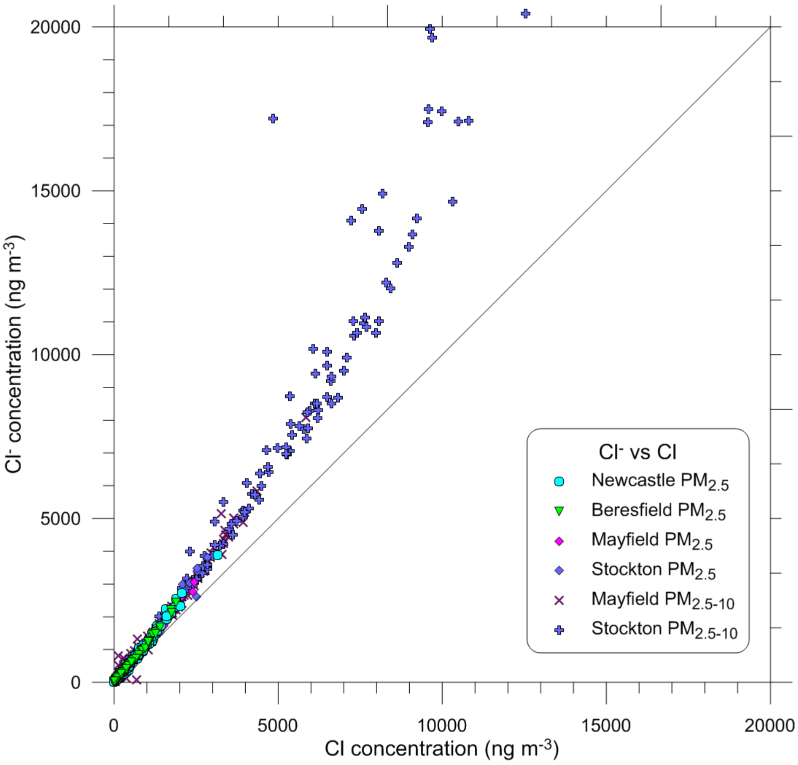

Figure 130: Comparison of chloride ion (Cl^-) concentrations determined by ion chromatography and elemental chlorine (Cl) concentrations determined by ion beam analysis

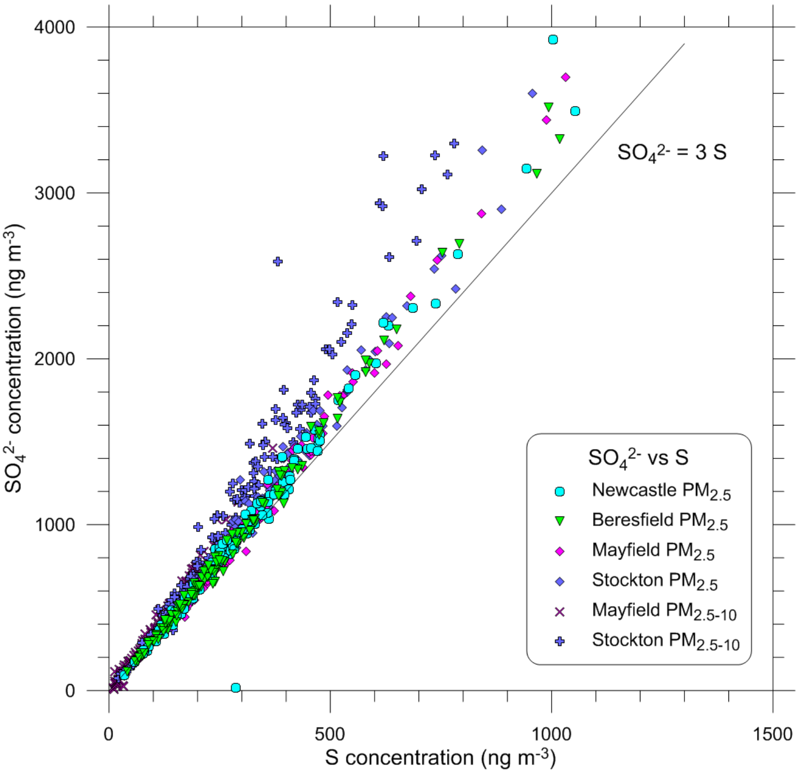

Figure 131: Comparison of sulfate ion (SO$_4^{2-}$) concentrations determined by ion chromatography and elemental sulfur (S) concentrations determined by ion beam analysis

The ratio of 3 is the ratio of the species molecular weights.

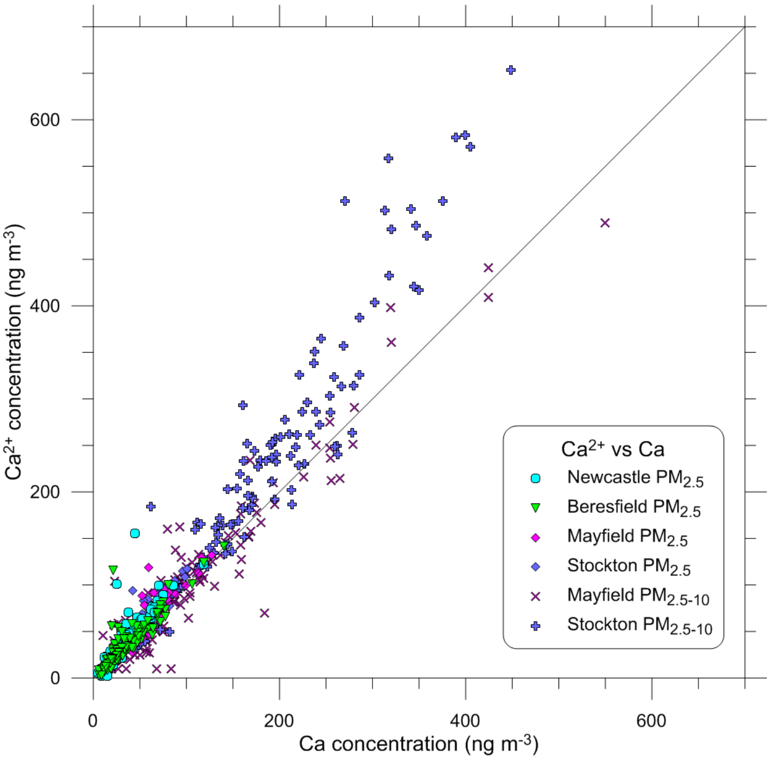

Figure 132: Comparison of calcium ion (Ca^{2+}) concentrations determined by ion chromatography and elemental calcium (Ca) concentrations determined by ion beam analysis

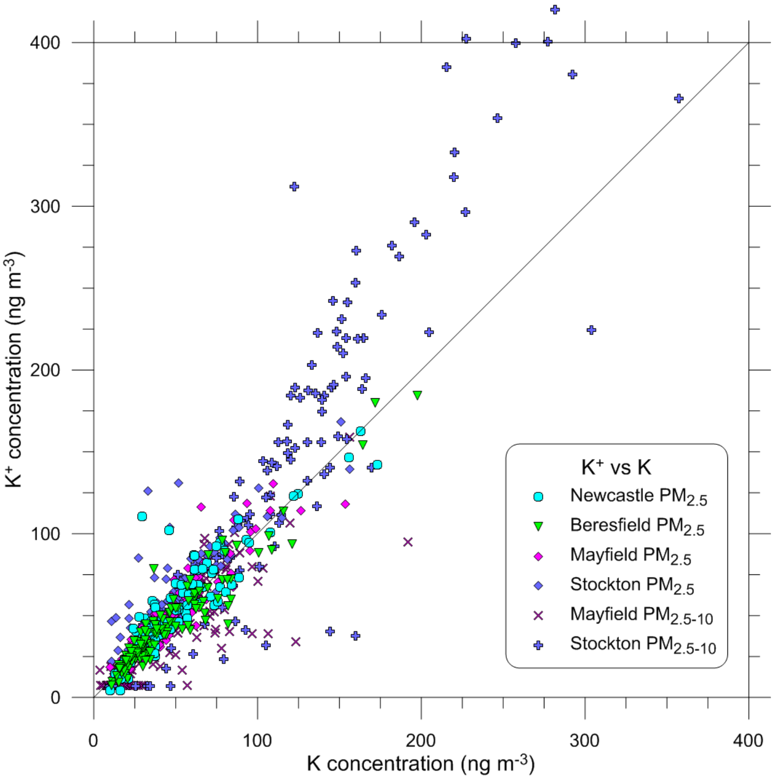

Figure 133: Comparison of potassium ion (K^+) concentrations determined by ion chromatography and elemental potassium (K) concentrations determined by ion beam analysis

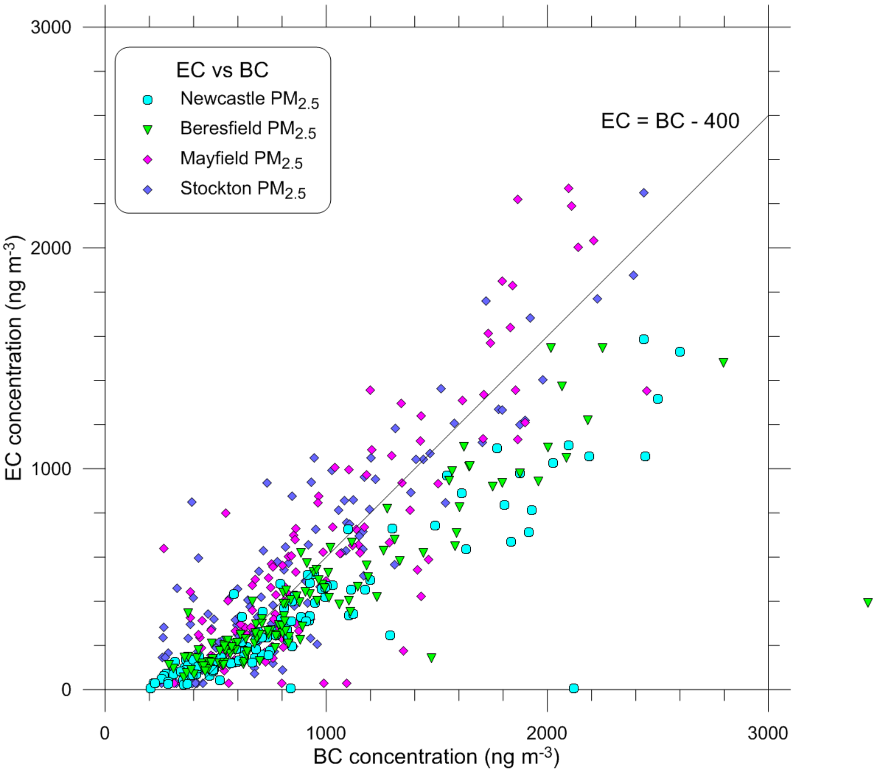

Figure 134: Comparison of elemental carbon (EC) concentrations determined by the thermal optical carbon analyser and equivalent black carbon (EBC) concentrations determined by the laser integrated plate method

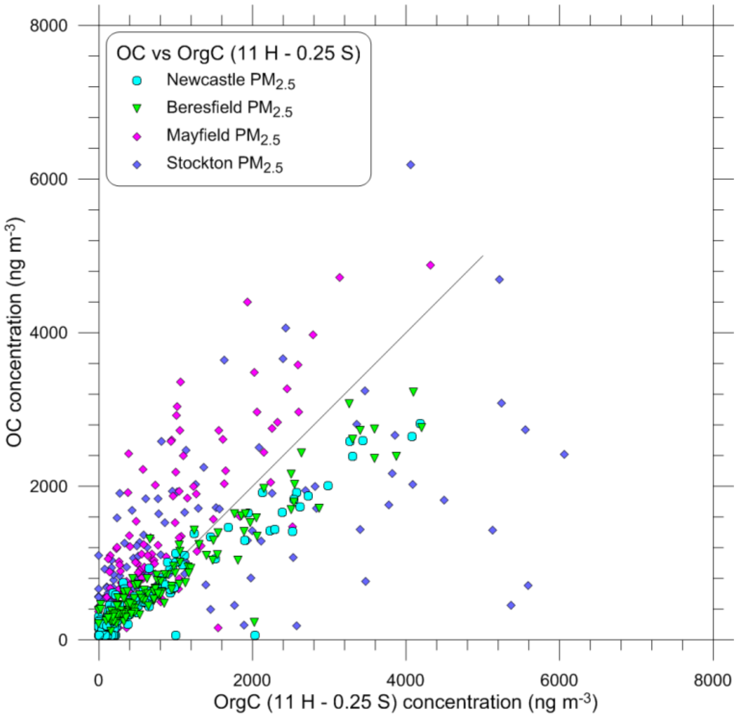

Figure 135: Comparison of organic carbon (OC) concentrations determined by the thermal optical carbon analyser and organic carbon (OrgC) concentrations determined from elemental hydrogen and sulfur concentrations in the method described by Malm et al. (1994)

Appendix C – PMF fingerprints by site

The factor fingerprints presented in Sections 6 and 8 were discussed by factor. In this appendix, the fingerprints are presented by site. For each site, one figure is given showing all the factor fingerprints for that site, and a second figure shows the distribution of each chemical species across factors.

The first of these figure shows the fingerprint information slightly differently than in the main body of the report, namely the contributions of each species are scaled so that the species making the largest contribution to that factor is given a value of 1.0. In contrast, in the main report, the absolute species concentrations are shown (in units of ng m^{-3}). The format used here makes it easier to determine the contributions of species relative to the most abundant species in a factor.

The second of the figures shows the percentage of each species in each factor and is the same as the dark red squares in figures such as Figure 53. However, the presentation of all factors together for each site makes it much easier to see how the species are distributed across factors.

The order of presentation of the results is

- $PM_{2.5}$ Newcastle
- $PM_{2.5}$ Beresfield
- $PM_{2.5}$ Mayfield
- $PM_{2.5}$ Stockton
- $PM_{2.5-10}$ Mayfield
- $PM_{2.5-10}$ Stockton.

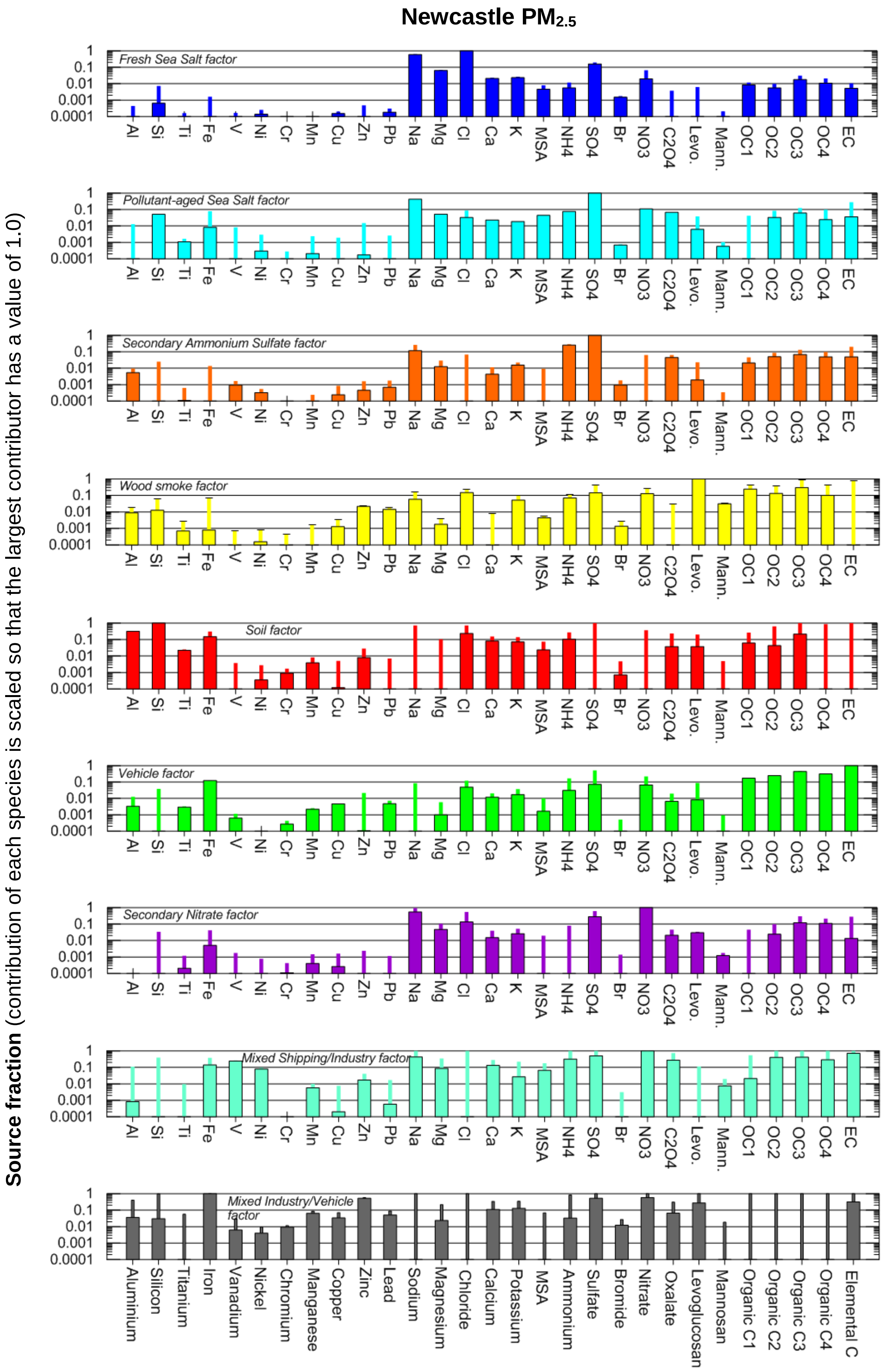
Newcastle PM2.5

Figure 136: Fingerprints of $PM_{2.5}$ factors at Newcastle from PMF analysis; broad bars show the contribution in the selected solution, narrow bars indicate uncertainty

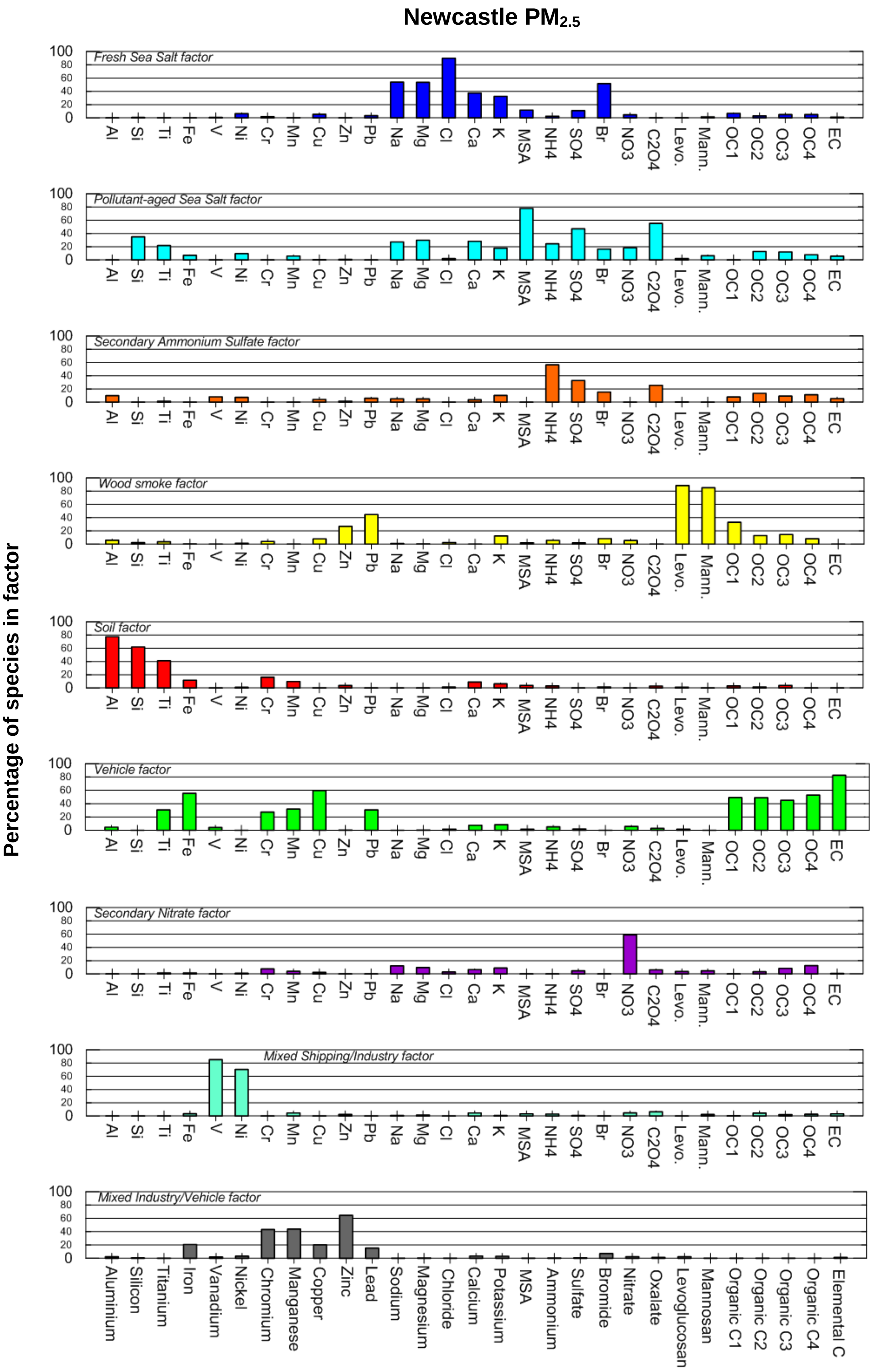

Figure 137: Percentage of each species in the $PM_{2.5}$ factors for Newcastle

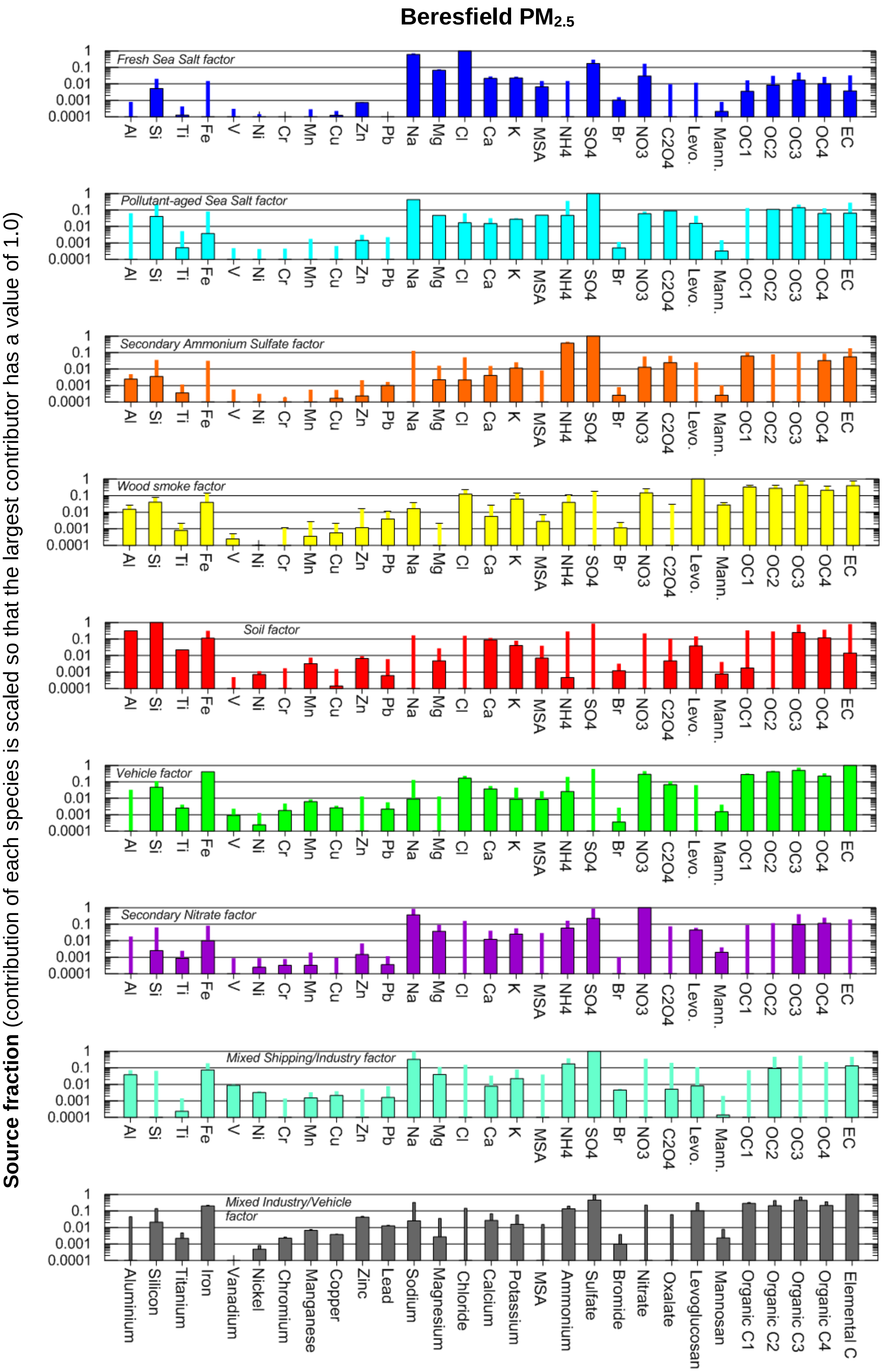

Figure 138: Fingerprints of $PM_{2.5}$ factors at Beresfield from PMF analysis; broad bars show the contribution in the selected solution, narrow bars indicate uncertainty

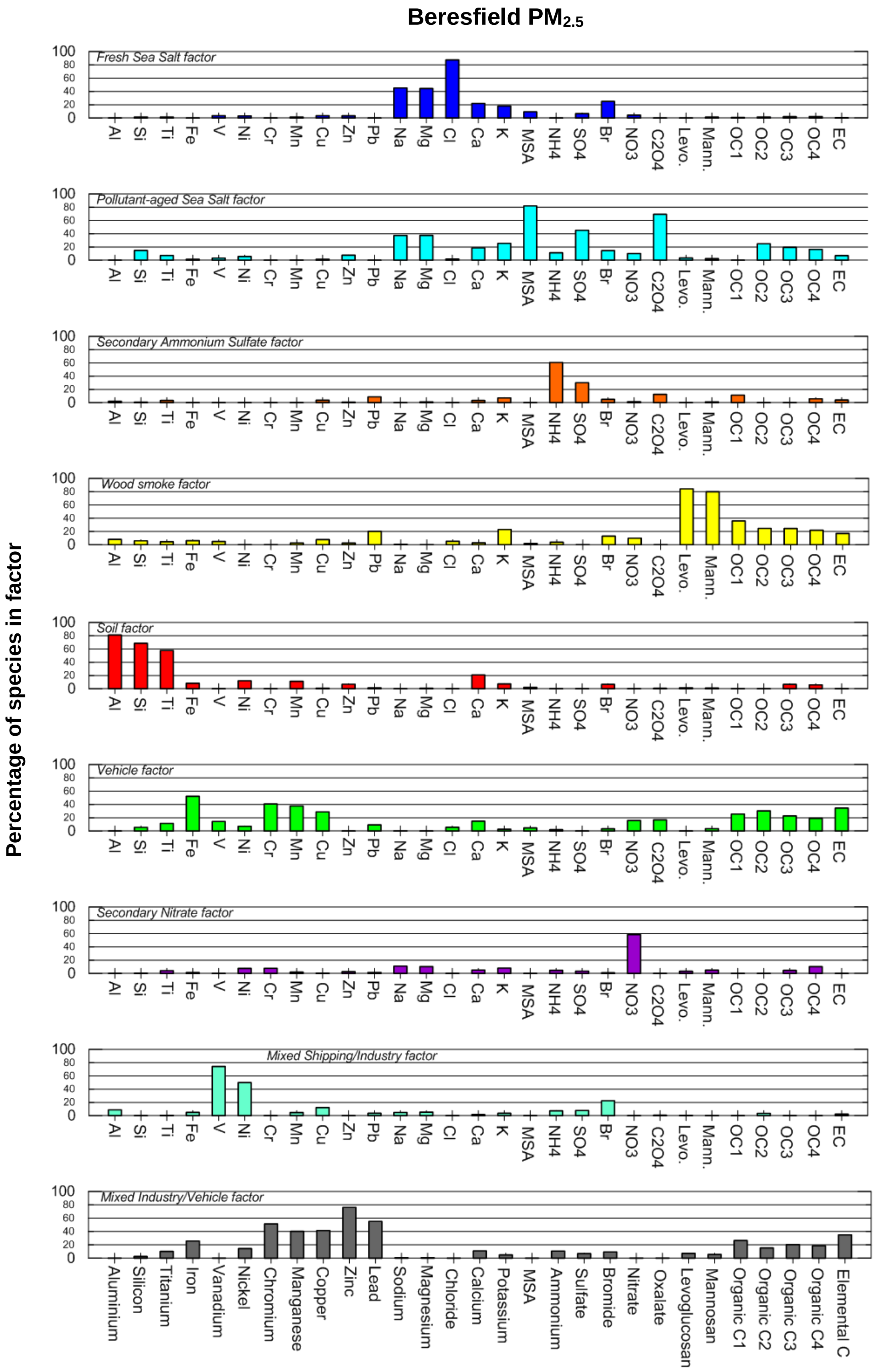

Figure 139: Percentage of each species in the $PM_{2.5}$ factors for Beresfield

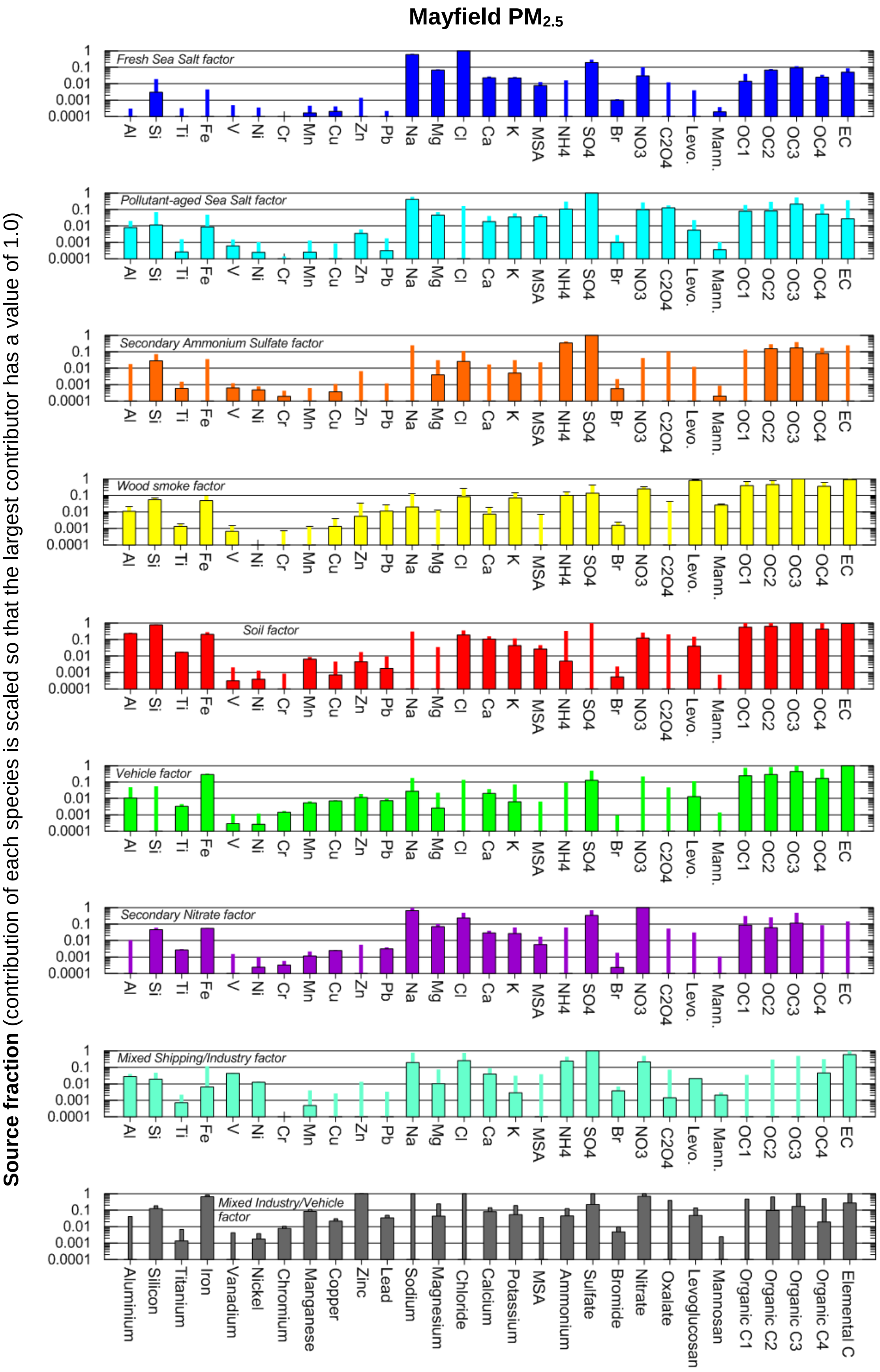

Figure 140: Fingerprints of $PM_{2.5}$ factors at Mayfield from PMF analysis; broad bars show the contribution in the selected solution, narrow bars indicate uncertainty

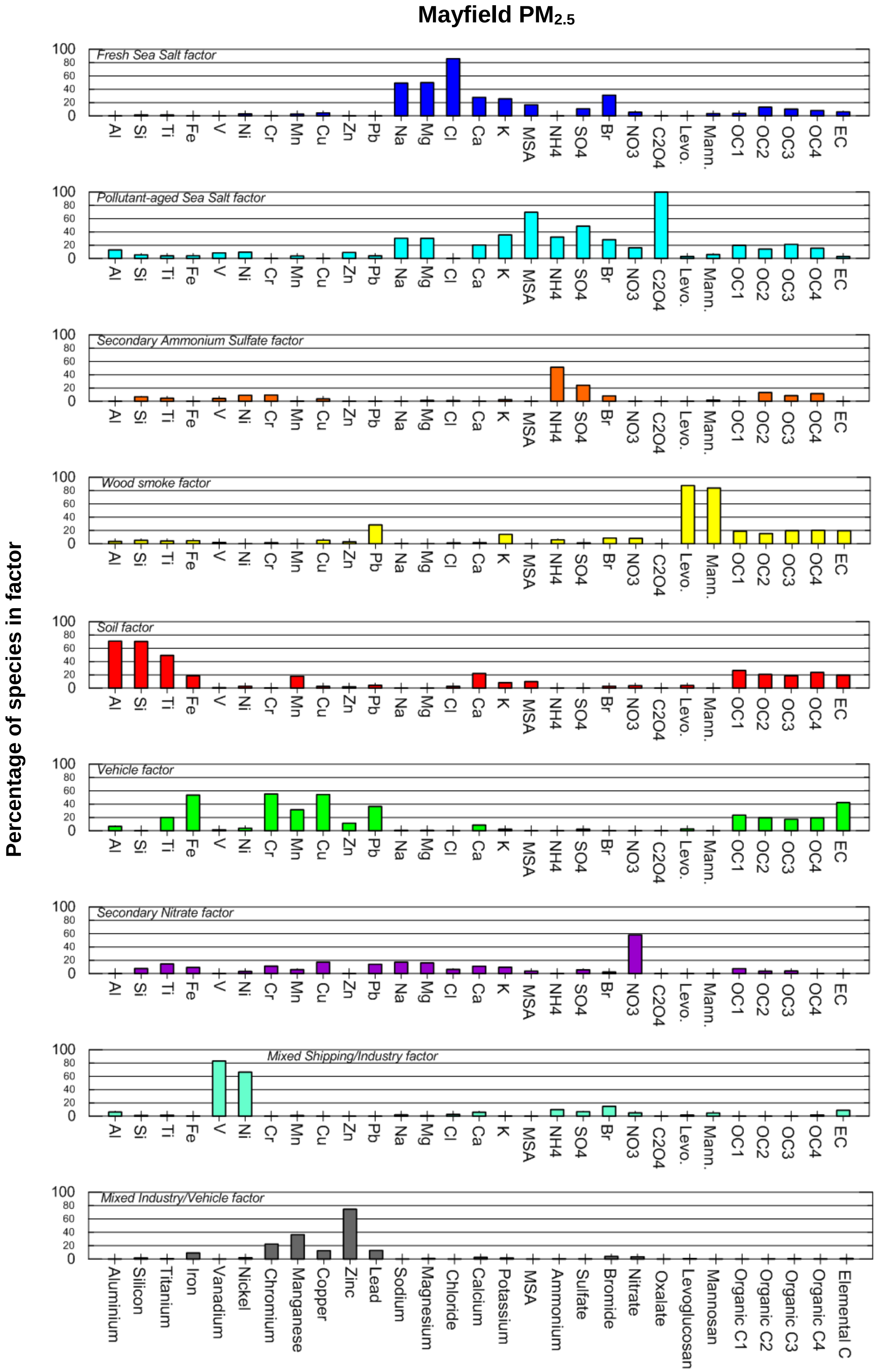

Figure 141: Percentage of each species in the $PM_{2.5}$ factors for Mayfield

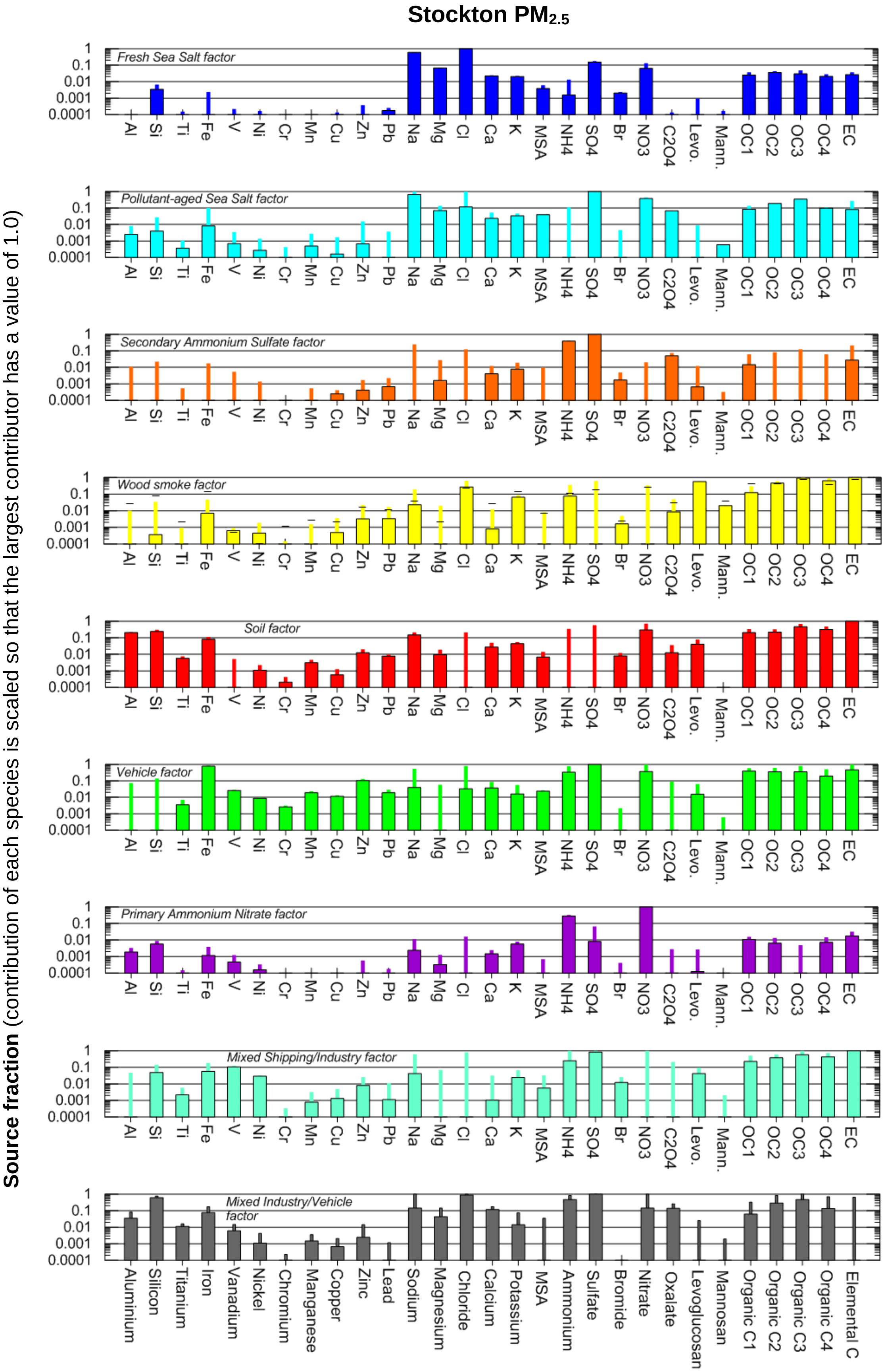

Figure 142: Fingerprints of $PM_{2.5}$ factors at Stockton from PMF analysis; broad bars show the contribution in the selected solution, narrow bars indicate uncertainty

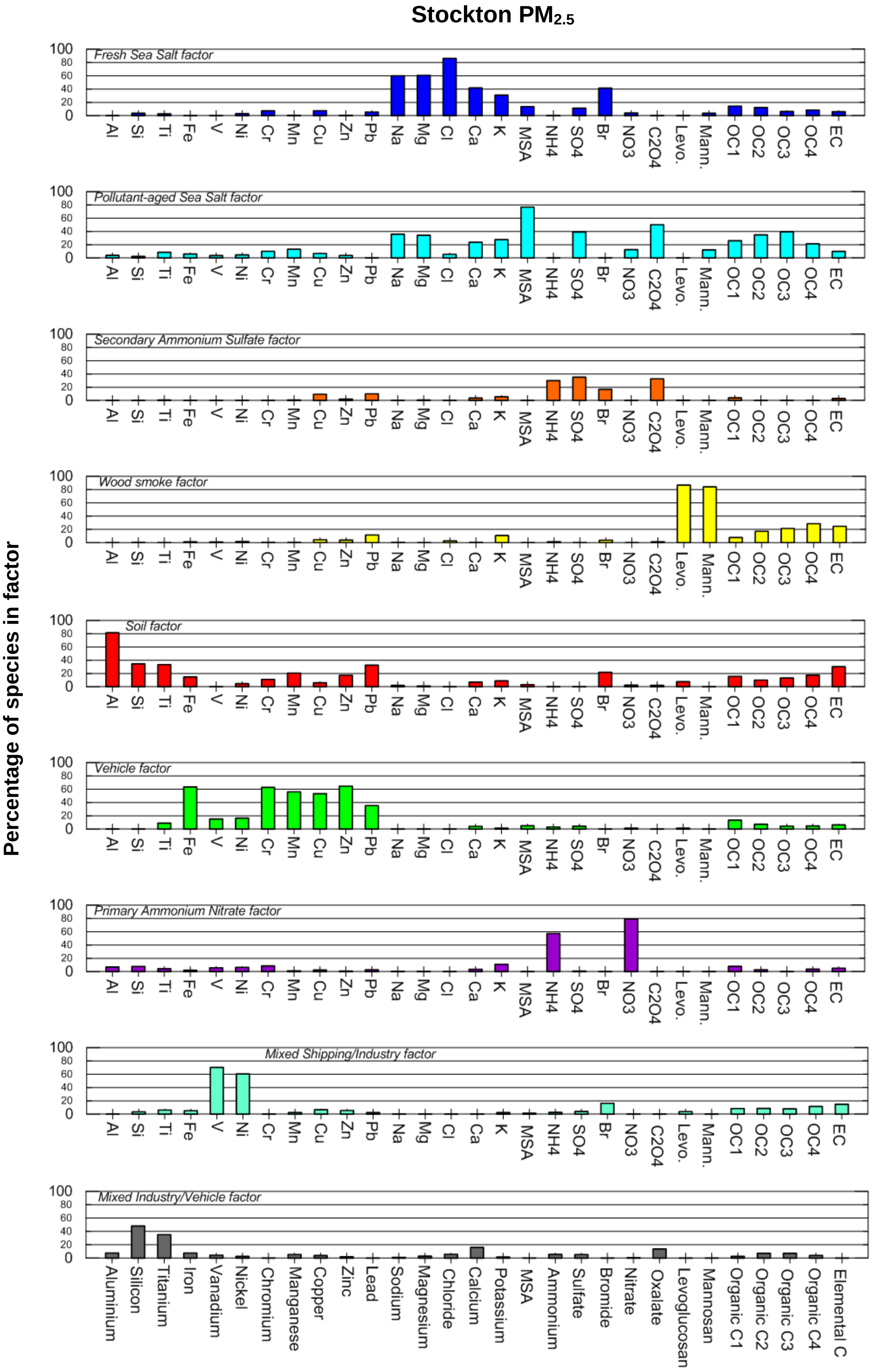

Figure 143: Percentage of each species in the $PM_{2.5}$ factors for Stockton

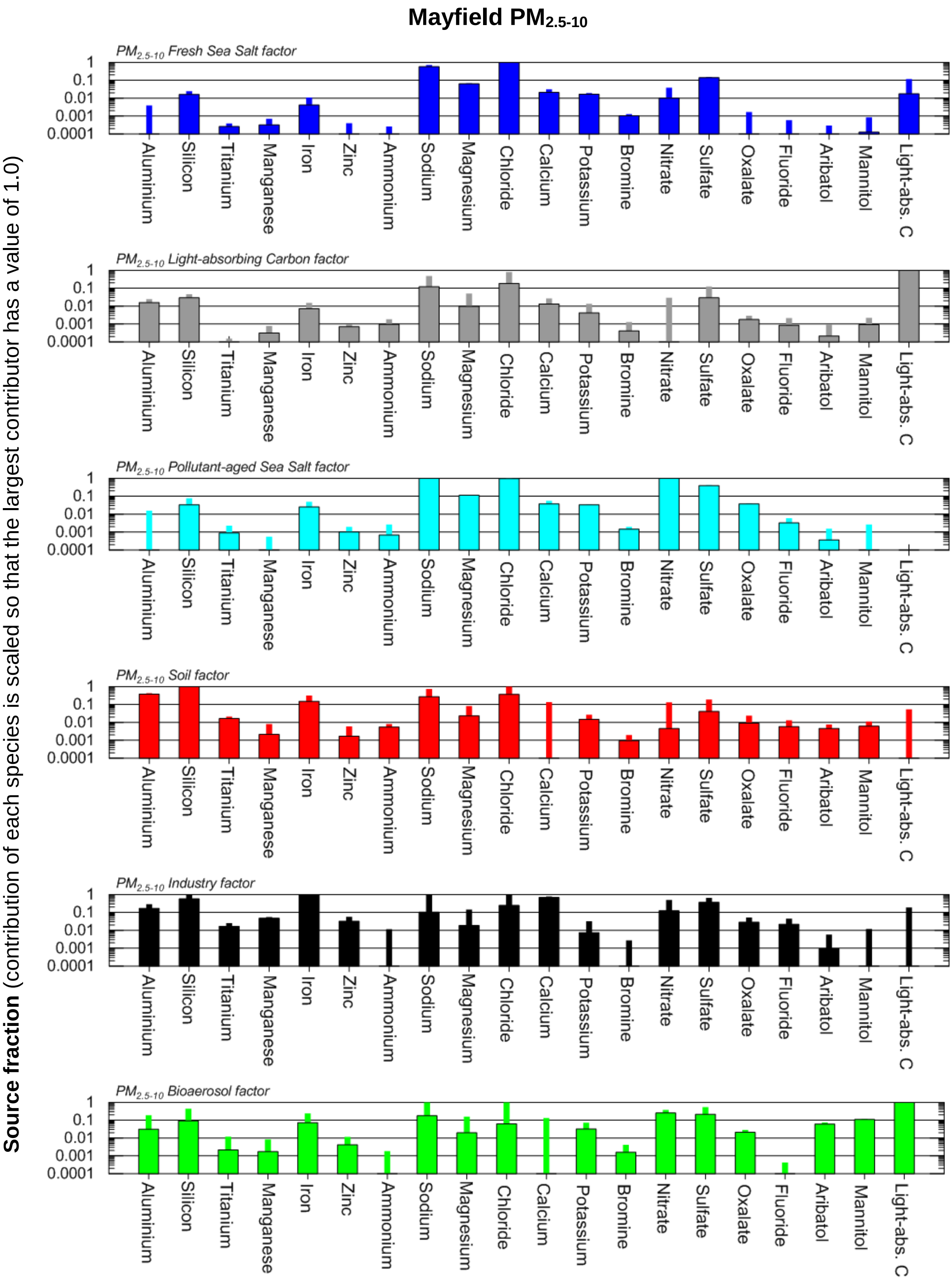

Figure 144: Fingerprints of $PM_{2.5-10}$ factors at Stockton from PMF analysis; broad bars show the contribution in the selected solution, narrow bars indicate uncertainty

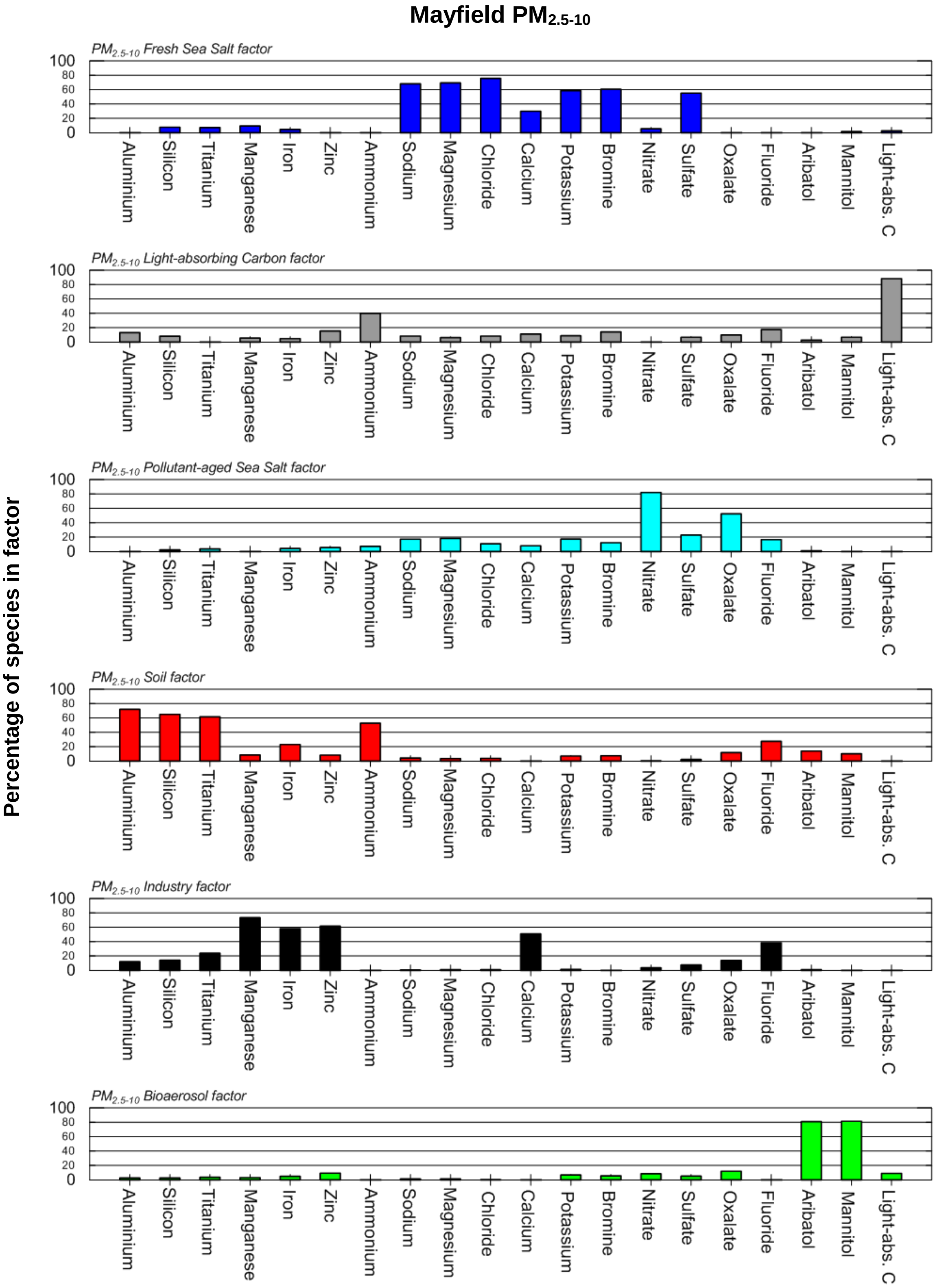

Figure 145: Percentage of each species in the $PM_{2.5-10}$ factors for Mayfield

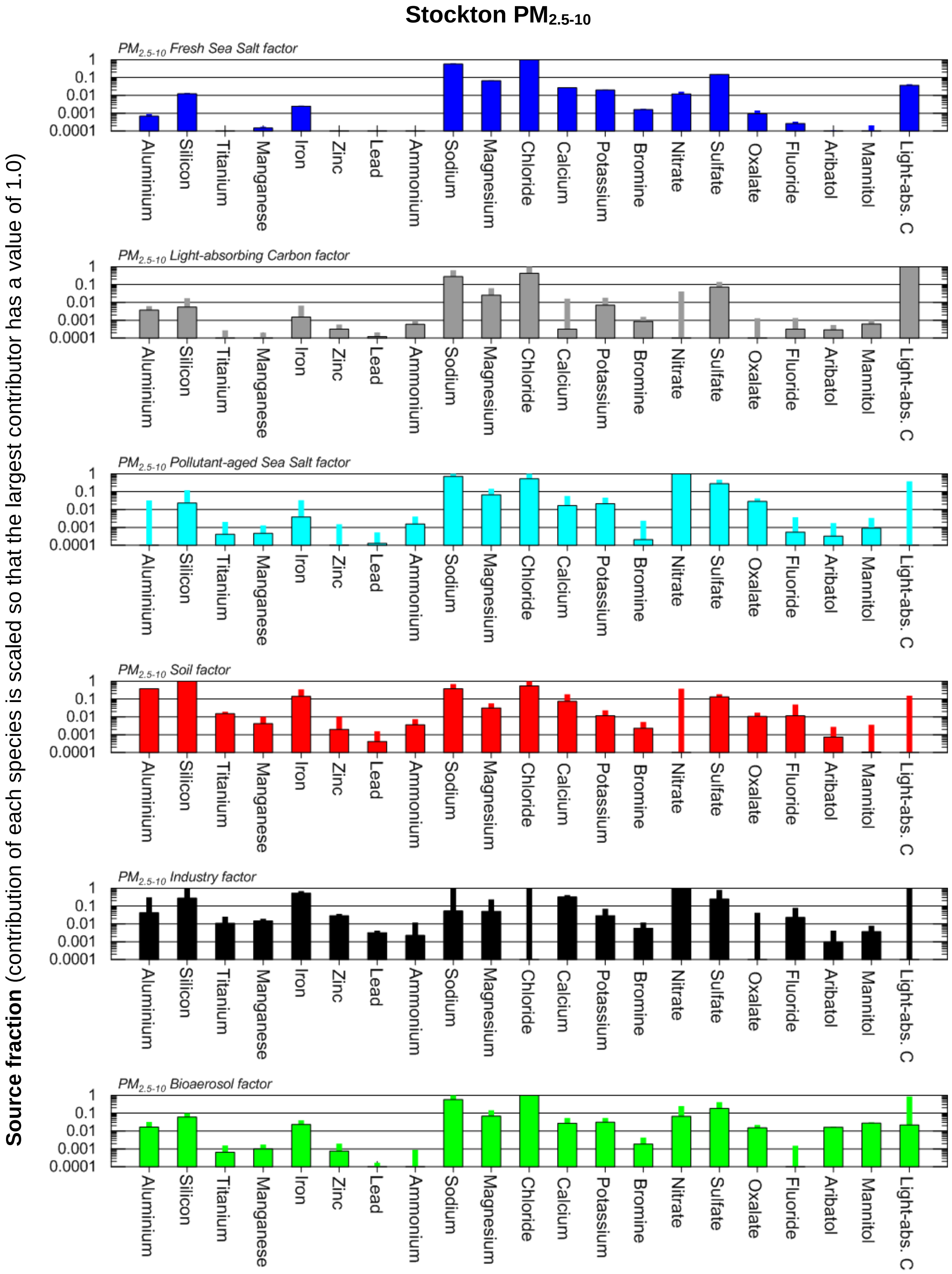

Figure 146: Fingerprints of $PM_{2.5-10}$ factors at Stockton from PMF analysis; broad bars show the contribution in the selected solution, narrow bars indicate uncertainty

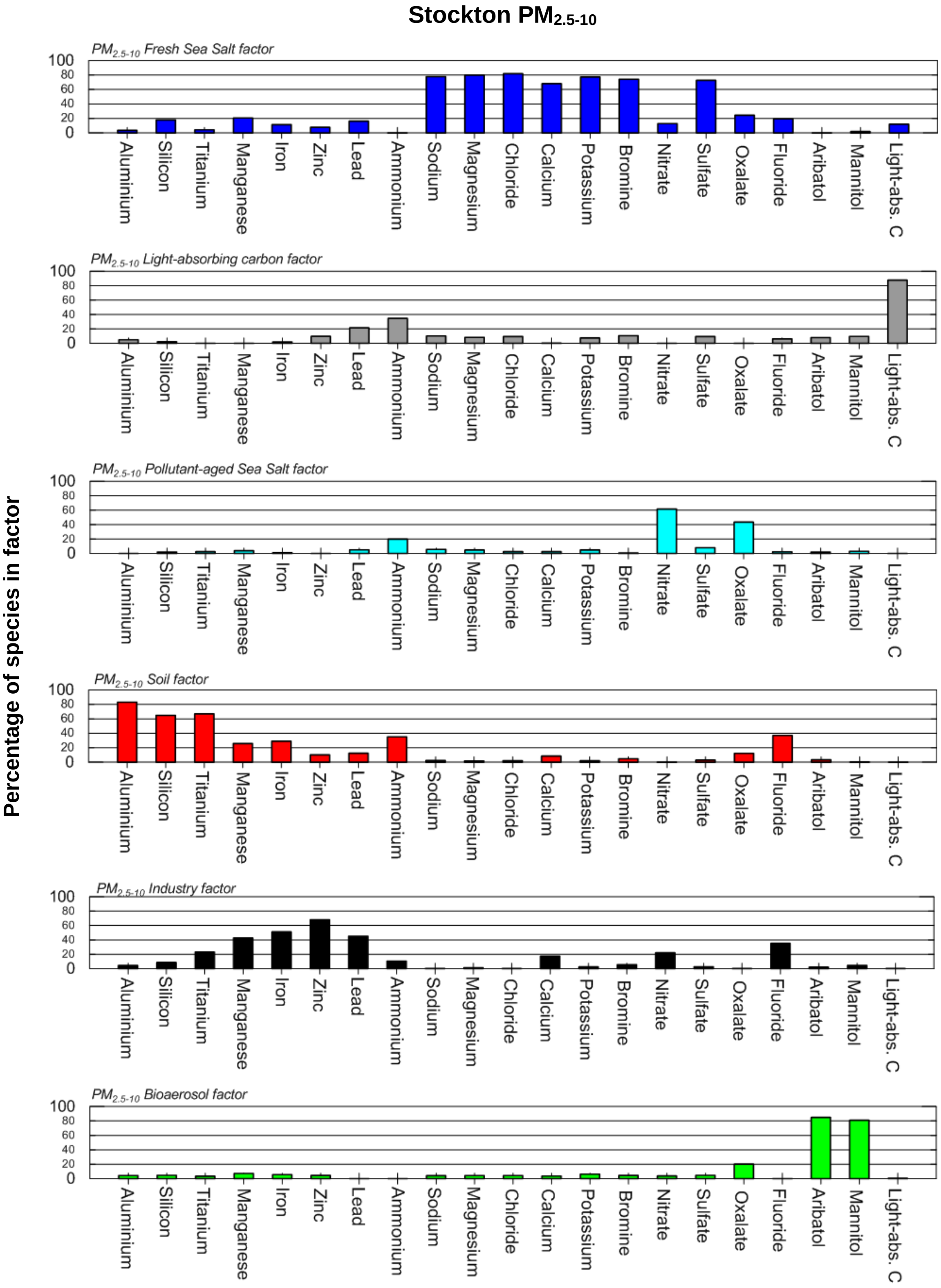

Figure 147: Percentage of each species in the $PM_{2.5-10}$ factors for Stockton

Appendix D – Uncertainty analysis (PMF)

The EPA PMF 5.0 software (Norris & Duvall 2014) used for the receptor modelling results presented in this report includes several methods for estimating the uncertainty in the analysis due to random errors and rotational ambiguity.

This appendix follows the recommendations of Paatero et al. (2014) on documenting the uncertainty estimates. A fuller description of the meaning of the uncertainty estimates is provided by Paatero et al. (2014) and Norris & Duvall (2014).

The displacement technique is a method for determining rotational uncertainty in the solution. Bootstrapping (BS) is a method for detecting and estimating disproportionate effects of a small number of observations on the solution and also, to a lesser extent on rotational ambiguity.

Newcastle $PM_{2.5}$ – EPA PMF v 5 diagnostics

Base run summary	
Number of base runs:	100
Base user-selected seed:	99
Number of factors:	10
Extra modelling uncertainty (%):	10

DISP summary	**Err.code**	**Max dQ**							
	0	0.000							
	Factor 1	**Factor 2**	**F 3**	**F 4**	**F 5**	**F 6**	**F 7**	**F 8**	**F 9**	**F 10**
dQmax = 4	0	0	0	0	0	0	0	0	0	0
dQmax = 8	0	0	0	0	0	0	0	0	0	0
dQmax = 15	0	0	0	0	0	0	0	0	0	0
dQmax = 25	1	0	0	0	0	0	0	0	0	1

Bootstrap summary of base run	
Number of bootstrap runs:	100
Bootstrap random seed:	99
Min. Correlation R-Value:	0.6

BS mapping:											
	Secondary nitrate	Wood smoke	Soil	Aged sea salt 1	Vehicles	Aged sea salt 2	Secondary ammonium sulfate	Fresh sea salt	Shipping	Industry	Unmapped
Boot Factor 1	100	0	0	0	0	0	0	0	0	0	0
Boot Factor 2	0	100	0	0	0	0	0	0	0	0	0
Boot Factor 3	0	0	100	0	0	0	0	0	0	0	0
Boot Factor 4	0	0	14	73	3	6	2	0	0	2	0
Boot Factor 5	1	1	2	0	90	1	0	0	0	5	0
Boot Factor 6	0	0	0	0	0	100	0	0	0	0	0
Boot Factor 7	0	0	0	0	0	1	99	0	0	0	0
Boot Factor 8	0	0	0	0	0	0	0	100	0	0	0
Boot Factor 9	0	0	0	0	0	0	0	0	100	0	0
Boot Factor 10	0	0	0	0	0	0	0	0	0	100	0

Beresfield $PM_{2.5}$ – EPA PMF v 5 diagnostics

Base run summary	
Number of base runs:	100
Base user-selected seed:	99
Number of factors:	10
Extra modelling uncertainty (%):	10

DISP summary	**Err.code**	**Max dQ**							
	0	0.000							
	Factor 1	**Factor 2**	**F 3**	**F 4**	**F 5**	**F 6**	**F 7**	**F 8**	**F 9**	**F 10**
dQmax = 4	0	0	0	0	0	0	0	0	0	0
dQmax = 8	0	0	0	0	0	0	0	0	0	0
dQmax = 15	0	0	6	5	0	0	5	0	0	0
dQmax = 25	0	0	14	8	0	0	14	1	4	1

Bootstrap summary of base run	
Number of bootstrap runs:	100
Bootstrap random seed:	99
Min. Correlation R-Value:	0.6

BS mapping:											
	Fresh sea salt	Wood smoke	Secondary nitrate	Vehicles	Industry	Shipping	Aged sea salt 2	Aged sea salt 1	Secondary ammonium sulfate	Soil	Unmapped
Boot Factor 1	100	0	0	0	0	0	0	0	0	0	0
Boot Factor 2	0	100	0	0	0	0	0	0	0	0	0
Boot Factor 3	0	0	99	1	0	0	0	0	0	0	0
Boot Factor 4	0	0	0	100	0	0	0	0	0	0	0
Boot Factor 5	0	2	0	0	98	0	0	0	0	0	0
Boot Factor 6	0	5	1	1	6	85	1	0	0	0	0
Boot Factor 7	0	3	0	7	9	0	75	0	0	5	0
Boot Factor 8	0	0	0	0	1	0	0	99	0	0	0
Boot Factor 9	0	1	0	0	0	0	0	0	99	0	0
Boot Factor 10	0	0	0	0	0	0	0	0	0	100	0

Mayfield $PM_{2.5}$ – EPA PMF v 5 diagnostics

Base run summary	
Number of base runs:	100
Base user-selected seed:	99
Number of factors:	10
Extra modelling uncertainty (%):	10

DISP summary	**Err.code**	**Max dQ**							
	0	0.000							
	Factor 1	**Factor 2**	**F 3**	**F 4**	**F 5**	**F 6**	**F 7**	**F 8**	**F 9**	**F 10**
dQmax = 4	0	0	0	0	0	0	0	0	0	0
dQmax = 8	0	0	0	0	0	0	0	0	0	0
dQmax = 15	0	0	0	0	0	0	0	0	0	0
dQmax = 25	0	0	0	0	3	3	0	0	4	1

Bootstrap summary of base run	
Number of bootstrap runs:	100
Bootstrap random seed:	99
Min. Correlation R-Value:	0.6

BS mapping:											
	Wood smoke	Industry	Shipping	Fresh sea salt	Soil	Secondary ammonium sulfate	Secondary nitrate	Vehicles	Aged sea salt 2	Aged sea salt 1	Unmapped
Boot Factor 1	100	0	0	0	0	0	0	0	0	0	0
Boot Factor 2	0	99	0	0	1	0	0	0	0	0	0
Boot Factor 3	0	0	100	0	0	0	0	0	0	0	0
Boot Factor 4	0	0	0	100	0	0	0	0	0	0	0
Boot Factor 5	0	0	0	0	100	0	0	0	0	0	0
Boot Factor 6	0	0	0	0	2	97	0	1	0	0	0
Boot Factor 7	0	0	0	0	0	0	100	0	0	0	0
Boot Factor 8	0	0	0	0	1	0	0	99	0	0	0
Boot Factor 9	0	0	0	0	27	0	0	18	51	4	0
Boot Factor 10	0	0	0	0	0	0	0	0	0	100	0

Stockton $PM_{2.5}$ – EPA PMF v 5 diagnostics

Base run summary	
Number of base runs:	100
Base user-selected seed:	99
Number of factors:	10
Extra modelling uncertainty (%):	10

DISP summary	**Err.code**	**Max dQ**							
	0	-0.004							
	Factor 1	**Factor 2**	**F 3**	**F 4**	**F 5**	**F 6**	**F 7**	**F 8**	**F 9**	**F 10**
dQmax = 4	0	0	0	0	0	0	0	0	0	0
dQmax = 8	13	12	0	0	0	0	0	13	0	0
dQmax = 15	15	13	0	0	0	0	0	15	0	0
dQmax = 25	20	14	1	0	4	2	0	23	0	0

Bootstrap summary of base run	
Number of bootstrap runs:	100
Bootstrap random seed:	99
Min. Correlation R-Value:	0.6

BS mapping:											
	Aged sea salt 1	Shipping	Aged sea salt 2	Soil	Industry	Ammonium nitrate	Wood smoke	Secondary ammonium sulfate	Fresh sea salt	Vehicles	Unmapped
Boot Factor 1	100	0	0	0	0	0	0	0	0	0	0
Boot Factor 2	0	100	0	0	0	0	0	0	0	0	0
Boot Factor 3	0	0	100	0	0	0	0	0	0	0	0
Boot Factor 4	0	0	0	100	0	0	0	0	0	0	0
Boot Factor 5	0	0	0	1	99	0	0	0	0	0	0
Boot Factor 6	0	0	0	0	0	100	0	0	0	0	0
Boot Factor 7	0	0	0	0	0	0	100	0	0	0	0
Boot Factor 8	24	4	2	0	0	0	0	69	0	1	1
Boot Factor 9	0	0	0	0	0	0	0	0	100	0	0
Boot Factor 10	0	0	0	0	0	0	0	0	0	100	0

Mayfield $PM_{2.5-10}$ – EPA PMF v 5 diagnostics

Base run summary	
Number of base runs:	100
Base user-selected seed:	99
Number of factors:	6
Extra modelling uncertainty (%):	10

DISP summary	**Err.code**	**Max dQ**				
	0	-0.023				
	Factor 1	**Factor 2**	**Factor 3**	**Factor 4**	**Factor 5**	**Factor 6**
dQmax = 4	0	0	0	0	0	0
dQmax = 8	0	0	0	0	0	0
dQmax = 15	0	0	0	0	0	0
dQmax = 25	0	0	0	0	0	0

Bootstrap summary of base run	
Number of bootstrap runs:	100
Bootstrap random seed:	99
Min. Correlation R-Value:	0.6

BS mapping:							
	Soil	Industry	Bioaerosol	Pollutant-aged sea salt	Light-absorbing carbon	Fresh sea salt	Unmapped
Boot Factor 1	100	0	0	0	0	0	0
Boot Factor 2	0	100	0	0	0	0	0
Boot Factor 3	0	0	100	0	0	0	0
Boot Factor 4	0	0	0	100	0	0	0
Boot Factor 5	0	0	0	0	100	0	0
Boot Factor 6	0	0	0	0	0	100	0

Stockton $PM_{2.5-10}$ – EPA PMF v 5 diagnostics

Base run summary	
Number of base runs:	100
Base user-selected seed:	99
Number of factors:	6
Extra modelling uncertainty (%):	10

DISP summary	**Err.code**	**Max dQ**				
	0	-0.012				
	Factor 1	**Factor 2**	**Factor 3**	**Factor 4**	**Factor 5**	**Factor 6**
dQmax = 4	0	0	0	0	0	0
dQmax = 8	0	0	0	0	0	0
dQmax = 15	0	0	0	0	0	0
dQmax = 25	0	0	0	0	0	0

Bootstrap summary of base run	
Number of bootstrap runs:	100
Bootstrap random seed:	99
Min. Correlation R-Value:	0.6

BS mapping:							
	Bioaerosol	Pollutant-aged sea salt	Soil	Industry	Fresh sea salt	Light-absorbing carbon	Unmapped
Boot Factor 1	100	0	0	0	0	0	0
Boot Factor 2	0	100	0	0	0	0	0
Boot Factor 3	0	0	100	0	0	0	0
Boot Factor 4	0	1	4	90	1	4	0
Boot Factor 5	0	0	0	0	100	0	0
Boot Factor 6	0	0	0	0	0	100	0

Appendix E – Trajectory modelling method

Back trajectory modelling was undertaken for selected periods to assess the movement of air masses prior to their moving over the study area. Case study periods selected for analysis included periods with elevated particle concentrations and periods when certain factors had higher contributions. The back trajectory analysis was undertaken using the National Oceanic and Atmospheric Administration (NOAA) Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) model. HYSPLIT has been widely used identify the source–receptor relationship for air pollutants using backward trajectories analysis. It has been used for a range of events including wildfire smoke transport, dust storm episodes, nuclear incidents and volcanic eruptions (Draxler & Rolph 2015).

To provide high-resolution meteorological input data for HYSPLIT, regional meteorological modelling was undertaken using the Advanced Research version of the Weather Research and Forecast model (WRF-ARW, Skamarock et al. 2008). The WRF-ARW model was set up with three nested domains (Figure 148), with the Domain 1 (27km horizontal resolution) run supporting 72-hour back trajectories, the Domain 2 (9km resolution) run supporting 48-hour back trajectories, and the Domain 3 (3km resolution) run supporting 24-hour back trajectory analysis.

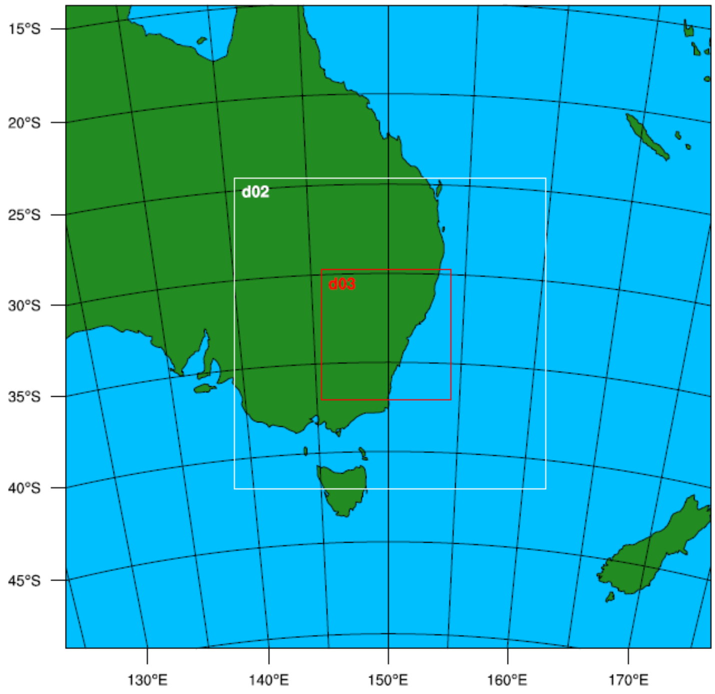

Figure 148: Domain configuration for WRF-ARW model simulations

A total of 50 vertical levels were considered in the model, of which 35 levels were placed below 700hPa for better interpolation of the boundary layer. Model physics included WRF Single-Moment (WSM) 3-class simple ice scheme, Kain-Fritsch (new Eta) cumulus parameterization scheme, Mellor-Yamada-Janjic (Eta) TKE scheme for boundary layer processes, Monin-Obukhov (Janjic Eta) Similarity scheme for surface-layer, RRTM (Rapid Radiative Transfer Model) scheme for longwave radiation and Dudhia scheme for shortwave radiation, and the NOAH land surface model for surface processes.

The WRF-ARW model was conducted as various split runs for episode studies, while each run was integrated for 60 hours (with the first 12 hours of simulation treated as a spin-up period) then the split outputs were combined together for analyses. Initial and boundary conditions were adopted from ERA-Interim data (global atmospheric reanalysis from the European Centre for Medium-Range Weather Forecasts – ECMWF) available at 0.75-degree horizontal resolution. Boundary conditions were updated at 6-hour intervals during the period of model integration. Then, the HYSPLIT model was driven by WRF simulated atmospheric fields to generate backward trajectories using the LHPCS sampling sites as starting locations for the back trajectories.

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