

Error estimate

Beijing 2012-2013

Once obtained the solution

- strong: Cl, K, Ca, Ti, Fe, SO₂₄, NO₃, NH₄, OC, and EC.
- weak: Na, Mg, Al, Si, V, Cr, Mn, Co, Ni, Cu, Zn, As, Br, Pb. PM_{2.5} was set as the total variable
- 10% extra uncertainty
- 6 factors
- Seed: 20

Error estimate – Base run

- BS (random errors)
 - DISP (rotational errors)
 - BS-DISP (random+rotational)
-
- Paatero, P., Eberly, S., Brown, S.G., Norris, G.A. Methods for estimating uncertainty in factor analytic solutions (2014) Atmospheric Measurement Techniques, 7 (3), pp. 781-797.
 - Brown, S.G., Eberly, S., Paatero, P., Norris, G.A. Methods for estimating uncertainty in PMF solutions: Examples with ambient air and water quality data and guidance on reporting PMF results (2015) Science of the Total Environment, 518-519, pp. 626-635.

Output error estimate

1. Random errors (Bootstrapping).
2. Rotational errors (Displacement)
3. Both (BS-DISP)

Modelling errors difficult to estimate, and they are not minimized by large datasets

If uncertainties are not well specified, use only BS-DISP or BS

The screenshot displays the EPA PMF software interface. The 'Base Model Runs' tab is active, showing configuration for 30 runs with 8 factors. The 'Error Estimation' section is set to 'Base Model Displacement Method' with a selected base run of 29. The 'Base Model Bootstrap Method' is also set to 'Base Model Displacement Method' with a selected base run of 29, a block size of 43, and 20 bootstraps. The 'Base Model BS-DISP Method' table is visible, listing various species and their S/N ratios. The 'Factor Names' table at the bottom shows the composition of each factor, with Run 29 being a mixture of heavy oil, non-exhaust, mineral, industrial, aged sea soil, exhaust, nitrate, and sulfate. The 'Run Progress' bar at the bottom indicates the current status of the runs.

Displacement	Species	Cat	S/N
<input checked="" type="checkbox"/>	PM	Strong	0.0
<input type="checkbox"/>	EC	Strong	10.0
<input type="checkbox"/>	OC	Strong	9.8
<input type="checkbox"/>	NH4	Strong	5.4
<input type="checkbox"/>	OI	Strong	3.5
<input type="checkbox"/>	NO3	Strong	9.7
<input type="checkbox"/>	SO4	Red	10.0
<input type="checkbox"/>	Al	Strong	4.7
<input type="checkbox"/>	Ca	Strong	6.5
<input type="checkbox"/>	Fe	Strong	9.1
<input type="checkbox"/>	K	Strong	2.7
<input type="checkbox"/>	Mg	Strong	7.7
<input type="checkbox"/>	Na	Strong	8.2
<input type="checkbox"/>	S	Strong	9.2
<input type="checkbox"/>	Li	Strong	9.1
<input type="checkbox"/>	Ti	Strong	1.7

Factor Names	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6	Factor 7	Factor 8
Run 29	Heavy oil	Non-exhaust	Mineral	Industrial	Aged sea soil	Exhaust	Nitrate	Sulfate
Run 30	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6	Factor 7	Factor 8



Bootstrapping diagnostic

- Random errors, partially evaluates the rotational ambiguity
- not influenced by the user-specified sample uncertainties.
- >80% mapped factors



EPA PMF

Model Data | Base Model | Rotational Tools | Help

Base Model Runs | Base Model Results | Base Model DISP Results | Base Model Bootstrap Results | Error Estimation Summary

Bootstrap Box Plots | Bootstrap Summary

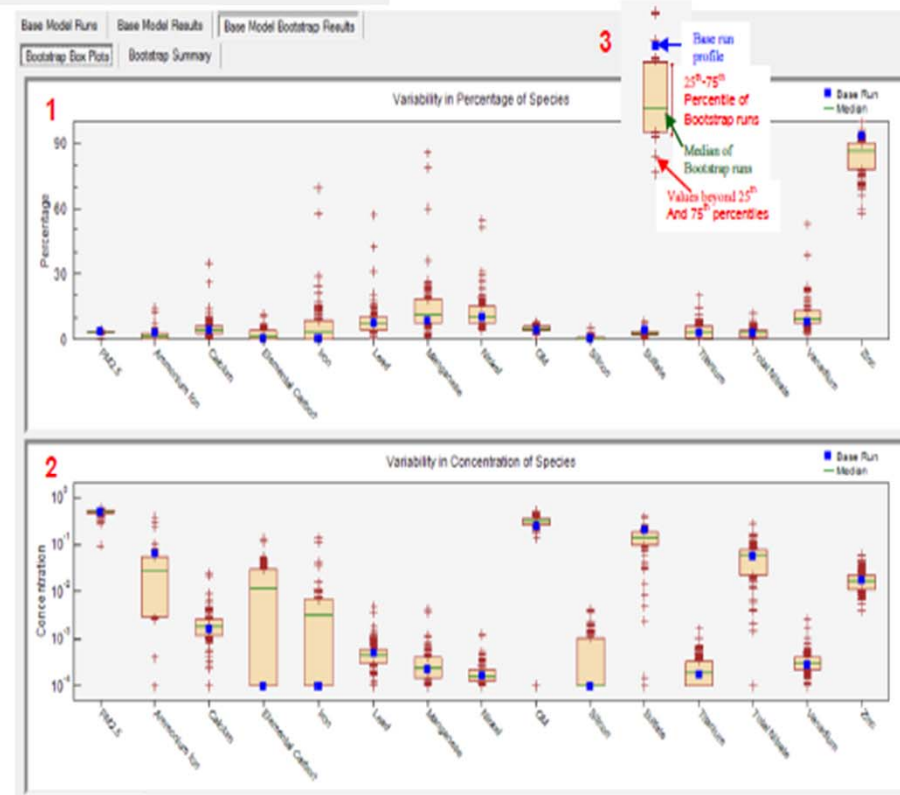
Base model run number: 29
 Number of bootstrap runs: 20
 Bootstrap random seed: 33
 Min. Correlation R-Value: 0.6
 Number of factors: 8
 Extra modeling uncertainty (%): 7

Mapping of bootstrap factors to base factors:

	Heavy oil	Non- exhaust	Mineral Industrial	Aged sea salt	Exhaust Nitrate Sulfate	Unmapped
Boot Factor 1	20	0	0	0	0	0
Boot Factor 2	0	20	0	0	0	0
Boot Factor 3	0	0	20	0	0	0
Boot Factor 4	0	0	0	20	0	0
Boot Factor 5	0	0	0	0	20	0
Boot Factor 6	0	1	0	0	19	0
Boot Factor 7	0	0	0	0	0	20
Boot Factor 8	0	0	0	1	0	19

Q (Robust) Percentile Report:

Min	25th	Median	75th	Max
5611	6214	6464	6663	6978



Bootstrap base run

The screenshot shows the EPA PMF software interface. The 'Base Model Bootstrap Method' section is highlighted with a red box. It contains the following settings:

- Selected Base Run: 3
- Block Size: 5 (with a 'Suggest' button)
- Number of Bootstraps: 20
- Min. Correlation R-Value: 0.6 (with a 'Run' button)

The 'Base Model Run Summary' table shows the results of 30 runs. The first three runs are highlighted in blue, indicating convergence. The 'Displacement Species' table shows the correlation of various species with the factors. The 'Factor Names' table shows the names of the factors for each run.

Run Number	Q (Robust)	Q (True)	Converged
1	699.4	699.4	Yes
2	699.4	699.4	Yes
3	699.4	699.4	Yes
4	699.4	699.4	Yes
5	699.4	699.4	Yes
6	699.4	699.4	Yes
7	699.4	699.4	Yes
8	699.4	699.4	Yes
9	699.4	699.4	Yes
10	699.4	699.4	Yes
11	699.4	699.4	Yes
12	699.4	699.4	Yes
13	699.4	699.4	Yes
14	699.4	699.4	Yes
15	699.4	699.4	Yes
16	699.4	699.4	Yes
17	699.4	699.4	Yes
18	699.4	699.4	Yes
19	699.4	699.4	Yes
20	699.4	699.4	Yes
21	699.4	699.4	Yes
22	699.4	699.4	Yes
23	699.4	699.4	Yes
24	699.4	699.4	Yes
25	699.4	699.4	Yes
26	699.4	699.4	Yes
27	699.4	699.4	Yes
28	699.4	699.4	Yes
29	699.4	699.4	Yes
30	699.4	699.4	Yes

Displacement	Species	Cat	S/N
<input checked="" type="checkbox"/>	Na	Weak	0.3
<input type="checkbox"/>	Mg	Weak	2.0
<input type="checkbox"/>	Al	Weak	3.7
<input type="checkbox"/>	Si	Weak	0.8
<input type="checkbox"/>	S	Bad	10.0
<input type="checkbox"/>	Cl	Strong	9.7
<input type="checkbox"/>	K	Strong	9.7
<input type="checkbox"/>	Ca	Strong	9.8
<input type="checkbox"/>	Ti	Strong	3.2
<input type="checkbox"/>	V	Weak	0.0
<input type="checkbox"/>	Cr	Weak	0.9
<input type="checkbox"/>	Mn	Weak	4.1
<input type="checkbox"/>	Fe	Strong	9.9
<input type="checkbox"/>	Co	Weak	0.0
<input type="checkbox"/>	Ni	Weak	0.1

Factor Names	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6
Run 3	Coal combustion	Secondary nitrate	Biomass burning	Secondary sulfate	Soil	Traffic
Run 4	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6

BS summary

EPA PMF

Model Data | Base Model | Rotational Tools | Help

Base Model Runs | Base Model Results | Base Model Bootstrap Results | Base Model DISP Results | Error Estimation Summary

Bootstrap Box Plots | Bootstrap Summary

Base model run number: 3
 Number of bootstrap runs: 20
 Bootstrap random seed: 33
 Min. Correlation R-Value: 0.6
 Number of factors: 6
 Extra modeling uncertainty (%): 10

Mapping of bootstrap factors to base factors:

	Coal combustion	Secondary nitrate	Biomass burning	Secondary sulfate	Soil	Traffic	Unmapped
Boot Factor 1	20	0	0	0	0	0	0
Boot Factor 2	0	20	0	0	0	0	0
Boot Factor 3	0	0	20	0	0	0	0
Boot Factor 4	0	0	0	19	0	1	0
Boot Factor 5	0	0	0	0	20	0	0
Boot Factor 6	0	0	0	0	0	20	0

Q(Robust) Percentile Report:

Min	25th	Median	75th	Max
484	611	635	663	754

Bootstrap run uncertainty statistics:

Coal combustion

Species	Base Run Profile	Within IQR	Bootstrap Runs:				
			Mean	Std. Dev.	5th	25th	Median
Na	2.0549E-002	Yes	9.8763E-002	1.7253E-001	0.0000E+000	0.0000E+000	0.0000E+000
Mg	1.0606E-002	Yes	6.8721E-003	6.5992E-003	0.0000E+000	1.0861E-004	5.9493E-003
Al	3.7713E-002	No	2.6637E-002	1.3771E-002	5.2390E-003	1.2527E-002	2.9080E-002
Si	6.5109E-002	No	3.7369E-002	2.1629E-002	2.9284E-003	1.6183E-002	4.3265E-002
Cl	2.2799E+000	Yes	2.7032E+000	2.8333E-001	2.1684E+000	2.4653E+000	2.7801E+000
K	2.2301E-001	No	2.9380E-001	1.3180E-001	3.6714E-002	2.2890E-001	2.7252E-001
Ca	8.1797E-002	No	5.7433E-002	2.9784E-002	1.1103E-002	3.2196E-002	5.9560E-002
Ti	1.8899E-003	Yes	1.1337E-003	9.8068E-004	0.0000E+000	1.0495E-005	1.2985E-003
V	0.0000E+000	Yes	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
Cr	3.7675E-004	No	5.4399E-004	2.7265E-004	5.8605E-006	4.0487E-004	5.5712E-004
Mn	5.7108E-003	Yes	6.6713E-003	2.5097E-003	2.4645E-004	5.1324E-003	6.6626E-003
Fe	4.9068E-002	Yes	6.8832E-002	4.8230E-002	0.0000E+000	3.8483E-002	7.3317E-002
Co	0.0000E+000	Yes	6.2051E-005	1.1258E-004	0.0000E+000	0.0000E+000	5.8285E-006
Ni	0.0000E+000	Yes	4.4676E-005	8.1023E-005	0.0000E+000	0.0000E+000	0.0000E+000
Cu	8.1042E-003	Yes	7.6276E-003	2.2249E-003	3.6827E-003	5.3758E-003	8.3443E-003
Zn	1.0541E-001	Yes	1.1126E-001	3.1304E-002	2.7764E-002	1.0213E-001	1.1798E-001
As	0.0000E+000	Yes	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
Br	8.0782E-003	Yes	8.5738E-003	1.4001E-003	6.1348E-003	7.2873E-003	8.6834E-003
Pb	6.2906E-002	Yes	7.2379E-002	2.3150E-002	1.4658E-002	5.9253E-002	7.2297E-002
SO42-	1.2929E+000	Yes	1.0450E+000	1.2429E+000	0.0000E+000	0.0000E+000	5.4756E-001
NO3-	3.5019E+000	Yes	2.6175E+000	1.6094E+000	6.7685E-003	1.4107E+000	2.5542E+000
NH4+	2.5401E+000	No	2.1041E+000	7.3168E-001	9.6724E-001	1.6120E+000	1.9273E+000
OC	9.7538E-001	Yes	1.5333E+000	1.0411E+000	8.3670E-002	6.7275E-001	1.5181E+000
EC	4.8311E-002	Yes	2.0033E-001	2.4705E-001	0.0000E+000	3.9418E-013	7.0127E-002
PM2.5	9.7420E+000	Yes	9.0369E+000	3.0845E+000	3.8304E+000	6.5128E+000	8.3249E+000

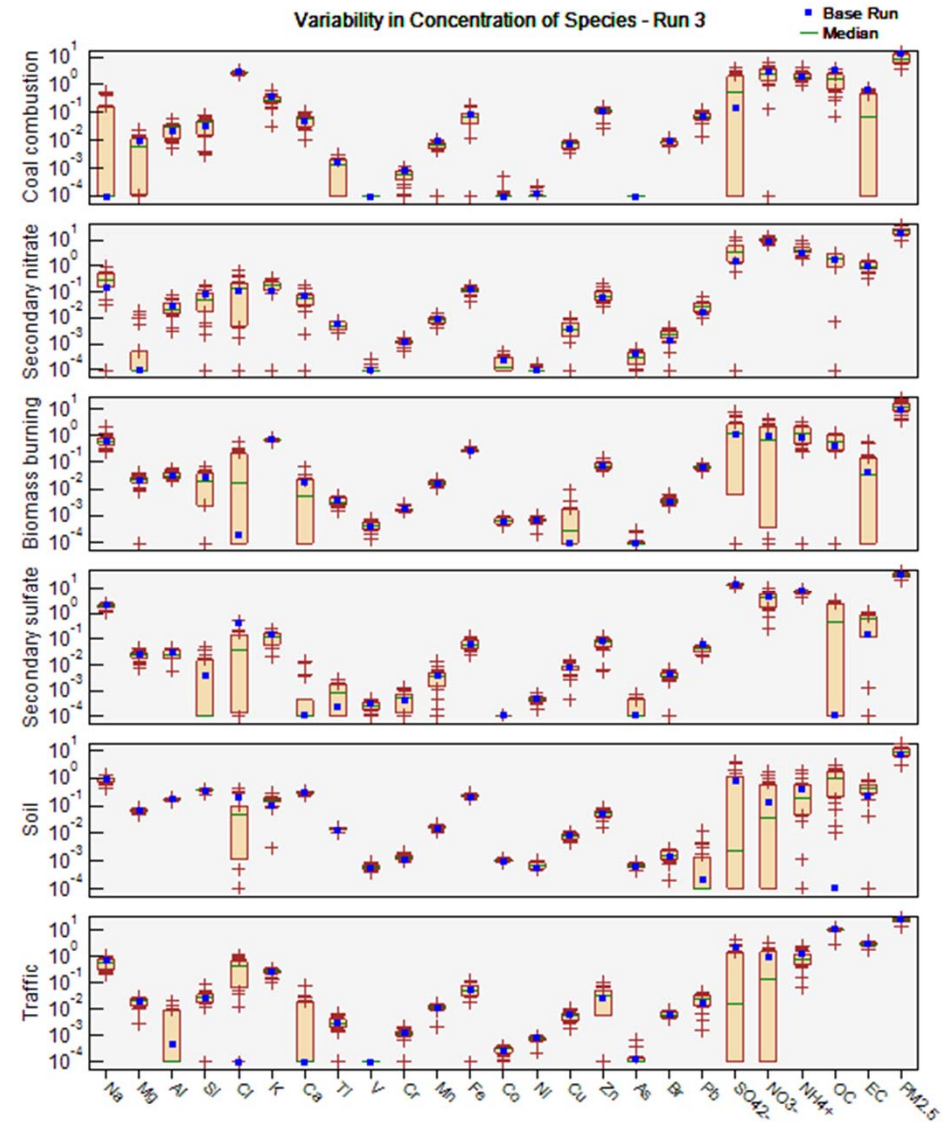
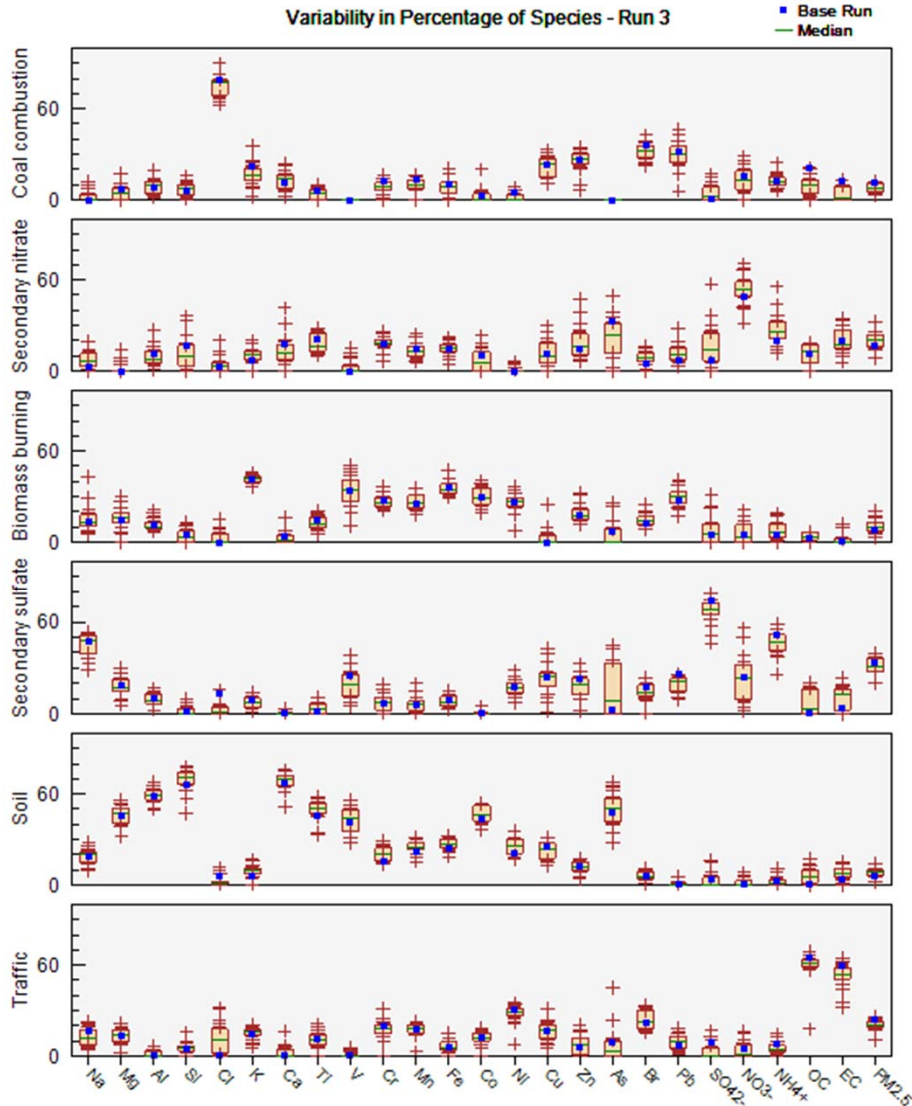
Secondary nitrate

Species	Base Run Profile	Within IQR	Bootstrap Runs:				
			Mean	Std. Dev.	5th	25th	Median
Na	4.1846E-001	Yes	3.5479E-001	2.5892E-001	0.0000E+000	1.6886E-001	3.0433E-001
Mg	0.0000E+000	Yes	2.4760E-003	5.4103E-003	0.0000E+000	0.0000E+000	0.0000E+000
Al	2.5735E-002	Yes	2.8410E-002	1.8545E-002	3.1161E-003	1.4795E-002	2.2649E-002

Help

BS box plots

Species with base run outside the IQR need evaluation

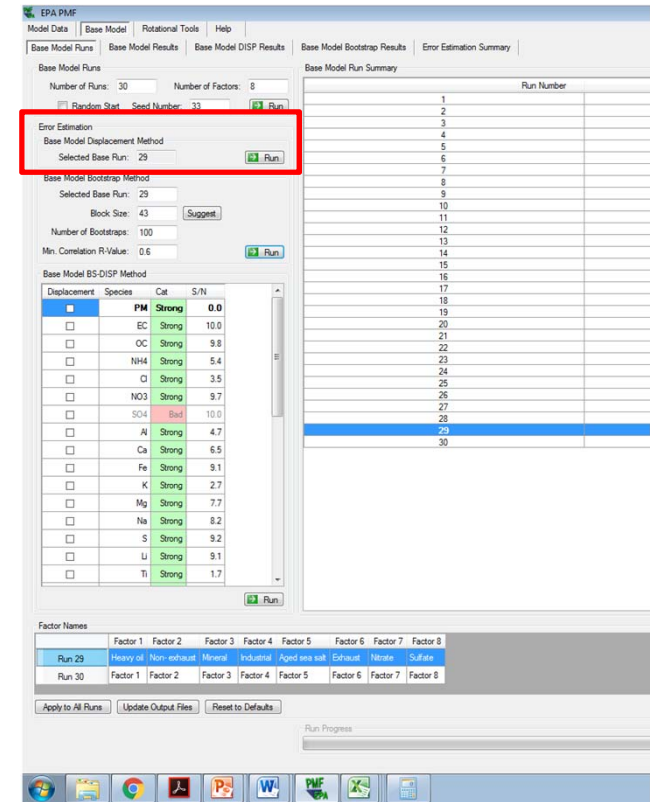


DISP

Only on strong species.
 Valid only if data uncertainties
 are reliable
 Invalid if $Q/Q_{exp} > 10$

Diagnostics:

- Error code: 0
- Second value $< 1\%$
- Number of swaps



Case 1. Small Errors	Case 2. Realistic Errors	Case 3. Simple Errors + 1 extra factor modeled
0 -0.111	0 0.000	0 -2.557
0 0 0 0	0 0 0 0	6 5 3 0 14
0 0 0 0	0 0 0 0	8 6 4 1 19
0 0 0 0	0 0 0 0	8 7 4 1 20
0 0 0 0	0 0 0 0	8 8 5 1 22



Displacement

- Assesses the largest range of source profile values without an appreciable increase in the Q-value
- For example, if 20 species are in a data set and a 7-factor model has been fitted, then the DISP method will estimate $20 \times 7 = 140$ intervals for each dQmax value.
- The model generates results for the following dQMax values: 4, 8, 15, and 25. Plots are only shown for dQmax of 4

The screenshot shows the EPA PMF software interface. The 'Base Model DISP Results' tab is active. A red box highlights the 'Base Model Displacement Method' section, which includes a 'Selected Base Run' dropdown set to 29 and a 'Run' button. Below this is a table of species displacement results.

Displacement	Species	Cat	S/N
<input checked="" type="checkbox"/>	PM	Strong	0.0
<input type="checkbox"/>	EC	Strong	10.0
<input type="checkbox"/>	OC	Strong	9.8
<input type="checkbox"/>	NH4	Strong	5.4
<input type="checkbox"/>	O	Strong	3.5
<input type="checkbox"/>	NO3	Strong	9.7
<input type="checkbox"/>	SO4	Weak	10.0
<input type="checkbox"/>	Al	Strong	4.7
<input type="checkbox"/>	Ca	Strong	6.5
<input type="checkbox"/>	Fe	Strong	9.1
<input type="checkbox"/>	K	Strong	2.7
<input type="checkbox"/>	Mg	Strong	7.7
<input type="checkbox"/>	Na	Strong	8.2
<input type="checkbox"/>	S	Strong	9.2
<input type="checkbox"/>	Li	Strong	9.1
<input type="checkbox"/>	Ti	Strong	1.7

At the bottom of the interface, there is a table of factor names for Run 29 and Run 30.

Factor Names	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6	Factor 7	Factor 8
Run 29	Heavy oil	Non-exhaust	Mineral	Industrial	Aged sea salt	Exhaust	Nitrate	Sulfate
Run 30	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6	Factor 7	Factor 8

DISP results

- 4 txt files generated (one for each dQmax)
- In each file, there is a line with two numbers, followed by four lines of data. In the first line, the first value is an error code: 0 means no error; 6 or 9 indicates that the run was aborted; 6 indicates there were too many swaps, and 9 indicates Q decreased too much. If this first value is non-zero, the DISP analysis results are considered invalid. The second value is the largest observed drop of Q during DISP.
- Below the first line is a four-line table that contains swap counts for factors (columns) for each dQmax level (rows). The first row is for dQmax = 4, the second row dQmax=8, the third dQmax=15 and the fourth dQmax=25. The swap counts are a key indicator of the stability of a PMF solution and swaps at dQmax = 4 or the first row in the table indicate that the solution should not be interpreted.

	0	-0.015
0	0	0
0	0	0
0	2	1
1	9	4

DISPres1.txt

=0 <1% (otherwise it was not a global minimum)

6f_DISPres1: Bloc de notas

Archivo Edición Formato Ver Ayuda

0	0	-0.015			
0	0	0	0	0	0
0	0	0	0	0	0
0	2	1	2	0	3
1	9	4	6	1	7

factors

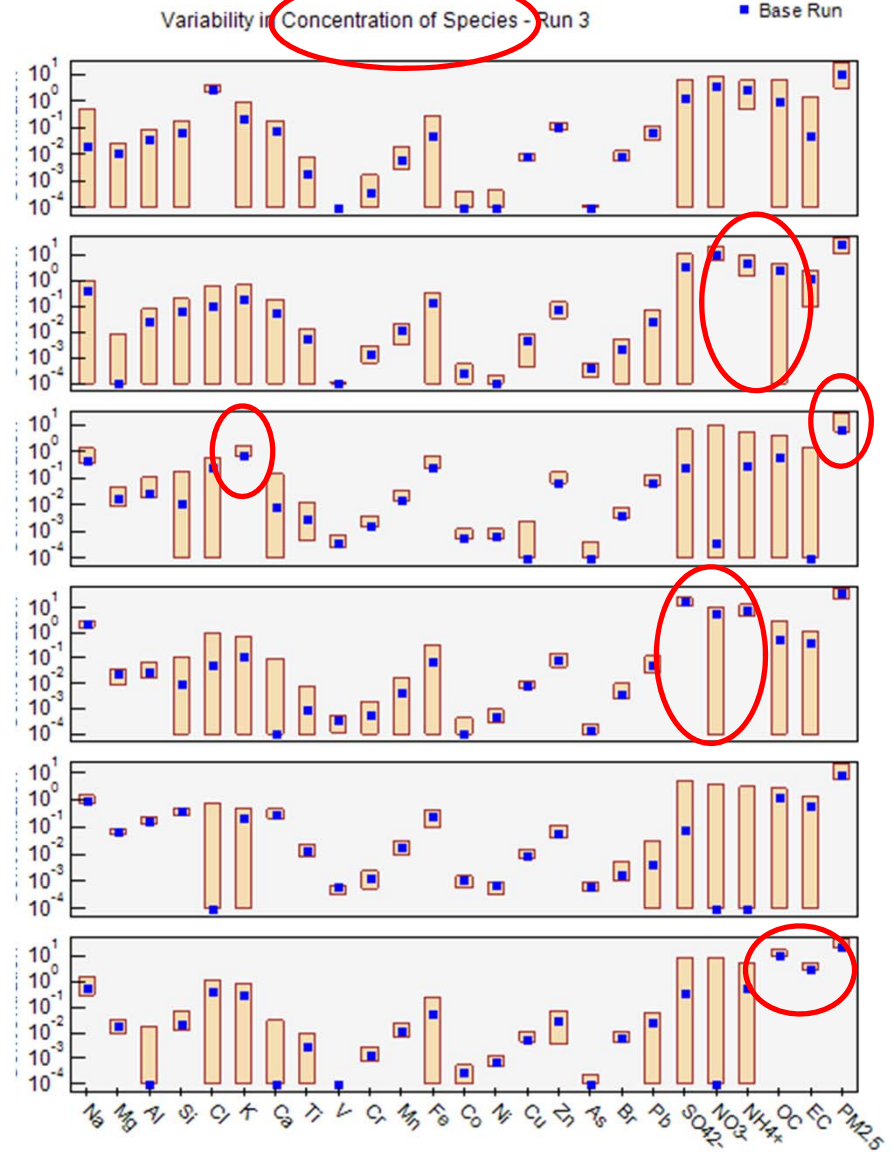
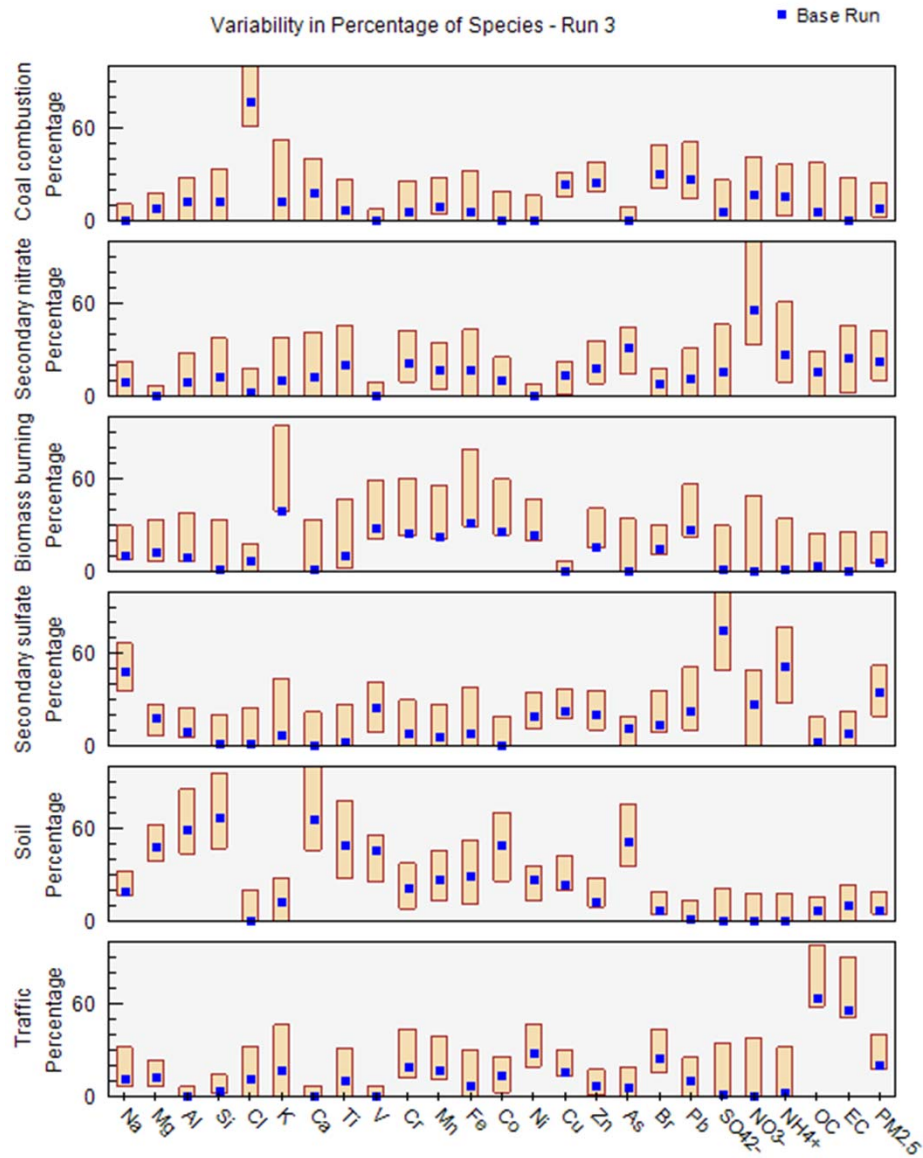
0.00000E+00	0.00000E+00	0.36258E+00	0.16112E+01	0.74664E+00	0.29333E+00
0.00000E+00	0.00000E+00	0.85038E-02	0.86904E-02	0.52903E-01	0.98530E-02
0.00000E+00	0.00000E+00	0.18424E-01	0.15908E-01	0.12515E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.24725E+00	0.12105E-01
0.21387E+01	0.00000E+00	-0.11352E-15	0.00000E+00	0.00000E+00	-0.16233E-15
0.00000E+00	0.00000E+00	0.67734E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	-0.72599E-18	0.00000E+00	-0.23703E-25	0.20063E+00	-0.16314E-19
0.00000E+00	-0.74138E-18	0.48127E-03	0.00000E+00	0.78294E-02	0.00000E+00
0.00000E+00	0.00000E+00	0.26015E-03	0.11572E-03	0.31990E-03	0.00000E+00
0.00000E+00	0.60598E-03	0.15104E-02	0.00000E+00	0.53472E-03	0.79752E-03
0.26314E-02	0.31792E-02	0.13596E-01	0.00000E+00	0.87318E-02	0.72483E-02
-0.12254E-16	0.00000E+00	0.24200E+00	0.00000E+00	0.90784E-01	0.00000E+00
0.00000E+00	0.00000E+00	0.51186E-03	0.00000E+00	0.56508E-03	0.55116E-04
0.00000E+00	0.00000E+00	0.53203E-03	0.28104E-03	0.33932E-03	0.51803E-03
0.55038E-02	0.40191E-03	0.00000E+00	0.60574E-02	0.68132E-02	0.46162E-02
0.77652E-01	0.33606E-01	0.63261E-01	0.43343E-01	0.38737E-01	0.35498E-02
0.00000E+00	0.17803E-03	0.00000E+00	-0.53889E-19	0.45405E-03	0.00000E+00
0.56773E-02	0.00000E+00	0.30019E-02	0.24781E-02	0.10566E-02	0.42132E-02
0.33266E-01	0.00000E+00	0.51553E-01	0.24174E-01	-0.74245E-19	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.11134E+02	-0.41297E-16	0.00000E+00
-0.50713E-15	0.66076E+01	0.00000E+00	-0.18024E-14	0.00000E+00	0.00000E+00
0.48952E+00	0.14829E+01	-0.18095E-16	0.44621E+01	0.00000E+00	0.00000E+00
0.00000E+00	-0.11876E-14	0.00000E+00	0.00000E+00	0.00000E+00	0.94964E+01
-0.32456E-17	0.99727E-01	0.00000E+00	0.00000E+00	0.00000E+00	0.26317E+01
0.30323E+01	0.11362E+02	0.57497E+01	0.21347E+02	0.53832E+01	0.19782E+02
0.10000E+01	0.10000E+01	0.10000E+01	0.10000E+01	0.10000E+01	0.10000E+01
0.48502E+00	0.10071E+01	0.13397E+01	0.29933E+01	0.14615E+01	0.14494E+01
0.24150E-01	0.84587E-02	0.44576E-01	0.36555E-01	0.84498E-01	0.32541E-01
0.80066E-01	0.79066E-01	0.10960E+00	0.70473E-01	0.24325E+00	0.17829E-01
0.17711E+00	0.19501E+00	0.17525E+00	0.10610E+00	0.50078E+00	0.73016E-01
0.37118E+01	0.64600E+00	0.60867E+00	0.88399E+00	0.70764E+00	0.11356E+01
0.89997E+00	0.66024E+00	0.16297E+01	0.74406E+00	0.48002E+00	0.80078E+00
0.17706E+00	0.18291E+00	0.14854E+00	0.96891E-01	0.44473E+00	0.30580E-01
0.76319E-02	0.13102E-01	0.13082E-01	0.73221E-02	0.22308E-01	0.87399E-02
0.93671E-04	0.11059E-03	0.74463E-03	0.51560E-03	0.70129E-03	0.92188E-04
0.16922E-02	0.28146E-02	0.39934E-02	0.19444E-02	0.24731E-02	0.28792E-02
0.17842E-01	0.21843E-01	0.35691E-01	0.16914E-01	0.28995E-01	0.24774E-01
0.26800E+00	0.35375E+00	0.65382E+00	0.31139E+00	0.42880E+00	0.24761E+00
0.41801E-03	0.54879E-03	0.12914E-02	0.41329E-03	0.15206E-02	0.55606E-03
0.43281E-03	0.20101E-03	0.12307E-02	0.91588E-03	0.94802E-03	0.12355E-02
0.10689E-01	0.78065E-02	0.22846E-02	0.12488E-01	0.14574E-01	0.10254E-01
0.15943E+00	0.14861E+00	0.16910E+00	0.14993E+00	0.11615E+00	0.72645E-01
0.11745E-03	0.56315E-03	0.42743E-03	0.23638E-03	0.95378E-03	0.23310E-03
0.13061E-01	0.48237E-02	0.81013E-02	0.94702E-02	0.50233E-02	0.11547E-01
0.11795E+00	0.71695E-01	0.13097E+00	0.11624E+00	0.31153E-01	0.58259E-01
0.60654E+01	0.10736E+02	0.68367E+01	0.24065E+02	0.48784E+01	0.79826E+01
0.82949E+01	0.20531E+02	0.97803E+01	0.97152E+01	0.36706E+01	0.75253E+01
0.59058E+01	0.99258E+01	0.55331E+01	0.12656E+02	0.29085E+01	0.52296E+01
0.61198E+01	0.46719E+01	0.39761E+01	0.29979E+01	0.25414E+01	0.16264E+02
0.14293E+01	0.23864E+01	0.13337E+01	0.11272E+01	0.12152E+01	0.47247E+01
0.27258E+02	0.47553E+02	0.28445E+02	0.57829E+02	0.21094E+02	0.45030E+02

species

4 matrixes

- (1) the profile matrix upper bound, in concentration units;
- (2) the profile matrix lower bound, in concentration units;
- (3) the profile matrix upper bound, in % species units;
- (4) the profile matrix lower bound, in % species

DISP box plots



Coal combustion Secondary nitrate Biomass burning Secondary sulfate Soil Traffic

DISP intervals

Small DISP range for tracers

Down to zero for:

- NO₃ in Sulfate

- Ions and C in Soil

BB likely contributes more (K)

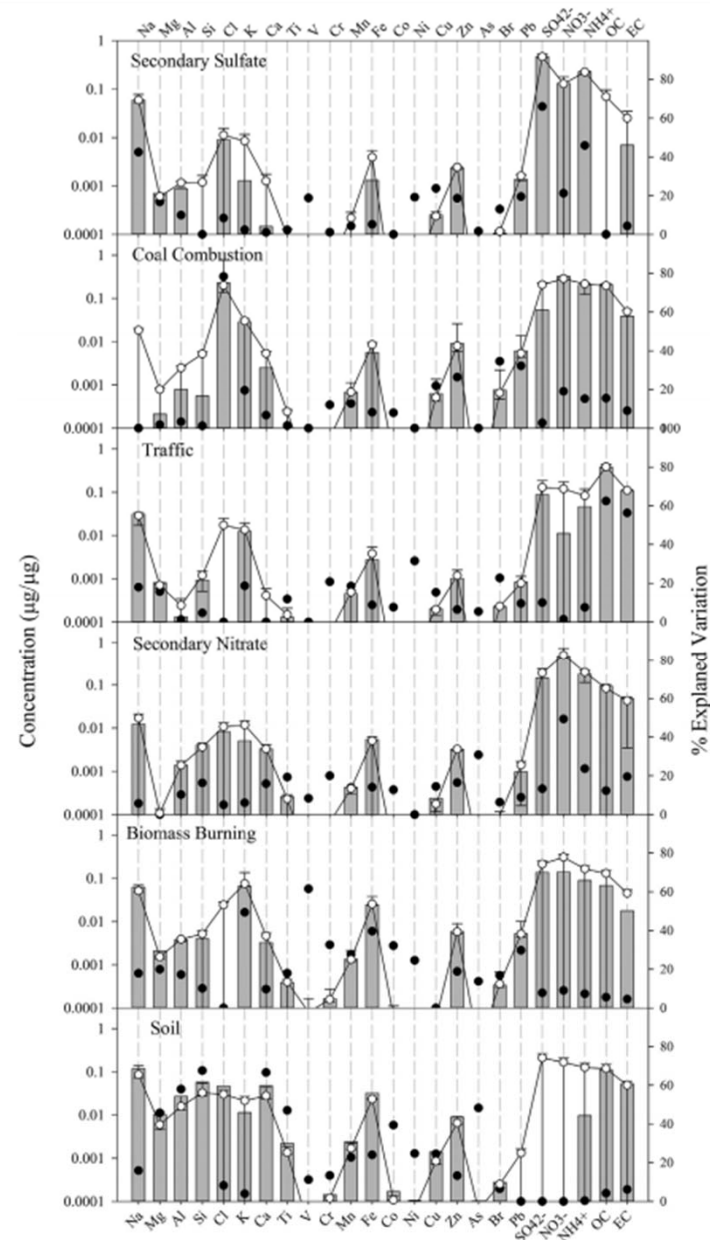


Fig. 2. The source profiles (bars represent mass contribution, open circles represent the mean DISP values with the error bars providing the confidence intervals, the lines are drawn to guide the eye, y-axis on the left; filled circles represent contribution in percentage, y-axis on the right).

BS-DISP

- Only key and major species
 - Long computation times
1. Each DISP defines the span of rotationally accessible space.
 2. Each BS resample moves this space around, randomly in different directions.
 3. Taken together, all the replications of the rotationally accessible space, in random locations, represent both the random uncertainty and the rotational uncertainty.

The screenshot displays the BS-DISP software interface with the following sections:

- Base Model Runs:** Number of Runs: 20, Number of Factors: 6, Seed: random, Run button.
- Error Estimation:** Base Model Bootstrap Method, Selected Base Run: 10, Block Size: 22, Number of Bootstraps: 100, Min. Correlation R-Value: 0.6, Run button.
- Base Model BS-DISP Method:** A table with columns Displacement, Species, Cat, and S/N. The 'Zinc' row is selected.
- Base Model Displacement Method:** Selected Base Run: 10, Run button.
- Factor Names:** A table with columns Factor 1 through Factor 6. Run 10 is selected.
- Base Model Run Summary:** A table with columns Run Number and values 1 through 20. Run 10 is highlighted.

Displacement	Species	Cat	S/N
<input type="checkbox"/>	Titanium	Strong	1.4
<input checked="" type="checkbox"/>	Total Nitrate	Strong	1.9
<input type="checkbox"/>	Vanadium	Weak	0.9
<input checked="" type="checkbox"/>	Zinc	Strong	2.0

Run Number
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20

Factor Names	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6
Run 10	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6
Run 11	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6
Run 12	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6



BS-DISP diagnostic

Ideally

- N° of runs+1
- <1%
- Zero values
- 0 in first row

Model Data | Base Model | Rotational Tools | Help

Base Model Runs | Base Model Results | Base Model Bootstrap Results | **Base Model BS-DISP Results** | Base Model DISP Results

BS-DISP Box Plots | **BS-DISP Summary**

101	-0.190	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0

The five values in the first line are:

(1) k = # of cases in the file (includes both the full-data case and the accepted (not rejected) resamples). If no cases were excluded, k should be equal to the number of bootstraps * number of factors * number of species selected for BS-DISP.

(2) Largest decrease of Q. A large value is not alarming in itself, it only says that there was at least one resample where a deeper minimum appeared.

(3,4,5) # of cases with: /drop of Q / swap in best fit / swap in DISP/

Below the first line is a table (four lines) which contains swap counts for factors (columns) for each dQmax level (rows), which are in descending order dQmax=0.5, 1, 2, 4. If swaps are present in the first line for the lowest dQmax, it indicates the solution is not well constrained, and should not be used.

Detailed BS-DISP results are included in the *_BSDISPresi-4.txt files (corresponding to the four dQmax levels) in the output folder.

Note: BS-DISP intervals include effects of random errors and rotational ambiguity. For modeling errors, if user misspecifies standard deviation of data, BS-DISP results are more robust than for DISP since the DISP phase of BS-DISP does not displace as strongly as DISP by itself.

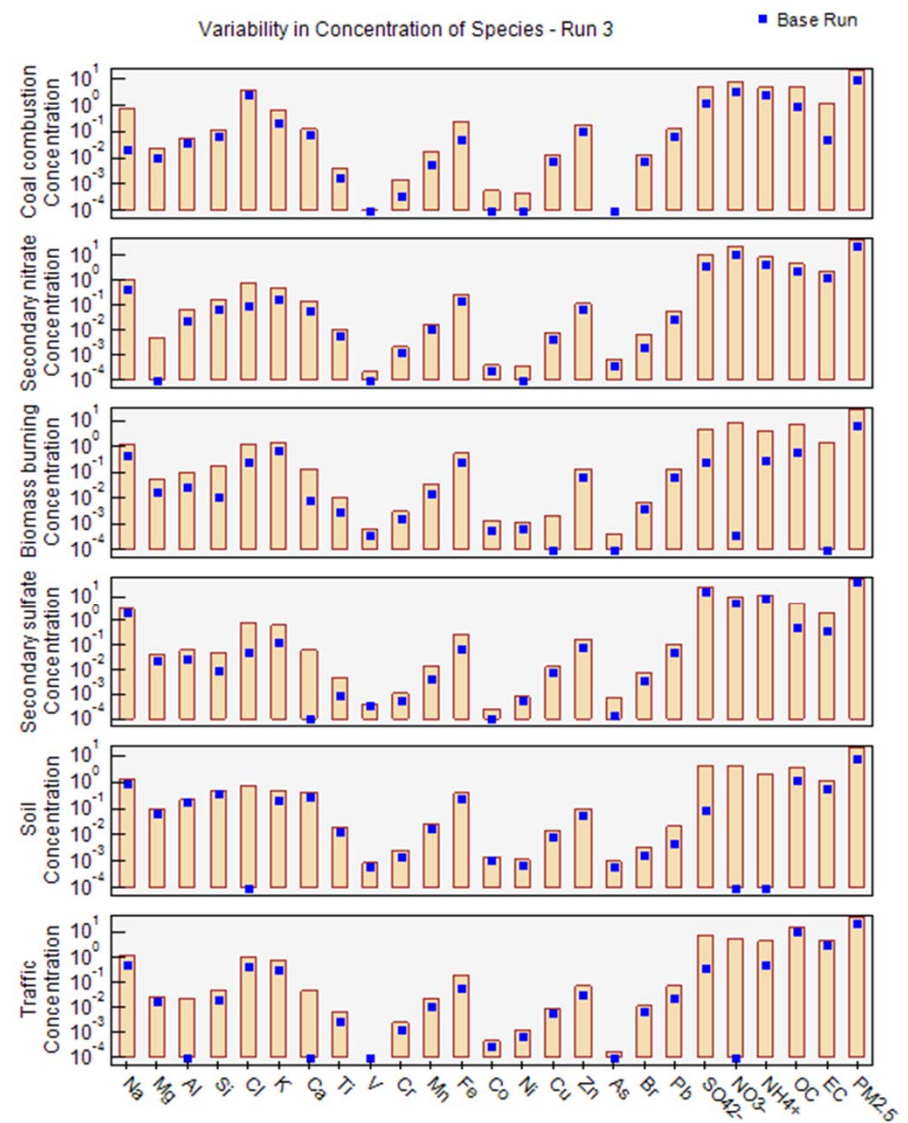
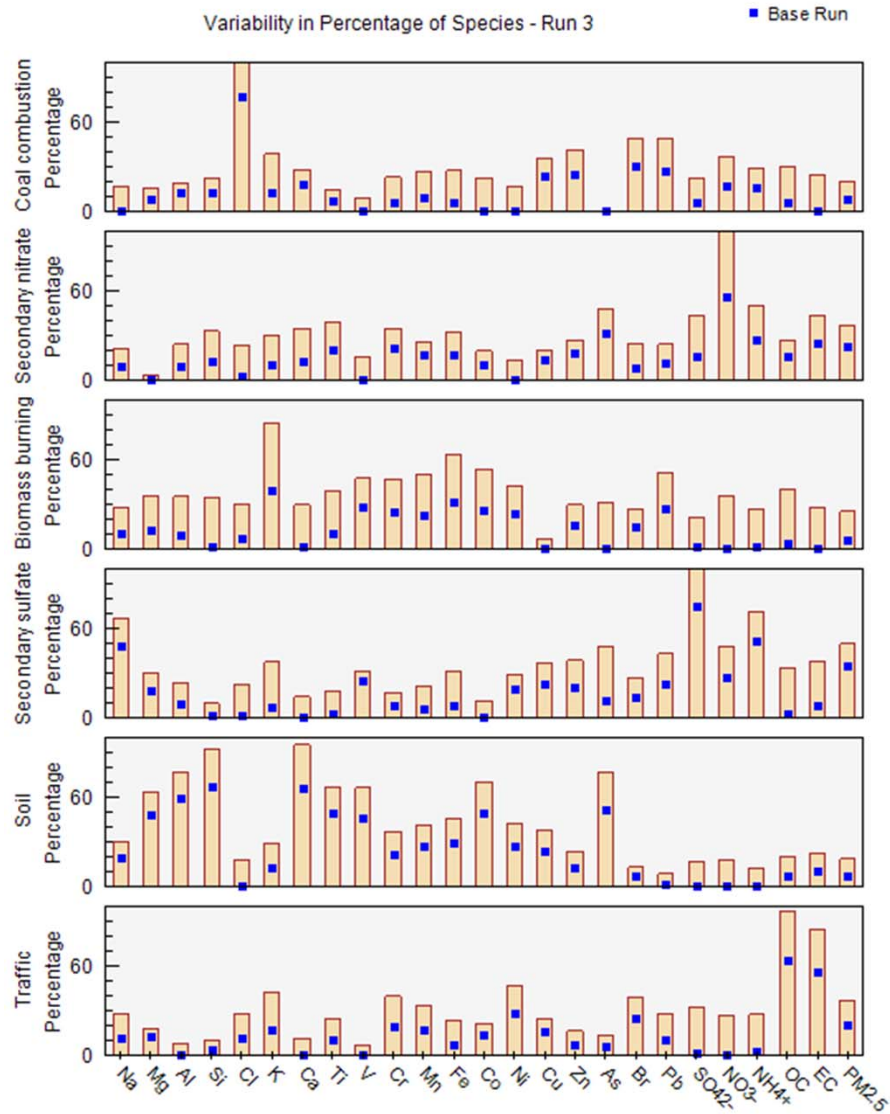


BS-DISP: three examples

51 -0.209 0 0 0	39 -21.149 8 0 4	11 -0.461 0 0 135
0 0 0 0	0 0 0 0	7 40 27 1 54
0 0 0 0	1 0 2 1	9 52 44 1 71
0 0 0 0	1 0 2 1	18 59 53 1 93
0 0 0 0	2 1 4 1	26 67 66 1 113



BS-DISP



Coal combustion Secondary nitrate Biomass burning Secondary sulfate Soil Traffic

BS-DISP summary

EPA PMF

Model Data | Base Model | Rotational Tools | Help

Base Model Runs | Base Model Results | Base Model Bootstrap Results | Base Model DISP Results | Base Model BS-DISP Results | Error Estimation Su

BS-DISP Box Plots | BS-DISP Summary

	3	-0.069	0	1	17
0.5	0	0	2	0	2
1	0	1	4	0	3
2	1	4	6	0	3
4	2	10	14	2	9

The five values in the first line are:

(1) # of cases used in BS-DISP, i.e., the base run plus the number of accepted (not rejected) resamples. If all cases were accepted, then this value will be the number of bootstraps + 1.

(2) Largest decrease of Q. A large value is not alarming in itself, it only says that there was at least one resample where a deeper minimum appeared.

(3,4,5) # of cases with: /drop of Q / swap in best fit / swap in DISP phase/

Below the first line is a table (four lines) which contains swap counts for factors (columns) for each dQmax level (rows), which are in descending order dQmax=0.5, 1, 2, 4. If swaps are present in the first line for the lowest dQmax, it indicates the solution is not well constrained, and caution used when interpreting the solution.

Detailed BS-DISP results are included in the *_BSDISPres1-4.txt files (corresponding to the four dQmax levels) in the output folder.

Note: BS-DISP intervals include effects of random errors and rotational ambiguity.

Error Estimation summary

