

We want to thank the reviewers for their support of the paper and their helpful comments and suggestions which have helped to improve our manuscript. We provide a point by point response to review.

Response to Anonymous Referee #1

General comments:

This study conducted a preliminary assessment of the impacts of multiple temporal-scale variations in PM data (using Kolmogorov-Zurbenko filter) on chemical species and source apportionment results, and tried to determine what processes/sources are responsible for the main variation characteristics. The method in this manuscript might be useful in the future PM source apportionment and air pollution studies. However, there are a few questions that are needed to be addressed before considering acceptance of this work by Atmospheric Chemistry and Physics.

1. The authors should clarify the physical meaning of the four different TS components.

Response: We have explained the physical meaning of the four TS components. The revised manuscript now have:

“ $X_{(intra-day)}$, is concentration dataset of the intra-day component that relates to fast-acting, local emission sources, and local-level processes. $X_{(diurnal)}$ is concentration dataset of the diurnal component that reflects the source diurnal variation. $X_{(synoptic)}$ is concentration dataset of the synoptic component that is influenced by weather patterns and short-term fluctuations in emissions. $X_{(baseline)}$ is concentration dataset of the baseline component that might link to seasonal or long-term scale variation in emissions, climate, policy, etc.”.

2. The authors should further clarify the different results from Figure 1 and Figure 2.

For example, as shown in Figure 1, it seems that only variations of secondary inorganic

species (e.g., SO_4^{2-} , NO_3^- , NH_4^+) are more influenced by baseline TS component, and the relative influence by synoptic TS component was higher compared to baseline TS component. However, the results indicated by Figure 2 show that baseline TS component dominates the concentrations of $\text{PM}_{2.5}$ and chemical species.

Response: According to Table 1, synoptic TS component is the largest contributor to the total variance of the three ions concentrations, followed by baseline TS component for SO_4^{2-} and NH_4^+ and diurnal TS component for NO_3^- concentrations. Synoptic TS component had higher relative contributions to the total variance of secondary species compared to baseline TS component. However, Figure 1 shown the synoptic TS component not only increased the secondary species concentrations (>0) but decreased the values (<0) during the sampling campaign resulting in the small influence on the average concentrations of secondary species. Baseline TS component had higher concentration levels of secondary species although it had a little impact on the variations of secondary species. The baseline TS component has a small influence on the variations of species, including OC, EC, Ca, Fe. Figure 1 shown higher concentration levels of baseline TS component than the other three TS components, suggesting the baseline TS component is the bigger contributor to the species (OC, EC, Ca, Fe) average concentrations. Therefore, the results shown in Figures 1 and 2 were consistent that baseline TS components dominated the average concentrations of $\text{PM}_{2.5}$ and chemical species.

Table 1. Relative contributions (%) of the different TS components to the total variance of PM_{2.5} and chemical species concentrations.

	NO ₃ ⁻	SO ₄ ²⁻	NH ₄ ⁺	OC	EC	Ca	Fe	SOC	PM _{2.5}
Intra-day (%)	5	4	4	9	17	40	20	9	9
Diurnal (%)	36	18	17	23	47	45	32	20	36
Synoptic (%)	32	48	54	56	28	10	32	62	32
Baseline (%)	27	31	26	12	8	5	16	9	24

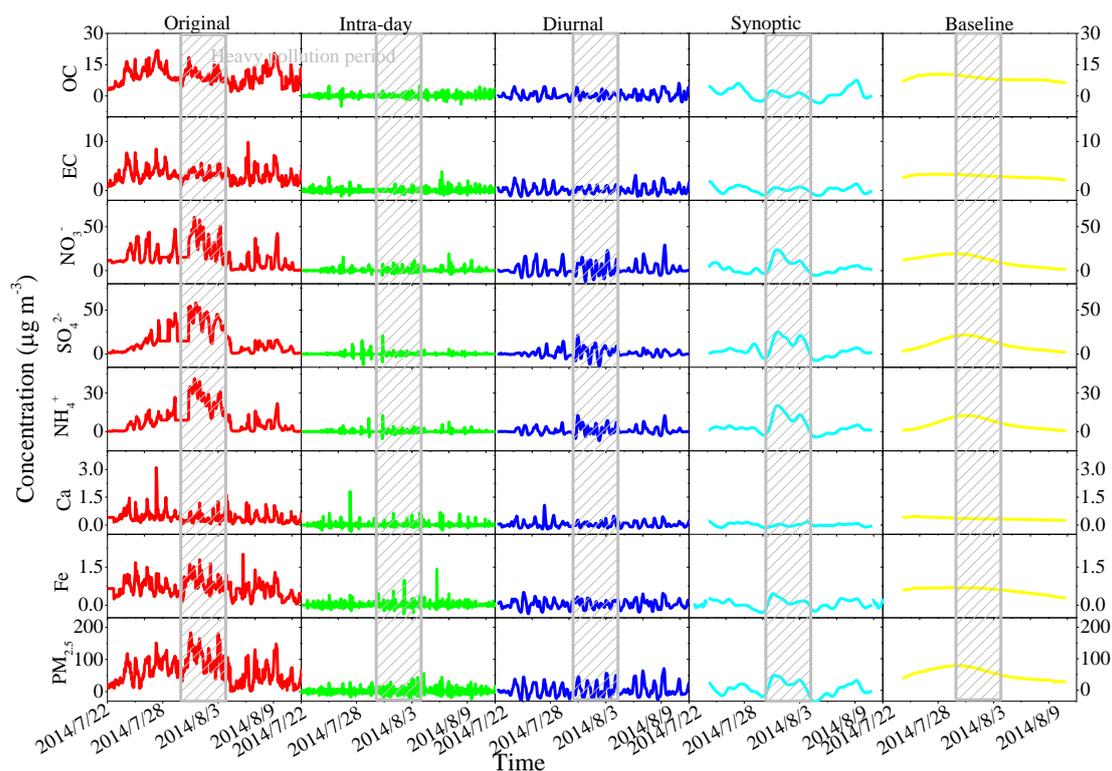


Figure 1. The variance of PM_{2.5} and chemical species concentrations influenced by intra-day (period less than 12 h), diurnal (12-24 h), synoptic (2-21 days), and baseline (greater than 21 days) temporal-scale (TS) components, for the period of 22 July 2014 to 13 Aug 2014 at Beijing, China. The variation of species that originated from primary sources mainly was influenced by diurnal TS components. The variation of ions and OC (partly from the secondary formation) that originated from secondary formation primarily were affected by synoptic TS component. The vertical gray lines demarcate the heavy pollution period.

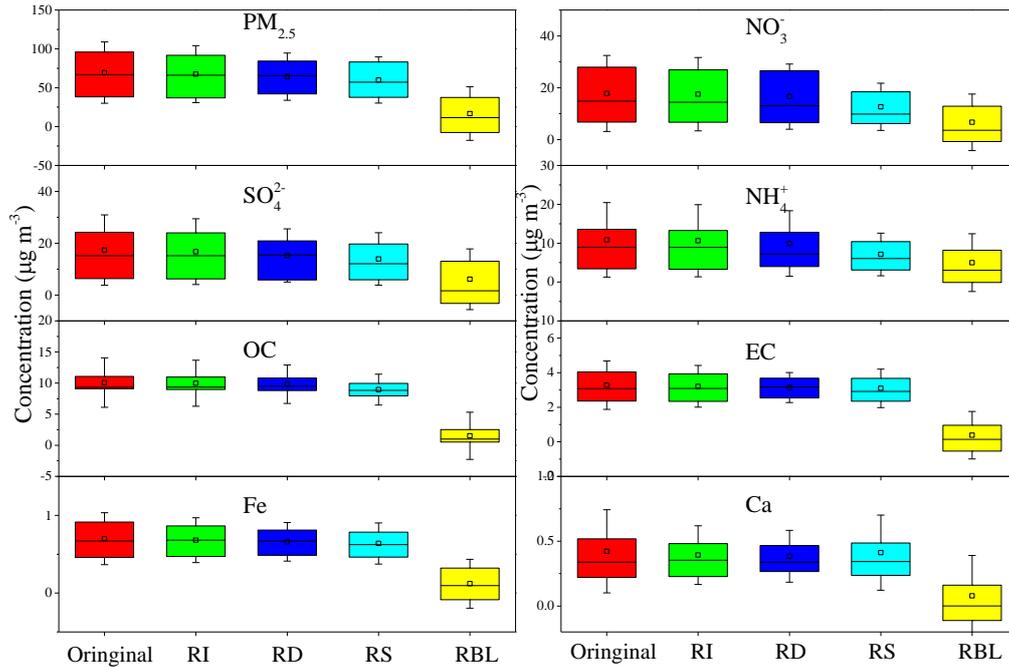


Figure 2. The influence of different TS components on the average concentrations of $PM_{2.5}$ and chemical species (Beijing site). The baseline TS component dominated the $PM_{2.5}$ and chemical species average concentrations. The figure shows box plots of individual chemical species from the original, RI, RD, RS, and RBL datasets. Cubes denote the average and dashes denote the median concentration. The whiskers are the standard deviation. (RI: intra-day removed dataset, RD: diurnal removed dataset, RS: synoptic removed dataset, RBL: baseline removed dataset).

3. The different source profiles obtained from ME-2 look not quite good in the source apportionment results part. For example, chemical species profiles for coal combustion and vehicle emissions look quite similar both in Figure 3 and Figure S6; and there are high OC fractions exist in the “Nitrate source”. The authors should verify their source apportionment results and give more robust results and explanations.

Response: Given that coal combustion, vehicle emissions, and crustal dust are collinearity sources that have similar profiles (Shi et al., 2009; Shi et al., 2011; Zhang et al., 2013), and that the absence of marker species (Si, Al, etc.) in the source profiles increased their collinear and uncertainties (Peng et al., 2016), these lead to difficulties

in completely separating the three sources. We identified vehicle emissions and coal combustion according to the criterion that OC and EC fraction in vehicle emissions are higher than the values in coal combustion. We also analyzed the correlations of time series between source contributions and gaseous pollutants (SO_2 , NO, NO_2) and diurnal patterns of source contribution (Figure S8). Correlation analysis showed vehicle emission has a significant correlation with NO (ranging from 0.1 to 0.3, $p < 0.01$) and NO_2 (ranging from 0.2 to 0.3, $p < 0.01$). Correlation between coal combustion and SO_2 ranged from 0.4 ($p < 0.01$) to 0.6 ($p < 0.01$), for the four datasets. For the results of the original dataset, vehicle emissions exhibited a relatively high contribution to $\text{PM}_{2.5}$ during the nighttime, suggesting that diesel vehicles appeared and emitted pollutants during the nighttime (Gao et al., 2016). Coal combustion showed a stable diurnal trend, and crustal dust has high contributions from 0:00 to 12:00. The diurnal pattern of secondary formation primarily dominated by nitrate that peaked in the early morning and at nighttime (Xu et al., 2014). Source diurnal trends estimated from RI dataset similar with results from original dataset, implying the small influences of intra-day TS component on the source diurnal trends. For the results from RS dataset, secondary formation (sulfate source) presented a broad peak during the daytime and might link to photochemical processes of sulfate. For results from RD and BL datasets, it is an expected result that all of four sources did not show obvious diurnal trends after removing the diurnal TS component.

The result that high OC fractions exist in the “nitrate source” is similar to other reporters (Xie et al., 2008; Huang et al., 2017; Masiol et al., 2017; Srivastava et al., 2018). PMF does not need source profiles as model input but require receptor data. It is possible that one factor includes multiple sources and combine other chemical components in the factor profile except for the source markers (Canepari et al., 2009; Lee et al., 2009). We exhibited the percentage fraction (%) of source profiles to make them more distinguishing (Figure 3 and S11).

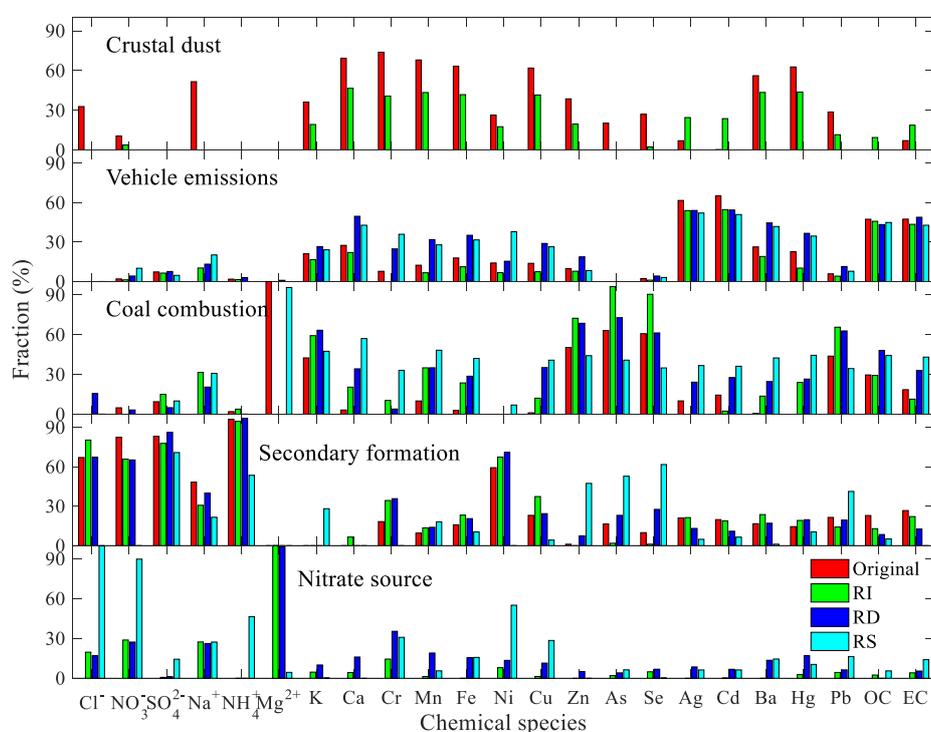


Figure 3. The influence of different TS components on source determination (Beijing site). Crustal dust was not identified from the RD and RS datasets. Nitrate source and sulfate source were identified from the RS dataset. RBL dataset was investigated by PCA analysis instead of ME-2 due to the dataset has some negative values. Note: The factor 4 solution was generated by removing the synoptic dataset and represents the sulfate source.

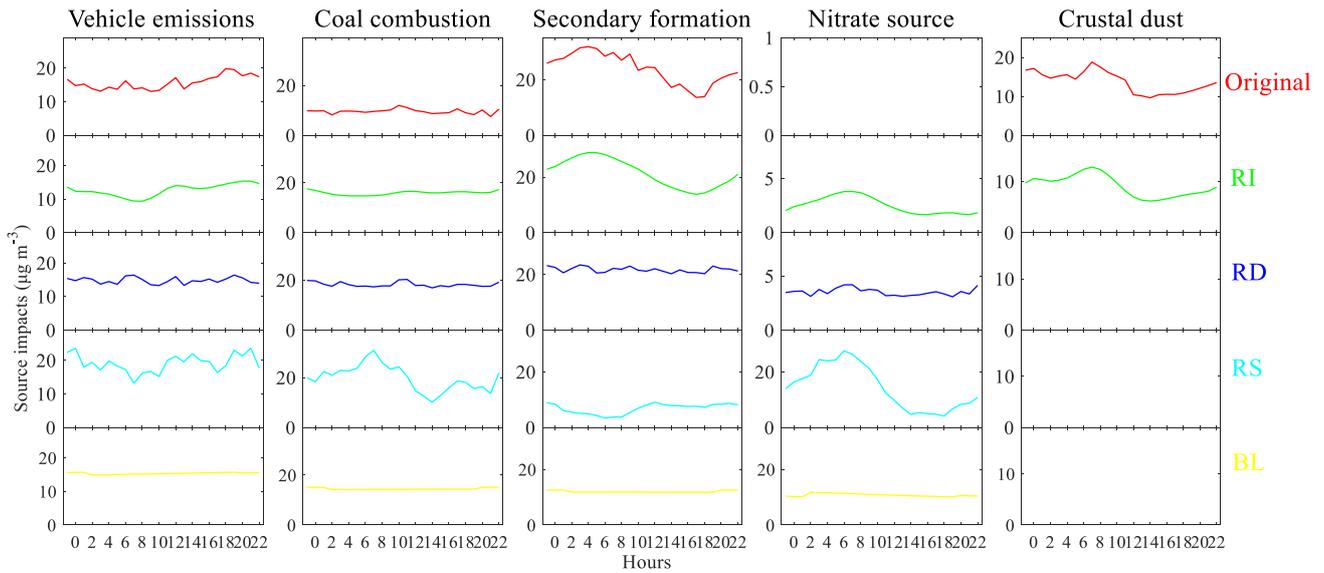


Figure S8. Diurnal trend of Source impacts for each source (vertical columns) and each dataset (horizontal rows) (Beijing site). The blanks mean that the source has not been identified.

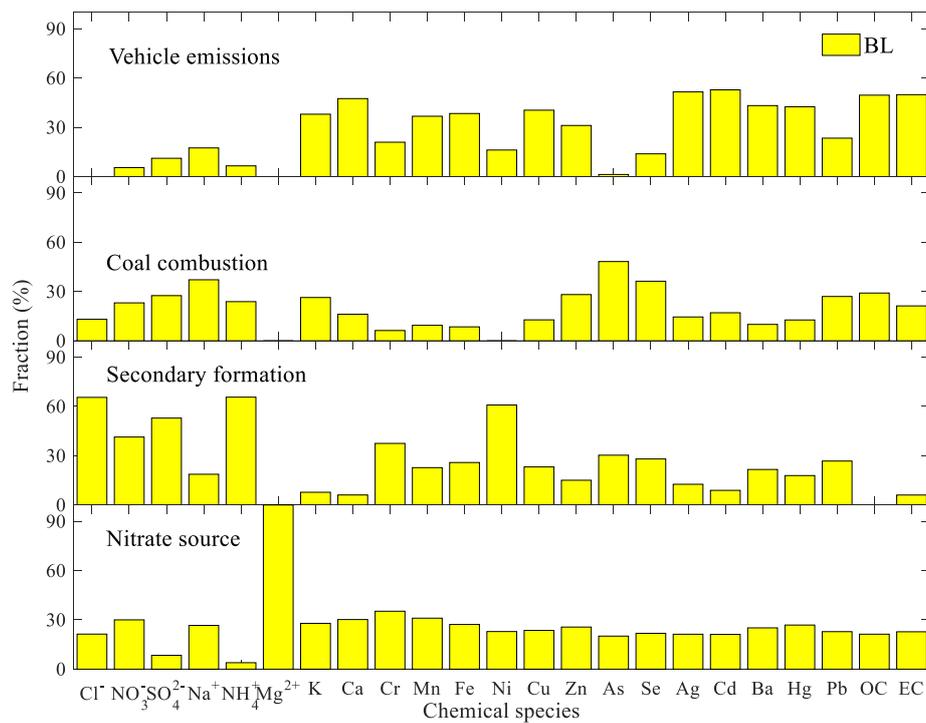


Figure S11. The factor profiles obtained from ME-2 from baseline dataset (Beijing site).

4. The authors should carefully check their manuscript. There are some mistakes and inconsistencies in the context and figures. Grammar modification is needed.

Response: In this work, Original, RI, RD, RS, and BL datasets were run by ME-2,

respectively. RBL dataset was investigated by PCA due to negative values (about 40%) of the RBL dataset and non-negative requirement of ME-2. The discussion about the BL and RBL datasets has been checked and revised to make it clearer. The grammar on the manuscript and supplemental material also has been corrected.

Specific comments:

1) Page 4 Line 55: change to “such as local emission sources and weather conditions”.

Response: The sentence has been changed to “Variations in aerosol concentrations and chemical species reflect influences from multiple factors, such as local emission sources and weather conditions, etc.”

2) Page 4 Line 78: change “key drivers” to “one of the key drivers”?

Response: The “key drivers” has been changed to “one of the key drivers”.

Revisions made in the manuscript:

“Pollution sources are one of the key drivers of aerosol pollution.”.

3) Page 9 Line 158-172: please clearly definite the abbreviations, such as Q_{main} , Q_{aux} , a_{kj} .

Response: The explanation for three abbreviations has been added to the revised manuscript. Q_{enh} is the object function that the model aims to minimize it. Q_{main} is the main part of object function that from main or data fitting equations. Q_{aux} is the auxiliary part of object function from the auxiliary equations. a_{kj} is the target factor loading that f_{kj} is pulled toward by employing the auxiliary equation.

Revisions made in the manuscript:

“Auxiliary equations are included as additional terms Q_{aux} in an enhanced object function Q_{enh} (Amato et al., 2009; Amato and Hopke, 2012), the equation can be written as follows:

$$Q_{enh} = Q_{main} + Q_{aux} \quad (3)$$

Q_{main} is the main part of object function that from main or data fitting equations. Q_{aux} is the auxiliary part of object function from the auxiliary equations. The task of ME-2 is to calculate a minimum Q_{enh} value or balance the minimization of the values Q_{main} and Q_{aux} in the iterative process (Paatero and Hopke, 2009). The term Q_{main} is described as follows:

$$Q_{main} = \sum_{i=1}^m \sum_{j=1}^n (e_{ij}/\sigma_{ij})^2 \quad (4)$$

where σ_{ij} is the uncertainty in the j^{th} species for the i^{th} sample; e_{ij} has the same meaning as is described in Eq.(2).

The typical auxiliary equation, pulling equation, can be written as follows:

$$Q_{aux} = \frac{(f_{kj} - a_{kj})^2}{\sigma_{kj}^{aux^2}} \quad (5)$$

where σ_{kj}^{aux} is the uncertainty connected to the pulling equation or softness of the pull. f_{kj} is the element of factor loading. a_{kj} is the target factor loading that f_{kj} is pulled toward by employing the auxiliary equation.”

4) Page 10 Line 185: The authors should clarify what m values (the length of the moving average window) they used and what should be considered.

Response: The parameters m and k control the separating frequency according to the

Eq.(8). It needs to find the m and k that produce a separating frequency (w) closest to a given separating frequency (w_0). In this work, the wavelet analysis method used to analyze the periodicities and determine the separating frequency (w_0) for KZ filter. Because the study of finding appropriate m and k for a given separating frequency has been conducted and confirmed in many previous works, this work referred to the KZ filter parameters reported by the Hogrefe et al. (2000) study that selected $KZ_{3,3}$, $KZ_{13,5}$, and $KZ_{103,5}$. More details of parameter m have been added into the revised manuscript.

Revisions made in the manuscript:

“For the KZ filter, the first thing is to analysis the time series of pollutants in the periodicities and determine the separating frequency (w_0) for KZ filter. Then the next step is to select the appropriate parameters m and k that produce a separating frequency (w) closest to the w_0 . The study of finding appropriate m and k for a given separating frequency has been conducted and confirmed in many previous works (Rao et al., 1997; Hogrefe et al., 2000; Wise and Comrie, 2005; Hogrefe et al., 2006; Tchepel et al., 2010). The wavelet analysis method analyzed the $PM_{2.5}$ and chemical species’ periodicities before decomposing their concentrations time series. The results of wavelet analysis suggested that the periodicities of $PM_{2.5}$ and chemical species are mainly 4-8 h (<12 h), 16-32 h, and 128-256 h (6-10 day) (Figure S1, see the Supporting Information), which were similar to the results reported by Hogrefe et al. (2000). It suggested the separating frequencies in this works were closed to the values reported by Hogrefe et al. (2000). This work referred to the KZ filter parameters reported by the Hogrefe et al. (2000) study that selected $KZ_{3,3}$, $KZ_{13,5}$, and $KZ_{103,5}$. The separating frequency of $KZ_{3,3}$, $KZ_{13,5}$ and $KZ_{103,5}$ are about 0.09, 0.015 and 0.002 h^{-1} , respectively, and the corresponding

periods are 11, 64 and 510h, respectively.”

5) Page 10 Line 186: Grammar mistakes. Please revise the sentence “Then the y_t as the input data and calculate according to Eq.(6).”

Response: The sentence has been changed to “Then the first y_t ($y_t^{(1)}$) acts as the input data for the second y_t ($y_t^{(2)}$).

6) Page 10 Line 190: Grammar mistakes. Please revise the sentence “ $y_t(k)$ is removed the variations that frequency lower than w (cutoff frequency)”.

Response: The sentence has been changed to “ $y_t^{(k)}$ is the moving average without the variations of frequency lower than w (separating frequency)”.

7) Page 11 Line 202: change “was” to “were”.

Response: It has been changed in the revised manuscript.

Revisions made in the manuscript:

“The results of wavelet analysis suggested that the periodicities of PM_{2.5} and chemical species are mainly 4-8 h (<12 h), 16-32 h, and 128-256 h (6-10 day) (Figure S1, see the Supporting Information), which were similar to the results reported by Hogrefe et al. (2000).”.

8) Page 11 Line 202: Please give more descriptions in Figure S1. For example, what do the color bars and black lines represent?

Response: This is now more clearly stated in the revised manuscript and revised SI:

Figure S1 shown the wavelet power spectrum for the PM_{2.5} and chemical species time series. The black line encloses regions suggested the corresponding periods were the significant periodicities of the species. In figure S1, the regions enclosed by black line occurred at the periods about 4-8 h, 16-32h, and 128-256h.

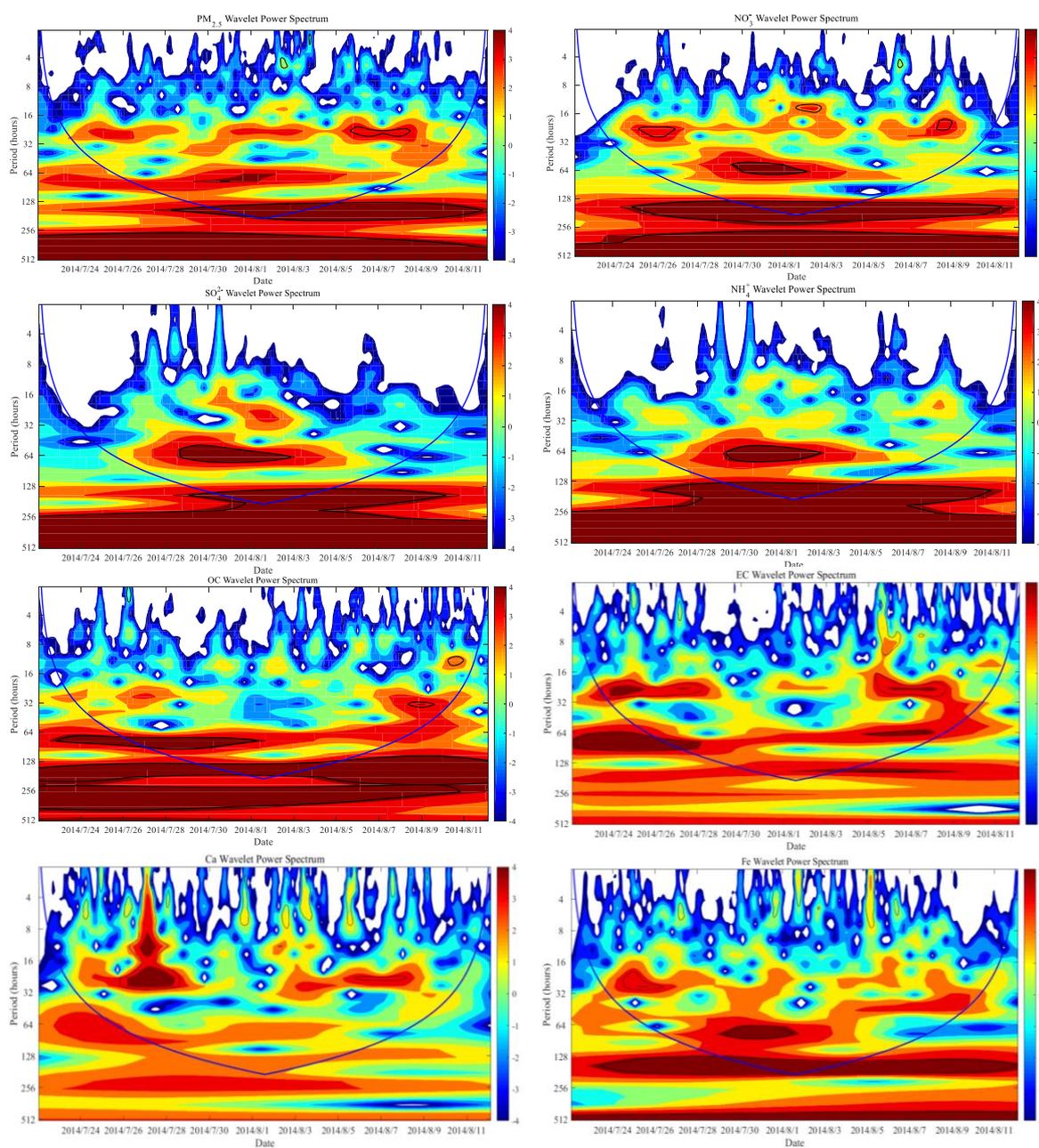


Figure S1. The wavelet variance diagrams of PM_{2.5} and chemical species from original data (Beijing site). The black line encloses regions of greater than 95% confidence, suggesting the corresponding periods (y axis) are the significant periodicities of the species. The blue line outside regions indicates the "cone of influence", where edge effects become important. The regions outside the blue line are

not considered, although they are enclosed by the black line. The color bar presents real part of the wavelet transform that related to wavelet power.

9) Page 11: please clarify why different lengths of the moving average window (e.g., 3, 13, 103) were used in the X(intra-day), X(diurnal), and X(synoptic) calculation. And how was the w value determined? What about the criteria?

Response: The explanation has been discussed in the above response (question (4)) and revised manuscript. The intra-day, diurnal, and synoptic TS components present different frequencies component, and their separating frequencies are different. Due to the parameters m and k control the separating frequency, different m and k were used to calculate the X(intra-day), X(diurnal), and X(synoptic). Good parameters m and k will produce a separating frequency (w) closest to a given separating frequency (w_0) and is characterized by the energy at the TS component of interest do not mix energies from different TS components. Because the study of finding appropriate m and k for a given separating frequency has been conducted and confirmed in many previous works (Rao et al., 1997; Hogrefe et al., 2000; Wise and Comrie, 2005; Hogrefe et al., 2006; Tchepel et al., 2010), this work referred to the KZ filter parameters reported by the Hogrefe et al. (2000) study that selected $KZ_{3,3}$, $KZ_{13,5}$, and $KZ_{103,5}$. The more explanation has been discussed in the above response (question (4)) and revised manuscript.

10) Page 14 Line 268: Remove the word “had”.

Response: It has been removed in the revised manuscript.

Revisions made in the manuscript:

“synoptic TS component had the largest amplitude and the largest relative contributions to the total variance of SO_4^{2-} (48%) and NH_4^+ (54%) concentrations”.

11) Page 14 Line 280 and 282: Please show the data/figure for other elements in the table/figure in the manuscript or in the supplementary materials.

Response: For other elements, diurnal and synoptic/intra-day TS components had the larger amplitudes and were the larger contributors to the total variance of the concentrations (Figures S2 and S3, Table S1).

Revisions made in the manuscript and SI:

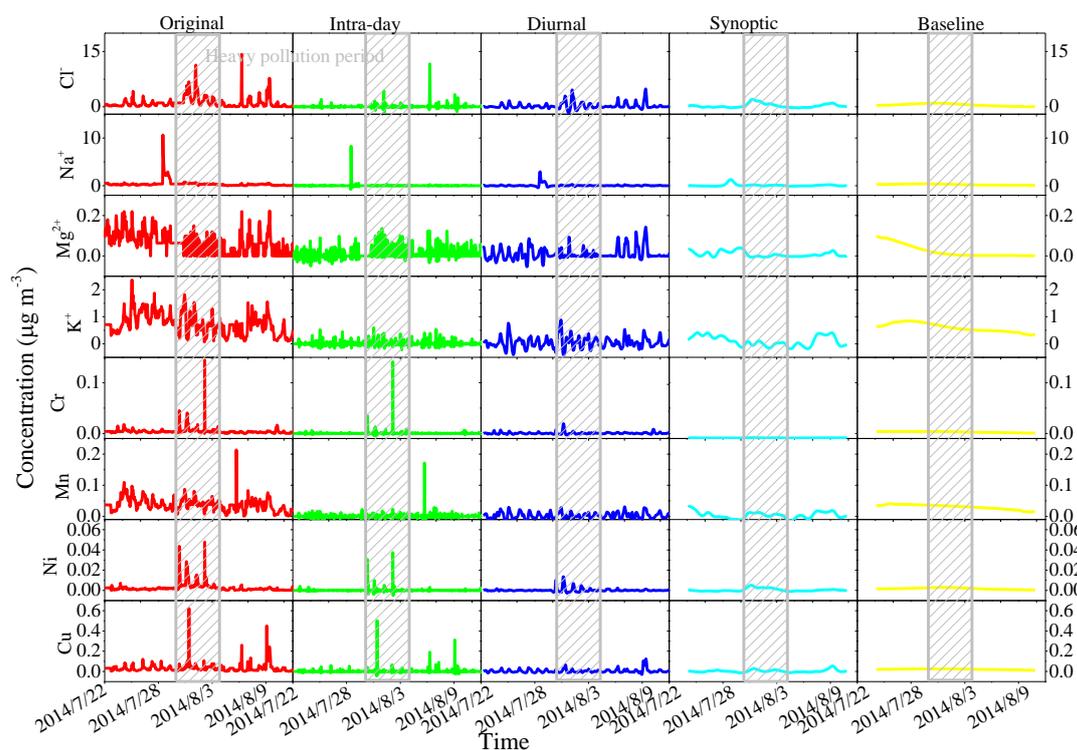


Figure S2. Variance of chemical species (Cl^- , Na^+ , Mg^{2+} , K^+ , Cr , Mn , Ni , and Cu) concentrations influenced by intra-day (period less than 12 h), diurnal (12–24 h), synoptic (2–21 days), and baseline (greater than 21 days) temporal-scale (TS) components, for the period of 22 July 2014 to 13 Aug 2014 at Beijing, China. The vertical gray lines demarcate the heavy pollution period.

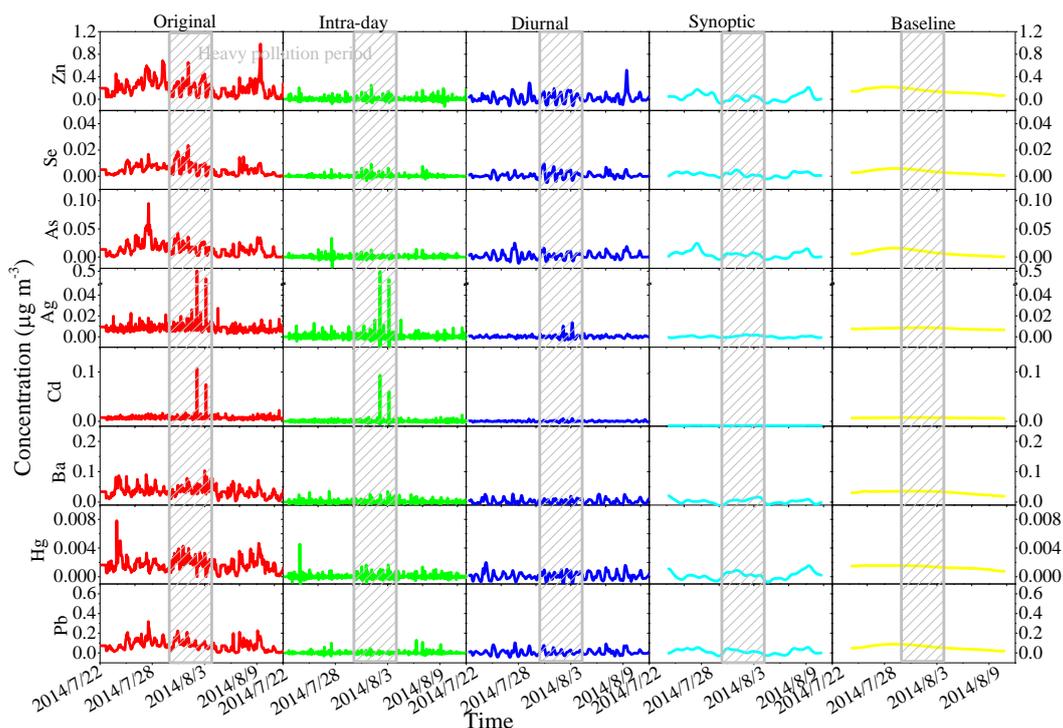


Figure S3 Variance of chemical species (Zn, Se, As, Ag, Cd, Ba, Hg, and Pb) concentrations influenced by intra-day (time period less than 12 h), diurnal (12-24 h), synoptic (2-21 days), and baseline (greater than 21 days) temporal-scale (TS) components, for the period of 22 July 2014 to 13 Aug 2014 at Beijing, China. The vertical gray lines demarcate the heavy pollution period.

Table S1. Relative contributions (%) of the different TS components to the total variance of chemical species concentrations (Beijing site).

	Intra-day (%)	Diurnal (%)	Synoptic (%)	Baseline (%)
Cl ⁻	32	46	17	5
Na ⁺	54	25	17	3
Mg ²⁺	31	31	6	32
K	10	40	29	21
Cr	86	9	3	2
Mn	27	30	28	15
Ni	52	28	15	5
Cu	66	23	10	1
Zn	11	46	29	14
As	11	35	32	22
Se	13	44	20	22
Ag	99	1	0	0
Cd	94	4	1	1
Ba	21	40	24	14
Hg	17	38	38	8
Pb	12	38	27	23

12) Page 15 Line 293: delete “s” in the word “contributions”

Response: The “contributions” has been changed to “contribution” in the revised manuscript.

Revisions made in the manuscript:

“Therefore, species with similar TS component contribution trends may have similar sources or influencing factors.”.

13) Page 15 Line 297: add “e.g.” before “NO₃-”.

Response: The “e.g.” has been added in the revised manuscript.

Revisions made in the manuscript:

“partial statistical analysis and AAE analysis were performed on the PM_{2.5} and source markers (e.g., NO₃⁻, SO₄²⁻, NH₄⁺, Ca, Fe, OC, and EC) from five ambient datasets”.

14) Figure 2: Please revise the sentence “Presented are box plots of individual chemical species from the original, RI, RD, RS, and RBL datasets.”

Response: The sentence has been changed to “The figure shows box plots of individual chemical species from the original, RI, RD, RS, and RBL datasets”.

15) Table S3: Please definite the abbreviation “Q_{the}”.

Response: The Table S3 has been changed to Table S4. Q_{the} is the theoretical Q. The definition of “Q_{the}” has been added in Table S4.

Table S4. The Q values of each solution obtained by ME-2 (Beijing site).

	Q	Q _{the} ^a
Original	12593	9940
RI	10732	9353
RD	9873	9712
RS	10847	8002

^aQ_{the}: the theoretical Q.

16) Figure S3: Please revise “BL” to “RBL”.

Response: RBL dataset had negative values and was analyzed using PCA instead of ME-2 due to this non-negative requirement. The BL dataset was estimated by ME-2 to study the source impacts from the BL TS component. The caption of Figure S3 has been revised and changed to Figure S7.

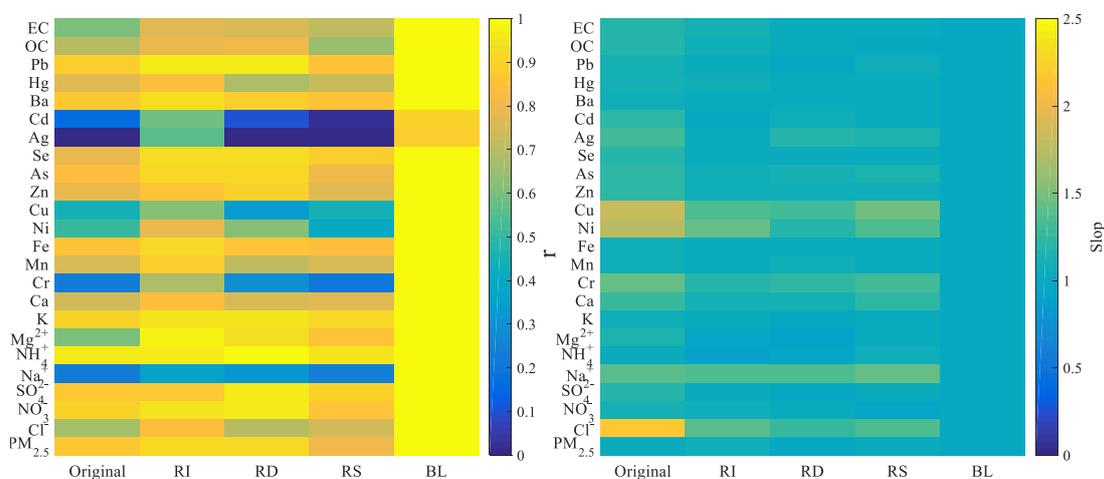


Figure S7. The performance of ME-2 from five datasets (Beijing site). (Left): the slops between model and measured concentrations of chemical species and PM_{2.5}. (RI: intra-day removed dataset, RD: diurnal removed dataset, RS: synoptic removed dataset, BL: baseline dataset) (Right)The correlation coefficients between modeled and measured concentrations of chemical species and PM_{2.5}.

17) Page 17 Line 337: Remove comma after “Fe”.

Response: The comma has been removed.

Revisions made in the manuscript:

“For original dataset run, 13 out of 23 chemical species (e.g., SO₄²⁻, OC, EC, Fe) obtained slop values ranged from 0.80 to 1.20”.

18) Page 17 Line 346: It should be “RBL”, but not “BL”.

Response: RBL dataset had negative values and was analyzed using PCA instead of

ME-2 due to this non-negative requirement. The BL dataset was estimated by ME-2 to study the source impacts from the BL TS component.

19) Page 17 Line 345-347”: Please further explain why “the precision of results from RBL dataset is the best than other four runs” with “slop and r values (larger than 0.89 of all species close to 1)”.

Response: The BL dataset was run by the ME-2. The precision of results from original, RI, RD, and RS datasets was not well as the BL run the due to ME-2 not fitting all of the spikes in the dataset. The BL dataset smoother than the other four datasets (Figure S5), resulting in the higher precision of results from BL dataset.

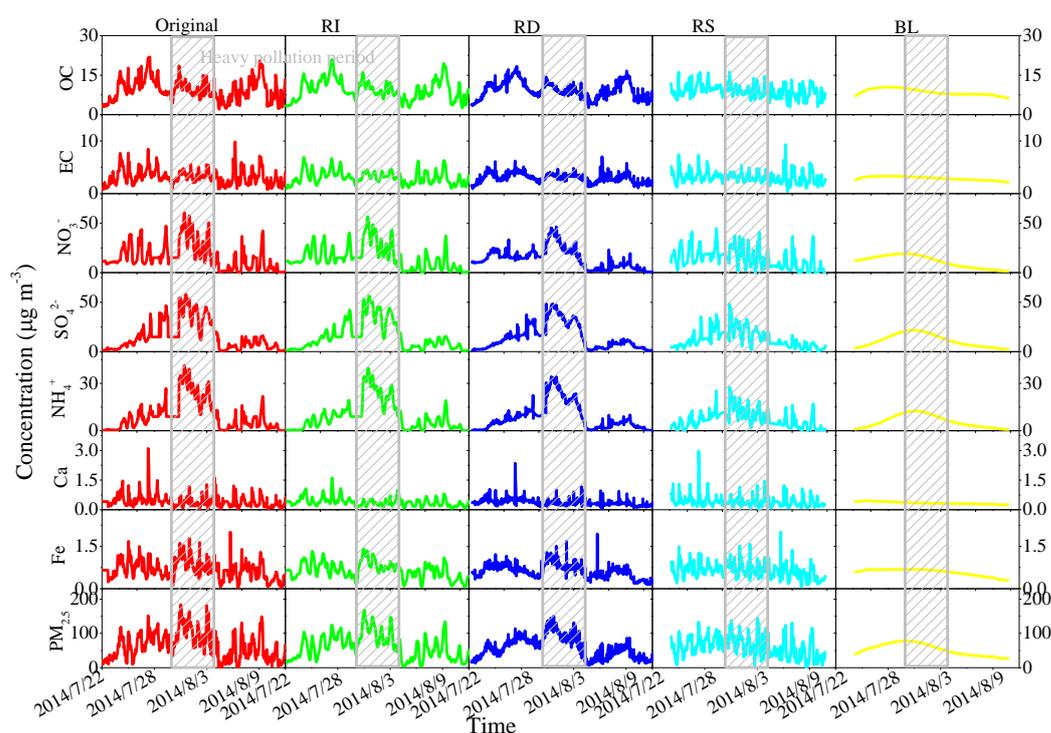


Figure S5. The variance of PM_{2.5} and chemical species concentrations from original, RI, RD, RS and BL datasets, for the period of 2 July 22, 2014, to Aug. 13, 2014, in Beijing, China. (RI: intra-day removed dataset, RD: diurnal removed dataset, RS: synoptic removed dataset, BL: baseline dataset). The vertical gray lines demarcate the heavy pollution period.

20) Page 18 Line 358-362: The context about results for RD and RS dataset are not consistent with those shown in Figure 3. Please check Figure 3 and the figure caption.

Response: For RD and RS dataset, crustal dust was not identified by ME-2. The color of RD and RS results have been revised in Figure 3 (see above).

21) Figure S4: The vertical gray lines didn't correctly present the heavy pollution period selected "from 30 July to 4 August 2014" (see Line 427 on Page 21).

Response: Figure S4 changed to Figure S9. The position of vertical gray lines has been revised in Figure S9.

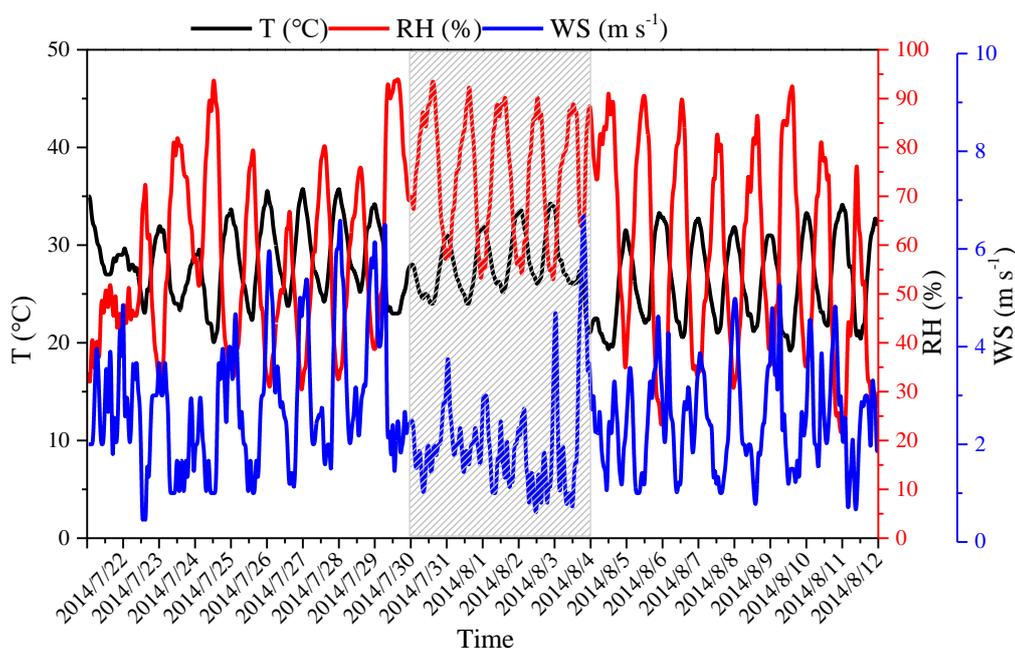


Figure S9. Time series of the temperature, RH and wind speed (Beijing site). The vertical gray lines demarcate the heavy pollution period.

22) Table 3: Please clarify the data in the parentheses and outside the parentheses.

Response: The explanation has been added in Table 3. The data in the parentheses and outside the parentheses are the absolute values of average source contribution ($\mu\text{g m}^{-3}$)

and percentages of average source contribution (%), respectively.

Table 3. Average source contributions to PM_{2.5} (µg m⁻³) estimated by ME-2 from the BL datasets.

	Vehicle emission	Coal combustion	TPS ^a	Secondary formation	Nitrate source	TSS ^b
During the entire sampling period	15.4 ^c (29%)	14.5 (28%)	29.9 (57%)	12.0 (23%)	10.8 (20%)	22.8 (43%)
Pollution period	17.6 (29%)	17.9 (29%)	35.6 (58%)	22.4 (36%)	3.6 (6%)	26.0 (42%)

^aTPS is the total contributions of crustal dust, vehicle emissions, and coal combustion. ^bTSS is the total contributions of secondary formation and nitrate source. ^cThe data in the parentheses and outside the parentheses are the absolute values of average source contribution (µg m⁻³) and percentages of average source contribution (%), respectively.

23) Page 23 Line 461: Please change “BL” to “RBL”, and check other places. It seems the authors used “BL” incorrectly in the last part of the manuscript...

Response: In section 3.2 and 3.3, we want to examine the source impacts from the BL TS component by employing ME-2 on the BL dataset.

24) Page 23 Line 470: Please change “same” to “similar”.

Response: The “same” has been changed to “similar” in the revised manuscript.

Revisions made in the manuscript:

“TPS and TSS obtained similar impact percentages from the entire period and pollution period”.

25) Page 24 in the conclusion part: Please use uniform and consistent abbreviations for “baseline removed datasets”, e.g., “RBL”, “RB”, “BL”

Response: Thank you for pointing this out. All of the abbreviations have been checked

and revised. The “RB” in line 528 has been changed to RBL. Please see the revised manuscript and supporting information.

Reference:

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