

**Referee Comments – Significant contributions of biomass burning to PM<sub>2.5</sub>-bound aromatic compounds: insights from field observations and quantum chemical calculations (<https://doi.org/10.5194/egusphere-2024-3678>)**

**General Overview:**

The manuscript (egusphere-2024-3678) presents an interesting study investigating the sources and formation mechanisms of aromatic compounds, specifically focusing on polycyclic aromatic compounds (PAHs), oxygenated PAHs (OPAHs), and nitrated phenols (NPs) in the atmosphere of Dongying, a city in the Yellow River Delta. The topic of this study falls within the scope of the journal Atmospheric Chemistry and Physics (ACP). The authors present data from field observations and analyze the data with a source apportionment model and quantum chemical calculations. The authors provide insights and helpful information for reducing emissions of aromatic compounds in Dongying and other places with similar atmospheric environments. This manuscript is generally laid out well and shows its academic value. This manuscript is recommended to be published after addressing the concerns and comments below with minor revisions.

**Major Concern:**

- Lines 277 – 281: The 2 sentences seem to contradict each other. The first sentence says that there is not significant diurnal variation, while the second sentence says that there is a significant nighttime increase compared with daytime. It would be great if these 2 sentences could be explained in more detail or modified to make sure that the statements throughout this manuscript are consistent with each other.

**Minor Concerns:**

- Line 30: What is heating season? Does it mean winter or from which months to which months? It would be great to be clear in the description for the readers to avoid confusion.
- Lines 32 – 33: Is the term “positive matrix factorization” the full form of the acronym PMF? If so, please clarify this in the text for readers to know what PMF stands for later in the text.

- Line 34: Is the term “density functional theory” the full form of the acronym DFT? If so, please clarify this in the text for readers to know what DFT stands for later in the text.
- Line 39: What is the definition of a petrochemical city in this study? What specifically are the cities being referred to in this sentence? It seems that the city Donying is the only focus throughout this study.
- Line 104: It is strongly encouraged that a map with the sampling site and the land use information of surrounding areas labeled is provided.
- Line 118: How was this quarter of filter obtained and quantified to make sure it is actually a quarter (25%)? If it is based on the surface area of the filter, then the weight of sample collected on each quarter of the filter might be different and could be confirmed by weighing to quantify the amount of sample, which might deviate from the presumed 25%. The accuracy of the analysis should be enhanced by taking this deviation into account. No matter if this step of weighing each quarter of filter is taken or not, the description should be clarified in the manuscript.
- Lines 133 – 150: It would be more reader-friendly if those kinds of 13 different PAHs, 8 different OPAHs, 9 different NPs, and 8 water-soluble inorganic ions are summarized as a list in a table instead of putting them in a paragraph. Readability of an article helps readers find useful information easily and thus potentially increases the opportunity of citations for this article in the future.
- Line 169: Is the quartz filter a “fiber” filter or a “membrane” filter? Please double check.
- Lines 169 – 170: What is the purpose of this pretreatment procedure for the filters? Is it trying to remove adsorbed contaminants on the surfaces of quartz fiber filters? If so, it would be great to mention that for clarity.
- Lines 119 and 172: If it is a fiber filter rather than a membrane filter, the word "membrane" is suggested to be removed.
- Line 184: Starting from Line 184 moving forward, do the numbers represent mean plus or minus one standard deviation or two standard deviations or something else? It would be great if they are mentioned explicitly.
- Lines 189 – 190: Is there any information or data supporting this statement of simply attributing all the increases of measured gaseous air pollutants to the increased burning activities? Are there any relevant data showing that other emission sources of the pollutants remain unchanged or unimportant during the study periods? Could

other factors such as meteorology be attributable to such increases as well? Since there are many factors influencing the trends of pollutants, the discussion here is suggested to be expanded. If the authors believe that the discussion is already covered in a later section of this article, please also mention that explicitly to avoid confusion.

- Lines 193 – 194: Is there solar radiation information to support this statement of ascribing the variation of gaseous pollutants before heating?
- Lines 195 – 196: There are variations in PM<sub>2.5</sub> concentration throughout the sampling period according to Figure 1(d). It might not be appropriate to oversimplify the analysis of the trend by simply looking at the average value over a period of several days and by saying that the concentrations remain unchanged, especially when the data of time series are available.
- Line 201: Why is 1.6 used to convert OC to OM? Are there studies in the literature to refer to? If so, please add citations.
- Line 204: If the average values are to be mentioned, Table 1 rather than Fig. 1(b) and (c) should be referred to. If Fig. 1 is to be referred to, it should be Fig. 1(d) so that there are data of the species mentioned.
- Lines 204 – 205: The total concentrations and proportions of secondary inorganic aerosols are both mentioned initially, but only the average of proportion (35%) is mentioned in the following statement of the same sentence. It would be great if the information of concentration is also mentioned.
- Lines 211 – 213: Are there any studies in the literature to support the statement that OC is generated from both primary emissions and secondary formation, while EC is predominantly derived from primary sources? If so, please add citations.
- Lines 213 – 215: Are there any studies in the literature to support the statement that the significant increase in the concentration of OC alongside a stable OC/EC ratio suggests that the sources of carbonaceous aerosols in this study include both primary emissions and secondary formation processes? If so, please add citations.
- Lines 215 – 219: Is  $r = 3$  for potassium ion (K<sup>+</sup>) considered as high? Are there any studies in the literature to support the statement? If so, please add corresponding citations.
- Table 1 and Table 2: Does N mean the number of samples? It would be great if the definition of N for the tables could be explicitly mentioned. Similar to the comment on Line 184, do the numbers for temperature, relative humidity, gaseous pollutants,

PAHs, etc. represent mean plus or minus one standard deviation or two standard deviations or something else? It would be great if they are mentioned explicitly. For the numbers in the parentheses, do they mean minimum to maximum or 5<sup>th</sup> percentile to 95<sup>th</sup> percentile? It would be great if they are explicitly mentioned. What does NA mean? Does it mean lower than the limit of detection or the limit of quantification? If so, what are the corresponding limit of detection and limit of quantification?

- Line 223: What are SOR and NOR in Fig. 1(c)? Please define them.
- Line 230: Please define r, p, and n in Fig. 3. Is simple linear regression or any other type of regression analysis used here? Please clarify.
- Lines 246 – 247: The pattern aligns with observations from other locations in previous studies. Is there any analysis or explanation for the results? Is this pattern due to the diel variations of mixing heights or other factors?
- Lines 249 – 250: The dominance of BbF was found to be consistent with the previous research. Is there any reason to potentially explain this?
- Lines 253 – 254: The average during the heating period is higher than that before the heating period, but the maximum value before the heating period is higher than that during the heating period. Is there any potential explanation for the higher maximum before heating?
- Lines 255 – 257: Is this observation due to mixing height or other factors?
- Lines 260 – 264: Is there any explanation for such difference compared with other cities?
- Lines 274 – 275: What is the relation between Before heating, During heating, autumn, and winter? Some clarifications might be needed to enhance the readability.
- Line 277: To help clarify the definitions of terms used, it might be helpful if the dates defined for autumn, winter, summer, and spring are mentioned so that readers can more easily follow the flow of the description and compare with the “before heating” and “during heating” in this study, which have been defined clearly.
- Lines 281 – 283: Are there any data supporting the statement that the relative nine NPs molecular composition in PM<sub>2.5</sub> remained consistent throughout the observation period? It does not seem to be delivered in Fig. 4 or Fig. 5.
- Lines 283 – 286: The relative percentage is hard for the readers to observe by simply looking at Fig. 4 and Fig. 5 because the data shown are in concentrations rather than

percentages. It would be great if the figures showing relative percentages could be provided, either in the supplementary information document or the main article, for the discussion.

- Lines 286 – 294: Is there any explanation for the similarities and differences while comparing with the results from other cities?
- Line 298: In the Fig. 4, it shows “Before heating” and “During heating” while the caption shows autumn and winter. What are the definitions of autumn and winter here? Please be consistent with the terminology or clearly state the relation between different terms to avoid confusion.
- Line 303: If the whiskers in Fig. 5(a), (b), and (c) denote the 25<sup>th</sup> and 75<sup>th</sup> percentiles, what are the boxes for the box-whisker plots? Usually, the boxes show the 25<sup>th</sup> and 75<sup>th</sup> percentiles as well as the median values while the whiskers show either the 5<sup>th</sup> and 95<sup>th</sup> percentiles or minimum and maximum values. Please double check the values used in the Fig. 5. Additionally, what do the error bars indicate in Fig. 5(d), (e), and (f)? Do they indicate one standard deviation or 75<sup>th</sup> percentile or 95<sup>th</sup> percentile or maximum?
- Fig. 6: The numbers and text in Fig. 6(a), (b), and (c) are hard to read due to the small size. Fig. 6(a), (b), and (c) are suggested to be enlarged for readability.
- Line 334: Does “PMF” mean positive matrix factorization? It should be defined first before the acronym is used.
- Line 338: Does autumn mean before heating and winter mean during heating? Please clearly describe the relation between different terms or use the same terminology throughout the article to be consistent.
- Lines 369 – 372: Is there any explanation for the reason why the contribution from secondary formation is higher before heating?
- Lines 393 – 394: Should the DFT be a subscript?
- Lines 403 – 404: Does supplementary material mean the same thing as supplementary information mentioned in Line 396? If so, please use consistent terminology to avoid confusion.
- Line 411: Is there any reason to consider only the *para*-H for the formation of 4NP?
- Lines 440 – 441: Is there any S atom involved in the mechanisms?

**Technical Comments:**

- Line 46: The phrase “by the presence benzene ring” seems to be intended to mean “by the presence of benzene ring” but missed the word “of”.
- Line 156: The word “theotry” seems to be a typographical error of “theory”.
- Line 201: The word “component” seems to be a typographical error of “components” since the plural form should be used.
- Line 249: The word “accounting” seems to be a typographical error of the phrase “accounting for”.
- Line 310: The word “substantial” seems to be a typographical error of “substantially”.
- Lines 453 and 458: The word “OPAH” seems to be a typographical error of “OPAHs”.
- Line 455: The phrase “in comparison to before heating” seems to be intended to mean “in comparison to those before heating” but missed the word “those”.