This manuscript investigates O_3–NO_x–VOC sensitivity and O_3 formation mechanisms in Zhengzhou (2019–2021) using a combination of online VOC measurements, OBM, CMAQ-DDM, source apportionment, PMF, and machine-learning (ML)/SHAP interpretation. While the dataset is valuable and the research direction is meaningful, the manuscript suffers from inconsistent methodology, unclear descriptions of model configurations, uncertainties and machine learning, no comparisons between different analytical models for the O_3 formation mechanism, and very vague data interpretation. The manuscript is long and unreadable. Therefore, I suggest the manuscript be rejected.

Major Comment:

1. In Section 3, "Results and Discussion", there is a substantial focus on O_3 source apportionment (CMAQ) and VOCs source apportionment (PMF). Unfortunately, how these contents are linked to the research question "O_3-NO_x-VOC sensitivity" is weak. For example, the authors claim that traffic and industry dominate both O_3 and VOCs. But there is no justification for "X% of O_3 from traffic" and "how O_3 responds if traffic NO_x/VOCs are reduced".

   In addition, there is no cross-method comparison. A combined table is highly recommended to show the section contributions across PMF, CMAQ-DDM, and OBM RIR/EKMA. As a result, the manuscript reads like a report by stacking results (sensitivity diagnostics + VOC and O_3 source apportionment + ML/SHAP), but with limited discussion.
2. The CMAQ simulation suggests that transportation and industry dominate MDA8 O_3 contributions, while the PMF result indicates that vehicle, solvent, and industrial sources contribute most VOCs. The current discussion is very vague: "transportation should be prioritized," "more aggressive control is required," etc. However, what is the take-home message for policy translation? There are no recommended emission-reduction scenarios (e.g. -30% traffic VOCs, -30% industrial NO_x, different VOC/NO_x ratios by sector) and no quantitative estimate of the expected O_3 under those scenarios.
3. Machine-learning setup and data leakage risk are not clearly addressed. The authors use XGBoost and RF with grid search and cross-validation (CV), and report training/test metrics in Table S4. However, essential methodological details are missing. How are training and test sets defined—random split or chronological split for this time-series dataset? What CV scheme is used (k-fold, blocked time-series CV)? Does CV account for temporal ordering?
4. What is the inherent relationship between the VOCs/NO_x ratio method for determining O_3 sensitivity, modelling results from OBM and CMAQ, and radical budgets?
5. How do the results of XGBoost relate to those of other methods? Why is XGBoost analysis not mentioned at all in the Section 4 Summary and Conclusions? How do the authors come up with the claim that the ML method should be advised in the future in the subsection Limitations and future research directions in Line 986?
6. The role of biogenic VOCs is mentioned but not fully clarified in terms of O_3 formation and control. Biogenic VOCs are explicitly identified as a separate PMF factor with isoprene as tracer, and OBM RIR shows that biogenic VOCs have non-negligible reactivity,

especially on polluted days. Emissions used in CMAQ also include biogenic VOCs via MEGAN. On the one hand, the authors claim that the contribution of biogenic sources to VOC is small (Line 724). On the other hand, they claim that the contribution of biogenic VOCs to local O_3 is high (Lines 840-850). So, I wonder what the overall role of biogenic VOCs in the O_3–NO_x–VOC sensitivity and O_3 formation mechanism is.

Minor Comment:

1. The period simulated by the CMAQ model was not mentioned in the methodology.
2. What is the rationale for studying warm seasons? Could you provide any justification and supporting references?
3. Lines 141-143: Could you provide any reference for the study city of Zhengzhou?
4. Lines 212-215: "PO_3^S(X) and PO_3^S (X-ΔX) refer to the simulated O_3 yields…" Are you sure "yield" is the right terminology here? Why does the author later state that "The net O_3 production rate (PO_3^S)" in Lines 215-216?
5. The CMAQ result shows transportation can contribute 64% to O_3 (Fig.4), but the PMF result shows vehicles contribute only 31% to VOCs. This apparent discrepancy needs justification. Presumably, VOCs and NO_x emissions from transportation are equally important for O_3 formation. Therefore, the role of NO_x emissions needs to be discussed.
6. Why does Table S5 show a negative correlation (Kendall's, -0.305) between VOCs and O3, while the RIR indicates a positive correlation (Fig.9)? Shouldn't this discrepancy require some explanations?
7. Table S4: The rationale for selecting XGBoost over RF is well justified.
8. A strong positive correlation between O_3 and alkenes is observed in SHAP (Fig.2), whereas Spearman's analysis reveals the opposite relationship (Table S6, -0.054**). Please standardise the terminology for "olefins" (Fig.2) or "Alkene" (Table S6)!
9. Line 427: "160 160 μg/m³ and 160 μg/m³ are categorised as light pollution and moderate pollution"? Could you please carefully check if this is CORRECT?
10. Fig.9: What are "AVOCs", "ALKA", "ALKE", "ARO"? What is the relationship between them? Which subsets of compounds belong to AVOCs? Why is there no further discussion of the contribution and sensitivity of VOCs from different sources to O_3?

Technical Comment:

1. Fig.2 The font is too small to read.
2. Line 351: What is the full name of "XGBoost"?
3. Line 386: Should it be "SHAP" instead of "Shapley"?
4. Table S3: What do "DISP" and "BS" mean? What is the meaning of BS mapping < 80%?
5. Fig.S3: A full description needs to be provided for "E/X" in the manuscript for the first time and figure captions.
6. Line 712: "Zhengzhou comprises vehicle emissions (31%), solvent use (24%), and industrial processes (21%)". But in Table S8, the corresponding values are 32.4%, 24.8% and 18.3%.

7. Lines 1135-1137: Make sure the font style is consistent throughout.
8. Please be consistent in the use of subscripts and full names or abbreviations for proper nouns.