Comments:

This study employs machine learning techniques to investigate the patterns and driving factors underlying the fluctuations in isoprene levels — a crucial precursor to surface ozone — using extensive historical datasets. The analysis demonstrates good agreement with previous short-term modeling results, while also emphasizing that vegetation expansion and temperature increases linked to climate change are key drivers of long-term variability. Moreover, by extending the model projections to the year 2100 and integrating them with a detailed chemical box model, the researchers estimated future surface ozone levels. Their results indicate a significant rise in ozone concentrations if NOx emissions are not effectively controlled. Importantly, these conclusions were obtained using a data-driven approach that differs from conventional atmospheric chemical transport models, highlighting the robustness and novelty of the findings. I recommend acceptance for publication in ACP after minor revisions.

1. The superior performance of T-training suggests that reliable simulations can be achieved for grid cells or cities with existing isoprene observations. Furthermore, could this method also be applied to regions lacking monitoring data?

2. The decrease in vehicle emissions seems to significantly influence isoprene concentrations at traffic sites in London, as further supported by the comparison with benzene. Have prior studies presented similar evidence or discussed this effect?

3. Please include the calculation formulas for R^2 and NMAE.

4. Some input variables have varying spatial resolutions. How were these differences addressed, and what were the primary criteria for selecting these variables?

5. In the PINN-ResMLP model, an additional loss term was incorporated into the training process. Was the training stable across different sites, and how did the model

loss change accordingly?

6. Please ensure that the use of abbreviations is consistent between the main text and the appendix tables, such as Radiation vs. SSRD and U10 vs. u10.

7. Please supply additional details regarding the isoprene measurement instruments used at each site.

8. Please include a definition of SHAP in the Methods section.

9. In the simulation of future scenarios with NOx reduction, please specify the basis or reference for the assumed reductions of 49.7% and 89.2%.

10. Please add the full names of LAI and NDVI in the caption of Figure 1.

11. Additionally, since Figure 2 includes multiple algorithm abbreviations, it would be beneficial to define them in the caption for improved clarity.

12. Line 162: provide the full term for R^2.

13. Line 129: add a reference.