General Comments

The manuscript has improved substantially since the first review, particularly regarding literature coverage, discussion of model limitations, and treatment of NO_2 chemistry. However, several conclusions remain stronger than warranted by the evidence presented. The remaining concerns primarily involve overinterpretation of atmospheric significance, the strength of the toxicity claims derived from QSAR predictions, and limited integration of recent experimental literature on heterogeneous oxidation and nighttime nitrate-radical chemistry. These issues appear addressable through a focused revision and do not require fundamental changes to the overall structure of the manuscript. Addressing the remaining concerns would substantially strengthen the scientific impact of the work and help establish it as a more robust and meaningful contribution to the field. I therefore recommend major revision to address the comments below.

Major Comments

1) The manuscript continues to draw conclusions regarding atmospheric residence time, long-range transport, air-quality model underestimation, and regulatory relevance that are not supported by the computational framework employed. The MD simulations provide molecular-level information on adsorption behavior in an idealized system but do not constrain atmospheric lifetimes, transport, or large-scale environmental impacts. These statements should be removed, substantially qualified, or supported by additional quantitative atmospheric analysis.

2) Although the revised manuscript acknowledges the limitations of QSAR predictions, the title, abstract, and conclusions continue to imply demonstrated toxicity amplification and environmental risk amplification. Because the toxicity analysis remains based entirely on predictive models without experimental validation, product yields, or exposure estimates, the results should be presented consistently as *predicted changes in toxicity indicators* rather than demonstrated increases in environmental risk. Ensure that conclusions clearly distinguish computational findings from broader atmospheric implications.

3) The treatment of nighttime oxidation chemistry remains incomplete. The manuscript draws atmospheric conclusions regarding the fate and transformation of 2,4-DNP while providing only limited consideration of NO_3 radical chemistry, despite its recognized importance in the nighttime processing of phenolic compounds. This omission limits the atmospheric interpretation of the proposed reaction framework. The discussion should more clearly place the results within the broader context of known nighttime oxidation processes and relevant experimental studies demonstrating NO_3-driven formation of nitrocatechols, oligomers, and brown carbon in phenolic systems (Rana and Guzman, ACS Earth Space Chemistry, 2026, DOI: 10.1021/acsearthspacechem.6c00226) and heterogeneous oxidation pathways in phenolic aldehydes (Rana and Guzman, ACS Physical Chemistry Au, 2026, DOI: 10.1021/acsphyschemau.6c00106)

4) The kinetic discussion remains largely based on comparison of bimolecular rate constants. Inclusion of pseudo-first-order loss estimates, representative atmospheric oxidant concentrations, or simple lifetime calculations would substantially strengthen the connection between the computed kinetics and atmospheric significance.