

Comment on “i_NRACM: Incorporating ¹⁵N into the Regional Atmospheric Chemistry Mechanism (RACM) for assessing the role photochemistry plays in controlling the isotopic composition of NO_x, NO_y, and atmospheric nitrate” by Michalski et al.

General Comments:

Michalski and coauthors have expanded an existing chemical mechanism designed for air pollution chemistry to consider the heavy isotope of nitrogen (¹⁵N) as it proceeds through the NO_x and NO_y cycles. Although they have made significant assumptions due to lack of experimental data, they have demonstrated the feasibility of using the tool to simulate idealized and real-world cases. They finally make the argument that incorporating this scheme in a 3-D air quality model will enable researchers to use δ¹⁵N data to constrain NO_x emissions, a major challenge facing the air pollution community. Broadly, I think the elements of the study are exceptionally well-designed and chosen, particularly the progression from simplified box model examples to more complicated scenarios and finally one real-world case. I also thank the authors for a well-scoped and executed introduction and methods that helped me understand much better the pertinent issues with and potential gains from a better understanding of NO_y isotope abundance. This may be one of those frustrating reviews that reveal the ignorance and misunderstandings of the reviewer, but hopefully the authors will find these comments useful for the success of the paper. My suggestions involve mostly matters of presentation.

The manuscript is overlong and could stand another read-through focused on eliminating redundant text and moving details to the SI. Section 2.4 for example, could be moved. I think upgrading section 2.4.4 out of section 2.4 is warranted. This section could also describe the Tuscon case.

Figures 1, 4, 5 can be moved to the SI.

A table is needed in the main text to summarize the scenarios in sections 3.1 and 3.2. It is too difficult to track what reactions are included or excluded from the different cases and quite frustrating to interpret axes like Fig. 12 where two different cases are subtracted. Fig 12 and Fig. 14 require y-axis labels.

Another suggestion includes moving sections 3.3.1-3.3.4 to the SI and instead using an abbreviated table to report the initial conditions and emissions of each scenario, with only the most important compounds from Table S8 (e.g. NO, NO₂, HNO₃, PAN, (and isotopes) and total VOC).

Regarding the case in section 3.4, I agree with the other anonymous reviewer that 48 hours may be problematic as it appears to be within the dynamic phase of the 5-day simulation examples in section 3.3. It would be prudent to run the model out to 5 days or longer to get a sense for the steady-state that will be reached.

How were the emissions for the Tuscon case applied? What temporal assumptions were made? What is the sensitivity to this?

How are the assumptions with respect to the heterogenous reaction of N₂O₅ impacting the results in Fig. 19? What is the expected impact from developments to this part of the mechanism in the future?

Are there significant concentrations of ¹⁵NH₄ and ¹⁵NH₃ in the atmosphere? If so, can this impact the measured δ¹⁵N data for PM_{2.5} and PM₁₀?

Typos/Editorial Suggestions

1. Page 2, Line 18: “The final mechanism was **characterized...**”
2. Page 6, Line 26-28: I was confused about exactly how the alpha relates to the reaction shown. Is it isotope product over isotope reactant? Could you explain a bit more in the text please? Just an extra five words or so may do it.
3. Page 6, Line 28: I can't find this alpha in the SI. R238 and R238A have different alphas than this.
4. Table S2b: This is a difficult lift at this stage of the manuscript, but it would have been helpful if R238 were named R238b instead.
5. Page 11, Lines 30-34: I was confused by this assertion and the use of the terms *chemically equilibrated* vs *isotopically equilibrated*. The authors assert that HNO₃ is likely not able to exchange isotopes in the gas phase, but N₂O₅ and NO₃ are? How is HNO₃ not already chemically equilibrated in the mechanism as well, for example in R239a and R239b? I would have been better-served with a more precise definition of equilibration and
6. Page 27. Line 33: Recommend avoiding “weekly trend” throughout discussion and instead using something like “multi-day” trend. I don't think there's enough data here to establish weekly trends.