Reply on RC1
Huan Fang and Greg Michalski

Author comment on "Assessing the roles emission sources and atmospheric processes play in simulating δ15N of atmospheric NOx and NO3- using CMAQ (version 5.2.1) and SMOKE (version 4.6)" by Huan Fang and Greg Michalski, Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2020-415-AC1, 2021

All typo and grammatical errors were adjusted according to the comments. The responses to other comments are included below.

1. “... the authors themselves point out on page 4 (lines 11-15) the “unsatisfactory” nature of the 2020 paper’s approach so why is it justified to separately publish that?”, “It is of critical importance to address the significant overlap between this work and the cited companion paper of Fang & Michalski (2020) ...”

We decided to combine the companion paper with this manuscript in order to deal with the overlapping and completeness issue.

2. “... While I value the need to focus on the detailing the model specifics in a journal such as GMD, the manuscript here lacks any real interpretation, quantification of the sensitivity of the output to the model parameters and consideration of the implications of the predicted values compared to previous studies in the literature of interpreting the isotopic composition of NOx and nitrate ...

The more in detail interpretation and quantification of the output have been included in the revised manuscript (In section 3.2, 3.3, 3.5, and 3.7)

3. “Second, the model is compared with one set of observations of “d15N-NOx” in Indiana (within the domain of the model runs) ...”

The full simulation domain covers the whole Midwest while the sampling sites only locate in IN, IL, OH, and KY. As a result, the sampling site would have sufficient distance between the domain boundary to eliminate the bias near the domain boundary.

4. “Additionally, the measurements that are compared with are specifically d15N-NO2 and not d15N-NOx ...

Walters et al (2018) did include the d15N(NOx) values based on the measurements in Table 1 and 3.
"The first comparison is to the only direct measurements within the domain, which occurred in West Lafayette, IN. The $\delta^{15}$N(NOx) values were inferred from the measured $\delta^{15}$N(NO2) and the calculated $\delta^{15}$N(NO2) shift (Walters, Fang, & Michalski, 2018)."

5. “Third, the sensitivity to the starting emissions values should be evaluated ...”

The range of $d^{15}$N values for any source is generally a function of equilibrium, kinetics, or reaction progress happening in that source process. For example, automobiles show a wide range of both NOx amount and $d^{15}$N values going from cold start to normal driving, but once the catalytic converter is warm the values are relatively constant because the NOx reduction by the CC becomes constant. We are using the average to account for these effects and for simplicity. In future work hope to explicating model the sources variation in SMOKE or land surface models, but that is well beyond the scope of this work. Fig. S10 shows the uncertainties of $d^{15}$N values within the research area. For most of the grids, the uncertainties are less than 5 ‰, which is well below the difference in $d^{15}$N values between any two of the emission sources. For those regions dominated by biogenic source, the uncertainties in $d^{15}$N values are less than 10 ‰, which is also significantly below the difference in $d^{15}$N values between the emission from biogenic source and all the other sources.

6. “Fourth, one of the key conclusions of this work is that changes in the polluted boundary layer (PBL) are critical to transport and dispersion of NOx such that the pattern of $d^{15}$N- NOx is importantly changed based on the PBL height. I’m not convinced the results shown support this conclusion ...”

The more in detail interpretation and quantification of the relationship between $d^{15}$N and PBL height has been included in section 3.3 of the revised manuscript.

7. “Fifth, “the role of deposition” section and comparison of $d^{15}$N-NOx with $d^{15}$N-NO3- seems out of place in this work ...”

CMAQ simulated the $d^{15}$NOx effect by NOx removal using enhanced deposition. These “emission + mixing + enhanced deposition” simulations were not imposing an isotope effect related to dry/wet deposition, rather they are an attempt to show how “lifetime chemistry” alters NOx $d^{15}$N values by removing NOx before it can be transported significant distances.

8. “Finally, it needs to be addressed why in this work there are only 8 NADP sites being compared with, while it appears that 82 measurement sites are included in FM2020?”

We decided to use the exact measurement from our lab at the 8 NADP site to validate the simulation, instead of using the values of literature review and compared with the simulation values at the grids contains the NADP site within the simulation domain.

9. “Title: Is it necessary to have the CMAQ, SMOKE and WRF versions as part of the title?”

The editor requested us to include the model’s name and the version number in the title.

10. “I would argue that atmospheric “processes” are not really being tested here, it’s really transport or meteorology ...”

Transport, mixing, dispersion, and deposition are all examples of atmospheric
processes