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Interactive comment on "Impacts of using reformulated and oxygenated fuel blends on the regional air quality of the upper Rhine valley" *by* J.-F. Vinuesa et al.

Anonymous Referee #2

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This paper describes results of modeling effects on O3, NOx, and total VOC levels due to vehicle fuel composition and emission changes in an ozone exceedences episode in the Rhine Valley. The description of the modeling methods appears to be reasonably clear, though some omissions are noted by Referee #1, and as discussed below some additional information about emissions also needs to be given. Assuming that there is no problems with the methodology (my expertise is atmospheric chemistry and chemical mechanisms, not emissions or regional modeling), the results are sufficient interest to merit publication if the presentation were adequate and sufficiently complete.

However, the presentation of the results could stand improvement in a number of respects, and additional information is needed to adequately interpret the results. I agree with Referee #1 that the discussion of the atmospheric chemistry of ozone formation could use improvement, though this, by itself should not be a basis for rejecting a modeling study such as this if sufficient information is presented to allow readers to interpret the results for themselves. However, I think some of the results presented were not particularly useful for understanding the results, and that other information or calculations, which were not presented, needs to be given.

The main difficulty in interpreting the results of the reformulation calculations is that several changes are being made at once, and information is insufficient to determine the effect of each change. The fuel reformulations result in changes in total mass and time and place of VOC and NOx emissions as well as in the chemical compositions of the emissions. Table 4 indicates that all three of the reformulations cause a reduction in total VOC emissions by roughly the same amount, that the two ETBE reformulations cause an increase in NOx by about the same amount but the "R2" reformulation causes NOx to decrease. It would have been useful had Table 4 indicate the total scenario-wide changes in NOx and VOC emissions as well as changes for different road types, so one could assess the relative total impacts. Table 1 indicates the general chemical compositions (presumably) reactivities of the fuels are somewhat different, but no indication is given concerning changes in compositions and reactivities of the exhausts. This could be significant because in general exhausts have different chemical compositions than the fuels themselves. As discussed below, it is difficult to understand the results for the ETBE fuels unless the exhausts are significantly different, or unless there is some other relevant information about the emissions differences for these fuels that is not presented.

If I understand the presentation correctly, the results indicate that the ETBE1 reformulation gives a considerably better improvement in O3 than ETBE2. This is despite the fact that there is relatively little difference in total mass emissions according to Table 4, and

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Table 2 indicates that ETBE1 is higher in aromatics, which one would think would result in higher ozone reactivity. However, although Table 2 also indicates that the two fuels are very similar in oxygenate content, Table 6 seems to imply (if I interpret it correctly) that there is much greater formaldehyde and higher aldehyde emission or formation in the scenario with ETBE2. Is this due to differences in the exhaust speciation? This is not adequately discussed.

In order to more clearly separate out the effects of the various changes in mass and reactivity, it would have been useful to carry out calculations where changes are made one at a time. For example, calculations where only the mass emissions but not the composition of the emissions were changed would have been useful to assess the effects of composition changes, and calculations where NOx is not changed would have been useful to assess effects of NOx changes. How would the ETBE and R2 scenarios have differed had they not had such differences in total NOx emissions?

The sensitivity studies where NOx or VOCs are changed by 10% were useful to indicate that ozone formation in this scenario tend to be VOC sensitive, and have NOx reduction disbenefits, at least according to the metrics used in this study. However, they should have separate out urban and regional impacts in this assessment, since one would think that while urban areas would be as found by these metrics, rural areas would show positive effects on NOx reduction and less VOC sensitivity, as referee #1 indicates. This would be quite unlike ozone sensitivity in regional scenarios in the United States if this whole region is as VOC sensitive as indicated by these metrics.

The differences between the results of this study and the previous work from this group (V2003) are potentially significant if the simulations are in fact comparable. However, the second paragraph on page 12083 indicate that the "emissions inventories and spatial resolution" of the two studies differ. They discount this as being significant, but I wonder whether this has been adequately established. It would have been better had they conducted a separate simulation using this model and inventory except that emissions only in the urban area are verified in order to provide a more direct comparison.

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If the results are similar to V2003 then this would be significant.

Some more minor comments that the authors should consider if the paper is to be revised prior to publication are as follows:

The definition of “RIM” and “RIA” are such that negative numbers means that the changes cause increases and positive numbers indicate decreases. It would have been less confusing throughout had positive numbers indicated increases, etc.

The fractional changes in fleet penetration shown on Tables 5, 6, and 8 and the effects of increase compared to decrease shown on Table 7 indicate near-linear effects of these changes. It seems to me it would be sufficient to state that these changes had nearly linear effects in the ranges considered, and not burden these tables with the additional numbers that do not really provide additional information beyond this fact. This would improve readability and save journal space.

I think in general the discussion should emphasize more the effects on ozone and less the effects on VOC and NOx. The latter would be more or less directly related to the effects on mass emissions, while the ozone impacts are the major interest of this type of calculation. This would also save journal space.

In a few places the term “COV” is used rather than VOC.

Overall, I think this is probably worth publishing after improving the discussion of the emissions changes on exhaust composition and reactivity and perhaps conducting additional simulations to clarify the effects of the various changes. Calculations are probably also needed to assess differences between the results of this work and their 2003 study.

Interactive comment on Atmos. Chem. Phys. Discuss., 5, 12067, 2005.