Comment: The manuscript "Comprehensive multiphase chlorine chemistry in the box model CAABA/MECCA: Implications to atmospheric oxidative capacity" by Soni et al. describes an expansion of the MECCA chemical mechanism to include chlorine chemistry. Using published data from India and the UK, the authors show how the inclusion of this additional chemistry leads to improved modelling results and present an interesting analysis of the oxidation chemistry in these two very different locations.

The manuscript is generally well written, although the English could benefit by some tweaking, and clearly laid out. I have only a few comments, and after the authors have addressed them, I recommend publication.

Response: We thank reviewer for the constructive comments to our manuscript. Please find our responses below in blue fonts. The discussion added/updated in the manuscript is presented by red color font.

1. My main suggestion is to change figures 2 and 6. I think it would make the whole paper much clearer if they both show the base model, the base model with added chemistry, and the measurements. To keep the figures in a manageable size I would suggest having all radical species in one figure and all non-radicals species in the other figure. Likewise, I suggest introducing earlier in the paper the three mechanisms that are now discussed only from section 4.3 onwards. In this way, it will be easier for the reader to understand how the model results have changed with the addition of the new Cl chemistry.

Response: As suggested, we have modified Figure 2 and 6 (which is now Figure 2, 3 in the revised manuscript). To manage the size of the figures and lay out the discussion clearly, we have moved Cl, $ClNO_2$, and ClONO to Figure 3 of the revised manuscript. In our view, introducing three simulations from Figure 2 or at the beginning of Section 4 would make the discussion a bit chaotic. Inf act, as the concentration of NO and NO_2 is constrained in the model simulations, the diurnal levels of NO, NO_2, and O_3 that are simulated by the three model runs will coincide with each other. As a result, noticable changes in the diurnal levels of NO_3 (which forms through the reaction of NO_2 + O_3) and N_2O_5 cant't be seen when the three model runs are shown together. Therefore, for better manuscript flow, we have defined the three simulations in Section 4.1 of the manuscript. We have also modified the names of the model runs in order to avoid any confusion, and in the revised version, the model runs are referred to as follows:

OLD=includes default chemistry already present in the model
NEW=chemistry already present in the model + newly added gas and aqueous phase chlorine chemistry
NOCL=OLD minus chlorine chemistry (i.e. without Cl chemistry).

The following line is added to clarify that OLD simulation also include some basic chlorine chemistry that was already present in MECCA before we started model development.
Lines 192-194: "OLD simulation also encompassed some basic chlorine chemistry that was part of the model prior to its update (full mechanism is also shown in supplement)."

2. line 36: I wouldn't say that the limitation in our understanding of Cl chemistry is "mostly" due to the limitations of the models. These processes are also understudied in laboratory/chamber experiments, not to mention that the database of ambient observations is rather limited.

Response: As suggested, the following line is added to reflect that chemistry of Cl compounds are understudied in laboratory/chamber experiments.

Line 39: "In addition, the chemistry of Cl compounds has been less studied using the laboratory/chamber experiments."

3. lines 125-127. I suggest moving to line 121 the explanation of why the winter season was chosen for the model simulations, and also add a note explaining why the Leicester and Delhi datasets were used for this study.

Response: The motivation of choosing winter season for model simulation is now moved as suggested (Lines 132-134 of revised manuscript).

4. figure 2: the isoprene mixing ratio in Leicester looks constant. I assume it is an estimate of some sort, and in an average sense that may be fine, but the profile is likely unrealistic. The authors should consider how this affect their results and the related discussion.

Response: The constant value shown in Figure 2 represents the observations, not the model. This is already mentioned in line 162 of the revised manuscript and is now also clarified in the Figure 2 caption. A diurnal cycle of measured isoprene is not available for Leicester, and therefore, the mean value is used to illustrate that the modeled isoprene varies around the observed mean level.

5. line 211: "indicating", rather than "representing"?

Response: In the revised manuscript, "representing" is now replaced by "indicating".

6. line 219: "Cl- concentrations"?

Response: Yes, we have updated as suggested.

7. line 226: why are the rate constants for OH + X reactions not taken from MECCA, like those for Cl + X reactions?

Response: The rate constants for nearly all the OH+X reactions were already published in Soni et al., 2022, and those were based on another box model, NCAR's master mechanism. Hence, they were directly taken from that reference. However, as correctly pointed out by the reviewer, the rate constants do vary in different models. Therefore, in the revised manuscript, all the rate constants are taken from MECCA only, and the calculations are revised accordingly (Line 279, Figure 5).

8. figure 3, and related discussion: the model suggests that the gas phase reaction Cl + NO2 can be a significant source of ClNO2. As far as I am aware, most studies indicate the aqueous-phase reaction as the major (if not only) source of ClNO2, so this may be a potentially interesting/important finding. Can the authors expand the discussion on this point? For instance, how well is this reaction known? Have previous studies considered it?

Response: We agree with the reviewer, and similarly, reviewer #1 also pointed out that the contribution from the gas-phase reaction $Cl+NO_2$ is thought to be negligible compared to the aqueous-phase reaction of $Cl^- + NO_2^+$ in the formation of $ClNO_2$. The chemistry presented over the Delhi environment is quite unusual during wintertime, such as the nighttime negligible and daytime peak levels of NO_3 and N_2O_5. Measurements of such an unusual diurnal pattern of N_2O_5 are also reported in a recent study by Haslett et al., 2023 (which is discussed in the revised manuscript, Lines: 177-179). Though gas-phase reaction $Cl + NO_2$ is discussed in the literature (Burkholder et al. 2015, Qiu et al., 2019), however, to the best of our knowledge, such an unusually higher contribution of the gas-phase $Cl+NO_2$ reaction as compared to the aqueous-phase reaction of $Cl^-+NO_2^+$ has not been reported in any study (discussed in the revised manuscript, Lines: 247-250). In fact, the detailed budget of $ClNO_2$ considering a comprehensive set of gas and aqueous-phase reactions of involved reactions along with showing the importance of different production and loss mechanisms of $ClNO_2$ in distinct urban environments are not presented anywhere in the literature. In this regard, our results provide more comprehensive insights and highlight the implications of these different reactions in urban environments.

9. figure 4, and related discussion: I find it a bit odd that Cl is so important for the AOC in Leicester when the model predicts significant concentrations of Cl only around 8am. Likewise the levels of Cl in Delhi during the night are expected to be very small. Perhaps the authors should comment on this point.

Response: (Considering the reviewer is pointing towards Figure 5 (showing AOC) and related discussion)

As reviewer pointed, it is correct that the model predicts significant concentrations of Cl at around 8 am over Leicester. Since morning time (7-9 h LT) strong contribution is included in the mean value of AOC during daytime (6-16 h LT), higher Cl reactivity throughout the day lead to stronger contribution from Cl in daytime (6-16 h LT) AOC in Leicester. In addition, results reveal a significant change in AOC in Leicester with the changes in reaction rate coefficient of $ClNO_2 + Cl^-$ reaction. For example, morning-time AOC dropped from 74% to 58.1%. A new section (4.4) has been added to the manuscript discussing the changes occurring due to the reaction rate coefficient of the A6 reaction.

As per reviewer's second point, "Likewise the levels of Cl in Delhi during the night are expected to be very small", Cl concentration is zero during the night as expected which is clearly seen in Figure 3a.

10. lines 251-257: it is not clear to me how the base model differ from the base model without chlorine chemistry. Up until this point I was under the impression that chlorine chemistry was not

present in the "original" MECCA. Can you please clarify here, and in the Introduction if necessary, what are the differences in the various mechanisms?

Response: Some basic chlorine reactions were already included in MECCA before we initiated this work (full mechanism is included in supplement). To prevent any confusion, we have modified the simulation names as discussed in response to comment (1). Additionally, we have added following line for further clarification.

Line 192-194 : "OLD simulation also encompassed some basic chlorine chemistry that was part of the model prior to its update (full mechanism is also shown in supplement)."