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Interactive comment on "Nighttime O(^{1}D) distributions in the mesopause region derived from SABER data" *by* Mikhail Yu. Kulikov and Mikhail V. Belikovich

Anonymous Referee #1

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The manuscript applies a new source of O(1D) proposed by Kalogerakis (2019) to data from SABER to estimate the nighttime O(1D) population distributions for the years 2003-2005. The motivation of the study is to provide information for subsequent evaluation of nighttime O(1D) influence on the chemistry of the mesopause region. The manuscript reports that depending on the time of year, monthly averaged O(1D) distributions may have a pronounced maximum localized in height and latitude. The nightly averaged O(1D) concentrations may reach number densities as high as 300 cm-3.

The strength of the manuscript is that it is a clearly written paper related to a topic currently debated in the literature and its motivation to provide helpful information to

better understand mesopause chemistry is justified. The weakness of the manuscript is that the calculation of [O(1D)] has major flaws and inconsistencies.

The fact that there are no measurements of [O1D] near the mesopause means there is no direct comparison between results from observations and calculated estimates. As a consequence, the details of the calculation of [O(1D)] must be considered very carefully.

There are several problems with the calculations reported in this manuscript:

(a) The SABER profiles for oxygen atoms used in the calculations are inconsistent with the new source of O(1D) and not appropriate for this type of calculation. These oxygen atom profiles come from a model which assumes 100% single-quantum relaxation by oxygen atoms from OH(9) to OH(8) to get the global energy budget near balance (Mlynczak et al., 2018). The yield of the new mechanism from OH(9) to OH(8) is less than 1.2/6.2 or $\sim$20% according to Table 1 of the manuscript. Applying the results of the SABER single-quantum model to calculate [O(1D)] is in contradiction with the new multi-quantum O(1D) source. In addition, using the single-quantum approach described in Mlynczak et al. (2018) was recently shown to give inconsistent results with SCIAMACHY data (Fytterer et al., ACP, 2019).

(b) The SABER inputs for hydrogen atoms used in the calculations suffer from the same problem as discussed in (a) above. The best-fit results for [H] calculated by the multi-quantum model of Fytterer et al. (2019) are 50% larger than the single-quantum SABER model. The hydrogen atom population distributions are also strongly affected from uncertainty in ozone, to be discussed next.

(c) The SABER inputs for ozone are not well constrained. In order to get the global energy budget near balance, Mlynczak et al. (2018) made an arbitrary adjustment reducing the daytime ozone values between 65 and 100 km by 25%, and also considered the possibility of nighttime ozone being too high. Both [H] and [O3] directly affect the calculation of [O(1D)] and any systematic errors are multiplied.

(d) There are at least three very different values in the recent literature for the rate coefficient of OH(9) + O (Kalogerakis, 2019; Fytterer et al., 2019; Zhu and Kaufmann, GRL, 2018). The choice of this rate coefficient directly affects the calculations. The manuscript ignores these possibilities and their effect on the estimated [O(1D)]. For example, at a mesopause temperature of 190 K, the manuscript adopts a rate coefficient for OH(9) + O of 3.05 x 10(-10) cm3s-1, whereas Zhu and Kaufmann (2018) determined a best-fit value of 2.3 x 10(-10) cm3s-1. This choice implies ∼33% larger [O(1D)] for the calculation reported in the manuscript.

In contrast to the assertion of the manuscript, the SCIAMACHY data and latest SABER atomic oxygen data reveal significant systematic differences at all latitudes and seasons (Zhu and Kaufmann, 2018). Below 87 km, the SABER atomic oxygen dataset is 40% lower on average than SCIAMACHY. This may be attributed to a very unrealistic, rate coefficient for quenching of OH(8) by O2 used in the SABER single-quantum model (approximately a factor of 50 smaller than the corresponding quenching rate of OH(9) by O2). Above 90 km, the difference between the two datasets is reversed and the SABER atomic oxygen is 10-30% higher than SCIAMACHY. Additionally, the SABER photochemical model for ozone does not take into account the loss of ozone through reaction with atomic oxygen, which affects retrieved atomic oxygen on the order of 30% at atomic oxygen peak altitudes. All these differences summarized in the discussion above directly propagate into the calculation of [O(1D)], which cannot be directly validated by observations.

In conclusion, several important parameters used for the calculation of [O(1D)] in this manuscript are flawed and inconsistent with the multi-quantum source of O(1D), and therefore lead to inaccurate results and large systematic errors.

Other Minor Comments ——————————— Line 37 “. . .A-band is well. . .”

Line 57 Delete “good” — it is redundant

Line 92 “. . .detailed analysis. . .”

Line 99 “. . .grateful to the. . .”

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