This paper presents some very interesting data and analysis from a study in Beijing using state-of-the-art measurements of OH, HO_2, and RO_2. Similar to a few other recent studies, the authors find that RO_2 concentrations and instantaneous ozone formation rates are both underestimated by 0-D models under high NOx conditions.

The authors define the instantaneous rate of ozone production using Equation 11:

$$P(O_3) = (k_{HO2+NO}[HO_2][NO] + k_{RO2+NO}[RO_2][NO]) - (k_{OH+NO2+M}[OH][NO_2][M] + k_{RO2+NO2+M}[RO_2][NO_2][M])$$

Similar definitions of $P(O_3)$ were used in Shirley et al. (2006), Sheehy et al. (2010), Dusanter et al. (2009), and Whalley et al. (2018), in contrast to the simpler earlier definitions which only included the first two terms on the right hand side of the equation, e.g., Kleinman et al. (1994), Thornton et al (2002), and Ren et al. (2003).

The last two terms are included to account for the fact that O_3 is not actually formed if an NO_2 molecule formed by the reaction of NO with HO_2 or RO_2 is then immediately removed by reaction with OH to form HNO_3 or with RO_2 to form a peroxy nitrate. The problem with this definition is that those two NO_2 removal reactions are just two of several Ox loss reactions, where $[Ox] = [O] + [O_3] + [NO_2] + [O(^1D)] + 2[NO_3] + 3[N_2O_5]$. For example, the reaction of $O(^1D)$ with H_2O is just as much of an Ox loss mechanism as is the reaction of NO_2 with OH. Including only one Ox loss term in the definition of $P(O_3)$ is confusing and not quite accurate. It would be much simpler and more accurate to just define the rate of gross Ox production as

$$P(O_X) = k_{HO2+NO}[HO_2][NO] + k_{RO2+NO}[RO_2][NO]$$

and to separately define L(Ox), which would include the rates of the reactions $OH + NO_2$, $O(^1D) + H_2O$, $O_3 + HO_2$, etc. The net rate of peroxy nitrate (RO_2NO_2) formation or loss could also be included.

It is worth noting that truly defining the *instantaneous* formation rate of ozone (rather than Ox) necessitates accounting for variations in j_{NO2}, e.g. $P(O_3) = j_{NO2}[NO_2] - k[NO][O_3]$. The difficulty of evaluating this expression and its limited utility, especially on days with variable j_{NO2} (due to clouds), underscore the advantage of considering Ox rather than O_3.

Please note the similar open comments made for Dusanter et al., (2009):

https://acp.copernicus.org/preprints/8/S5350/2008/acpd-8-S5350-2008.pdf

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