

Dear Anonymous Referee #2,

we thank you very much for your time and effort spent to provide your comments.

1. Why is the nighttime PSS value in Fig4 so abnormal? Is it the problem of box model simulation?"

In order to address this question, some details of the calculation need to be considered. In PSS the time derivative of the system is assumed to be zero, so the production and loss terms are equal. For NO_2 this results in $j_{\text{NO}_2}[\text{NO}_2] = k_1[\text{NO}][\text{O}_3] \frac{p}{k_B T} \Rightarrow [\text{NO}]_2 \sim \frac{[\text{NO}][\text{O}_3]}{j_{\text{NO}_2}}$. So $[\text{NO}_2]$ is inversely proportional to the photolysis frequency, which tends to zero during nighttime. This leads to an unstable behavior of PSS in absence of sunlight.

2. Why is the ensemble mean value of SMC so different from the PPS calculation at 12 o'clock in Fig6?

We investigated this and found multiple occurrences in the extrapolation example where the ensemble becomes unstable and entropy is reduced. This is also visible in the plot in Figure 6 where the red curve is disconnected due to discarded points as mentioned in 4.1. We added this discussion to section 4.1 (L 235ff):

This threshold is set to

$$H(\bar{x}_n) < \log(K) \Leftrightarrow R^* < K$$

as there are effectively less particles left to sample from than samples to be drawn. After a low entropy incident, the ensemble may require a few iterations to converge again. Considering this effect and discarding additional points may increase the data accuracy while lowering data coverage. Throughout this analysis no additional points were discarded. In applications the amount of low entropy events may be reduced using an increased ensemble size which requires a longer runtime.