

We thank the reviewer for the insightful comment. The reviewer is correct that surface ozone concentrations before 2015 were predicted using the LSTM model trained using data during 2015–2020. Therefore, it is essential to clarify the prediction uncertainty of the HrSOD product during 2005–2014. We would address this issue both theoretically and practically in the following:

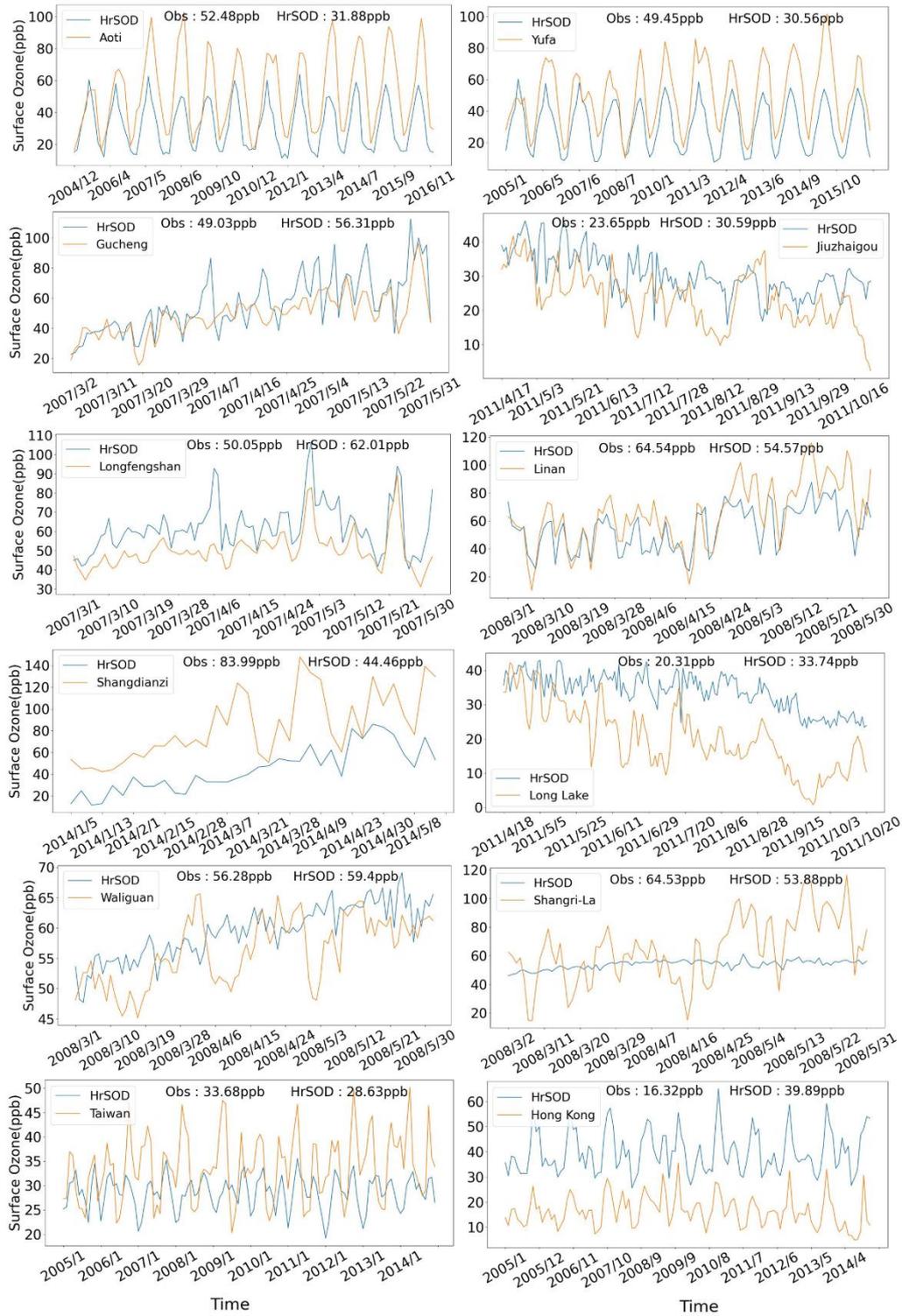
First, deep/machine learning models reproduce changes in dependent variables through capturing the complex nonlinear relationships between them and the predictors. This means if the underlying mechanisms controlling changes in dependent variables do not change, the trained deep/machine learning models can always stand irrespective of the time. This is the prerequisite that deep/machine learning models are used in amounts of retrospective research (e.g., Liao et al., 2020; Liu et al., 2020). In the case of the HrSOD product, there is no evidence that there was a significant shift of surface ozone production mechanisms locally before and after 2015 in China (Wang et al., 2017).

Second, though there were much fewer observations of surface ozone concentrations before 2015 in China, we successfully collected some site records (Table R1) at different time-steps, which were mostly obtained in 2014 (946 stations). Notably, there were several sites with long-term monthly observations, including 18 stations in Hong Kong during 2005–2014, and seven stations in Taiwan during 2005–2014. Figure R1 shows that the HrSOD estimates were generally consistent with those site observations at the daily and monthly scales in terms of the magnitude, the trend and the variability. The specific statistical metrics are summarized in Table R1. It should be noted that the HrSOD has a spatial resolution of 0.1° which would inevitably bring errors when directly compared with the site-level measurements (i.e., scale mismatch). Figure R2 shows the HrSOD performance across China at the hourly time-scale, which suggests the LSTM model trained using data after 2015 could well capture the spatio-temporal patterns of surface ozone concentrations before 2015 at the site level.

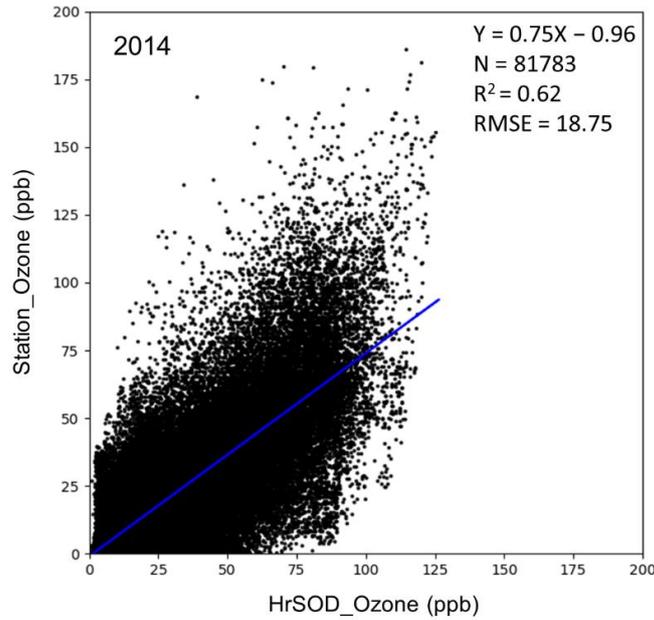
**Table R1.** Validation of ozone monitoring concentrations and HrSOD from different stations at different time scales from 2005 to 2017.

Site	Location	Study Period	Metric	Sample Size	R <sup>2</sup>	RMSE (ppb)	Reference/Source
Aoti	40.00°N, 116.41°E	2004–2017	Monthly	122	0.55	26.23	Cheng et al., 2019
Yufa	39.52°N, 116.31°E	2004–2017	Monthly	120	0.67	22.36	Cheng et al., 2019
Gucheng	39.13°N, 115.67°E	2007/3–2007/6	[O <sub>3</sub> ] MDA8	91	0.52	15.22	Ni et al., 2018
Lin'an	30.20°N, 119.70°E	2008/3–2008/6	[O <sub>3</sub> ] MDA8	94	0.61	17.42	Ni et al., 2018
Shangdianzi	40.65°N, 117.10°E	2004/1–2014/6	[O <sub>3</sub> ] MDA8	36	0.43	46.00	Ma et al., 2016
Longfengshan	44.70°N, 127.60°E	2007/3–2007/6	[O <sub>3</sub> ] MDA8	93	0.59	14.48	Ni et al., 2018
Shangri-La	28.01°N, 99.72°E	2008/3–2008/6	[O <sub>3</sub> ] MDA8	91	0.09	24.49	Ni et al., 2018
Waliguan	36.30°N, 100.90°E	2008/3–2008/6	[O <sub>3</sub> ] MDA8	93	0.25	5.92	Ni et al., 2018
Jiuzhaigou	33.27°N, 103.92°E	2011/4–2011/11	Daily	158	0.15	10.58	Qiao et al., 2012
Long Lake	33.04°N, 103.93°E	2011/4–2011/11	Daily	171	0.47	15.17	Qiao et al., 2012
Taiwan	Region	2005–2014	Monthly	121	0.08	8.32	Schultz et al., 2017
Hong Kong	Region	2005–2014	Monthly	119	0.59	24.18	EPD
China	Country	2014/6–2014/12	Hourly	81783	0.62	18.75	CNEMC

MDA8: maximum daily average 8-hour ozone; EPD: Environmental Protection Department in Hong Kong (<https://www.epd.gov.hk/epd/english/top.html>); CNEMC: China National Environmental Monitoring Centre (<http://www.cnemc.cn/>).

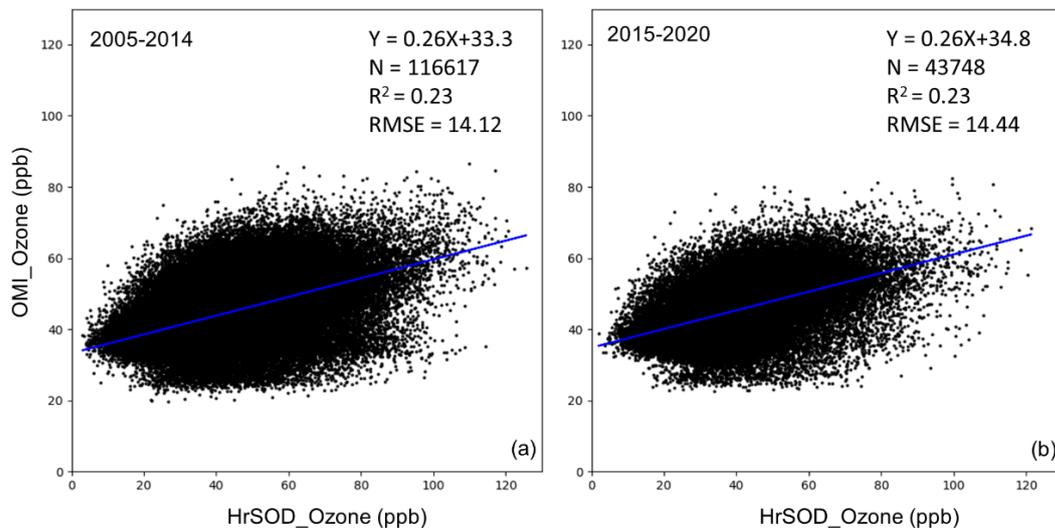


**Figure R1.** The temporal dynamics of both observed surface ozone concentrations and the corresponding HrSOD estimates at different stations mostly before 2015.



**Figure R2.** Comparison of observed hourly surface ozone concentrations and HrSOD estimates across China in 2014.

Third, we further compared the HrSOD with the OMI remote sensed surface ozone concentrations. Although the OMI surface ozone concentration product has been criticized for its low accuracy (Shen et al., 2019), it had consistent performance before and after 2015 both spatially and temporally. Thus, the OMI surface ozone concentration product can serve as a benchmark to evaluate the consistency of the HrSOD product. Figure R3 shows the HrSOD product has a highly congruous performance against the OMI product during 2005–2014 ( $R^2 = 0.23$ ,  $RMSE = 14.12$  ppb) and 2015–2020 ( $R^2 = 0.23$ ,  $RMSE = 14.44$  ppb). Therefore, we can conclude that the HrSOD product has a robust performance both before and after 2015, which means the uncertainty around the product is also comparable during the two periods.



**Figure R3.** Comparisons of HrSOD against the OMI remote sensed surface ozone

concentrations across China before **(a)** and after 2015 **(b)**. The blue lines represent linear regression lines.

The above analysis and discussion will be added into the main text in the future revised version.

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