Estimation of Surface-level Ozone Concentration Using TROPOMI Data and Source-sink Analysis over China

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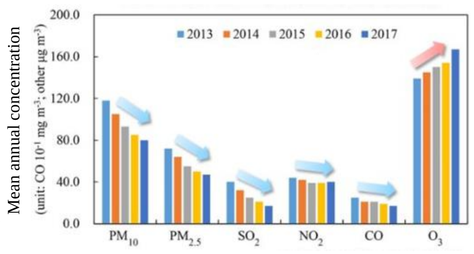
Introduction

- Ozone in the lower troposphere(or near surface)can cause photochemical smog, reduces agricultural yield and has an adverse effect on human health (Gharibzadeh et al., 2021). At present, it has become the main culprit of atmospheric environment pollution in many cities in summer and autumn(Fig. 1), second only to $PM_{2.5}$.
- When it is not easy or accurate to obtain surface-level ozone concentration directly by remote sensing, the source-sink analysis can effectively help estimate surface-level O_3 concentration data.
- The chemical, photochemical, atmospheric movement relationships among the factors in the various sources and sinks is quiet complicated. LGBM algorithm (Fig. 2), supports more efficient parallel training, has faster running speed(Fig.3), lower memory consumption, better accuracy and can quickly process massive data. In addition, there are good results achieved in some similar studies(Kang Yoojin, et al., 2021).
- Furthermore, this study can provide high-resolution estimation results, because it based on TROPOMI data which has a higher spatial resolution (5.5km×3.5km) than other satellite sensors that have provided the column density information of air pollutants.



Data from Bulletin of China's Environmental Status of China

Fig. 1. Interannual comparison of concentrations of six air pollutants in 74 cities in China

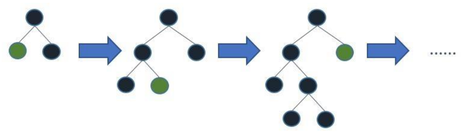


Fig. 2. Growth by leaf algorithm with depth limitation

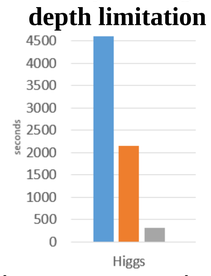


Fig. 3. Time cost comparison between different models, lower=better

blue: xgboost; rad: xgboost_approx; grey: LightGBM

Methods

The model estimates the surface-level O_3 concentration while maintaining its highest resolution and accuracy. The overall process of surface O_3 concentration estimation is summarized in Fig. 4, including source-sink analysis of surface ozone, estimation model development, model verification and analysis.

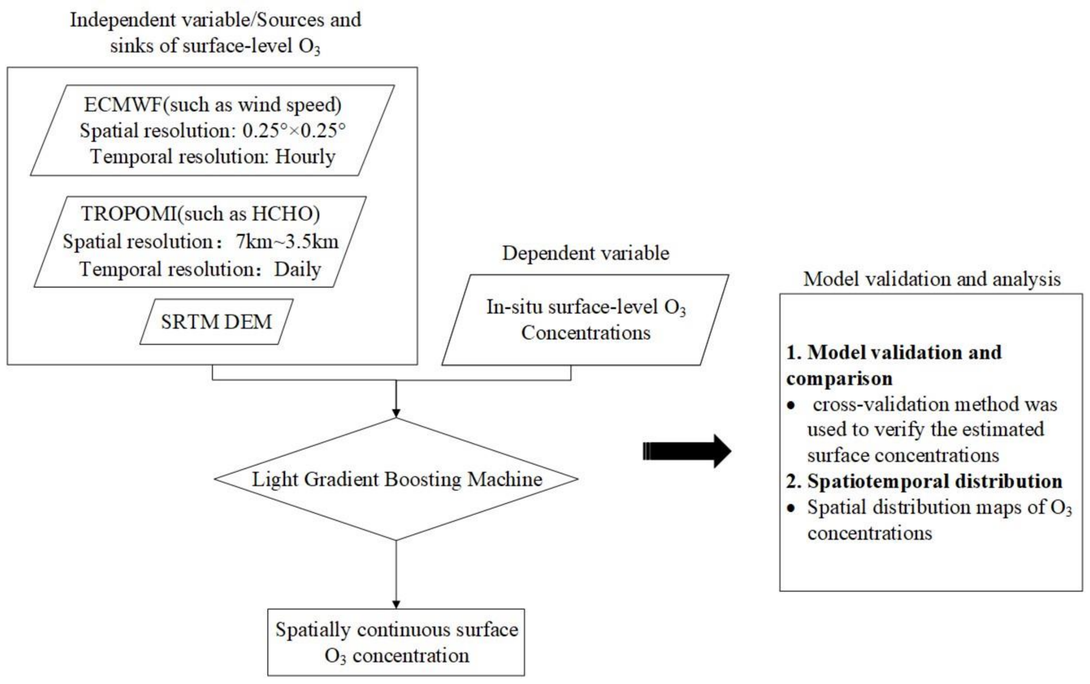


Fig. 4. Process flow diagram for estimation of surface O_3 concentrations

Source-sink Analysis

Tab. 1. Sources and sinks of surface O_3 and related influence factors

Source	Influence Factors of Source	Sink	Influence Factors of Sink
Stratospheric injection	Total O_3 column; Divergence of ozone flux; Tropospheric effective potential energy; Solar radiation; Boundary layer height; Pressure at the top of the ozone layer	**Surface failure (deposition)**	DEM; Humidity; Surface pressure; Skin temperature; Wind speed; Surface roughness
Chemical formation in the ambient atmosphere	NO_2 concentration; SO_2 concentration; O_3 concentration; HCHO concentration; CO concentration; Humidity; Surface pressure; Skin temperature; Wind speed; Friction velocity; Solar radiation; Water concentration	**Chemical decomposition in the ambient atmosphere**	NO_2 concentration; SO_2 concentration; O_3 concentration; HCHO concentration; CO concentration; Humidity; Surface pressure; Skin temperature; Wind speed; Friction velocity; Solar radiation; Water concentration
Interregional transport(Both source and sink)	Wind speed; Surface roughness; Humidity; Surface pressure; Skin temperature; Friction velocity; DEM		

Results

- We ran the model in summer(June, July and August) of this year(Fig. 5). These months are the warmest months of the year and have the highest ozone concentration at ground level.

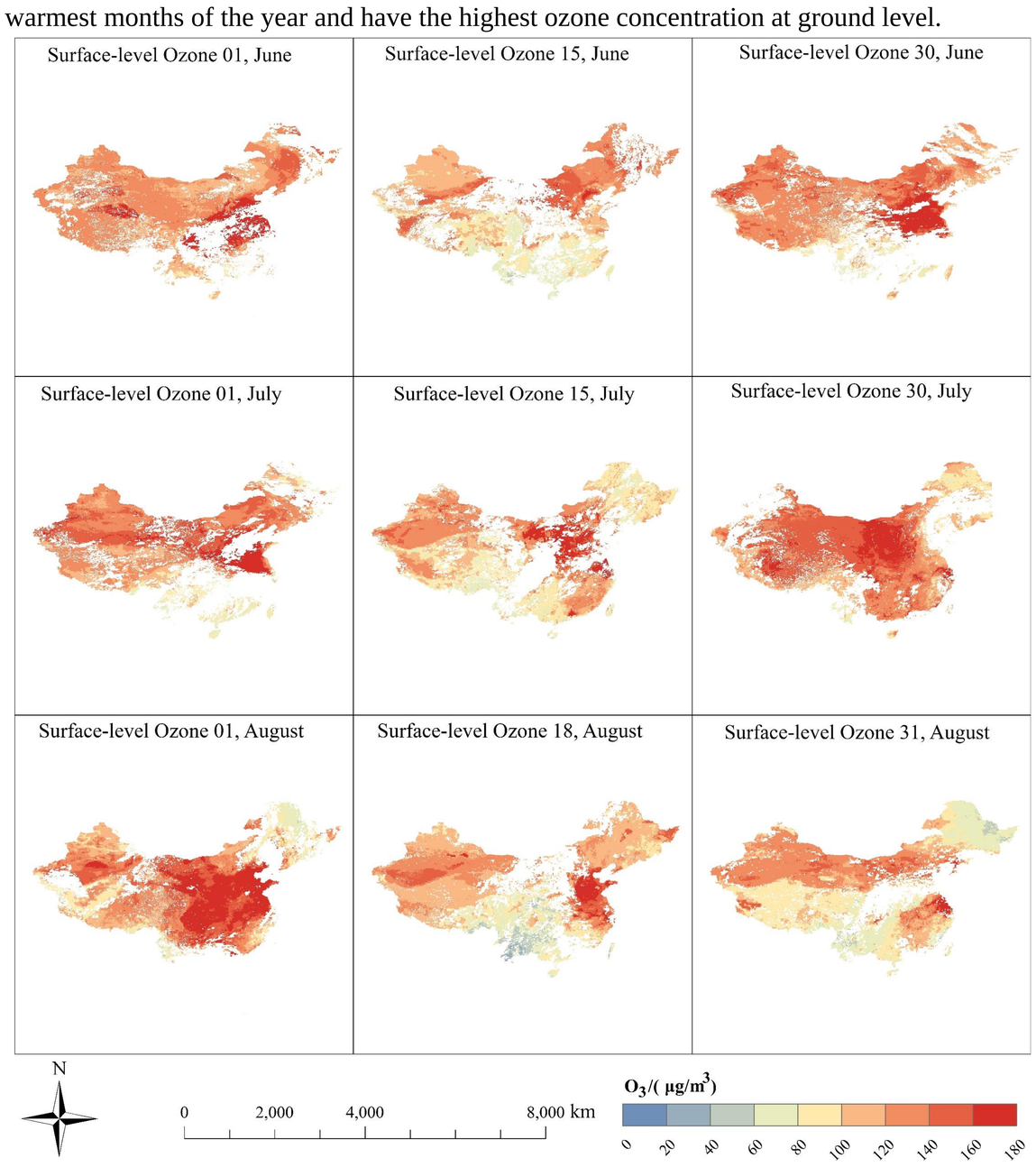


Fig. 5. Spatial and temporal distribution of surface ozone concentration in summer 2021.

The trend from blue to red indicates a higher level of ozone at ground level.

- We cross-verify the model result data with ground base station observation data (Fig. 6).

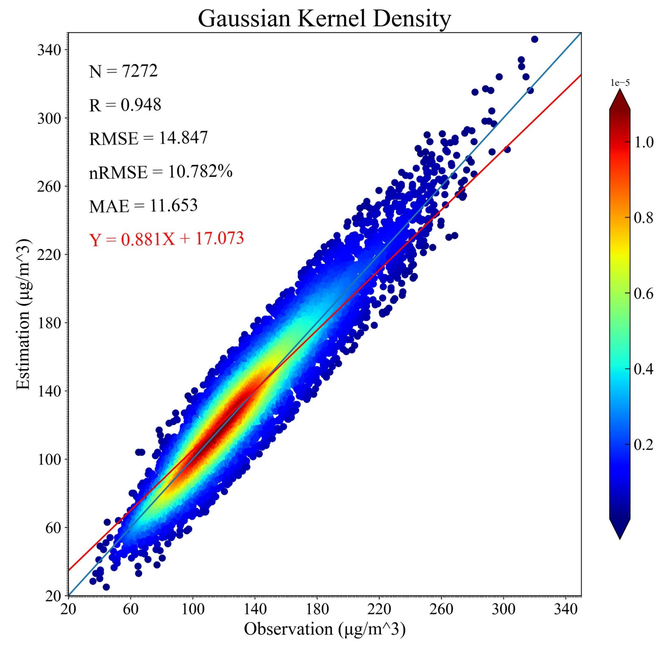


Fig. 6. Results of cross validation of surface ozone estimation model.

The blue line (Y=X) is the diagonal line; The red line (Y=0.881X+17.073) is the fitting line of all points in the figure.

References

Gharibzadeh, M. , and A. A. Bidokhti . "The interaction of ozone and aerosol in a semi-arid region in the Middle East: Ozone formation and radiative forcing implications." Atmospheric Environment 245.118015(2020):1-16.

Kang Yoojin, et al."Estimation of surface-level NO2 and O3 concentrations using TROPOMI data and machine learning over East Asia." Environmental Pollution 288.(2021): doi:10.1016/J.ENVPOL.2021.117711.

Conclusion

- In this study, a surface-level ozone concentration estimation model was developed. Due to the limited temporal-spatial resolution of TROPOMI, the spatial resolution can reach 0.05° and the temporal resolution is daily (i.e., 13:30 local time) of the result data.
- By analyzing the source and sink of surface ozone(Tab. 1), it is clear that ozone concentration in ambient air influenced by background value, regional and local chemical generation, surface failure, regional and local chemical removal and Interregional transport comprehensively.
- The time series comparison showed that surface-level ozone concentration exceeded the standard in some areas of China in summer, especially in the economically developed areas such as Beijing-Tianjin-Hebei and Yangtze River Delta.
- With 7272 points used for validation, the R, RMSE, nRMSE and MBE is 0.948, 14.847, 10.782% and 11.653 of the proposed ozone concentration estimation model, respectively. The results show that the model can effectively reflect the actual situation of surface-level O_3 concentration in some degree.