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## Supplement of

## Retrieving ground-level $PM_{\rm 2.5}$ concentrations in China (2013–2021) with a numerical-model-informed testbed to mitigate sample-imbalance-induced biases

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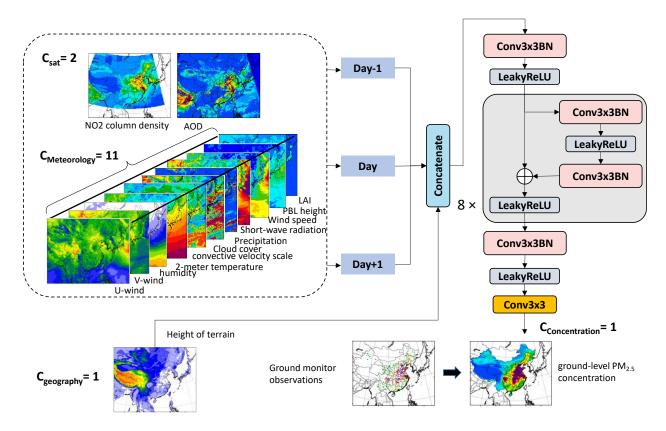
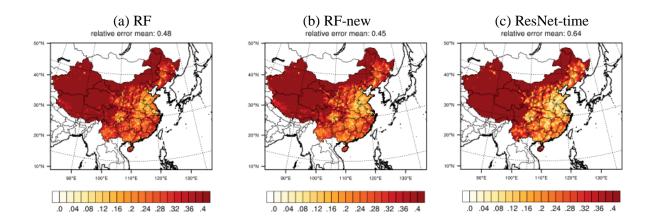
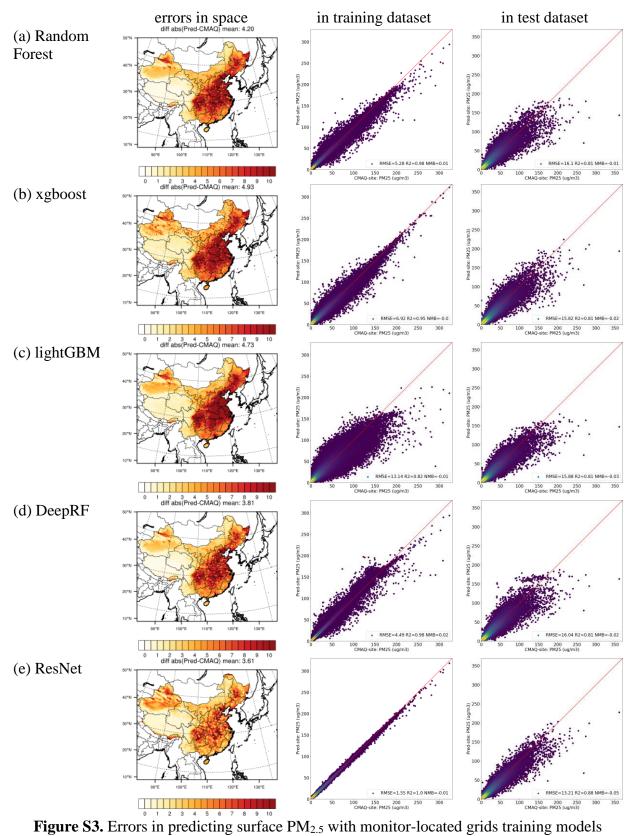
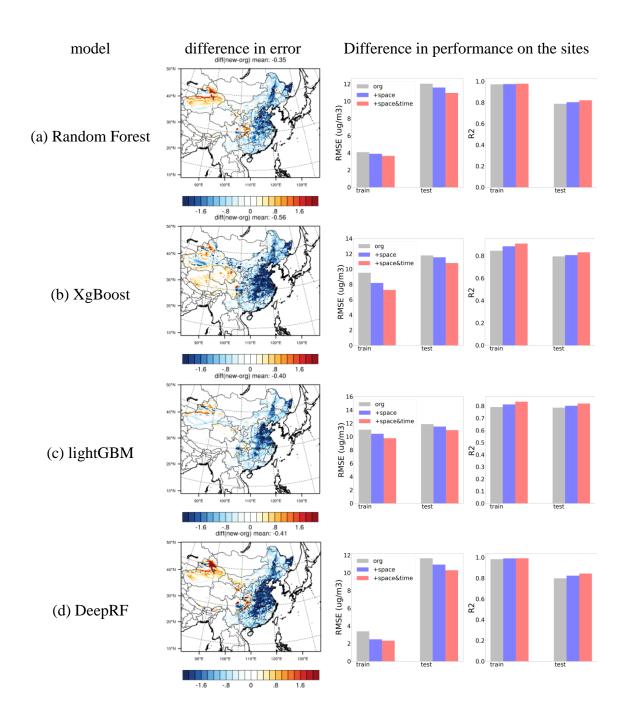


Figure S1. ResNet model structure

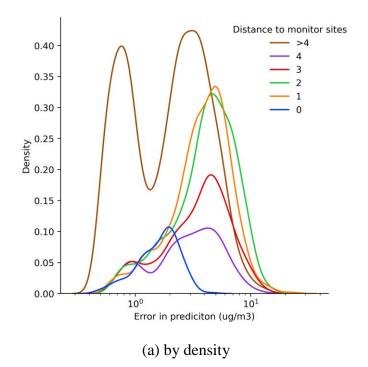


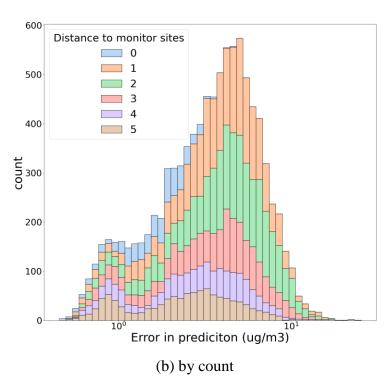
**Figure S2.** Comparison of relative errors in predicting ground-level  $PM_{2.5}$  using RF, RF-new, and ResNet-time models with the testbed.



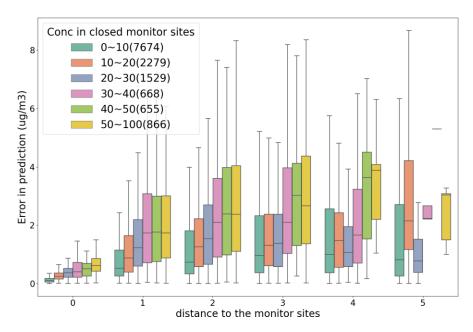


**Figure S4.** Improvement after implementing the features in surrounding grid cells (compared to each baseline model without spatiotemporal-neighbourhood features)

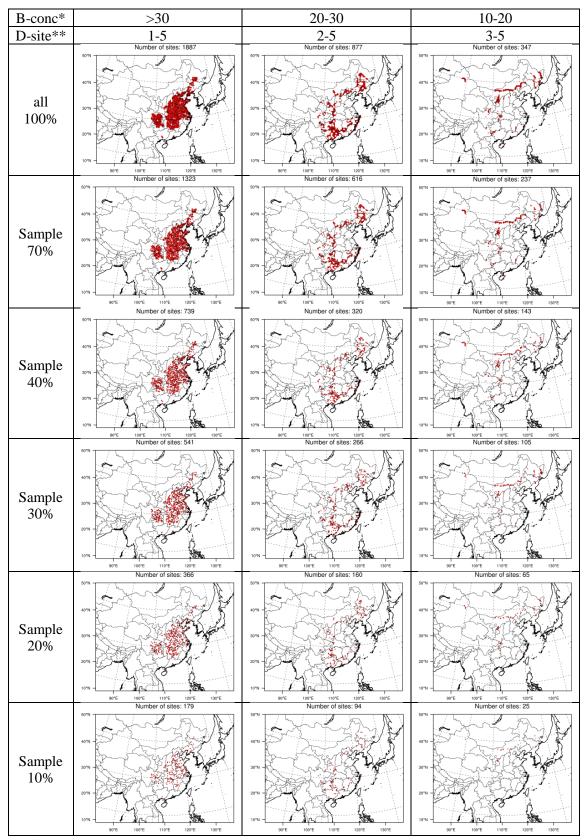




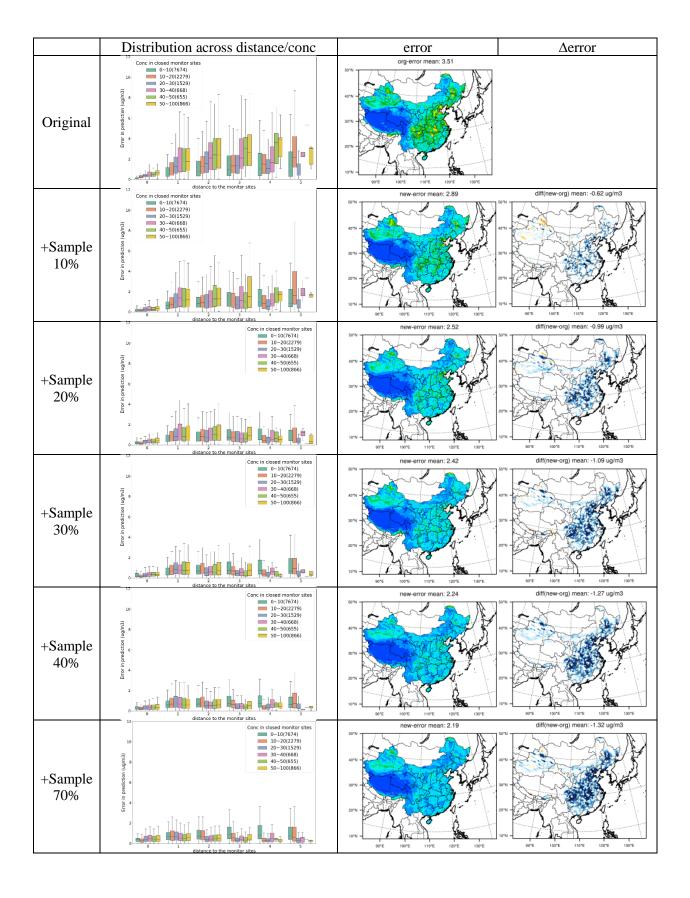
**Figure S5.** Error distribution across the distance to monitor sites (D-site) based on ResNet-time model

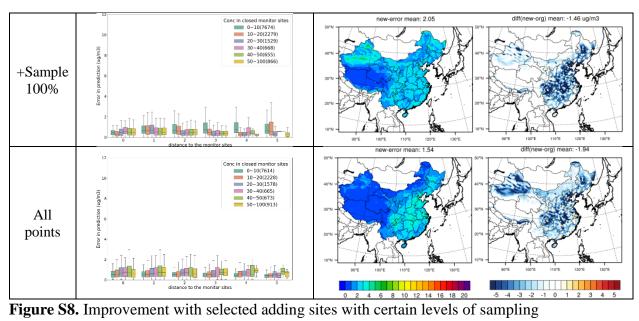


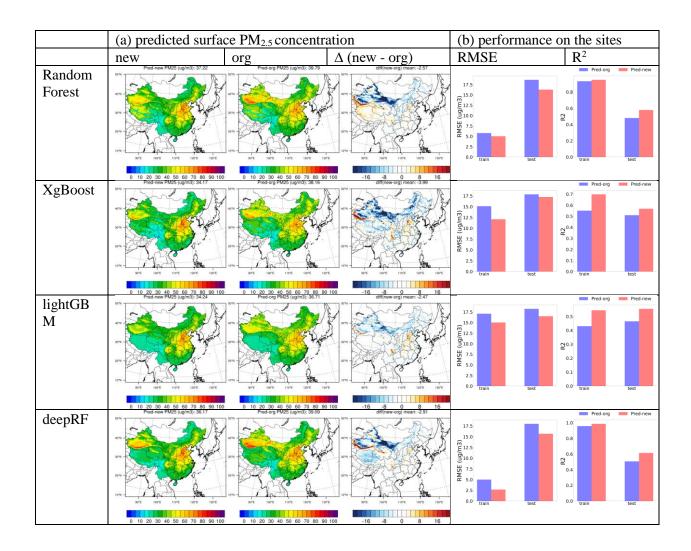
**Figure S6.** Error distribution across the monitor concentrations (B-conc) based on ResNet-time model



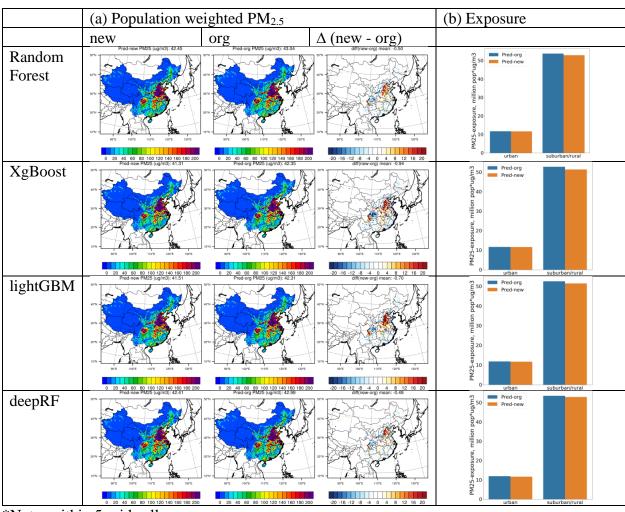
**Figure S7.** Spatial distribution of selected adding sites with certain levels of sampling (B-conc: conc in closed monitor sites; D-site: distance from monitor sites)







**Figure S9.** Improved performance with inclusion of spatiotemporal-neighbourhood features trained with real measurement dataset



\*Note: within 5 grid cells

Figure S10. Uncertainties in estimation of PM2.5-related exposure across China

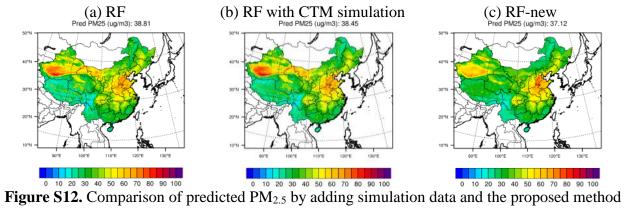
## (a) performance in scenarios with adding points across distance to monitor sites deepRF XgBoost lightGBM ResNet RF-add XgBoost-add lightGBM-add deepRF-add ResNet-add 20 RMSE (ug/m3) Ó 2 3 Distance to monitor sites (by number of grid cells) 1 (b) +sample new sites during 2017-2021 Location of sites Prediction Pred PM2.5: 13.95 ug/m3 difference in errors diff(new-org) mean: -0.32 ug/m3

**Figure S11.** Improvement with the inclusion of new sites after 2017 in testing with CMAQ simulations

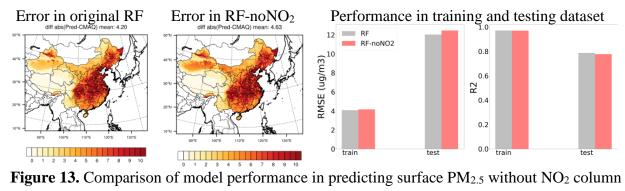
5 10 15 20 25 30 35 40 45 50

-2

\*black dot: original monitor sites (619)



in this study (2017 for example)



feature