The drivers and health risks of the unexpected surface ozone enhancements over the Sichuan basin, China in 2020

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Abstract

After a continuous increase in surface ozone (O3) level from 2013 to 2019, the overall summertime O3 concentrations across China showed a significant reduction in 2020. In contrast to this overall reduction in surface O3 across China, unexpected surface O3 enhancements of 10.2 ± 0.8 ppbv (23.4%) were observed in May-June 2020 vs. 2019 over the Sichuan basin (SCB), China. In this study, we use high resolution nested-grid GEOS-Chem simulation, the eXtreme Gradient Boosting (XGBoost) machine learning method, and the exposure–response relationship to determine the drivers and evaluate the health risks of the unexpected surface O3 enhancements. We first use the XGBoost machine learning method to correct the GEOS-Chem model-to-measurement O3 discrepancy over the SCB. The relative contributions of meteorology and anthropogenic emissions changes to the unexpected surface O3 enhancements are then quantified with the combination of GEOS-Chem and XGBoost models. In order to assess the health risks caused by the unexpected O3 enhancements over the SCB, total premature death mortalities are estimated. The results show that changes in anthropogenic emissions caused 0.9 ± 0.1 ppbv of O3 reduction and changes in meteorology caused 11.1 ± 0.7 ppbv of O3 increase in May-June 2020 vs. 2019. The meteorology-induced surface O3 increase is mainly attributed to an increase in temperature and the decreases in precipitation, specific humidity and cloud fractions over the SCB and surrounding regions in May-June 2020 vs. 2019. These changes in meteorology combined with the complex basin effect enhance biogenic emissions of volatile organic compounds (VOCs) and nitrogen oxides (NOx), speed up O3 chemical production, and inhibit the ventilation of O3 and its precursors, and therefore account for the surface O3 enhancements over the SCB. The total premature mortality due to the unexpected surface O3 enhancements over the SCB has increased by 89.8% in May-June 2020 vs. 2019.
Keywords: Ozone; Health risk; Emissions; Meteorology; Chemical model; Machine learning

1. Introduction

Surface ozone ($O_3$) is largely generated from its local anthropogenic (fossil fuel and biofuel combustions) and natural (biomass burning (BB), lightning, and biogenic emissions) precursors such as volatile organic compounds (VOCs), nitrogen oxides ($NO_x$), and carbon monoxide (CO) via a chain of photochemical reactions (Cooper, 2019; Sun et al., 2018). Additional portion of surface $O_3$ is transported from long-distance regions or from stratosphere (Akimoto et al., 2015; Wang et al., 2020b). Surface $O_3$ is one of the most harmful air pollutants that threatens human health and corps production (Fleming et al., 2018; Lu et al., 2020; Sun et al., 2018; Van Dingenen et al., 2009). Exposure to ambient $O_3$ pollution evokes a series of health risks including stroke, respiratory disease (RD), hypertension, cardiovascular disease (CVD), and chronic obstructive pulmonary disease (COPD) (Brauer et al., 2016; Lelieveld et al., 2013; Li et al., 2015; Liu and Wang, 2018; Lu et al., 2020; Wang et al., 2020c). Lu et al., 2020 estimated that the premature RD mortalities attributable to ambient $O_3$ exposure in 69 Chinese cities in 2019 reached up to 64,370.

Surface $O_3$ variability is sensitive to both emissions and meteorological changes (Liu and Wang, 2020a, b; Lu et al., 2019c). Meteorological conditions affect surface $O_3$ variability indirectly through changes in natural emissions of its precursors or directly via changes in wet and dry removal, dilution, chemical reaction rates, and transport flux (Li et al., 2019a; Lin et al., 2008; Liu and Wang, 2020a; Lu et al., 2019d). A reduction in temperature can lessen $O_3$ production by slowing down the chemical reaction rates (Fu et al., 2015; Lee et al., 2014; Liu and Wang, 2020a) or reducing the biogenic VOCs and $NO_x$ emissions (Guenther et al., 2006; Im et al., 2011; Tarvainen et al., 2005). A dryer meteorological condition can result in an increase in surface $O_3$ level (He et al., 2017; Kalabokas et al., 2015; Liu and Wang, 2020a). Depending on which process dominates the influence of planetary boundary layer height (PBLH) on surface pollutants, a higher PBLH can either reduce surface $O_3$ level by diluting $O_3$ and its precursors into a larger volume of air (Sanchez-Coyollo et al., 2006; Wang et al., 2020d) or increase surface $O_3$ level by transporting more $O_3$ from upper troposphere or lessening NO abundance for $O_3$ titration (He et al., 2017; Liu and Wang, 2020a; Sun et al., 2009). Precipitation has been verified to decrease surface $O_3$ level through the wet removal of its precursors, and clouds reduce surface $O_3$ level by decreasing the oxidative capacity of the atmosphere and enhancing scavenging of atmospheric oxidants (Lelieveld and Crutzen, 1990; Liu and Wang, 2020b; Shan et al., 2008; Steinfeld, 1998). A higher wind speed can decrease surface $O_3$ level by a fast ventilation of $O_3$ and its precursors (Lu et al., 2019c; Sanchez-Coyollo et al., 2006).

Emissions of air pollutants affect surface $O_3$ variability by perturbing the abundances of hydroperoxyl ($HO_2$) and alkylperoxyl ($RO_2$) radicals which are the key atmospheric constituents in formation of $O_3$ (Liu and Wang, 2020b). Many previous studies have verified a nonlinear relationship between $O_3$ and its precursors (e.g., Atkinson, 2000; Liu and Wang, 2020b; Lu et al., 2019d; Sun et al., 2018; Wang et al., 2017). If surface $O_3$ formation regime lies within the VOCs limited region, reductions in VOCs emissions will result in a reduction in surface $O_3$ level. Similarly, if surface $O_3$ formation regime lies within the $NO_x$ limited region, reductions in $NO_x$ emissions will result in a reduction in surface $O_3$ level (Atkinson, 2000; Wang et al., 2017). If surface $O_3$ formation regime lies within transitional region, reductions in either VOC or $NO_x$ emissions will result in a
reduction in surface O₃ level. Atmospheric aerosols can affect surface O₃ level through either heterogeneous reactions of reactive gases (Li et al., 2018; Lou et al., 2014; Lu et al., 2012; Stadtler et al., 2018) or affecting the solar radiation for gases photolysis and oxidation (Li et al., 2011; Lu et al., 2019c; Lu et al., 2019d; Xing et al., 2017).

Understanding the drivers of surface O₃ variability has a strong implication for O₃ mitigation purpose (Chen et al., 2020; Lu et al., 2019c; Sun et al., 2018). China has experienced a continuous increase in surface O₃ level despite the implementation of control measures on NOₓ since 2013 (Liu and Wang, 2020a; b; Lu et al., 2018; Lu et al., 2020). Many studies have attempted to determine the drivers of high-O₃ events occurred in specific region and time across China. Most of these studies focus on the most densely populated and highly industrialized areas in eastern China, whereas the studies in the rest part of China are still limited (Liu and Wang, 2020a, b; Lu et al., 2019a; Lu et al., 2019b; Lu et al., 2012; Wang et al., 2020a; Wang and Lu, 2019; Wang et al., 2017). As China has a vast territory with a wide range of emission levels and meteorological conditions, O₃ variability and its drivers may vary both temporally and geographically, so the results from one region are not likely to be applied nationally. In addition, previous studies typically use state-of-the-art chemical transport models (CTMs) with sensitivity simulations to quantify the drivers of O₃ variability, e.g., fixed meteorology but varied emission levels to quantify the influences of emission changes or vice versa (Liu and Wang, 2020a, b; Lu et al., 2019a). However, uncertainties in local meteorological fields, emission estimates, and model mechanisms can lead to a discrepancy in CTMs that may affect the accuracy of O₃ predictions and their sensitivities to changes in emissions and meteorology (Lu et al., 2019c; Young et al., 2018). This is in particular for the Sichuan basin (SCB), one of the most industrialized and populated cities cluster in western China, where large discrepancies between measured and modelled surface O₃ are found due to the complex terrain (Lu et al., 2019c; Wang et al., 2020d).

After a continuous increase in surface O₃ level from 2013 to 2019, the summertime (May-August) O₃ concentration across China showed a significant reduction in 2020 (Figure 1 (d)). In this study, we use high resolution nested-grid GEOS-Chem simulation, the eXtreme Gradient Boosting (XGBoost) machine learning method, and the exposure–response relationship to determine the drivers and evaluate the health risks of the unexpected surface O₃ enhancements. We first use the XGBoost machine learning method to correct the GEOS-Chem model-to-measurement O₃ discrepancy over the SCB. The relative contributions of meteorology and anthropogenic emissions changes to the unexpected surface O₃ enhancements are then quantified with the combination of GEOS-Chem and XGBoost models. In order to assess the health risks caused by the unexpected O₃ enhancements over the SCB, total premature death mortalities are also estimated.

2. Methods and data
2.1 Surface O₃ data and auxiliary data over the SCB

China has identified nine city clusters that lead the populations and developments of economy, society, and culture across China. The SCB contains the fourth-largest cities cluster in China after the Yangtze River Delta (YRD), the Pearl River Delta (PRD), and the Beijing-Tianjin-Hebei (BTH) cities clusters. The location of the SCB city cluster is shown in Figure S1. With Chongqing and Chengdu as the dual core cities, more than a dozen cities including Mianyang, Deyang, Yibin, Nanchong, Dazhou, and Luzhou over the SCB have achieved rapid economic development and
industrial upgrading. As the region with the strongest economic strength and best economic foundation in western China, the SCB region has many industries such as energy and chemical industry, electronic information, food processing, equipment manufacturing, eco-tourism, and modern finance. As one of the most densely populated and highly industrialized regions in China combined with the basin terrain which is favorable to the accumulation of air pollutants, the SCB is a newly emerging region of severe air pollution in China (Lu et al., 2019b; Lu et al., 2012).

Surface O₃ measurements over the SCB are available from the China National Environmental Monitoring Center (CNEMC) network (http://www.cnemc.cn/en/, last access: 2 July 2021). The CNEMC network has routinely measured the concentrations of CO, O₃, NO₂, SO₂, PM₁₀, and PM₂.₅ at 122 sites in 22 key cities over the SCB since 2015. The mean geolocation, population, the number of measurement site, and data range of each city are summarized in Table 1. The altitude of these cities ranges from 0.3 to 4.3 km (above sea level, a.s.l.) and the population ranges from 822 to 32,054 thousand. The number of measurement site in each city ranges from 2 to 21. Surface O₃ measurements at all measurement sites are based on similar differential absorption ultraviolet (UV) analyzers. The hourly mean time series of surface O₃ concentrations have covered the period from January 2015 to present at all measurement sites in the 22 cities. After removing unreliable measurements with the filter criteria used in (Lu et al., 2020) (Section S1), we average the O₃ concentrations at all measurement sites in each city to form a city representative O₃ dataset. O₃ metric used in this study is on maximum 8-h average (MDA8) basis.

Since the vertical distributions of tropospheric HCHO and NO₂ are weighted heavily toward the lower troposphere over polluted regions, many studies have used tropospheric column measurements of these gases to represent near-ground conditions (Streets et al., 2013; Sun et al., 2021b; Sun et al., 2018). In this study, the tropospheric NO₂ and HCHO columns from the TROPOMI Level 3 products are used for investigating the changes in O₃ precursors in May-June 2020 vs. 2019. TROPOMI overpasses China at approximately 13:30 local time (LT) with a ground pixel size of 7 km × 7 km. Pixels with quality assurance values of less than 50% for HCHO and 75% for NO₂ are not included in present work.

2.2 GEOS-Chem nested-grid simulation

We use the high resolution nested-grid GEOS-Chem model version 12.2.1 to simulate surface O₃ over the SCB (Bey et al., 2001). Simulations are conducted at a horizontal resolution of 0.25° × 0.3125° over the nested domain (70°-140°E, 15°-55°N) covering China and surrounding regions. The boundary conditions for the nested-grid GEOS-Chem simulation are archived from the global simulation at 2° × 2.5° resolution (Sun et al., 2021a; Sun et al., 2021b; Yin et al., 2020; Yin et al., 2019) We spun up the model for one year to remove the influence of the initial conditions. We first run global simulation at 2° × 2.5° resolution and then interpolate the restart file on 1 January 2018 into high resolution (0.25° × 0.3125°) for the nested domain to initialize the nested model simulation from January 2019 to June 2020.

The simulations were driven by GEOS-FP meteorological field at the native resolution of 0.25° × 0.3125° and 47 layers from surface to 0.01 hPa at the top. The PBLH and surface meteorological variables are implemented in 1-hour interval and other meteorological variables are in 3-hour intervals. The time step applied in the model for transport is 5 minutes and for chemistry and emissions is 10 minutes (Philip et al., 2016) The non-local scheme for the boundary layer mixing
process is from (Lin and McElroy, 2010), wet deposition is from (Liu et al., 2001), and dry deposition is generated with the resistance-in-series algorithm (Wesely, 1989; Zhang et al., 2001). The photolysis rates are from the FAST-JX v7.0 photolysis scheme (Bian and Prather, 2002). Chemical mechanism follows the universal tropospheric-stratospheric Chemistry (UCX) mechanism (Eastham et al., 2014). The GEOS-Chem simulation outputs 47 layers of O₃ and other atmospheric constituents over China with a temporal resolution of 1 hour.

We use the Community Emissions Data System (CEDS) inventory for global anthropogenic emissions at the latest 2017 level, which is overwritten by the Chinese anthropogenic emissions with the Multi-resolution Emission Inventory (MEIC) in 2019 (Hoesly et al., 2018; Li et al., 2017; McDuffie et al., 2020; Zheng et al., 2018). Anthropogenic emissions are fixed for 2019 and 2020. Global BB and biogenic emissions were from the Global Fire Emissions Database (GFED v4) inventory (Giglio et al., 2013) and the Model of Emissions of Gases and Aerosols from Nature (MEGAN version 2.1) inventory (Guenther et al., 2012), respectively. Soil NOₓ emissions (Hudman et al., 2010; Lu et al., 2021) and lightning NOₓ (Murray et al., 2012) emissions are calculated online in the model.

2.3 Correction of GEOS-Chem discrepancy with machine learning method

We used the XGBoost machine learning method to correct the GEOS-Chem model-to-measurement O₃ discrepancy over the SCB following (Keller et al., 2021). The same methodology has also been applied in our companion study examining ozone changes over the eastern China from 2019 to 2020 (Yin et al., 2021). It uses the Gradient Boosting Decision Tree (GBDT) framework to iteratively train the GEOS-Chem model-to-measurement discrepancy to improve the model predictions in a stagewise manner. XGBoost method minimizes the loss function by adding a weak learner for the purpose of optimizing the objective function. The optimization objective function used in XGBoost model is expressed as,

\[ L^{(t)} = \sum_{i=1}^{n} [l(y_i, \hat{y}_i^{(t-1)}) + g_i f_t(x_i) + \frac{1}{2} h_i f_t^2(x_i)] + \Omega(f_t) \]  

\[ g_i = \partial_{\hat{y}_i^{(t-1)}} l(y_i, \hat{y}_i^{(t-1)}) \]  

\[ h_i = \partial^2_{\hat{y}_i^{(t-1)}} l(y_i, \hat{y}_i^{(t-1)}) \]

where \( g_i \) and \( h_i \) are first and second order gradients of the loss function, respectively. \( L^{(t)} \) represents the optimization objective function to be solved at the \( t \)-th iteration. \( l(y_i, \hat{y}_i^{(t-1)}) \) is the loss function representing the difference between the prediction for the \( i \)-th sample at the \((t-1)\)-th iteration and the real values \( y_i \). Function \( f(t) \) is the amount of change at the \( t \)-th iteration. Overall, the objective function consists of a two-order Taylor approximation expansion of the loss function and the regularization term (\( \Omega(f_t) \)), which penalizes the complexity of the model and prevents overfitting of the model. Compared to traditional GBDT method, XGBoost method has the following advantages: (1) effectively handles missing values; (2) prevents overfitting; (3) reduces computing time by using parallel and distributed computing methods.

Since GEOS-Chem model-to-measurement discrepancy is usually site-specific, we train a separate XGBoost model for each site. Similar to the method of (Keller et al., 2021), we use a full seasonal cycle of hourly measurements in 2019 at each site as the learning samples, and GEOS-
Chem input of emissions and meteorological parameters, output concentrations of atmospheric constituents, and time information as training input data. In order to incorporate emissions and meteorological factors that affect O3 production properly, we have included the GEOS-Chem simulated concentrations of 43 atmospheric chemical constituents, emissions of 21 atmospheric chemical constituents, 10 meteorological parameters, and 4-time parameters (e.g., hour, day, month, and year) into the data training. All these training input data are summarized in Table S1 and have been standardized as equation (2) in section S2. We choose a learning rate of 0.35, maximum tree depth of 6, L1 and L2 regularization terms of 0 and 1, the loss function of mean square, and evaluation metric of root-mean-square error (RMSE) in the data training.

We use k-fold cross-validation method to test the performance of the XGBoost model (\(k=1–n\)). First, all sample data are randomly and uniformly divided into \(k\) groups, where one group is taken as the test dataset and the remaining \(k-1\) groups are taken as the training dataset. We then start to train the model and use the test dataset to evaluate the performance of the trained model. We repeated this process for \(k\) times by using different groups of datasets as the test data. The training model is finally determined if all the \(k\) groups of experiments show similar performances. This method ensures the stability and robustness of XGBoost model and avoid overfitting. In this study, a 10-fold cross-validation method is applied, i.e., we divide the O3 measurements in 2019 into 10 groups of sub data: the training dataset accounts for 90% and the test dataset accounts for the remaining 10% of the total sample data. We also attempted to use 60% and 80% of the sample data as the training dataset and do not find significant influences on the results, indicating the robustness of the XGBoost training model.

### 2.4 Quantifying meteorological and emissions contributions

We have used the GEOS-Chem only and the combination of GEOS-Chem and XGBoost model (hereafter GEOS-Chem-XGBoost) to quantify the contributions of meteorology and anthropogenic emissions to the unexpected surface O3 enhancements over the SCB in 2020, following (Yin et al., 2021). For the GEOS-Chem method, since the anthropogenic emissions are fixed, the simulated O3 differences between 2020 and 2019 can be attributed to changes in meteorological conditions, which is calculated as,

\[
G_{\text{Met}} = G_{2020} - G_{2019}
\]  

(4)

The contribution of anthropogenic emissions changes can then be quantified as,

\[
G_{\text{Emis}} = (\text{Meas}_{2020} - \text{Meas}_{2019}) - G_{\text{Met}}
\]  

(5)

where \(G_{\text{Met}}\) and \(G_{\text{Emis}}\) represent the meteorology and anthropogenic emissions contributions, respectively. \(\text{Meas}_{2019}\) and \(\text{Meas}_{2020}\) represent O3 measurements in 2019 and 2020, respectively. \(G_{2019}\) and \(G_{2020}\) represent GEOS-Chem O3 simulations in 2019 and 2020, respectively.

Since the GEOS-Chem-XGBoost model has corrected the GEOS-Chem model-to-measurement discrepancy in 2019, we assume it can provide accurate predictions to the surface O3 measurements in 2020 if the anthropogenic emissions were unchanged. This assumption is valid since the probability density functions (PDFs) of key O3 precursors and meteorological parameters for the training data within a full seasonal cycle of 2019 cover the variation ranges of these factors in May-June 2020 (Figures S2 and S3). For predicting O3 evolutions in 2020, all input parameters except anthropogenic emissions fed into each GEOS-Chem-XGBoost model are updated to match the measurements in 2020, while anthropogenic emissions are fixed at the 2019 levels. As a result,
the differences between the GEOS-Chem-XGBoost predictions for 2020 and the 2020 measurements are attributed to the changes in anthropogenic emissions (equation (6)). The meteorology induced contributions are then obtained as equation (7) by subtracting the anthropogenic emissions induced contributions.

\[
XG_{\text{Emis}} = \text{Meas}_{2020} - XG_{2020}
\]  
(6)

\[
XG_{\text{Met}} = (\text{Meas}_{2020} - \text{Meas}_{2019}) - XG_{\text{Emis}}
\]  
(7)

where the acronyms are similar to those in equations (4) and (5) but for GEOS-Chem-XGBoost method. By correcting the model-to-measurement discrepancy, GEOS-Chem-XGBoost model is expected to provide a more accurate \(O_3\) sensitivity to changes in both meteorology and anthropogenic emissions as will be discussed later.

2.5 Health risks evaluation

We have assessed the total premature mortalities including all nonaccidental causes, hypertension, CVD, RD, COPD, and stroke attributed to ambient \(O_3\) exposure in all cities over the SCB in 2019 and 2020. We first calculated the \(O_3\) induced daily premature mortalities based on the exposure–response relationship described in Cohen et al., 2004, which have been used in many subsequent studies (Anenberg et al., 2010; Liu et al., 2018; Wang et al., 2021). We then added up the daily premature mortalities within May-June or the whole year to get the total \(O_3\) induced premature mortalities in the respective periods. The population data used in this study include all age groups, which may result in higher daily mortalities than expected (Liu et al., 2018; Wang et al., 2021). According to (Cohen et al., 2004), the daily premature mortalities attributable to ambient \(O_3\) exposure can be estimated by the following equation (Cohen et al., 2004),

\[
\Delta x = \begin{cases} 
0, & \text{if } C_{\text{meas}} - C_{\text{thres}} \leq 0 \\
C_{\text{meas}} - C_{\text{thres}}, & \text{if } C_{\text{meas}} - C_{\text{thres}} \geq 0
\end{cases}
\]  
(8)

\[
\Delta M = y_0[1 - \exp(-\beta \Delta x)] \times \text{Pop}
\]  
(9)

where \(\Delta M\) represents the daily premature mortalities due to ambient \(O_3\) exposure. The city representative daily mean \(O_3\) concentration \(C_{\text{meas}}\) is an average of all measurements in each city. Variable \(y_0\) is the daily baseline mortality rate for each disease averaged from all ages and genders. We follow the method of (Wang et al., 2021) and use the daily \(y_0\) value for each disease from the latest China Health Statistical Yearbook in 2018. \(\beta\) represents the increase in daily mortality as a result of each 10 \(\mu g/cm^3\) (~ 5.1 ppbv) increase in daily \(O_3\) concentration, which is often referred to as the concentration response function (CRF) in previous studies. We collected the CRF values from those used in (Yin et al., 2017) and (Wang et al., 2021). \(\Delta x\) represents the incremental \(O_3\) concentration relative to the threshold concentration \(C_{\text{thres}}\) of 35.1 ppbv, which is obtained from (Lim et al., 2012) and (Liu et al., 2018). \(\text{Pop}\) represents the population exposed in the ambient \(O_3\) pollution, which is available from the seventh nationwide population census in 2020 provided by National Bureau of Statistics of China. The daily \(y_0\) and \(\beta\) values for all non-accidental causes, hypertension, CVD, RD, COPD, and stroke are summarized in Table S2.

3 Unexpected surface \(O_3\) enhancements over the SCB in 2020

Figures 1(a)-(b) show the May-June mean MDA8 \(O_3\) concentrations at all measurement sites over the SCB in 2019 and 2020. The May-June mean MDA8 \(O_3\) concentrations averaged over all
cities in the SCB region in 2019 and 2020 are 48.1 ppbv and 58.3 ppbv, which are 11.0 ppbv lower and 1.2 ppbv higher than those averaged over all Chinese cities in the same period, respectively. As the most densely populated and highly industrialized region in western China, the land use, industrialization, infrastructure construction, and urbanization over the SCB have expanded rapidly in recent years, resulting in the highest anthropogenic emissions of O₃ precursors and highest surface O₃ levels in the region (Figure S4). Although the O₃ levels in the SCB cities cluster are lower than those in the three most developed city clusters in eastern China, i.e., the BTH, the Fenwei Plain (FWP), and the YRD city clusters, the SCB region has been classified by the MEE as a newly pollution region for O₃ mitigation (Sun et al., 2021b; Wang et al., 2020a; Wang and Lu, 2019; Zou et al., 2019). Situated in the basin with stationary meteorological fields combined with high anthropogenic emissions, the SCB cities cluster is potential to become a new region with frequent high-O₃ events after BTH, FWP, and YRD.

We find significant O₃ enhancements by 10.2 ± 0.8 ppbv (23.4%) (mean ±1σ standard deviation) averaged over all cities in the SCB in May-June 2020 vs. 2019 levels (Figure 1(c)). The largest enhancements are observed in the most densely populated areas around the megacities Chongqing and Chengdu (11.8 ± 0.6 ppbv (29.9%)). These year-to-year O₃ enhancements over the SCB are record high in the 2015-2020 period, following an increasing change rate of 1.2% yr⁻¹ from 2015 to 2017 and then a decreasing change rate of −0.7% yr⁻¹ from 2017 to 2019. These surface O₃ enhancements mainly reflect regional emissions and meteorology changes in the SCB and surrounding regions since the lifetimes of surface O₃ and most of its precursors are too short to undergo long range transport.

The significant O₃ enhancements over the SCB in May-June 2020 vs. 2019 are opposite to the overall decrease in surface O₃ levels across China in the same period (Figure 1(d)). After a continuous increase in surface O₃ levels from 2013 to 2019 by approximately 5% yr⁻¹ (Figure 1(d)), the MDA8 O₃ averaged over all cities outside the SCB across China in May-June 2020 vs. 2019 levels showed a significant reduction of 5.3 ± 0.5 ppbv (8.3%). Such O₃ reductions are widespread in the eastern China, especially in the BTH, FWP, and YRD regions, and we have investigated their drivers in a separate study (Yin et al., 2021).

### 4 Model performance assessment

We use the metrics of normalized root-mean-square error (NRMSE), normalized mean bias (NMB), and Pearson correlation coefficient (R) to assess the performance of the GEOS-Chem-XGBoost model. For each measurement site, we analysed these metrics for both training (blue) and test (red) datasets as shown in Figure S5. We define the NRMSE as the RMSE normalized by the difference between the 95th and 5th percentile concentrations, and NMB as the mean bias normalized by average concentration at the given measurement site. The formulas of above metrics are summarized in Section S2.

The GEOS-Chem-XGBoost model predictions for surface O₃ over the SCB show no bias when evaluated against the training data, with NMB of 0.01, NRMSEs of less than 0.1, and R between 0.93 – 1.0. Compared to the training data, the performances on the test data show a higher variability, with an average NMB of −0.04, NRMSE of 0.22, and R of 0.83. We find no significant difference in prediction performance between clean (less than the Cthres defined in section 2.5) and polluted measurement sites. A number of factors likely contribute to relatively poorer statistical results at
some sites such as Ganzizhou, Leshan, and Suining. First, the training data of these sites may include
certain temporal events that are not easily generalizable, such as unusual emissions activity (e.g.,
BB, fireworks, closure of nearby point source) or weather patterns that are not properly observed,
which might be prone to overfitting. In addition, the differences in surface O3 variabilities between
the training data and the test data at these sites are relative larger than other sites, which can
contribute to a relative poorer performance.

We use the SHapely Additive exPlanations (SHAP) approach to examine how the GEOS-
Chem-XGBoost model uses the input variables to make a prediction. The SHAP approach is based
on game-theoretic Shapley values and represents a measure of each predictor’s responsibility for a
change in the model prediction (Lundberg and Lee, 2017). The SHAP values are computed
separately for each model prediction, which offer detailed insight into the importance of each input
variable to this prediction while also consider the role of variables interactions (Keller et al.,
2021; Lundberg et al., 2020). Figure 2 shows the SHAP value distribution for all the major O3
predictors averaged over all cities in the SCB. The results show that all variables that are expected
to be associated with O3 formation can affect model O3 prediction. Generally, the temperatures (at
the surface, 2 m height, and 10 m height) are the most important predictors for the GEOS-Chem
model-to-measurement discrepancy over the SCB, followed by the uncorrected GEOS-Chem
simulated O3, reactive nitrogen (e.g., NO2, Peroxyacetyl nitrate (PAN)), atmospheric oxidants (Ox,
hydrogen peroxide (H2O2)), fine aerosols, VOCs (Isoprene, C3H8), hour of the day, and
meteorological variables including horizontal and vertical wind speeds (u10m, v10m). All of these
factors have tight connections to surface O3 formation over the SCB and it is thus not surprising that
the GEOS-Chem model-to-measurement discrepancies are most sensitive to them (Seinfeld and
Pandis, 2016).

We have compared the performances of GEOS-Chem and GEOS-Chem-XGBoost in capturing
the measured surface O3 levels. Figure 3 (a) shows the time series of measured and model predicted
O3 concentrations averaged over all cities in the SCB region. Figure 3 (b) shows histogram of the
differences between the GEOS-Chem-XGBoost predictions and the measurements. The GEOS-
Chem simulations generally capture the daily variability of MDA8 O3 over the SCB, but they show
a high bias of 7.8 ± 5.0 ppbv (17.5%) across all measurement sites within the SCB region. The
discrepancy can be mainly attributed to uncertainties in the horizontal transport and vertical mixing
schemes simulated by the GEOS-Chem model at a relatively coarse spatial resolution compared to
the measurements at a single point, and also associated with the errors in emission estimates,
chemical mechanism, and the sub-grid-scale local meteorological processes. Especially, errors of
O3 predictors with high SHAP values are more likely to result in large model-to- measurement
discrepancy. For example, GEOS-Chem model overestimates the correlations between surface O3
concentration and temperature (Figure S7 (a)), indicating that this overestimation of O3-to-
temperature sensitivity is one of the major factors contributing to higher GEOS-Chem model O3
predictions.

By iteratively training and correcting the GEOS-Chem model-to-measurement discrepancy in
O3-to-temperature sensitivity, the correlations between temperature and surface O3 concentration
predicted by the GEOS-Chem-XGBoost model were in good agreement with the measurements
(Figure S7 (a)). With respect to the performance of reproducing the sensitivities of O3 to other
meteorological parameters such as humidity, cloud fraction, and precipitation, the GEOS-Chem-
XGBoost model is also better than the GEOS-Chem (Figure S7 (b)-(d)). After correcting the errors
in all O₃ predictors, the GEOS-Chem-XGBoost model significantly improves the prediction of surface O₃ concentrations in all cities over the SCB compared to the GEOS-Chem (Figure S8). It shows a bias of 0.5 ± 0.3 ppbv for all O₃ measurements in 2019 over the SCB. As a result, the overall GEOS-Chem-XGBoost model performance is acceptable and can support further investigation of the drivers of the unexpected surface O₃ enhancements over the SCB in May–June 2020.

5 Attribution
5.1 Separation of meteorological and anthropogenic emissions contributions

We quantify the surface O₃ enhancements in May–June 2020 over the SCB to changes in anthropogenic emissions and meteorological conditions according to equations (6) and (7). Differences between the measured and GEOS-Chem-XGBoost predicted O₃ in May–June 2020, as indicated by the shadings in Figure 4(a), represent the anthropogenic emissions-induced O₃ changes in 2020 vs. 2019. Mean contributions driven by changes in anthropogenic emissions and meteorological conditions are summarized in Figure 4(b). Due to the different change rates in anthropogenic emissions in May and June in 2020 (see section 5.3), the changes in anthropogenic emissions caused an overall increase in surface O₃ level in May but a reduction in surface O₃ level in June (Figure 4(a)). For the May–June mean contributions averaged over all cities in the SCB, changes in anthropogenic emissions caused 0.9 ± 0.1 ppbv of O₃ reduction and changes in meteorology caused 11.1 ± 0.7 ppbv of O₃ increase, which correspond to −8.0% and 108% of relative contributions to the total O₃ enhancement (10.2 ± 0.8 ppbv) over the SCB in May–June 2020, respectively. As a result, the anthropogenic emissions induced O₃ reductions are dominantly overwhelmed by the meteorology induced O₃ increases, leading to the unexpected O₃ enhancements over the SCB in 2020.

We compare the meteorology and anthropogenic emissions induced contributions to the unexpected surface O₃ enhancements estimated by the GEOS-Chem-XGBoost model with those by the GEOS-Chem model only (Figure 4(b)). Both methods show that changes in meteorology contribute significantly to the O₃ enhancements, while the absolute magnitudes differ slightly from each other. For example, the anthropogenic emissions induced O₃ reduction calculated with the GEOS-Chem model only is 0.94 ppbv, while the value for GEOS-Chem-XGBoost model is 1.36 ppbv. By taking the subtraction in equation (5) and the average over all cities, the propagation of systematic model discrepancies that are common to all measurements sites was effectively minimized, which can mitigate the difference in attribution results between the GEOS-Chem and GEOS-Chem-XGBoost methods. However, as demonstrated in Figure S8, model discrepancies may differ between regions and time. Therefore, the GEOS-Chem-XGBoost approach is expected to provide a more accurate and consistent estimate on O₃ change attribution than the GEOS-Chem model alone.

5.2 Meteorological contribution

Figure 5 shows the terrain elevations and May–June mean wind fields and surface pressures over the SCB and surrounding regions. The terrain altitudes, at a resolution of 3 × 3 arc-minute, indicate a rapid change in altitude from the Tibetan Plateau (4.0–5.0 km) and Yunan-Kweichou Plateau (2–3 km) to the SCB (0.5 km). The SCB is located in the saddle between the Tibetan and
Yunnan-Kweichou Plateau (Chen et al., 2009; Sun et al., 2021c). Figure 5 (b) are the May-June mean wind fields at 500 m overlaid with surface pressure available from GEOS-FP fields at 0.25° × 0.3125° resolution. In May-June, the Tibetan High formed over the middle region of the Tibetan Plateau with the western Pacific Subtropical High shifts westward to the west of the SCB (Chen et al., 2009). The southwesterly East Asian summer monsoon generates a cyclonic pattern over the southeast part of the SCB. Driven by large-scale circulations, southwesterly flow enters the east part of the SCB near the northwest edge of the Yunnan-Kweichou Plateau, while strong northwesterly flow enters the SCB near the east edge of the Tibetan Plateau. The interaction of these two flows results in a convergent zone of northward jet stream over the east part of the SCB due to the westward shift of the Western Pacific Subtropical High and the blocking effect of topography. Furthermore, strong instability of vertical convection could originate over the basin and move toward the east part of the SCB as dry air continuously entered the upper layer over the SCB (Chen et al., 2009). This process makes it a favorable region for trapping air pollutants within the SCB region (Chen et al., 2009; Liu et al., 2003).

Figure 6 shows the May-June mean differences in vertical velocity, precipitation, temperature, specific humidity, cloud fraction, and PBLH between 2020 and 2019. In May-June 2020, the northwest, central western and southern China experienced anomalous strong droughts (https://quotsoft.net/air/), leading to a significant increase in temperature and decreases in precipitation, specific humidity and cloud fractions compared to the 2019 levels (Figure 6). These changes in meteorological conditions could enhance the natural emissions of O₃ precursors and speed up O₃ chemical production. Meanwhile, the SCB basin effect inhibited the ventilation of O₃ and its precursors, which further enhanced the O₃ accumulations over the SCB. As a result, we conclude that the meteorological anomalies combined with the complex basin effect caused the surface O₃ enhancements over the SCB in 2020. Although higher PBLH over the SCB in May-June 2020 vs. 2019 may reduce surface O₃ levels by diluting O₃ and its precursors into a larger volume of air, this reduction effect was overwhelmed by the aforementioned enhancement effect. There is no strong evidence for the change in the horizontal transport from other regions (Figure 5(b)) and the vertical transport from the free troposphere to the surface (Figure 6 (a)) over the SCB in May-June 2020 vs. 2019 (Lefohn et al., 2012; Skerlak et al., 2014; Stohl et al., 2003; Wang et al., 2020a; Wang and Lu, 2019; Wang et al., 2020b; Wang et al., 2020c; Wirth and Egger, 1999). It is worth noting that, with similar meteorological anomalies in May-June 2020 vs. 2019, the O₃ enhancements were not observed in the northwest China such as Xinjiang and Inner Mongolia Provinces, and southern China such as the Pearl River Delta (PRD) region, which is also one of the nine well-developed city clusters in China with severe air pollution. This can be partly attributed to low anthropogenic emissions of O₃ precursors in northwest China (Zheng et al., 2018); and that strong exchange between the land and sea in the coastal regions driven by the summer monsoon facilitates the ventilation of O₃ and its precursors in the PRD region. Furthermore, the meteorology induced O₃ enhancements are probably overwhelmed by the anthropogenic emissions induced O₃ reductions in the northwest and southern China.

5.3 Emissions contribution

To suppress the spread of coronavirus pandemic 2019 (COVID-19) across China and above, the Chinese government sealed off several cities starting in January 2020; implementing a few
measures such as closing local businesses and halting public transportation at an unprecedented scale (Li et al., 2019b; Steinbrecht et al., 2021; Yin et al., 2021). These prevention measures quickly spread nationwide. Although the COVID-19 lockdowns in all cities have been removed before May, there are still restrictions on public transportation, businesses, social activities and industrial manufactures, which could cause domestic anthropogenic emissions reductions in both HCHO and NO$_2$. Furthermore, the MEE continues the mitigation of NO$_x$ emissions following the 2018–2020 Action Plan on Defending the Blue Sky, and has also implemented The 2020 Action Plan on VOCs Mitigations in 2020. This new Action Plan issues a number of control measures including implementation of stringent VOCs emission standards, replacement of raw and auxiliary materials with low VOCs content, and mitigation of unorganized emissions. Driven by the above factors, the TROPOMI observed tropospheric HCHO and NO$_2$ over China in May-June 2020 vs. 2019 reduced by 2.0 ± 0.3% (averaged for all Chinese cities) and 1.1 ± 0.2%, respectively. Due to the relative short lifetime of both HCHO and NO$_2$ in troposphere, these reductions mostly reflect local emissions changes. These reductions in domestic anthropogenic emissions dominated the significant reduction of summertime MDAA8 O$_3$ across China in 2020 vs 2019.

We have used the HCHO/NO$_2$ ratios following the method of (Sun et al., 2018) to investigate the O$_3$ production regime over the SCB region. The results show that the satellite observations of HCHO/NO$_2$ ratios in May-June in most cities over the SCB have indicated a shift toward high values from 2019 to 2020 but the O$_3$ chemical sensitivity in 2020 still lies within the transitional regime (Jin et al., 2017; Jin and Holloway, 2015; Figure S9). Meanwhile, the O$_3$ chemical sensitivity in May 2020 is similar to that in June, indicating that the O$_3$ variability in May-June 2020 is sensitive to both NO$_x$ and VOCs. The recently available Chinese anthropogenic emissions statistic data provided by the MEE show that the anthropogenic VOCs over the SCB has decreased by 5.0% and 3.5% in May and June in 2020 relative to the 2019 level, respectively. The anthropogenic NO$_x$ in the same period has increased by 1.5% and decreased by 1.7%, respectively (Zheng et al., 2021). The increase in anthropogenic NO$_x$ in May 2020 vs. 2019 is attributed to an increase in NO emissions from power plant sector, which was not affected by the post-lockdown restrictions for suppressing the spread of COVID-19 (Table S3). For the May-June aggregation, the anthropogenic VOCs and NO$_x$ over the SCB have decreased by 4.3% and 0.3%, respectively (Zheng et al., 2021). These independent analyses on anthropogenic emissions explain the different predicted O$_3$ changes due to anthropogenic emissions alone in May (increase) versus June (decrease) in the SCB.

In contrast to the widespread reductions in both HCHO and NO$_2$ across the BTH, FWP, and YRD regions, we find notable increases in both HCHO and NO$_2$ in the SCB in May-June 2020 vs. 2019 levels. The tropospheric HCHO and NO$_2$ columns averaged over all cities in the SCB region have been increased by (2.8 ± 0.3%) and (5.1 ± 0.5%) in 2020 vs. 2019 levels, respectively. Since both anthropogenic VOCs and NO$_x$ emissions in the SCB showed decreasing change rates in May-June 2020 vs. 2019, these regional increases in both HCHO and NO$_2$ could thus be attributed to natural emissions enhancements in both VOCs and NO$_2$ in the SCB. Indeed, natural emissions of biogenic VOCs and soil NO$_x$ calculated online in the GEOS-Chem model show increasing change rates in May-June 2020 vs. 2019 in the SCB and surrounding regions (Figure 7). These enhanced biogenic VOCs and NO$_x$ emissions are most likely driven by the hotter and dryer meteorological conditions in the SCB and surrounding regions (Figure 7).

Finally, we concluded that natural emissions enhancements of both NO$_x$ and VOCs induced by the unexpected meteorological anomalies could be accounted for the O$_3$ enhancements in May-June
2020 over the SCB, and their contributions have been included in the meteorology-driven ozone enhancement as discussed in Section 5.2. In present work, we were not able to determine which specific VOCs species are the most effective for O₃ enhancements and cannot quantify the relative contributions of VOCs and NOₓ enhancements to the O₃ enhancements in the SCB. A series of sensitivity studies might be able to address this important issue, but this is beyond the scope of present work.

6 Health risks for the O₃ enhancements over the SCB

Figure 8 presents the total premature mortalities from all non-accidental causes, hypertension, CVD, RD, COPD, and stroke attributable to ambient O₃ exposure in all cities over the SCB during May-June in 2019 and 2020. The statistical results for each city in 2019 and 2020 are summarized in Tables S4 and S5, respectively. The surface O₃ enhancements over the SCB in May-June 2020 vs. 2019 results in dramatically higher health risks. The estimated total premature mortalities from all non-accidental causes due to the surface O₃ enhancements in May-June 2020 over the SCB is 5455, which is 89.8% higher than that in the same period in 2019 (i.e., 2874). All above O₃ induced diseases over the SCB have significant increases in total mortalities in May-June 2020 vs. 2019. The highest health risk among these diseases is from CVD which is 741 in May-June 2019, followed by RD (236), COPD (231), and hypertension (223). This O₃ induced health risk rank over the SCB is consistent with those in the YRD, BTH, and PRD in previous studies (Liu et al., 2018; Lu et al., 2020; Yin et al., 2017; Wang et al., 2021). In May-June 2020, total mortalities from CVD, RD, COPD, hypertension, and stroke over the SCB reached to 1405, 450, 439, 418, and 46, respectively, due to significant O₃ enhancements. The change rates for these diseases are 89.6, 90.7, 90.1, 87.4, and 91.7%, respectively.

From a whole year view, the estimated total premature mortalities from all non-accidental causes due to surface O₃ exposure over the SCB in 2019 and 2020 are 16,772 and 18,301, respectively (Tables S4 and S5). All O₃ induced diseases within May-June 2019 account for about ~17.0% of those in the whole year 2019, and this percentage reaches up to ~30.0% in 2020 (Figure S10). The total premature mortalities from all non-accidental causes due to surface O₃ exposure over the SCB has increased by 1528 in the whole year 2020 vs. 2019 (Figure S11), which is 40.8% lower than that within May-June 2020 vs. 2019 (i.e., 2581). This indicates that the O₃ level over the SCB showed an overall decreasing change rate in all months except May-June in 2020 vs. 2019, which resulted in a decrease (by 1053) in O₃ induced diseases in the period.

We further investigated the O₃ induced diseases in the two most densely populated cities over the SCB (i.e., Chengdu and Chongqing) during May-June in 2019 and 2020. The premature mortalities from all O₃ induced diseases in 2020 vs. 2019 in each city are dependent on regional population, surface O₃ level, and enhancement level (equation (9)). With the largest populations and highest O₃ enhancements, the estimated total premature mortalities in Chengdu and Chongqing accounted for 46.9% of total O₃ induced mortalities over the SCB during May-June 2020 (Figure 8 (b)-(c)). Since the O₃ levels and enhancement in Chengdu are larger than those in Chongqing, the total O₃ induced mortalities in Chengdu are larger even with smaller population. The change rates for all O₃ induced diseases are about 75% in Chengdu and 160% in Chongqing during May-June 2020 vs. 2019, which are much higher than the enhancement of ozone levels in the two cities (29.9%). In order to reduce the O₃ induced health risk, strident O₃ control policies are necessary in
dramatically higher health risks. The estimated total premature mortalities due to the unexpected surface O₃ enhancements over the SCB during May-June 2020 is 5455, which is 89.8% higher than that in the same period in 2019 (i.e., 2874). We further investigated the O₃ induced diseases in the two most densely populated cities over the SCB (i.e., Chengdu and Chongqing) during May-June 2019 and 2020. With largest populations and highest O₃ enhancements, the estimated total premature mortalities in Chengdu and Chongqing accounted for 46.9% of total O₃ induced mortalities over the SCB. The change rates for all O₃ induced diseases are about 75% in Chengdu and 160% in Chongqing during May-June 2020 vs. 2019, which are much higher than the enhancement of ozone levels in the two cities (29.9 %). In order to reduce the O₃ induced health risks, strident O₃ control policies are necessary in densely populated cities.

**Code and data availability.** Surface O₃ measurements over the SCB are from http://www.cnemc.cn/en/. All other data are available on request of YS (ywsun@aiofm.ac.cn)

**Author contributions.** YS designed the study and wrote the paper. HY carried out the GEOS-Chem simulations and GEOS-Chem-XGBoost training and evaluation. XL designed the concept of health risk evaluation and revised the manuscript. BZ constructed the latest MEIC emission inventory. JN,
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**Competing interests.** None.

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### Table 1. Measurement sites in the SCB city clusters. All sites are organised alphabetically. Population statistics are based on the seventh nationwide population census in 2020 provided by National Bureau of Statistics of China.

| Name         | Longitude mean | Latitude mean | Altitude mean (km) | Population    | Number of sites | Time period      |
|--------------|----------------|---------------|--------------------|---------------|-----------------|-----------------|
| Abazhou      | 102.21°E       | 31.91°N       | 3.5                | 822,587       | 3               | 2015 - present  |
| Bazhong      | 106.75°E       | 31.85°N       | 0.8                | 2,712,894     | 4               | 2015 - present  |
| Chengdu      | 104.04°E       | 30.69°N       | 0.5                | 20,938,000    | 10              | 2015 - present  |
| Chongqing    | 106.51°E       | 29.58°N       | 0.4                | 32,054,200    | 21              | 2015 - present  |
| Dazhou       | 107.5°E        | 31.22°N       | 1.0                | 5,385,422     | 5               | 2015 - present  |
| Deyang       | 104.39°E       | 31.12°N       | 0.5                | 3,456,161     | 4               | 2015 - present  |
| Ganzizhou    | 101.96°E       | 30.05°N       | 3.5                | 1,107,431     | 2               | 2015 - present  |
| Guangan      | 106.63°E       | 30.48°N       | 1.7                | 3,254,883     | 6               | 2015 - present  |
| Guangyuan    | 105.85°E       | 32.44°N       | 2.1                | 2,305,657     | 4               | 2015 - present  |
| Leshan       | 103.76°E       | 29.57°N       | 0.5                | 3,160,168     | 4               | 2015 - present  |
| Liangshanzhou| 102.28°E       | 27.87°N       | 2.3                | 4,858,359     | 5               | 2015 - present  |
| Luzhou       | 105.43°E       | 28.9°N        | 0.3                | 4,254,149     | 4               | 2015 - present  |
| Meishan      | 103.85°E       | 30.07°N       | 0.8                | 2,955,219     | 6               | 2015 - present  |
| Mianyang     | 104.73°E       | 31.48°N       | 0.7                | 4,868,243     | 4               | 2015 - present  |
| Nanchong     | 106.09°E       | 30.8°N        | 0.3                | 5,607,565     | 6               | 2015 - present  |
| Neijiang     | 105.05°E       | 29.59°N       | 0.5                | 3,140,678     | 4               | 2015 - present  |
| Panzhihua    | 101.69°E       | 26.56°N       | 2.6                | 1,212,203     | 5               | 2015 - present  |
| Suining      | 105.71°E       | 30.58°N       | 0.5                | 2,814,196     | 4               | 2015 - present  |
| Yaan         | 103.01°E       | 29.99°N       | 3.1                | 1,434,603     | 4               | 2015 - present  |
| Yibin        | 104.62°E       | 28.78°N       | 2.0                | 4,588,804     | 6               | 2015 - present  |
| Zigong       | 104.75°E       | 29.35°N       | 0.3                | 2,489,256     | 6               | 2015 - present  |
| Ziyang       | 104.64°E       | 30.13°N       | 0.5                | 2,308,631     | 5               | 2015 - present  |
Figures

Figure 1 Surface O₃ enhancements over the SCB region in May-June 2020 vs. 2019. (a) Spatial distributions of May-June mean O₃ concentrations over the SCB region in 2019. Number (N) denotes available measurement sites for this year. We average the O₃ concentrations at all measurement sites in each city to form a city representative O₃ dataset. (b) Same as (a) but for 2020. (c) Differences between 2020 and 2019. (d) Trends in May-June mean ozone concentrations from 2015-2020 averaged for all Chinese cities (red) and for the SCB cities cluster (blue). Grey shadings represent the range of mean value ± 1σ STD across all cities. The base map of the figure is created by the Basemap package of Python.
Figure 2 Importance of input variables for the XGBoost model trained to correct the GEOS-Chem model-to-measurement $O_3$ discrepancy over the SCB. Shown are the distribution of the SHAP values for each variable averaged over all cities in the SCB, ranked by the average importance of each feature. Higher SHAP value indicates higher feature importance. Descriptions for all acronyms are listed in Table S1. For clarity, only the top 30 variables are shown. See Figure S6 for importance of all variables.
Figure 3 Measured and modelled O₃ variabilities over the SCB in 2019 (a). Measured, GEOS-Chem, and GEOS-Chem-XGBoost predicted O₃ values are denoted by black solid, grey dashed, and purple dashed lines, respectively. (b) Histogram of the differences between the GEOS-Chem-XGBoost predictions and the measurements.
Figure 4 (a) Comparison of the GEOS-Chem-XGBoost O₃ predictions to the 2020 measurements. Red (blue) shadings represent where GEOS-Chem-XGBoost predictions are higher (lower) than the actual measurements in 2020, indicating that changes in anthropogenic emission lead to O₃ increase (decrease) in 2020. All values shown are 7-day average for presentation purpose. (b) Attribution of surface O₃ enhancements over the SCB in May-June 2020 vs. 2019. Filled colored bars denote O₃ change as seen from measurements, and due to changes in anthropogenic emission and meteorological conditions estimated by the GEOS-Chem-XGBoost model and the GEOS-Chem model. Black vertical bars represent 1σ STD across cities.
Figure 5 Terrain elevations (a) and surface temperature and wind fields (b) over the SCB and surrounding regions. The spatial resolutions for (a) and (b) are 3 × 3 arc-minute and 0.25° × 0.25°, respectively. The white area in black line is Tibetan Plateau (with altitudes of 4–5 km a.s.l.), the yellow area in red line is the Yunnan-Kweichow Plateau (2–3 km a.s.l), the green area in circle is the SCB (0.5–1 km a.s.l). The base map of the figure is created by the Basemap package of Python.
Figure 6 May-June mean differences in vertical pressure velocity (a), precipitation (b), temperature (c), specific humidity (d), cloud fraction (e), and PBLH (f) between 2020 and 2019 over the SCB and surrounding regions. All these meteorological parameters are from the GEOS-FP dataset. The vertical pressure velocity is prescribed at the PBLH and others are at the surface. The base map of the figure is created by the Basemap package of Python.
Figure 7 May-June mean differences in O$_3$ precursors between 2020 and 2019. (a) TROPOMI observed HCHO, (b) biogenic VOCs, (c) TROPOMI observed NO$_2$, and (d) Soil NO$_x$. Biogenic VOCs and soil NO$_x$ are available from GEOS-Chem model online calculations. The base map of the figure is created by the Basemap package of Python.
Figure 8 Total daily mortality from all non-accidental causes, CVD, RD, COPD, hypertension, and stroke attributable to ambient O$_3$ exposure over the SCB during May-June in 2019 and 2020.