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Scenario-driven ozone projections and associated impact on mortality over Africa with an integrated machine learning framework

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Abstract

Ozone (O_3), a major tropospheric air pollutant, poses significant threats to public health and ecosystems, especially across Africa, where O_3 concentrations have experienced pronounced increases in recent decades. This study employs an interpretable machine learning (ML) model integrated with multi-source data to predict near-surface O_3 levels over Africa from 2020 to 2050 driven by climate change under four Shared Socioeconomic Pathways (SSPs). We quantitatively investigate the respective roles of climate-driven changes in meteorological conditions and biogenic isoprene emissions in affecting future O_3 variations. Results reveal that as a NO_x-limited region, increased biogenic isoprene emissions contribute to a slight reduction in O_3 levels (< 0.5 ppb). Conversely, favorable meteorological conditions elevate O_3 levels over Africa, with a maximum projected increase of 2.0 ppb in 2050 relative to 2020, dominating the O_3 variations driven by climate change. The low-emission SSP scenarios are projected to prompt less increases in O_3 levels than the high-emission SSPs. Moreover, elevated air temperatures associated with global warming magnify the health burden across Africa, as O_3 pollution acts as an additional stressor in a warming climate. This highlights the urgency for robust air pollution control and climate mitigation strategies to alleviate future health impacts in Africa.

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1. Introduction

Ozone (O_3) near the surface is a secondary air pollutant, primarily generated via the complex photochemical reactions involving precursors such as nitrogen oxides ($NO_x = NO + NO_2$) and volatile organic compounds (VOCs) under solar radiation. Since O_3 absorbs longwave radiation, it also acts as an important greenhouse gas that contributes to climate forcing (Myhre et al., 2017). Chronic exposure to elevated O_3 levels poses substantial threats to human health (Anenberg et al., 2010; Lelieveld et al., 2015), ecosystems (Yue et al., 2017; Mills et al., 2018), and climate change (Gaudel et al., 2018; Gao et al., 2022; Wang et al., 2023). Africa suffers a high burden of O_3 pollution in densely populated regions, where exhibit a rapid increase in daily maximum 8 h mean (MDA8) O_3 with an annual growth rate exceeding 3% (Sicard et al., 2023). Approximately more than 0.3 million premature deaths are attributed to O_3 pollution in 2019, which has become the second largest cause of death in Africa (Fisher et al., 2021; Lyu et al., 2023). Therefore, it is urgent to characterize the long-term variations of O_3 over Africa and identify their underlying driving factors.

Two thirds of countries in Africa lack ground-based observational data with sufficient temporal and geographic coverage, making it difficult to evaluate the air quality across the entire continent (Fajersztajn et al., 2014). Satellite O_3 products from the Total Ozone Mapping Spectrometer can provide long-time series of data. Combined these satellite measurements with the Global

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Modeling Initiative model, Ziemke et al. (2019) found a 4–5 DU (Dobson unit) increase in tropospheric column O_3 over Central Africa during the past four decades. Nevertheless, theses satellite retrievals still face spatial gaps and accuracy challenges, and cannot be directly used to estimate chemical and physical processes involved in O_3 production and loss (Colombi et al., 2021; Miyazaki et al., 2025). To complement the limitations of near-surface O_3 measurements, chemical transport models (CTMs) have been applied to simulate O_3 concentrations. Zunckel et al. (2006) found that the modelled near-surface O_3 mixing ratio over Southern Africa frequently exceeded 40 ppb, which may damage the local crops. Currently, artificial intelligence algorithms such as machine learning (ML) methods are widely applied in O_3 research due to their high computational efficiency and strong predictive performance, which can contribute to reducing the simulation biases inherent in traditional CTMs (Requia et al., 2020; Z. Liu et al., 2022; Wei et al., 2022; Li et al., 2023, 2024; Ni et al., 2024). For example, X. Liu et al. (2022) developed a 0.5° global monthly near-surface O_3 dataset for the period of 2003–2019 based on a cluster-enhanced ensemble ML method, and demonstrated that the average population-weighted MDA8 O_3 concentration in Northern Africa reached 53 ppb during the peak season, exceeding the global average of 47 ppb. Due to the severe O_3 pollution in Africa, the prediction of future O_3 concentrations is essential to providing scientific guidance for effective mitigation strategies.

The variation of O_3 largely depends on meteorological factors and synoptic

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conditions (Jacob and Winner, 2009; Doherty et al., 2013; Kavassalis and Murphy, 2017; Fu and Tian, 2019; Gong and Liao, 2019; Lu et al., 2019; Yang et al., 2022; Li et al., 2023, 2024). As documented in the Sixth Assessment Report of the Intergovernmental Panel on Climate Change (IPCC AR6), all global regions would experience intensified climate change, with the frequency, intensity, and duration of heatwaves are projected to increase by 2100 (IPCC, 2021). The frequency of high-temperature days in Africa is projected to increase substantially by the mid-21st century under the Shared Socioeconomic Pathway (SSP) 2-4.5 (26–59%) and SSP5-8.5 (30–69%) relative to the recent climatology of 1991–2010 (Iyakaremye et al., 2021). Such future climate changes under the various scenarios will further influence near-surface O_3 through altering meteorological factors (Colette et al., 2015; Wang et al., 2022). Turnock er al. (2022) applied the United Kingdom Earth System Model (UKESM1) to assess the impacts of future climate change on near-surface O_3, and found a modest reduction in annual mean O_3 levels by 2050 across Northern Africa (4%) and Southern Africa (2%) under the SSP3-7.0 scenario. Compound events involving extremely high temperatures and O_3 concentrations are projected to occur more frequently, with Africa experiencing the largest increase of compound-event days by more than 150 days in 2080s under the SSP5-8.5 scenario compared to the baseline of 1995–2014 (Ban et al., 2022). Utilizing three state-of-the-art earth system models, Brown et al. (2022) showed a multi-model average increase of O_3 by up to 4 ppb over urban

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areas of Africa during 2090–2100 under the SSP3-7.0 scenario.

Variations in meteorological parameters under the SSP scenarios can also influencing O_3 levels through perturbing natural emissions of precursors, such as those from vegetation, soil and lightning. As a dominant O_3 precursor, VOCs are largely emitted from terrestrial ecosystems (Kesselmeier and Staudt, 1999), with approximately 90% originating from biogenic sources (Guenther et al., 1995). Wang, Li et al. (2025) evaluated annual O_3 precursor emissions in 2019 over Southern Africa from different emission inventories, and demonstrated that biogenic VOCs (BVOCs) emissions exceeded those from other sources by a factor of 9 to 147. Among BVOCs, isoprene contributes the largest proportion of total emissions (Guenther et al., 2012). Notably, the African continent accounts for 20% of global isoprene emissions, with the evergreen tropical forests of Western and Equatorial Africa serving as a major source (Marais et al., 2012; Jaars et al., 2016; Sindelarova et al., 2022). Evidences indicate that BVOCs emissions are strongly modulated by meteorological conditions, such as air temperature, solar radiation, relative humidity, and precipitation (Zhang et al., 2008; Debevec et al., 2018; Yáñez-Serrano et al., 2020; Liu et al., 2021). Given the potentially increasing variability in future climate, isoprene emissions are becoming more uncertain in O_3 prediction, as it plays a crucial role in tropospheric chemistry, particularly in the formation of tropospheric O_3 (Fehsenfeld et al., 1992; Williams et al., 2009). Consequently, future changes in isoprene emissions in a warming climate are expected to further impact O_3

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concentrations across Africa.

Many previous studies predicted future O_3 under single scenario based on limited climate model simulations, without considering the impacts of climate change on O_3 variations, as well as the underlying changing meteorological conditions and natural precursor emissions. Also, the uncertainties in future meteorological parameters projected by a small number of climate models can also suffer specific model biases in O_3 predictions. In this study, we aim to quantify the impacts of future climate change on near-surface O_3 concentrations over Africa in the mid-21st century (average of 2045–2054) by employing a ML approach integrated with GEOS-Chem model simulations and multi-model simulations under four SSPs scenarios (SSP1-2.6, SSP2-4.5, SSP3-7.0, and SSP5-8.5) from the Coupled Model Intercomparison Project Phase 6 (CMIP6). Individual contributions of changing meteorological conditions and changing natural emissions (isoprene) under climate change are separately evaluated. The corresponding future health risk in Africa is also assessed. Details of the data, model description and methodology are elaborated in Sect. 2. Section 3 presents future projections of near-surface O_3 concentrations over Africa, relative contributions of driving factors, and assessment of the health risks. Key conclusions and potential uncertainties of this study are summarized in Sect. 4.

2. Materials and methods

2.1 GEOS-Chem model simulations

The historical near-surface O_3 concentrations over Africa (36°S–30°N,

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17.5°W–50°E) for the period 2000–2019 are simulated in the GEOS-Chem model version 13.4.1, which is driven by meteorological fields from the Modern-Era Retrospective analysis for Research and Applications version 2 (MERRA-2; Gelaro et al., 2017). The model simulation has a horizontal resolution of 2° latitude × 2.5° longitude, and includes 47 vertical layers from the surface up to 0.01 hPa. It incorporates fully coupled O_3-NO_x-hydrocarbon-aerosol chemical mechanisms (Park et al., 2004; Pye et al., 2009; Mao et al., 2013), with about 300 species participating in over 400 kinetic and photochemical reactions (Bey et al., 2001). Vertical mixing process within the planetary boundary layer is characterized using a non-local scheme (Lin and McElroy, 2010), and stratospheric O_3 chemistry utilizes the linearized O_3 parameterization scheme (LINOZ; McLinden et al., 2000).

Anthropogenic emissions of O_3 precursors, including non-methane VOCs (NMVOCs), NO_x and CO from 2000 to 2019 are derived from the Community Emissions Data System (CEDS) version 2021_04_21 (O'Rourke et al., 2021). Biogenic emissions are calculated online based on the Model of Emissions of Gases and Aerosols from Nature (MEGAN) version 2.1 (Guenther et al. 2012). Biomass burning emissions are obtained from the Global Fire Emissions Database (GFED) version 4 (van der Werf et al., 2017). NO_x emissions from soil sources are estimated online according to an updated version of the Berkeley–Dalhousie Soil NO_x Parameterization scheme proposed by Hudman et al. (2012). Lightning-induced NO_x emissions are calculated online following

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the algorithm developed by Ott et al. (2010) and Murray et al. (2012). Methane (CH_4) concentrations are prescribed using spatially interpolated monthly average observations from the National Oceanic and Atmospheric Administration (NOAA) Global Monitoring Division (GMD; Murray, 2016). Previous studies have shown that GEOS-Chem model well reproduces the magnitude and spatial distributions of observed O_3 concentrations across Africa (Han et al., 2018; Yan et al., 2019; Wang, Li et al., 2025).

2.2 CMIP6 multi-model outputs

The CMIP6 repository contains multi-model climate projections for various SSPs based on alternative scenarios of future emissions and land use changes (O'Neill et al., 2016). In this study, we collect meteorological variables from CMIP6 models under four different scenarios. SSP1-2.6 represents a low-forcing scenario that considers comprehensive climate mitigation strategies to effectively reduce greenhouse gas emissions and progress toward sustainable development goals. SSP2-4.5 is an intermediate-forcing scenario that follows the business-as-usual pathway. SSP3-7.0 corresponds to a medium-to-high forcing scenario. SSP5-8.5 denotes a high-forcing scenario aiming to achieve climate adaptation alongside rapid development through intensive utilization of fossil-fueled resources.

To perform a robust prediction of future near-surface O_3 concentrations in Africa, climate projections from 18 global climate models participating in CMIP6 are applied, including ACCESS_CM2, ACCESS-ESM1-5, CanESM5, CESM2-

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WACCM, CMCC-CM2-SR5, EC-Earth3, EC-Earth3-Veg, FGOALS-f3-L, FGOALS-g3, GFDL-ESM4, INM-CM5-0, IPSL-CM6A-LR, MIROC6, MPI-ESM1-2-HR, MPI-ESM1-2-LR, MRI-ESM2-0, NorESM2-LM, and NorESM2-MM. These models provide the major meteorological variables essential for predicting near-surface O_3, such as air temperatures (at 2m, 850 hPa, and 500 hPa), wind fields (at 850 hPa and 500 hPa), incoming shortwave radiation at the surface, near-surface relative humidity, precipitation rate, total cloud cover, and sea level pressure under the four different scenarios. In order to minimize the inconsistencies of initial conditions between CMIP6 models and MERRA-2 reanalysis data, the future meteorological fields under different scenarios from CMIP6 models are adjusted based on the differences between CMIP6 historical meteorological variables and MERRA-2 reanalysis data during 2000–2019 following H. Li et al. (2022, 2023, 2024). Additionally, to discuss the role of climate change in the projected variation of O_3 concentrations driven mainly by anthropogenic emissions, the monthly O_3 simulation outputs under four SSPs scenarios from 8 CMIP6 models are adopted, including BCC-CSM2-MR, FGOALS-g3, IPSL-CM6A-LR, MPI-ESM1-2-HR, MPI-ESM1-2-LR, MRI-ESM2-0, NorESM2-LM, and NorESM2-MM.

2.3 Machine learning model construction

As one of the traditional ML algorithms, Random Forest (RF) model can process high-dimensional data with lower computational costs compared to the CTMs (Breiman et al., 2001). This ensemble approach excels at dealing with

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nonlinear and complex relationships between input and target variables, and it provides stable and reliable predictions of O_3 in many previous studies (Wei et al., 2022; Xu et al., 2023). In this study, to predict future near-surface O_3 over Africa, we integrate a set of relevant features as predictors, including O_3 concentrations from GEOS-Chem model simulations, O_3 precursor emissions, meteorological variables, topography (TOPO), land cover (LC), normalized difference vegetation index (NDVI), and population density (POP). Considering the autocorrelation between O_3 and its covariates varies across space and time, the RF model also incorporates spatiotemporal information, including month of the year (MOY), longitude (LON) and latitude (LAT) across the Africa domain. The details of input data applied in this study are summarized in Table 1.

Here we firstly predict future biogenic isoprene emissions based on RF model, which are then used for predicting future near-surface O_3 concentrations across Africa. The RF model for isoprene is trained by the emission output from MEGAN2.1 in GEOS-Chem model, MERRA-2 meteorological variables, TOPO, LC, NDVI, POP, MOY, LAT, and LON over 2000–2009 and 2011–2019. The 2010 records are used to validate the performance of RF model, as that land surface air temperature over Africa reached its peak during 2000–2019, which facilitates future projections in a warming climate. This data splitting strategy ensures the critical information related to rising temperature trends is captured in both RF model training and testing phases. Based on trained RF model, the future monthly isoprene emissions from 2020 to 2054 under different climate

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scenarios (SSP1-2.6, SSP2-4.5, SSP3-7.0, and SSP5-8.5) in Africa are then predicted using future meteorological fields from CMIP6.

Secondly, to train the RF model for predicting future monthly near-surface O_3 concentrations in Africa, we composite O_3 simulations from GEOS-Chem model, emissions and concentrations of O_3 precursors, the ratio of VOCs emission to NO_x emission, MERRA-2 meteorological variables, and auxiliary data. The ratio of VOCs emission to NO_x emission is used to roughly determine the ozone formation regime. The samples over 2000–2009 and 2011–2019 are selected as training dataset and the remaining data over 2010 as testing data. We conduct two experiments to quantitatively estimate the direct (via altering meteorological conditions) and indirect (via altering biogenic isoprene emissions) effects of climate change on future O_3 in Africa. By feeding the varying meteorological parameters into the trained model while fixing isoprene emissions in 2020, the climate-driven O_3 variations through changing meteorological conditions are explored (O_3_MET). Both the isoprene projections and CMIP6 multi-model projections from 2020 to 2054 under four scenarios are fed to the trained RF model to predict O_3 (O_3_ALL), and the difference of O_3_ALL – O_3_MET represents the impacts of changing isoprene emissions under climate change (O_3_NAT).

The RF model's predictive performance was optimized through hyperparameter tuning. The best hyperparameters (n_estimators = 600, min_samples_split = 2, max_features = "sqrt", bootstrap = "True") of RF model

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for predicting isoprene emissions and O_3 concentrations are tuned separately by 10-fold cross-validation (Rodriguez et al., 2010). To assess the accuracy of RF model, statistical metrics such as coefficient of determination (R^2), mean absolute error (MAE), root mean square error (RMSE), and mean relative error (MRE) are calculated by comparing the outputs of RF model and GEOS-Chem model. Moreover, we employ the Shapley Additive explanation (SHAP) approach (Lundberg and Lee, 2017) to quantify the importance of individual factors determining the RF model's predictions. The SHAP provides a value that reflects the contribution of each input variable to specific predictions, and has been widely adopted in atmospheric environmental studies to enhance the interpretability of the ML model (Hou et al., 2022; Stirnberg et al., 2021).

2.4 Mortality burden assessment

Exposure to elevated temperatures and O_3 pollution, esacerbated by global warming, significantly increases human health risks. We assess the future mortality ratio (MR) attributable to ambient O_3 and temperature changes, respectively, under different scenarios in Africa from 2020 to 2054, using the following equations:

$$MR_{ozone} = \frac{\frac{\sum_i RR_{ozone,i}}{m}}{\frac{\sum_j RR_{ozone,j}}{n}} \tag{1}$$

$$MR_{temperature} = \frac{\frac{\sum_i RR_{temperature,i}}{m}}{\frac{\sum_j RR_{temperature,j}}{n}} \tag{2}$$

$$RR_{ozone} = exp^{(\beta_1(C-C_0))} \tag{3}$$

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$$RR_{temperature} = exp^{(\beta_2(T-T_0))} \quad (4)$$

where MR_{ozone} ($MR_{temperature}$) stands for the MR due to O_3 pollution (temperature) changes. $RR_{ozone,i}$ and $RR_{temperature,i}$ represent relative risks caused by O_3 and temperature exceedance in a future (2050–2054) month i, respectively. $RR_{ozone,j}$ and $RR_{temperature,j}$ denote relative risk caused by O_3 and temperature exceedance on a baseline (2020–2024) month j, respectively. m is the total number of months during future period, and n is the total number of months of baseline period. β_1 indicates the O_3 concentration response factor, with a value of 1.39×10^{-3} (95% confidence interval: 8.9597×10^{-4}, 1.8822×10^{-3}) per ppb (Wang, Yang et al., 2025). C_0 is the theoretical minimum risk exposure level (TMREL) for O_3 exposure, which ranges from 29.1 to 35.7 ppb as adopted in Global Burden of Disease (GBD) 2019 study (2020). Following Malashock et al. (2022), we use the medium value of 32.4 ppb in this study. C reflects the O_3 concentrations predicted by the RF model. β_2 signifies the temperature response factor, and each 1 °C increase in temperature over Africa is associated with a 1.3×10^{-2} (95% confidence interval: 0.4×10^{-2}, 2.2×10^{-2}) rise in mortality risk (Cromar et al., 2022). T_0 is the threshold value indicating minimum mortality temperature (MMT), an important indicator for characterizing the health impacts of global heating. The 50th percentile of temperature distribution corresponding to the MMT over Southern Africa was calculated to be 25 °C, which is used as the reference value for this study (Tobías et al., 2021). T reflects air temperature from the CMIP6 dataset. Similar calculation

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methodology has been applied in previous studies (Lee and Kim, 2016; Wang et al., 2022).

3. Results

3.1 Evaluation of machine learning model performance

We evaluate the ML model using a test dataset from year 2010. Figure 1(a) and (b) illustrates the consistency between RF model projections and GEOS-Chem model simulations for isoprene emissions and near-surface O_3 concentrations in Africa, respectively. The RF model exhibits a strong predictive capability in reproducing both isoprene emissions (R^2 = 0.97, MRE = 17%) and near-surface O_3 concentrations (R^2 = 0.94, MRE = 6%). These robust statistical metrics confirm the trained RF model's suitability for predicting future O_3 concentrations over Africa under a warmer climate.

The isoprene emissions simulated by GEOS-Chem model during 2000–2019 reveal apparent regional discrepancies across Africa (Figure 2a). The maximum isoprene emissions originate from evergreen broadleaf trees over Central Africa, which has the second largest tropical rainforest in the world. Southern Africa exhibits relatively lower isoprene emissions due to its sparse coverage of deciduous broadleaf trees. Northern Africa, dominated by desserts and semi-arid grasslands, contributes little to isoprene emissions. The isoprene projections estimated by the RF model perfectly capture the spatial distributions of isoprene emissions across Africa, with a correlation coefficient (R) between the RF projections and GEOS-Chem simulations of 0.99 and a normalized

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mean bias (NMB) of -0.2%. In addition, the O_3 concentrations from 2000 to 2019 simulated by GEOS-Chem model indicate that O_3 pollution is predominantly concentrated in Southern Africa, as well as parts of Northern Africa and Central Africa, with concentrations over 40 ppb (Figure 2b). The RF model accurately reproduces this spatial characteristic, which aligns well with the O_3 simulation results (R = 0.99, NMB = -0.02%).

To gain deeper insights into the driving factors behind RF model outputs, we utilize SHAP, an explainable artificial intelligence technique, to quantify the contribution of each feature to the projections of biogenic isoprene emissions (Figure 3a) and O_3 concentrations (Figure 3b) in Africa. The LC and NDVI are identified as the strongest positive drivers of isoprene emissions. This is consistent with the physics that biogenic isoprene is emitted mainly from terrestrial vegetation, and its emissions are directly influenced by LC types and the associated plant species. Among all meteorological variables, air temperature plays a dominate role in regulating isoprene emissions, exhibiting a positive correlation, in line with prior work (e.g., Singsaas and Sharkey, 1998). For O_3 concentrations, meteorological factors – relative humidity, air temperature, precipitation, cloud cover, and incoming solar radiation – exert substantial influence, with temperature and solar radiation positively associated with O_3 levels. Additionally, precursor emissions constitute a vital component in O_3 formation. The VOCs-to-NO_x emission ratio, used here as an indicator of O_3 production regime in this study, is also a critical determinant of projected O_3.

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3.2 Climate-driven changes in biogenic isoprene emissions

The projected changes in RF-predicted isoprene emissions over Africa in 2050 (averaged over 2050–2054) relative to 2020 (averaged over 2020–2024) are shown in Figure 4. The isoprene emissions show increasing trends under all four future scenarios. Shaped by the land cover characteristics in Africa, there is a distinct north-south spatial distribution pattern in the changes in isoprene emissions. Central Africa, as a major source of isoprene emissions, exhibits the largest increases in biogenic isoprene emissions across Africa, with a maximum growth rate exceeding 1.0 g/m^2/yr under four scenarios. In contrast, the land use type in Northern Africa is dominated by barren land, resulting in consistently low isoprene emission levels. Compared to the period of 2020–2024, the projected changes of isoprene in Northern Africa for 2050–2054 are less than 0.1 g/m^2/yr, while the isoprene emissions increase by 0.1–0.5 g/m^2/yr over Southern Africa under all SSPs.

According to the feature contributions derived by SHAP analysis, biogenic isoprene emissions largely depend on meteorological fields, with air temperature (at 2m) identified as the most critical factor (Figure 3a). A comparison of future meteorological variables between 2050–2054 and 2020–2024 under different scenarios demonstrates that near-surface air temperatures elevate throughout the entire African continent in 2050–2054, with SSP5-8.5 presenting the strongest warming (Figure 5). Therefore, isoprene emission rates are anticipated to rise, especially in the strong warming

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scenarios (i.e. SSP3-7.0 and SSP5-8.5). Besides, isoprene emissions show opposite responses to humid weather conditions and the enhancement of projected isoprene emissions induced by drought stress is particularly pronounced over Central and Southern Africa (Figure 6).

Figure S1 shows the spatial distributions of biogenic isoprene emission changes during 2050–2054 compared to 2020–2024 in March–April–May (MAM), June–July–August (JJA), September–October–November (SON), and December–January–February (DJF) under the four scenarios. The changes in isoprene emissions do not show obvious seasonality, but there are relatively larger increases in MAM and DJF than other seasons.

3.3 Climate-driven changes in future O_3 concentrations over Africa

Figure 7a shows the changes in annual mean near-surface O_3 concentrations in response to climate change under different scenarios, as projected by the RF model using future meteorological fields from 18 CMIP6 models (O_3_MET). The projected O_3 exhibits an overall increasing trend during 2050–2054 relative to 2020–2024, indicating a climate penalty on air quality over most African regions. Future increases in air temperature (Figure 5), along with reductions in relative humidity (Figure 6) and cloud cover (Figure 8) will enhance photochemical O_3 production, leading to substantial increases in O_3 levels, with maximum increases over 1.0 ppb, even reaching 2.0 ppb, under strong warming scenarios. Under the weak warming scenario SSP1-2.6, the climate-driven O_3 increases are relatively small, with increases of less than 1.0

ppb across Africa.

The ratio of VOCs-to-NO_x emissions is adopted to express the nonlinearity of O_3 formation to its precursor emissions. Previous studies have revealed that the O_3 formation regime in Africa is generally NO_x-limited (Ziemke et al., 2009; Bela et al., 2015). Figure S2 shows that the ratio of VOCs-to-NO_x emissions does not change from present-day to the mid-21st century, which demonstrates that future O_3 production is also NO_x-sensitive over Africa. In NO_x-limited regions, increases in biogenic isoprene emissions result in a slight decrease in O_3 levels by less than 0.5 ppb over Central and Western Africa in 2050 relative to 2020 (Figure 7b, O_3_NAT). The total effects of changing meteorological factors and biogenic isoprene emissions on O_3 variations are similar to that due to the changes in meteorological factors alone, as depicted in Figure 7c (O_3_ALL). In summary, the climate-driven changes in meteorological parameters exert a more dominant role in regulating future O_3 concentrations over Africa through changing physical and chemical processes, while the changing biogenic isoprene emissions exerts a minor role.

Climatology of meteorological fields over Africa has obvious seasonal characteristics, and the formation of near-surface O_3 is tightly coupled with climate-driven processes. Figures S3–S6 show the spatial distribution changes in seasonal O_3 concentrations influenced by meteorological fields and biogenic isoprene emissions under climate change. O_3 concentration increases the most during MAM, with a maximum rise reaching up to 3.8 ppb over Central and

Southern Africa under the SSP5-8.5 scenario (Figure S3). In contrast, parts of Southern Africa show a reduction of 0.2–1.0 ppb during SON under all scenarios (Figure S5), primarily related to a higher sea level pressure (Figure S7) and its negative correlation with O_3 levels (Figure 3b). Additionally, a decrease exceeding 0.5 ppb is expected across Central Africa in DJF under the strong warming scenarios (Figure S6), largely driven by the rapid increases in precipitation frequency (Figure S8). Moreover, increasing isoprene emissions also contribute to the decrease in O_3 concentrations by 0.2–0.5 ppb over Eastern and Central Africa during JJA (Figure S4).

3.4 Projection of mortality attributed to O_3 and temperature

Figure 9 shows the relative changes in future projected mortality burden in 2050 compared to that in 2020 corresponding to changes in O_3 concentrations and air temperatures across Africa under the four future scenarios. The mortality due to the changes in O_3 pollution driven by changes in meteorological factors and biogenic isoprene emissions are separately investigated. It is worth noting that the potential amplification or suppression effects of interactions between O_3 and temperature on mortality are not considered in this study.

Mortality ratios (MRs) over Africa are presented in 2050 relative to 2020, with temperature-related MRs ($MR_{temperature}$) increases much higher than those due to the climate-driven increases in O_3 exposure levels (MR_{ozone}), particularly under the SSP3-7.0 and SSP5-8.5 scenarios. This demonstrates that increases in extreme heat in a warmer future are projected to cause substantially more

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deaths than the climate-driven increases in extreme O_3 concentrations across Africa. The $MR_{temperature}$ ranges from 1.007 to 1.015, with an average of 1.0115. The MRs due to climate-driven O_3 changes related to the meteorological parameters ($MR_{ozone\text{-}met}$) show a slight increase from 1.0002 to 1.0006, as the climate getting warmer. In contrast, MRs attributed to climate-driven O_3 changes related to biogenic isoprene emissions ($MR_{ozone\text{-}nat}$) do not show any noticeable change under different scenarios, which exceed 1.0 only under the SSP3-7.0 scenario. Nevertheless, these suggest that environmental conditions for human health in Africa will be deteriorated in a warming climate with more frequent extreme heat together with intensified O_3 pollution.

4. Conclusion and discussions

Africa is a vast continent with a population accounting for more than one-eighth of total population in the world. In the process of rapid urbanization, industrialization, and motorization, the O_3 pollution across the continent has been exacerbating, which poses a serious threat to the public health. In this study, we predict future near-surface O_3 concentrations over Africa from 2020 to 2050 driven by climate change under four different scenarios (SSP1-2.6, SSP2-4.5, SSP3-7.0, and SSP5-8.5) based on an interpretable RF model integrated with multi-source data, such as GEOS-Chem model simulations, future meteorological fields from CMIP6 multi-model outputs, O_3 precursor emissions, topography, land use, population density, and spatiotemporal information.

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Biogenic isoprene emissions are strongly influenced by land use and climate change, which in turn modulate O_3 concentrations through atmospheric photochemical reactions. With rising air temperatures, the RF model-projected biogenic isoprene emissions across Africa are expected to increase in 2050 relative to 2020 under future climate scenarios. Owing to distinctive characteristics of vegetation coverage and composition, the most substantial increase of isoprene emissions occurs over Central Africa, where the maximum increase is projected to exceed 1.0 g/m^2/yr under the SSP2-4.5, SSP3-7.0, and SSP5-8.5 scenarios. In contrast, the isoprene emissions in Northern Africa show minimal variabilities.

The impacts of biogenic isoprene emissions and meteorological fields under future climate change on O_3 levels across Africa are separately quantified. In general, climate change has the potential to increase O_3 concentrations, known as the "O_3 climate penalty". Favorable meteorological conditions such as higher temperature and lower relative humidity facilitate the photochemical generation of O_3, with a maximum increase of 2.0 ppb in 2050 compared to 2020. In this NO_x-limited region, the simultaneously increased biogenic isoprene emissions lead to a slight O_3 decline (<0.5 ppb). Meteorological fields play a dominant role in shaping future O_3 levels over Africa than biogenic isoprene emissions. In addition, the low-emission scenarios (SSP1-2.6 and SSP2-4.5) are projected to prompt less increases in O_3 levels than the high-emission scenarios (SSP3-7.0 and SSP5-8.5). This study reveals that global

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warming will exacerbate the health risk associated with O_3 pollution across Africa. It further highlights that elevated air temperatures act as the primary driver of increased mortality ratios in Africa, while enhanced O_3 concentrations is an additional stressor as an adverse side effect of warming climate.

To assess the role of climate change in future O_3 variations, O_3 concentrations from the CMIP6 multi-model future predictions are obtained, which are driven by changes in anthropogenic emissions, climate and land use following SSPs scenarios. The spatial distributions of simulated differences in O_3 concentration over Africa between 2020 and 2050 are shown in Figure 10. Under the SSP1-2.6 and SSP2-4.5 scenarios, O_3 concentrations are predicted to decrease by less than 10 ppb, mainly resulting from reductions in anthropogenic emissions. However, O_3 concentrations are expected to increase under the SSP3-7.0 and SSP5-8.5 scenarios, with the rise up to 1–5 ppb across Africa, which are largely contributed by the climate change in a warming future.

In this study, the O_3 projections over Africa are subject to uncertainties and limitations arising from input datasets, GEOS-Chem model simulations, CMIP6 multi-model simulations of meteorology, and the RF model. First, land use, topography and population density data are held at present-day values when predicting future O_3 concentrations; these factors will change with climate and may bias projections. Second, the RF model training and performance strongly relies on the accuracy of GEOS-Chem simulation results. Although the GEOS-Chem model has been proven capable of capturing the temporal and spatial

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variations of global O_3, there remain certain uncertainties in its simulated O_3 concentrations over Africa. These uncertainties mainly stem from discrepancies in emission inventories, including anthropogenic, biogenic, biomass burning, and lightning sources (Han et al., 2018). Third, the CMIP6 multi-model meteorological fields used to represent future climate under different scenarios may suffer projection uncertainties and can introduce biases (Xu et al., 2021). Fourth, the contributions of selected features in this study reflect the aggregate study domain; future work should train region-specific RF models to estimate near-surface O_3 concentrations and quantify variable contributions at regional scales. Finally, dependencies among the RF model input features can confound attribution, which may potentially result in spurious interpretations (Silva and Keller, 2024). Furthermore, when quantifying future O_3 changes driven by biogenic emissions, only biogenic isoprene emissions are considered, which may have led to a low bias of the influence from biogenic emissions.

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Author contributions

HL and YY designed the research. HL performed the model simulations, analyzed data and wrote the initial draft. YY and HW helped edit and review the manuscript. All the authors discussed the results and contributed to the final manuscript.

Code and data availability

The GEOS-Chem model is available at https://zenodo.org/records/7254273. MERRA-2 reanalysis data can be downloaded at https://gmao.gsfc.nasa.gov/reanalysis/MERRA-2/. Multi-model projections of climate variables are from Scenario Model Intercomparison Project in Phase 6 of the Coupled Model Intercomparison Project https://esgf-node.llnl.gov/search/cmip6/. Land cover is derived from http://maps.elie.ucl.ac.be/CCI/viewer/download.php. Normalized difference vegetation index is obtained from https://www.ncei.noaa.gov/data/land-normalized-difference-vegetation-index/access/. Topography is collected from https://cgiarcsi.community/data/srtm-90m-digital-elevation-database-v4-1/. Population density is acquired from https://landscan.ornl.gov/landscan-datasets.

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Competing Interest

At least one of the (co-)authors is a member of the editorial board of Atmospheric Chemistry and Physics. The authors also have no other competing interests to declare..

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Table 1. Details of the data used in this study.

Dataset type	Variable	Description	Spatial resolution	Temporal resolution	Time period	Data source
O_3	O_3	Near-surface ozone concentrations	2°×2.5°	Monthly	2000–2019 (historical)	GEOS-Chem simulations
Meteorology	T_2m	Air temperature at 2 meters	2°×2.5°	Monthly	2000–2019 (historical) 2020–2054 (future)	MERRA-2 (historical) Adjusted CMIP6 (future)
	T_850	Air temperature at 850 hPa				
	T_500	Air temperature at 500 hPa				
	U_850	Zonal wind at 850 hPa				
	U_500	Zonal wind at 500 hPa				
	V_850	Meridional wind at 850 hPa				
	V_500	Meridional wind at 500 hPa				
	RH	Near-surface relative humidity				
	PRECP	Precipitation rate				
	CLT	Total cloud cover				
	RSDS	Incoming shortwave radiation at the surface				
	SLP	Sea level pressure				
Emission	NO_x	Nitric oxide from soil sources	2°×2.5°	Monthly	2019	CEDS (Anthropogenic) GFED4 (Biomass burning) MEGAN2.1 (Biogenic) NOAA GMD for CH_4
		Nitric oxide from lightning sources				
		Nitric oxide from anthropogenic sources			2000–2019 (historical) 2019 (future)	
		Nitric oxide from biomass burning				
	CO	Carbon monoxide from anthropogenic sources				
		Carbon monoxide from biomass burning				
	CH_4	Surface methane concentration				
	NMVOCs	Non-methane volatile organic compounds from anthropogenic sources				
		Non-methane volatile organic compounds from biomass burning				
		Non-methane volatile organic compounds from biogenic sources			2019 (historical) 2020–2054 (future)	
Land use	LC	Land cover	300 m×300 m	Monthly	2000–2019 (historical) 2019 (future)	ESA CCI
	NDVI	Normalized Difference Vegetation Index	0.05°×0.05°			AVHRR
Topography	TOPO	Digital elevation model	90 m×90 m	-	2010	SRTM
Population	POP	Population density	1 km×1 km	-	2010	Land Scan

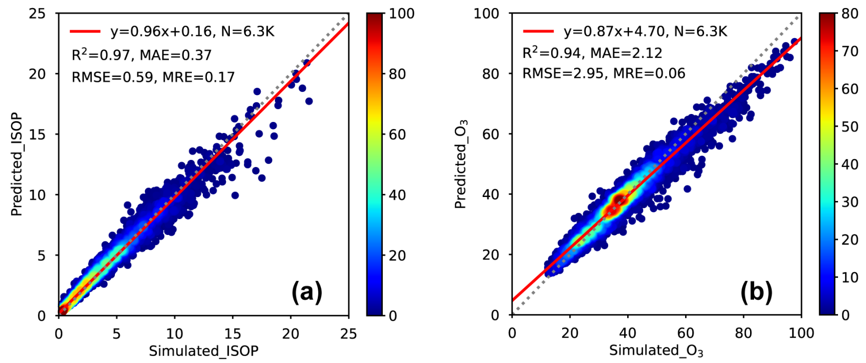

Figure 1. Density plot of GEOS-Chem model simulated vs. Random Forest model predicted monthly (a) biogenic isoprene emissions ($g/m^2/yr$) and (b) near-surface O_3 concentrations (ppb) in 2010 over Africa. The gray dotted and red lines are the 1:1 lines and linear regression lines, respectively. Statistical metrics including correlation of determination (R^2, unitless), root mean square error (RMSE, $g/m^2/yr$ or ppb), mean absolute error (MAE, $g/m^2/yr$ or ppb), and mean relative error (MRE, %) are given at the top of each panel.

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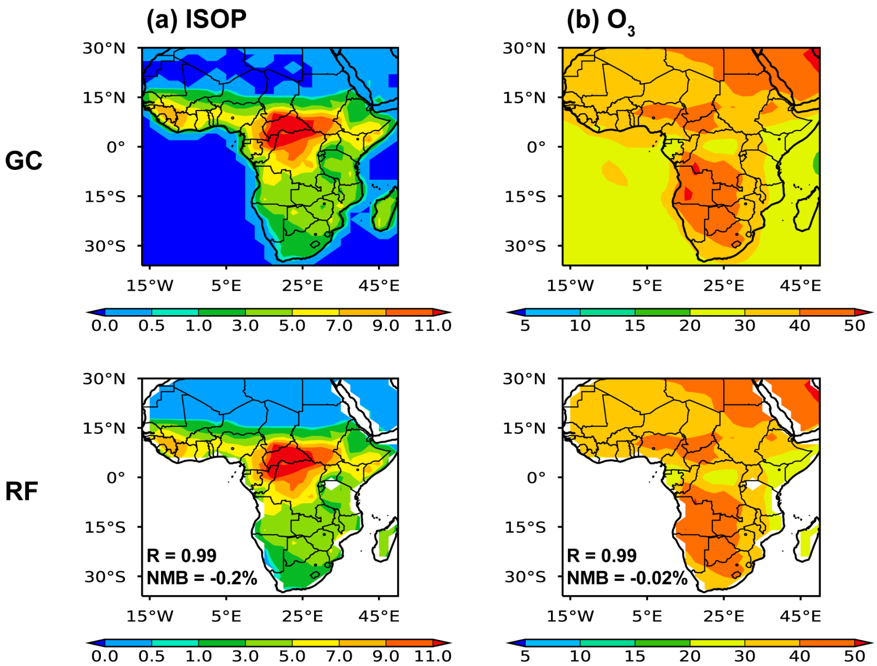

Figure 2. Spatial distributions of (a) biogenic isoprene emissions (ISOP, g/m^2/yr) and (b) near-surface O_3 concentrations (ppb) derived from GEOS-Chem model (GC) and Random Forest model (RF) over Africa in 2000–2019. The correlation coefficient (R) between simulated and predicted O_3 and the normalized mean bias (NMB= (Simulated − Predicted) / Predicted ×100 %) are given at the bottom left of panels.

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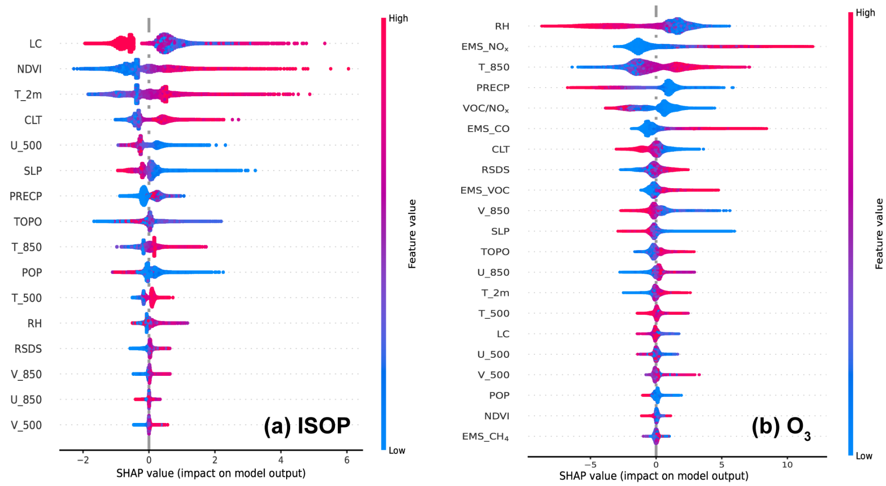

Figure 3. Main and interactive effects of major input features on projections of (a) biogenic isoprene emissions (ISOP) and (b) near-surface O_3 concentrations over Africa from Shapley Additive explanation (SHAP) analysis. The relative importance of selected independent features is shown in the descending order. A positive (negative) SHAP value suggests a positive (negative) contribution.

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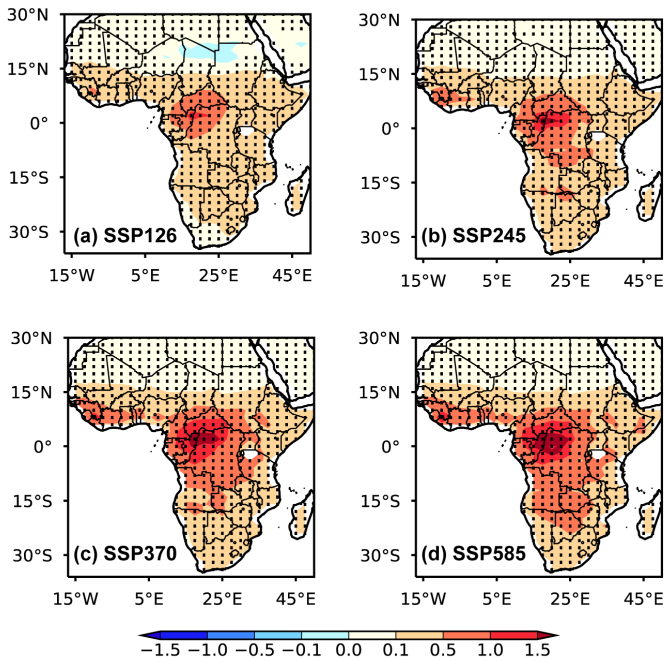

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1021 **Figure 4.** Spatial distributions of differences in scenario-driven biogenic
1022 isoprene emissions ($g/m^2/yr$) between 2050–2054 and 2020–2024 under (a)
1023 SSP1-2.6, (b) SSP2-4.5, (c) SSP3-7.0 and (d) SSP5-8.5 scenarios predicted
1024 by the RF model. The shaded areas indicate that the differences are statistically
1025 significant at the 90% confidence level.

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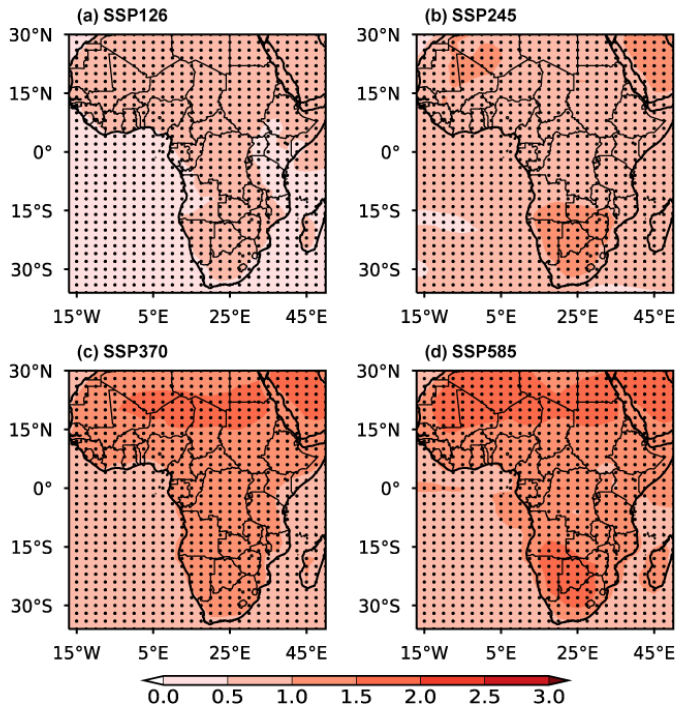

Figure 5. Spatial distributions of differences in the CMIP6 multi-model mean of air temperature at 2m (T_2m, K) between 2050–2054 and 2020–2024 over Africa under (a) SSP1-2.6, (b) SSP2-4.5, (c) SSP3-7.0 and (d) SSP5-8.5 scenarios. The shaded areas indicate that the differences are statistically significant at the 90% confidence level.

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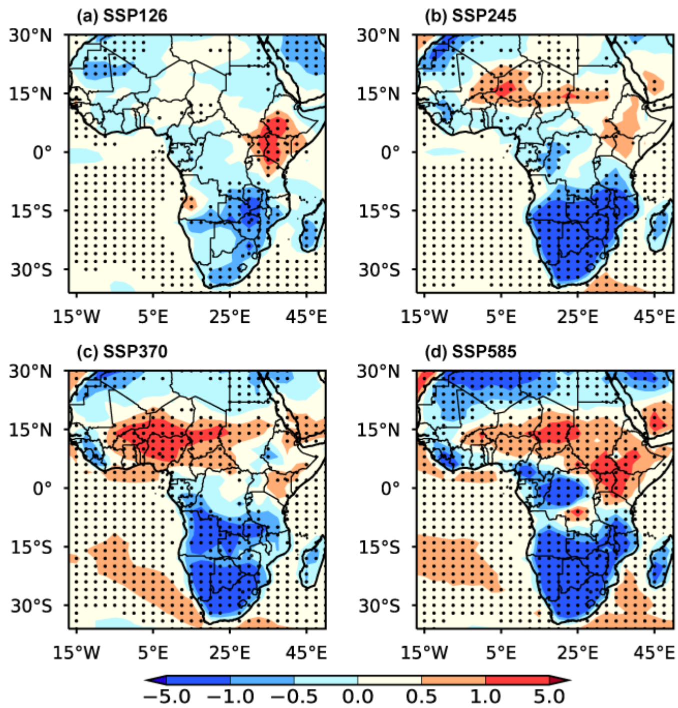

Figure 6. Spatial distributions of differences in the CMIP6 multi-model mean of relative humidity (RH, %) between 2050–2054 and 2020–2024 over Africa under (a) SSP1-2.6, (b) SSP2-4.5, (c) SSP3-7.0 and (d) SSP5-8.5 scenarios. The shaded areas indicate that the differences are statistically significant at the 90% confidence level.

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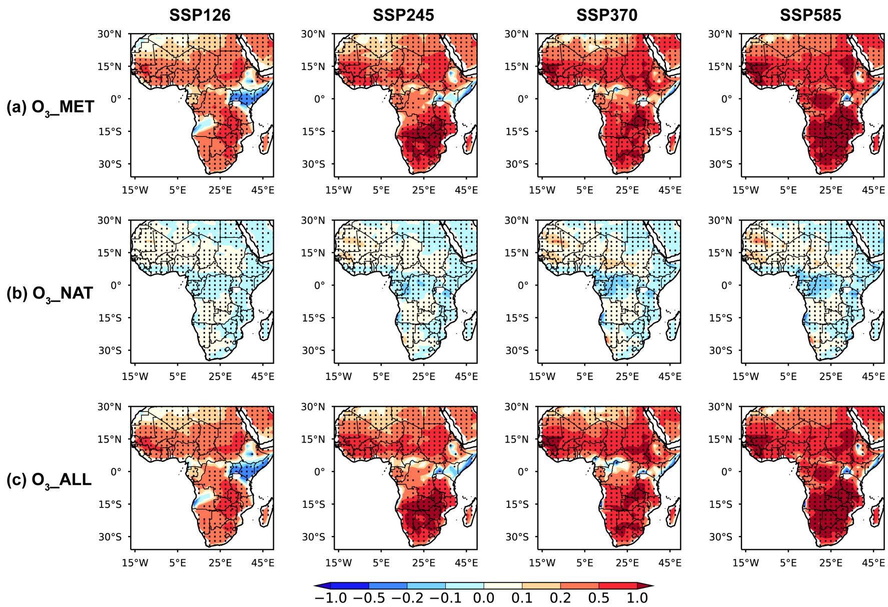

Figure 7. Spatial distributions of differences in RF-predicted near-surface O_3 concentrations (ppb) over Africa in response to (a) changes in meteorological fields (O_3_MET), (b) changes in biogenic isoprene emissions (O_3_NAT), and (c) both changes (O_3_ALL) between 2050–2054 and 2020–2024 under SSP1-2.6, SSP2-4.5, SSP3-7.0 and SSP5-8.5 scenarios. The shaded areas indicate that the differences are statistically significant at the 90% confidence level.

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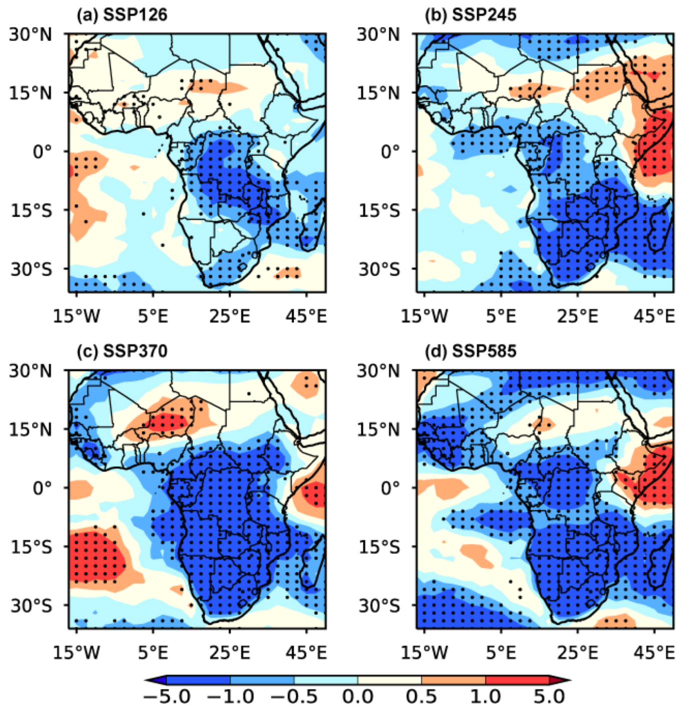

Figure 8. Spatial distributions of differences in the CMIP6 multi-model mean of total cloud cover (CLT, %) between 2050–2054 and 2020–2024 over Africa under (a) SSP1-2.6, (b) SSP2-4.5, (c) SSP3-7.0 and (d) SSP5-8.5 scenarios. The shaded areas indicate that the differences are statistically significant at the 90% confidence level.

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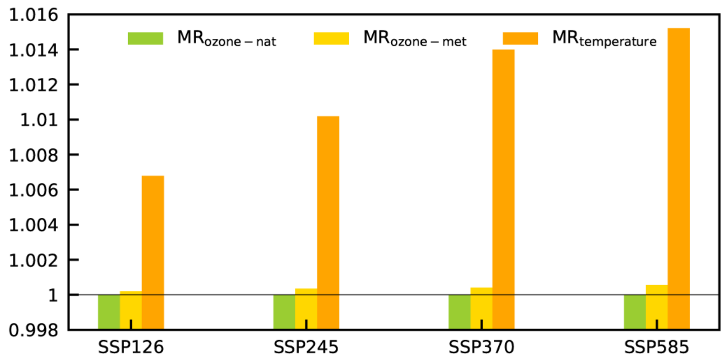

Figure 9. Mortality ratio over Africa due to climate-driven changes in O_3 levels related to natural emissions ($MR_{ozone\text{-}nat}$), O_3 levels related to meteorological fields ($MR_{ozone\text{-}met}$), and air temperature ($MR_{temperature}$) in 2050–2054 relative to 2020–2024 under SSP1-2.6, SSP2-4.5, SSP3-7.0 and SSP5-8.5 scenarios.

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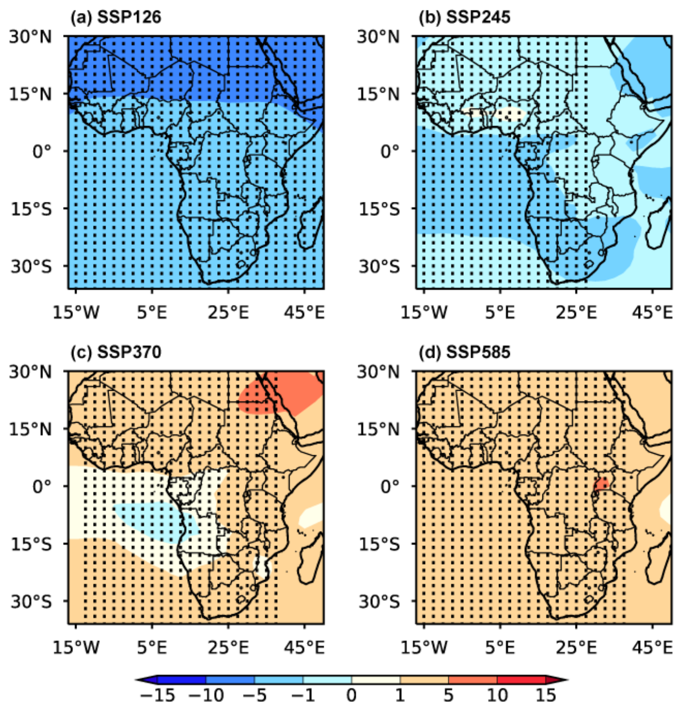

Figure 10. Spatial distributions of differences in near-surface O_3 concentrations (ppb) between 2050–2054 and 2020–2024 under (a) SSP1-2.6, (b) SSP2-4.5, (c) SSP3-7.0 and (d) SSP5-8.5 scenario obtained from CMIP6 multi-model simulations. The shaded areas indicate that the differences are statistically significant at the 90% confidence level.