CHAPTER II

LITERATURE REVIEW

As noted in Chapter I.3, complex interactions of O3 formation have been an interest in academics for over a century. Discovery and detection of O3 can be dated back to an isolated study conducted by Dr. Gordon Dobson in the early 1920s. This resulted in the first in-situ measurement of total column ozone (TCO) by comparing UV absorption at specific wavelengths (Dobson 1923). The establishment of the Dobson Unit (DU), the development of the Dobson Spectrophotometer, and discovery of the stratospheric O3 layer later enabled researchers to detect substantial depletions of Arctic stratospheric ozone, most notably the 1985 finding by (Farman, Gardiner, and Shanklin 1985). Later, was found that the Arctic contained higher levels of inorganic chlorine (Clₙ, such as HCl and ClONO₃), which, under temperatures below ~196 ± 4 K, undergo heterogeneous activation on polar stratospheric cloud (PSC) particles, converting them into reactive radicals (Cl, ClO) that catalyze ozone destruction (Webster et al. 1993). This activated chlorine enters catalytic ozone-destroying cycles that continue until chlorine reservoirs are depleted. While ozone depletion itself does not directly drive sea-level rise, Arctic ozone loss indicates polar stratospheric cooling, which can be linked to broader climate feedback such as ice-albedo and greenhouse warming, contributing indirectly to ice melt and sea-level rise (Girach et al. 2023; Minghu Ding et al. 2020; Nadzir et al. 2018). Ozone (O₃) primarily absorbs UV radiation but also plays a complex role in atmospheric chemistry by modulating the concentrations of other trace gases, such as reactive chlorine and nitrogen species, thereby acting as a catalytic agent within stratospheric cycles (Farman, Gardiner, and Shanklin 1985; Hansen 2007; S. He and Carmichael 1999; Webster et al. 1993; Zvyagintsev, Tarasova, and Kuznetsov 2008).

This literature review seeks to utilize as many resources as possible through professional CUB guidance, free Big Data sources, and course work to better understand overall surface O3. Due to its simplicity, it has many complexities with both short- and long-term trends occurring at coarse- and fine-resolutions. Due to the grandiose potential of computer science, this project follows two informal laws from computer science and military backgrounds: Keep It Stupid Simple and Proper Planning and Preparation Prevents Piss Poor Performance, or K.I.S.S and the 7P’s respectively. Providing streamlined access to data allows for numerous resources used for project implementation in a variety of fields. This thesis seeks to create a simple solution to high resolution surface mapping via thoughtful, out-of-the-box methods because of literature found regarding O3 models.

II.1. Search Methods

The literature synthesized utilized the University of Colorado, Boulder’s (CUB) vast academic resources to conduct a thorough investigation into O3 mechanisms and related processes to air pollutants. With access to prominent sources of academic literature via CUB’s library, EBSCOhost and Web of Science, numerous documents were selected from keywords found throughout literature consumed during course work. A python script accessed the API of each database with the following categorization of key-terms:

|  |  |
| --- | --- |
| TOPIC | Name |
| 1 | Ozone |
| 2 | Models |
| 3 | Ecology |
| 4 | Human |
| 5 | Risk |
| 6 | Prediction |
| 7 | Transport |

TABLE II.1

Used in conjunction with Table II.2, the main categories which this thesis covers can be used as key terms summarizing this thesis as well.

Combinations of the terms following Topic 1 (T1) in Table II.1 were utilized to construct patterns within the abstracts and titles of the literature to sort them into respective categories, in which many were reviewed by accessing the associated DOI with CUB credentials. For this thesis, 246 sources of unique documents pertaining to O3 were found among both databases:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Chapter | Set Combination | | EBSCO | WoS |
| I | All sets | | 29 | 196 |
| II | T1, T2, T6, T7 | | 436 | 964 |
| III | T1, T2, T6 | | 2,365 | 4,750 |
| VI | T1, T3, T4, T5, T7 | | 350 | 1,238 |
|  | | Thesis Count | | 246 |

Table 2

Total Count of literature sources selected and then utilized for this thesis. The full results of the coded literature can be found in Chapter VIII under Figures VIII.1-3.

This was captured by combining the topics O3 and Prediction with Ecology terms in the abstract to capture numerous disciplines like Environmental Sciences, Ecology, Meteorology, Atmospheric Sciences, Public Health, etc., which all have interest in surface O3 accumulation and have utilized relevant techniques helpful to this thesis (Abdullah et al. 2019a; Bashter et al. 2020; Bauer et al. 2004; De Marco et al. 2022; Ghozikali et al. 2015; Glaze 1986; Hakim et al. 2019; L. He et al. 2024; Heal et al. 2013; Jerrett et al. 2009; NIOSH 1994; Niu et al. 2022; Nuvolone, Petri, and Voller 2018; Serra et al. 2022; Turner et al. 2016).

Citations gathered from these searches were imported into python and Zotero for proper formatting and de-duplication. Many works utilized throughout this thesis, inclusive of the introduction, were from this process, though some works were also gathered during informational meetings and coursework. Certain works mentioned earlier e.g. (Dobson 1923; Farman, Gardiner, and Shanklin 1985; Tobler 1970; Webster et al. 1993; S. He and Carmichael 1999) and others published before 2000 e.g (Bojkov and Fioletov 1995; Davies and Schuepbach 1994; Goodchild 1992) were not excluded from the time frame for a few reasons: continued relevancy to further denote how long O3 chemistry and transport mechanisms have been grinding within the metaphorical academic cog (W. Chu et al. 2024; Cocchi, Fabrizi, and Trivisano 2005; De Marco et al. 2022; Glaze 1986; Honrath et al. 2017; Loughner et al. 2020; Mulholland et al. 1998), and they highlight methodologies applied in numerous works in the past decade, as further analyzed in this chapter. Literature was sorted into three main categories: Modelling, Transport, and Health.

A diagram of literature by tap

AI-generated content may be incorrect.FIGURE II.1

Result of separating literature into three main categories which best describe reasoning and content of this thesis. Estimating the correlation between literature gathered by the sets mentioned in Table II.1. This was done to gain a general understanding of what types of O3 literature exist can correlate to this thesis. Note, only 26 documents had keywords with a similar amount of all three topics. Some of these include researchers like Wang, Yiu, and Kim which model O3 for the public health related reasons.

Each category was based on a certain combination of keywords noted in Table 1. Modelling consisted of papers which mainly mentioned keywords from topics 1 and 2. Trasport represents topics 1 and 7. Health used the rest, with overlapping words and topics falling into remaining categories based on frequency of used words. A word cloud and plot of publications overtime shows the expected jump of literature pertaining to ozone modelling. This commenced a dictionary of similar key words in the gathered literature to look out for during the review. Out of the total documents filtered, around 900 documents were initially reviewed and separated into categories for which they may pertain in this thesis (Figure II.1). Topics covered in this section include the general formation of O3, utilization and/or development of surface O3 models in a modern technological world, and overall effects surface O3 can have on inorganic and organic processes. Literature was also gathered from colleagues and course work accomplished during the writing of this thesis.

This chapter seeks to conduct a full, yet brief analysis of O3 models today throughout numerous disciplines to develop in-depth knowledge of surface O3 reactions wherever they may occur. It was expected that appropriate models to use would be the same for most cases of complex adaptive system(s) (CAS). These systems generally contain numerous, similar predictive features with an undetermined unifying principle. As such, significant multi-collinearity within prominent features for CAS predictions is expected. Given numerous physical, chemical, and biological trends, this section seeks to provide a better understanding of where surface ozone reactions mainly occur and how they’ve been incorporated into models today.

II.2. Surface O3 Formation and Transport

The rate of O3 reactions overtime exhibit patterns at extremely close distances. Unlike most pollutants, surface O3 reactions tend to cyclically increase at distal locations from non-maintained and overly-maintained spaces (Y. Choi et al. 2012; D’Amico et al. 2024; Guan et al. 2023; Kim et al. 2016; Oltmans and Levy 1992; Zvyagintsev, Tarasova, and Kuznetsov 2008). Surface O3 formation tends to follow seasonal high and low concentrations, while steadily increasing in urban areas overtime due to interactions with solar radiation (UV) and VoCs (Alves et al. 2024; P. Chen et al. 2022; Guan et al. 2023; Perera et al. 2019; You et al. 2017). O3 trends cannot be modelled with something unable to consider complex systems, so this thesis seeks to utilize models beyond linear scopes. While linear regression is often used in combination with Principle Component Analysis (PCP) and Artificial Neural Networks (ANN) (Arsić et al. 2020; Moustris et al. 2012; Sousa et al. 2007; W. Sun et al. 2015), it was found to yield less accurate results than non-linear methods (Alessandro Fassò and Ilia Negri 2002; R. Wang et al. 2023; Yang et al. 2021; N. Zhao, Zhang, and Wang 2025). Model strengths, weaknesses, and potential contributions to the success of the end prediction established here are used for the final models in Chapter III.4.

The constituents and drivers of O3 might have a heavy effect on urban layouts where geophysical systems force higher temperatures to heavily populated areas. If the separation in urban density versus available green space is too great, surface ozone reactions trend towards areas of either well-kept high biological activity or areas at risk to natural hazards relating to heat and aerosol movement like storms, heat waves, and volcanic eruptions (Brown-Steiner and Hess 2011; Badia et al. 2023; Han et al. 2018; Kumari, Lakhani, and Kumari 2020; Platikanov et al. 2022). While the latter may not be found in most areas in the USNA, golf courses, urban parks, and similar anthropogenic constructions may experience the brunt of ozone concentrations due to these transport mechanisms (Al-Qassimi and Al-Salem 2020; Kong et al. 2023; F. Liu, Zhu, and Zhao 2008; Monks et al. 2015; You et al. 2017).

II.2.1. Complexities of Urban Surface O3

The rate of O3 reactions overtime should exhibit patterns at close distances, but the ideal distance for the proper representation of patterns regarding surface O3 have yet to be formally established (Abdullah et al. 2019b; Tong et al. 2017; Yuting Wang et al. 2023) due to the interaction of O3 molecules. Unlike most pollutants, surface O3 concentrations tend to cyclically increase with interactions within anthropogenic spaces (Y. Choi et al. 2012; D’Amico et al. 2024; Guan et al. 2023; Kim et al. 2016; Oltmans and Levy 1992; Zvyagintsev, Tarasova, and Kuznetsov 2008). Similarities across studies areas have revealed that surface O3 does follow seasonal high and low concentrations during Summer and Winter respectively; steadily increasing overtime in urban areas due to interactions with solar radiation and VoCs where Winter may not be as cold due to the overall geography of the AOI (Alves et al. 2024; P. Chen et al. 2022; Guan et al. 2023; Perera et al. 2019; You et al. 2017). In Chapter I, surface O3 formation was mentioned to be induced from stable tropospheric ozone cycles if the area is met with consistent high temperatures and presence of constituents, such as within PHOTUC.

Large populations can effectively contribute to O3 formations and are especially at risk to complex variations due to the large differentials in access to green space and industrialized zones (Pan et al. 2024; Cai, Zhuang, and Ren 2022; Meo et al. 2021). In addition, at low temperatures and combined with severely polluted, low photolysis days will typically denote lower ozone concentrations (C. Chen et al. 2021; S. He and Carmichael 1999; Jenkin and Clemitshaw 2000; Jiménez and Baldasano 2004; Kalabokas et al. 2008; Lee et al. 2009; M. Li et al. 2021; Manzini et al. 2024; Wie and Moon 2016; Zvyagintsev, Tarasova, and Kuznetsov 2008). The locations of these spaces don’t follow general, non-spatially related patterns, and pollutants which follow spatial non-heterogeneity at small distances must be properly related to the source. While linear regression is often used in combination with Principle Component Analysis (PCP) and Artificial Neural Networks (ANN) (Arsić et al. 2020; Moustris et al. 2012; Sousa et al. 2007; W. Sun et al. 2015), it was found to yield less accurate results than non-linear methods (Alessandro Fassò and Ilia Negri 2002; R. Wang et al. 2023; Yang et al. 2021; N. Zhao, Zhang, and Wang 2025).

II.2.2. Modern Numerical Models and Overcoming Adversity

By nature, applying a model for individual participants over some designated space and time is arduous work. Public health based O3 models are extremely effective at incorporating proper fields and values for persons of interest due to the amount of in-situ knowledge about the population and AOI. This thesis completes a high spatial resolution model of surface ozone values utilizing similar high-resolution techniques for three counties in Arizona using monitor locations instead of participants due to each other’s similarities as geo-atoms based on a location in time (Goodchild, Yuan, and Cova 2007). While Pina, Pimal, and Maricopa counties were chosen due to their population densities; this project results in reproducible functions for all areas with the appropriate materials due to innovations mentioned in Chapter I and III. Atmospheric conditions, constituents, model types, and depictions of surface O3 here build an expectation of the final predictive outputs to note both the accuracy and applicability of the SMaRK method in reference to the study area.

Trends and transportation mechanisms should appear in the final display over PHOTUC and be representative of the information seen in this section. The new revolution in Big Data and complex modeling schemes have allowed for methods outside typical linear scopes to introduce transport, anthropogenic, and thermodynamical mechanisms into their feature bases for urban locations (Chiacchiaretta et al. 2024; Gagliardi and Andenna 2020; Yu et al. 2018a). Modeling techniques for training, validation, prediction and implementation with the residual kriging method are noted and discussed further in the methods section. Studies such as (Congdon and Martin 2007; Demyanov et al. 2001; Mousavi et al. 2019; Seo, Kim, and Singh 2015) utilize CTM based methods to combine atmospheric dynamics and satellite imagery (Lin et. al., 2024). Some researchers like (De Marco et al. 2022; D. Gao et al. 2019; Javanmardi et al. 2017; Jerrett, Gale, and Kontgis 2010; Reid et al. 2012a; Schlink et al. 2006; Zhou et al. 2018) utilized statistical methods for public health to assign ozone exposures to individuals within a distance to nearest monitor methodology.

These must be done per study/cohort, and subsequent participants/locations within them. A study spanning numerous states, spans exponentially more counties and subsequent data points necessary for conclusive analysis.

II.3. CHEMICAL TRANSPORT MODELS

CTMs and ML ensembles represent distinct modeling paradigms; CTMs are process-based and mechanistic, while ML ensembles are data-driven. Recent studies demonstrate they can be effectively combined to improve surface ozone forecasting accuracy at coarse resolutions (HC Sun et al. 2021; Yu et al. 2018a; HC Sun et al. 2021; P. Cheng et al. 2022; Mo et al. 2021; X. Zhao et al. 2024) which can later be aggregated to a finer resolution. Typically, CTMs and ML ensembles sit at opposite ends of the modeling spectrum, but they can complement one another when studying pollutants such as surface ozone. ML ensembles don’t deal with spatial data; they’re combined with CTMs which are a mechanistic, 3D Eulerian framework accounting for some spatial variation through linear associations over a large trend predicted by the ensemble (Travis and Jacob 2019; Balamurugan, Balamurugan, and Chen 2022; Y. Cheng, He, and Huang 2021; Kang et al. 2021; Nelson et al. 2023; Smith et al. 2018; Tondini, Scilla, and Casari 2024; Wu, Tseng, and Huang 2024). Most CTMs around have 8-13 ppb +- 5ppb RMSE associated with them (Long et al. 2014; Travis and Jacob 2019; Q. Wang et al. 2022; Yu et al. 2018a; Zhou et al. 2018) stemming from the modifiable unit area problem (MAUP) when resampling outputs to the desired higher resolution.

CTMs separate emissions and transport mechanisms to later model the relations between surface measurements and satellite detections, typically incorporating valuable spatial information into the associated model’s overall error rather than accounting for this geospatial uncertainty (Konovalov et al. 2006; Lin et al. 2012; Miñarro et al. 2011; Rojas, Venegas, and Mazzeo 2016). What’s more, CTMs are computationally and temporally costly, with most models requiring extensive access to Big Data systems and expensive technology for proper depictions of surface trends (Brown, Waśniewski, and Zlatev 1995; Keller et al. 2017). CTMs using ML and AI methods for transport can be further improved by properly incorporating geospatial uncertainty from monitored data into them by way of residual kriging, making these costly systems more reliable and worthwhile given their typical inaccessibility. Their representations of transport rely on continuity equations like advection, convection, emissions, detailed gas‐ and/or aqueous‐phase, and more atmospheric equations and chemistry (Petetin et al. 2021); proper incorporation of numerical models are essential as uncertainties in general aerosol models are known to be exponentially greater (Lin et al. 2012; Miñarro et al. 2011; Rojas, Venegas, and Mazzeo 2016). CTMs typically use meteorology from remotely sensed data assimilations and chemical mechanisms of choice which simulate global to rural-scale concentrations at higher than average spatial-temporal resolutions. These are physically coherent fields suited to investigate long chemical lifetimes, transport, and stratosphere–troposphere cycles of certain chemicals, but extremely complex molecules like O3 usually yield the highest error. The general laws of physics applied within CTM are extracted and utilized in feature creation, discussed later in Chapter VI.

II.4. Statistical Regression

CTMs used to rely mainly on linear regression; a widely used statistical method used in regression and prediction (W. Sun et al. 2015; Ghazali et al. 2010; M. Wang et al. 2016; Starbuck 2023). Its simplicity, interpretability, and efficiency make it a valuable tool in geographic predictions involving binary classification problems such as land cover changes, habitat presence, or the classification of environmental hazards (Tucker 1979; Sousa et al. 2007; Dalezios 2017). Linear Regression is incredibly straightforward, typically going by the notation:

where m(x) is an indirect rise over run correlation between the independent variable and some feature, b is the y-intercept, and ε denotes the residual error that each point x deviates from the mean trend. Extending this same equation to multiple covariates initializes multi-linear regression:

wherein each represents a weighted value on which attributes to y(x) (Starbuck 2023). There are minimal interpretations to deviate from, and linear methods require next to no tuning unless additional weighing methods are used, but surface O3 requires more complexity.

Linear regression is a great starting point used for exploratory analysis and pre-determination of applicable features, but adaptive algorithms such as least absolute shrinking (LASSO) and similar weighted regularization methods (RIDGE) have become necessary to improve accuracy in numerous case studies using linear regression. RIDGE and LASSO methods represent weighted combinations of multi-linear or multiple-logistic regression to show a trend for a given variable. While working well for semi-complex systems, they can be too heavily constrained to begin with due to their basis in linear regression. Machine Learning and Artificial Intelligence methods work slightly more complexly, by learning weights during a bagging of samples into statistically related bins (often referred to as boosting).

II.5. MACHINE LEARNING

CTM models today use the combination of statistical trends and weighted boosting methods to learn from the metrological tendencies into the dataset via Machine Learning (ML). These garner accurate depictions of atmospheric physics and may utilize ML methods, but CTMs mechanically don’t learn from data. Rather, they are features for use in an ML model, and carry their own spatial uncertainties requiring corrections from the researcher (Yu et al. 2018a; Travis and Jacob 2019; Xiong et al. 2024). CTMs come at a high computational cost, often resulting in hundreds to thousands of CPU-hours for resolutions of 500m-1km. They are also dependent on emission inventories and parameterizations that carry additional uncertainties (K. Chen et al. 2021; Gilliland et al. 2008; Han et al. 2018; Jena et al. 2015; Konovalov et al. 2006; Kuo and Fu 2023). Utilizing these to represent 100m-300m of space is unsuitable due to the uncertainty in model error at these resolutions. CTMs are based on the standard representations of tropospheric–stratospheric chemistry with models like the MOZART-TS1 (Emmons et al. 2010), the Modal Aerosol Model with four modes (MAM4; Liu et al., 2016), and the multi-model reanalysis of Surface Ozone (MUSICA, Lin et al., 2021).

Most CTMs are tree-based algorithms, as they’ve more recently been found to better model chemical transport for O3 further discussed in Chapter V. O3 related literature using regression vs tree based correction ensembles mention the power of these learners, effects on error with unproper tuning and necessity for proper database management (Long et al. 2014; Q. Wang et al. 2022; Wen et al. 2021; Xiong et al. 2024). In their infancy, these models had trouble establishing proper trends for urban areas until further corrections were made within the CTMs themselves (Staehle, Rieder, and Fiore 2023; Saeipourdizaj et al. 2022; Monteiro et al. 2013; Djalalova et al. 2010). All statistical concepts within boosting ensembles are similar; sorting binned data via pre-determined constraints into trees for use in an overall ensemble to make a predictive algorithm and select an outcome given a set of features.

While complex in nature, these are extremely power representations of systems outside of linear scopes (Cao et al. 2024; Rafael et al. 2019; Q. Wang et al. 2022). The number of branches and decisions differ within each ensemble and can be tuned to represent different spreads of data (Keller et al. 2017; Gagliardi and Andenna 2020; Ko, Cho, and Rao 2022). The order in which trees are separated allows for a myriad of potential complex algorithms known as machine learning, where in each tree is based on trends established during the binning process. While normality and non-stochastic are preferred, these ensembles have parameters which account for this, further bolstering the need to learn these methods and incorporate them into this thesis. Boosting algorithms can be separated into two main categories: Sequential and Parrel. Both techniques work like series and parallel circuits in electrodynamics, with the former learning from an iterative binning of data and the latter learning by sorting all data at once and finding trends within subsets of created statistics.

II.5.1. SEQUENTIAL BOOSTING

Sequential bagging involves training base learners one after another, where each subsequent model tries to correct the errors made by its predecessor. Rather than drawing bootstrap samples independently, the model assigns higher weights to data points that were previously misclassified, ensuring that future learners focus on harder cases. This dependency creates a feedback loop, which allows the ensemble to iteratively improve its performance. While sequential bagging generally achieves higher accuracy, it can be more sensitive to noise and overfitting due to its focus on hard-to-classify examples.

Three main types of sequential boosting are used in this thesis. Adaptive boosting sequentially fits trees that focus on residual error by reweighing the data Gradient Boosting fits trees to linear residuals of prior trees via gradient descent of a chosen loss function. Extreme gradient boost (XGB) is the engineering goal to push the limit of computational resources for gradient boosted ensembles. XGB is one of the best performing algorithms utilized for machine learning, due to the many trees and tuning parameters it can yield; seeing positive results e.g. (Hu et al. 2022). The series nature of these processing steps limits the overall reproducibility of them on conventional machines. Computation times for sequential and parallel boosting strategies are compared in Chapter V.

II.5.2. PARALLEL BOOSTING

Parallel bagging is the classical approach to ensemble learning. Multiple base learners typically known as decision trees are simultaneously trained on independent samples of the overall dataset. Each model learns without being influenced by other models; regression is estimated through a majority averaging of predictions. Because the models are trained in parallel, this method benefits from faster training when computational resources support parallel processing. Naturally independent features help reduce overall variance, making parallel bagging especially effective in mitigating overfitting with large co-variance. This thesis uses the most common of parallel boosting techniques, Random Forest.

Random Forest (RF) ensemble learning methods are primarily used for classification and regression tasks. Their applications in geographic data sets have been extensively studied and validated due to their robustness, accuracy, and ability to handle complex datasets. Improvements in computer science alongside similar improvements in geographic practices have given rationale for using RF models in modern day geographic models and prediction systems. By nature, they exceed at handling high dimensionality datasets and complex trends (J. Wang et al. 2024; Runmei Ma et al. 2021; Wright and Ziegler 2017). RF models offer substantial advantages for complex geographic trends including high accuracy, robustness to noise, the ability to handle diverse data types, and account for non-linear relationships. However, they have limitations, like computational complexity, lack of spatial explicitness, and potential challenges in interpretability with many trees of large datasets. While there are other parallel boosting strategies, basic RF strategies were more than enough for this thesis. Other parallel boosting strategies are essentially minuet variations of the base RF ensemble.

II.6. ARTIFICIAL INTELLIGENCE

Before the development of GPU integration, all processing was done on the main computer processing unit (CPU), which is responsible for simultaneously running the rest of the computer and its systems. By incorporating a GPU into the training portion of the model, the CPU doesn’t have to work as hard and can focus on giving commands to the GPU, which does the rest to process the data. Recently, these implementations have seen high success when used to model complex trends such as PM2.5 emissions, disease transmission/hospitalizations, metrological processes, and land use classification (Adel El-Shahat 2018; Arsić et al. 2020; Braik et al. 2024; Binjie Chen et al. 2024; Faris, Alkasassbeh, and Rodan 2014; Seo, Kim, and Singh 2015). The full power of GPU integrated methods has allowed learning methods such as Neural Networks (NN)s to become the pinnacle of today’s modelling systems. NN is a layered, learning-driven architecture that excels at capturing high-dimensional, nonlinear relationships in data. It underpins many breakthroughs in modern AI by enabling scalable, end-to-end learning across diverse fields—from computer vision to healthcare.

II.6.2. Defining Complexity: Convolution and Recurrence

This project utilized a Multi-Layered Perceptron (MLPR), the most basic implementation of an NN in the sci-kit learn library. When trained utilizing the proper series of activation functions, layers, and ensemble learning methods, MLPR can make predictions not unlike the human brain (BJ Chen et al. 2024; S. Gao et al. 2021; T. Li et al. 2022). While there is a significant amount of math involved for determining activation functions and step sizes, the complexity of creating, tuning, and therefore utilizing neural networks in Geography is becoming more accessible. For instance, MLPRs are easy to implement, but lack specialized structure making them ideal for tabular or flattened data. While more complex models like Convolutional Neural Networks (CNN)s and Recursive Neural Networks (RNN) were experimented with, the lack of proper GPU access required this to be completed in future work. These models use the fully connected layers of MLPR with pooling and memory retention methods to either define convolutions across preset areas in the image or recurrence within indexed images to model complex spatial patterns via remote sensing.

CNNs are powerful for spatial patterns, especially in images. While they don’t model spatial patterns, they do incorporate corrected imagery as learners and make deductions based on the learned trend of related pixels, mimicking spatial thought by way of inheriting associated satellite corrections. Imagery is loaded into convolutional layers that scan inputs with weights commonly called kernels. These weights move across the image to detect local patterns given exact positioning of the kernal. RNNs are designed for temporal or sequential data, handling time dependencies. These maintain hidden states which enable the use of past information across an ordered sequence as opposed to a moving window. Combining CNN and RNN architectures form Hierarchical Convolutional Recurrent Neural Networks (HCRNN)s, combining kernel feature extraction with temporal sequencing to improve classification accuracy in multi-spectral, time-varying geospatial datasets. These offer power future directions for this thesis and the means to address numerous gaps in surface O3 literature; an MLPR combined with a spatial temporal regression of uncertainty can be though of a basic implementation of a HCRNN with geospatial kernals. These have seen high promise in surface O3 datasets and trend modelling, but still yield high geospatial error in dense urban locations (Arsić et al. 2020; Mandal et al. 2024; Kleinert, Leufen, and Schultz 2020; S. Gao et al. 2021; HT Sun et al. 2022).

II.7. Gaps in Surface ozone Literature

One of the most obvious gaps in literature is the full coverage of rasterized data depicting surface ozone values for the United States. As is with most cases regarding high resolution data, many specialized forms of surface ozone exist, but have yet to be incorporated into high-resolution raster models depicting universal surface trends, save a few case studies such as this thesis (Y. Choi et al. 2012; X. Lu et al. 2016; Mousavinezhad et al. 2023; Peng Liu et al. 2018; Pozzer, Schultz, and Helmig 2020; Reddy and Pfister 2016; Rui Zhu et al. 2023; Schnell and Prather 2017). Many high resolution models have been created for the EU, China, India, Iran, and other urbanized nations similarly concerned with the growing rate of surface ozone reactions (Dong et al. 2021; Z. Li et al. 2023; Tian et al. 2024; J. Wang et al. 2024; Y Wang et al. 2021). Urban based public health case studies tend to focus on personal exposures from environmental aspects related to O3. These typically assign O3 concentrations to wiling participants via advanced statistical modellings, with geo-located addresses to predict the expected exposure of the individual to surface O3 (Ghozikali et al. 2015, 2015; Jerrett et al. 2009; Malley et al. 2017; Niu et al. 2022; Tang et al. 2024; Tian et al. 2024; Turner et al. 2016).

The information provided by exposure studies such as these tend to be extremely informative for modeling due to their nature as a high-resolution dataset. These are usually built from estimated measurements like distance to the nearest monitor or road and aren’t used to make a full depiction of the area due to their basis in individual activity spaces. Most are difficult to create, as the movement of a human can drastically change their exposure to surface ozone in addition to other harmful pollutants, potentially co-funding with NOx and PM2.5 constituents (Balmes 2019; Jerrett et al. 2009; Malley et al. 2017; Niu et al. 2022; Turner et al. 2016). Due to the interactions with naturally occurring chemicals in Earth’s atmosphere explained in Chapter I, it is well known that anthropogenic sources and isoprene related VoC’s tend to yield the larges correlations with surface ozone reactions (You et al. 2017; R. Wang et al. 2023; Nelson et al. 2023; K. Ma et al. 2023; Q. Liu et al. 2022).

When exposed over long-terms, O3 has potential associations with hospitalization rates of upper and lower respiratory diseases, varies with age, gender, initial health of the individual, and promotes unnecessary/unregulated oxidative stress causing irreversible cognitive/immune system damage (Barzeghar et al. 2020; J. Choi et al. 2024; Crouse et al. 2015; Ghozikali et al. 2015; Heal et al. 2013; Im et al. 2023; Javanmardi et al. 2017; Nuvolone, Petri, and Voller 2018; Turner et al. 2016). Many other studies across the world have found minor to major associations between short-term exposure at the surface during seasonal cycles, having potential direct and indirect consequences which are still being discussed (S. Chen et al. 2023; L. Chu et al. 2023; Karimi et al. 2019; H. Ma et al. 2023; Orellano et al. 2020; Reid et al. 2012b; Tang et al. 2024; Tian et al. 2024; Shin et al. 2018). The trend makes sense due to the chemical volatility of O3, as oxidative stress becomes easier to achieve with O- as a product of unstable O3 in lieu of solely O2. The implications and harm surface O3 can have on both human health and the environment are further discussed in Chapter VI. Within ozone models for health-related risk, policy making, or similar cohort-based studies; air pollution along with growing worries of climate change, and associated health risks, have spurred the need for high resolution imagery at around 300m, which SMaRK can easily achieve.

The most notable gap in O3 literature is the same found with all ML/AI representations of geospatial data. Due to the revolution in Big Data and scientific technology, in-situ surface measurements are readily available across the globe (Emetere 2020; Gaudel et al. 2018). Researchers specializing in hybrid ML/AI methods for geospatial data don’t typically incorporate these in-situ measurements in the final prediction. Simply using them during the training process can establish an accurate trend based on corrections made by remote sensing satellites; however, these satellites don’t rely on ground-based observations. Chapter III later mentions that all remote sensing images are stemmed in corrected measurements of reflected light. When applied to coarse resolutions, these errors can be negligible due to the large area they’re meant to describe (about 1km and above). Remote Sensing data utilized for these also only represent total column estimates, not complex surface interactions. Chapter I revealed that chemical transport models (CTM)s, while accurate, at a high resolution ~500m-1km, and cover national boundaries, still depict some error regarding tropospheric chemicals in the upper and lower hemispheres of Earth when using remotely sensed imagery.

CONCLUSION

Models covered in this chapter helped better understand complex processes governing Ozone formation and transport. These are ultimately used by decision-makers of all scales and influence decisions surrounding efforts to mitigate the impacts of constituents attributing to surface O3 prominence (Balamurugan, Balamurugan, and Chen 2022; Watson et al. 2019; You et al. 2017). Given this information, it was expected that the dataset would need to be as complex as the reaction itself, requiring many features to accurately represent known interactions ozone has with natural and built environments (Jenkin and Clemitshaw 2000; Ziemke et al. 2011; Huang et al. 2017). Studies with a brief depiction, section, or which focus on surface O3 entirely suggest the best models suited for this project are tree-based and neural network models.

Many tropospheric ozone transport models assume constant distribution of the gas over the system in question and only result in predictions at a resolution of around 4km. CTM models are used in a wide variety of studies due to the robustness of the methodology; calculation expenses stem from the vast effort required to optimize the model pending on the complexity of the gas in question (Emetere 2020). For Ozone, these models are often complex but imperative to ensure a safe future for current and future generations. The health impacts and concerns associated with surface ozone exposure can’t rely CTM based models due to coarse results, which tend to under- or over- estimate ozone concentrations in the upper and lower and upper latitudes respectively (Long et al. 2014; Yu et al. 2018b).

Researchers have developed interpolated exposure rates via temporal analysis of extrapolated statistical learning models to create unique activity space exposures (De Marco et al. 2022; J. Lu and Yao 2023; Malley et al. 2017; Turner et al. 2016). Utilizing the geo-located point of a willing respondent or location of interest with metrological data of nearby environmental and urban aspects to capture the high variations of ozone concentrations. These are extremely fine resolution, depicting exposures in-terms of the populations exposed space (Jerrett et al. 2009; Balmes 2019; Niu et al. 2022). As the models in this thesis are to be trained on data gathered from similar satellite observations, the development of a large dataset which combines these techniques may improve exposure assignment times by reducing the amount of coding work necessary to add ozone as a variable of interest. This work could benefit numerous case studies in areas pertaining but not limited to; public health, surface chemistry/air quality, environmental health, atmospheric health, chemical transport trends, and others of similar methodologies.

Citations

Abdullah, Samsuri, Najihah Husna Ahmad Nasir, Marzuki Ismail, Ali Najah Ahmed, and Mohamad Nor Khasbi Jarkoni. 2019a. “Development of Ozone Prediction Model in Urban Area.” *International Journal of Innovative Technology and Exploring Engineering* 8 (10): 2263–67. doi:10.35940/ijitee.J1127.0881019.

Adel El-Shahat. 2018. *Advanced Applications for Artificial Neural Networks*. Croatia: IntechOpen. https://search.ebscohost.com/login.aspx?direct=true&AuthType=ip,sso&db=nlebk&AN=4007284&site=ehost-live&scope=site&authtype=ip,sso&custid=s8860338.

Alessandro Fassò and Ilia Negri. 2002. “Non-Linear Statistical Modelling of High Frequency Ground Ozone Data.” *Environmetrics* 13 (3). Wiley-Blackwell: 225–41.

Al-Qassimi, M, and SM Al-Salem. 2020. “Ozone (O3) Ambient Levels as a Secondary Airborne Precursor in Fahaheel Urban Area, the State of Kuwait.” *ATMOSPHERIC SCIENCE LETTERS* 21 (9). doi:10.1002/asl.983.

Alves, CA, MJS Feliciano, C Gama, E Vicente, L Furst, and A Leitao. 2024. “First Exploratory Study of Gaseous Pollutants (NO2, SO2, O3, VOCs and Carbonyls) in the Luanda Metropolitan Area by Passive Monitoring.” *ENVIRONMENTAL POLLUTION* 362 (December). doi:10.1016/j.envpol.2024.125015.

Arsić, Milica, Ivan Mihajlović, Djordje Nikolić, Živan Živković, and Marija Panić. 2020. “Prediction of Ozone Concentration in Ambient Air Using Multilinear Regression and the Artificial Neural Networks Methods.” *Ozone: Science & Engineering* 42 (1): 79–88. doi:10.1080/01919512.2019.1598844.

Badia, Alba, Veronica Vidal, Sergi Ventura, Roger Curcoll, Ricard Segura, and Gara Villalba. 2023. “Modelling the Impacts of Emission Changes on O3 Sensitivity, Atmospheric Oxidation Capacity and Pollution Transport over the Catalonia Region.” *EGUsphere*, March, 1–38. doi:10.5194/egusphere-2023-160.

Balamurugan, Vigneshkumar, Vinothkumar Balamurugan, and Jia Chen. 2022. “Importance of Ozone Precursors Information in Modelling Urban Surface Ozone Variability Using Machine Learning Algorithm.” *Scientific Reports* 12 (1). Nature Publishing Group: 5646. doi:10.1038/s41598-022-09619-6.

Balmes, John R. 2019. “Long-Term Exposure to Ozone and Cardiopulmonary Mortality: Epidemiology Strikes Again.” *American Journal of Respiratory and Critical Care Medicine* 200 (8). American Thoracic Society - AJRCCM: 958–59. doi:10.1164/rccm.201906-1105ED.

Barzeghar, V, P Sarbakhsh, MS Hassanvand, S Faridi, and A Gholampour. 2020. “Long-Term Trend of Ambient Air PM10, PM2.5, and O3 and Their Health Effects in Tabriz City, Iran, during 2006-2017.” *SUSTAINABLE CITIES AND SOCIETY* 54 (March). doi:10.1016/j.scs.2019.101988.

Bashter, I. I., M. A. Lasheen, E. M. Ahmed, O. S. Ahmed, and A. A. El-Ghazaly. 2020. “A Mathematical Model for Studying the Effect of the Atmospheric Boundary Layer on the Surface Ozone Variations at a Coastal Site.” *ARAB JOURNAL OF NUCLEAR SCIENCES AND APPLICATIONS* 53 (1): 97–109. doi:10.21608/ajnsa.2019.12283.1210.

Bauer, SE, Y Balkanski, M Schulz, DA Hauglustaine, and F Dentener. 2004. “Global Modeling of Heterogeneous Chemistry on Mineral Aerosol Surfaces: Influence on Tropospheric Ozone Chemistry and Comparison to Observations.” *JOURNAL OF GEOPHYSICAL RESEARCH-ATMOSPHERES* 109 (D2). doi:10.1029/2003JD003868.

Bojkov, Rumen D., and Vitali E. Fioletov. 1995. “Estimating the Global Ozone Characteristics during the Last 30 Years.” *Journal of Geophysical Research: Atmospheres* 100 (D8): 16537–51. doi:10.1029/95JD00692.

Braik, Malik, Alaa Sheta, Elvira Kovac-Andric, Heba Al-Hiary, Sultan Aljahdali, Walaa H. Elashmawi, Mohammed A. Awadallah, and Mohammed Azmi Al-Betar. 2024. “Predicting Surface Ozone Levels in Eastern Croatia: Leveraging Recurrent Fuzzy Neural Networks with Grasshopper Optimization Algorithm.” *WATER AIR AND SOIL POLLUTION* 235 (10). doi:10.1007/s11270-024-07378-w.

Brown, John, Jerzy Waśniewski, and Zahari Zlatev. 1995. “Running Air Pollution Models on Massively Parallel Machines.” *Parallel Computing* 21 (6). Elsevier BV: 971–91. doi:10.1016/0167-8191(95)00002-6.

Brown-Steiner, B, and P Hess. 2011. “Asian Influence on Surface Ozone in the United States: A Comparison of Chemistry, Seasonality, and Transport Mechanisms.” *JOURNAL OF GEOPHYSICAL RESEARCH-ATMOSPHERES* 116 (September). doi:10.1029/2011JD015846.

Cai, LY, MZ Zhuang, and Y Ren. 2022. “Spatiotemporal Characteristics of NO2, PM2.5 and O3 in a Coastal Region of Southeastern China and Their Removal by Green Spaces.” *INTERNATIONAL JOURNAL OF ENVIRONMENTAL HEALTH RESEARCH* 32 (1): 1–17. doi:10.1080/09603123.2020.1720620.

Cao, RH, YX Xiao, YB Dong, FW Zhang, K Shi, and ZY Wang. 2024. “Using Complex Systems Theory to Comprehend the Coordinated Control Effects of PM2.5 and O3 in Yangtze River Delta Industrial Base in China.” *STOCHASTIC ENVIRONMENTAL RESEARCH AND RISK ASSESSMENT* 38 (10): 4027–41. doi:10.1007/s00477-024-02791-3.

Chen, Binjie, Qiming Zheng, Weiwei Sun, Gang Yang, Tian Feng, and Yumiao Wang. 2024. “Geo-STO3Net: A Deep Neural Network Integrating Geographical Spatiotemporal Information for Surface Ozone Estimation.” *IEEE TRANSACTIONS ON GEOSCIENCE AND REMOTE SENSING* 62. doi:10.1109/TGRS.2024.3358397.

Chen, CH, TF Chen, SP Huang, and KH Chang. 2021. “Comparison of the RADM2 and RACM Chemical Mechanisms in O3 Simulations: Effect of the Photolysis Rate Constant.” *SCIENTIFIC REPORTS* 11 (1). doi:10.1038/s41598-021-84629-4.

Chen, KY, PF Wang, H Zhao, P Wang, AF Gao, L Myllyvirta, and HL Zhang. 2021. “Summertime O3 and Related Health Risks in the North China Plain: A Modeling Study Using Two Anthropogenic Emission Inventories.” *ATMOSPHERIC ENVIRONMENT* 246 (February). doi:10.1016/j.atmosenv.2020.118087.

Chen, PL, XY Zhao, O Wang, M Shao, XX Xiao, SS Wang, and QG Wang. 2022. “Characteristics of VOCs and Their Potentials for O3 and SOA Formation in a Medium-Sized City in Eastern China.” *AEROSOL AND AIR QUALITY RESEARCH* 22 (1). doi:10.4209/aaqr.210239.

Chen, SS, XQ Wang, DH Li, JW Zhao, JJ Zhang, YZ Zhang, XJ Zhang, and XH Kan. 2023. “Association Between Exposure to Ozone (O3) and the Short-Term Effect on Tuberculosis Outpatient Visits: A Time-Series Study in 16 Cities of Anhui Province, China.” *JOURNAL OF MULTIDISCIPLINARY HEALTHCARE* 16: 2045–55. doi:10.2147/JMDH.S412394.

Cheng, PY, A Pour-Biazar, AT White, and RT McNider. 2022. “Improvement of Summertime Surface Ozone Prediction by Assimilating Geostationary Operational Environmental Satellite Cloud Observations.” *ATMOSPHERIC ENVIRONMENT* 268 (January). doi:10.1016/j.atmosenv.2021.118751.

Cheng, Y, LY He, and XF Huang. 2021. “Development of a High-Performance Machine Learning Model to Predict Ground Ozone Pollution in Typical Cities of China.” *JOURNAL OF ENVIRONMENTAL MANAGEMENT* 299 (December). doi:10.1016/j.jenvman.2021.113670.

Chiacchiaretta, P, E Aruffo, A Mascitelli, C Colangeli, S Palermi, S Bianco, and P Di Carlo. 2024. “Inland O3 Production Due to Nitrogen Dioxide Transport Downwind a Coastal Urban Area: A Neural Network Assessment.” *SUSTAINABILITY* 16 (15). doi:10.3390/su16156355.

Choi, J, DK Henze, MO Nawaz, and CS Malley. 2024. “Source Attribution of Health Burdens From Ambient PM2.5, O3, and NO2 Exposure for Assessment of South Korean National Emission Control Scenarios by 2050.” *GEOHEALTH* 8 (8). doi:10.1029/2024GH001042.

Choi, Y., H. Kim, D. Tong, and P. Lee. 2012. “Summertime Weekly Cycles of Observed and Modeled NOx and O3 Concentrations as a Function of Land Use Type and Ozone Production Sensitivity over the Continental United States.” *Atmospheric Chemistry & Physics Discussions* 12 (1). Copernicus Gesellschaft mbH: 1585–1611. doi:10.5194/acpd-12-1585-2012.

Chu, LZ, K Chen, Q Di, S Crowley, and R Dubrow. 2023. “Associations between Short-Term Exposure to PM2.5, NO2 and O3 Pollution and Kidney-Related Conditions and the Role of Temperature-Adjustment Specification: A Case-Crossover Study in New York State\*.” *ENVIRONMENTAL POLLUTION* 328 (July). doi:10.1016/j.envpol.2023.121629.

Chu, Wanghui, Hong Li, Yuanyuan Ji, Xin Zhang, Likun Xue, Jian Gao, and Cong An. 2024. “Research on Ozone Formation Sensitivity Based on Observational Methods: Development History, Methodology, and Application and Prospects in China.” *Journal of Environmental Sciences* 138 (April): 543–60. doi:10.1016/j.jes.2023.02.052.

Cocchi, D, E Fabrizi, and C Trivisano. 2005. “A Stratified Model for the Assessment of Meteorologically Adjusted Trends of Surface Ozone.” *ENVIRONMENTAL AND ECOLOGICAL STATISTICS* 12 (2): 195–208. doi:10.1007/s10651-005-1041-6.

Congdon, Christopher, and Jay Martin. 2007. “On Using Standard Residuals as a Metric of Kriging Model Quality.” In *48th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference*. Honolulu, Hawaii: American Institute of Aeronautics and Astronautics. doi:10.2514/6.2007-1928.

Crouse, DL, PA Peters, P Hystad, JR Brook, A van Donkelaar, RV Martin, PJ Villeneuve, et al. 2015. “Ambient PM2.5, O3, and NO2 Exposures and Associations with Mortality over 16 Years of Follow-Up in the Canadian Census Health and Environment Cohort (CanCHEC).” *ENVIRONMENTAL HEALTH PERSPECTIVES* 123 (11): 1180–86. doi:10.1289/ehp.1409276.

Dalezios, Nicolas R., ed. 2017. *Environmental Hazards Methodologies for Risk Assessment and Management*. First published. London: IWA Publishing.

D’Amico, F, D Gullì, T Lo Feudo, I Ammoscato, E Avolio, M De Pino, P Cristofanelli, et al. 2024. “Cyclic and Multi-Year Characterization of Surface Ozone at the WMO/GAW Coastal Station of Lamezia Terme (Calabria, Southern Italy): Implications for Local Environment, Cultural Heritage, and Human Health.” *ENVIRONMENTS* 11 (10). doi:10.3390/environments11100227.

Davies, TD, and E Schuepbach. 1994. “Episodes of High Ozone Concentrations at the Earth’s Surface Resulting from Transport Down From the Upper Troposphere and Lower Stratosphere - A Review and Case-Studies.” *Atmospheric Environment* 28 (1): 53–68. doi:10.1016/1352-2310(94)90022-1.

De Marco, Alessandra, Hector Garcia-Gomez, Alessio Collalti, Yusef Omidi Khaniabadi, Zhaozhong Feng, Chiara Proietti, Pierre Sicard, Marcello Vitale, Alessandro Anav, and Elena Paoletti. 2022. “Ozone Modelling and Mapping for Risk Assessment: An Overview of Different Approaches for Human and Ecosystems Health.” *Environmental Research* 211 (August): 113048. doi:10.1016/j.envres.2022.113048.

Demyanov, V., S. Soltani, M. Kanevski, S. Canu, M. Maignan, E. Savelieva, V. Timonin, and V. Pisarenko. 2001. “Wavelet Analysis Residual Kriging vs. Neural Network Residual Kriging.” *Stochastic Environmental Research and Risk Assessment* 15 (1): 18–32. doi:10.1007/s004770000056.

Djalalova, I, J Wilczak, S McKeen, G Grell, S Peckham, M Pagowski, L DelleMonache, et al. 2010. “Ensemble and Bias-Correction Techniques for Air Quality Model Forecasts of Surface O3 and PM2.5 during the TEXAQS-II Experiment of 2006.” *ATMOSPHERIC ENVIRONMENT* 44 (4): 455–67. doi:10.1016/j.atmosenv.2009.11.007.

Dobson, Gordon. 1923. “Measurements of the Sun’s Ultra-Violet Radiation and Its Absorption in the Earth’s Atmosphere.” *Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character* 104 (725): 252–71. doi:10.1098/rspa.1923.0107.

Dong, C, R Gao, X Zhang, H Li, WX Wang, and LK Xue. 2021. “Assessment of O3-Induced Crop Yield Losses in Northern China during 2013-2018 Using High-Resolution Air Quality Reanalysis Data.” *ATMOSPHERIC ENVIRONMENT* 259 (August). doi:10.1016/j.atmosenv.2021.118527.

Emetere, Moses Eterigho. 2020. *Introduction to Environmental Data Analysis and Modeling*. Lecture Notes in Networks and Systems Ser, v. 58. Cham: Springer International Publishing AG.

Emmons, L. K., S. Walters, P. G. Hess, J.-F. Lamarque, G. G. Pfister, D. Fillmore, C. Granier, et al. 2010. “Description and Evaluation of the Model for Ozone and Related Chemical Tracers, Version 4 (MOZART-4).” *Geoscientific Model Development* 3 (1). Copernicus GmbH: 43–67. doi:10.5194/gmd-3-43-2010.

Faris, Hossam, Mouhammd Alkasassbeh, and Ali Rodan. 2014. “Artificial Neural Networks for Surface Ozone Prediction: Models and Analysis.” *POLISH JOURNAL OF ENVIRONMENTAL STUDIES* 23 (2): 341–48.

Farman, J. C., B. G. Gardiner, and J. D. Shanklin. 1985. “Large Losses of Total Ozone in Antarctica Reveal Seasonal ClOx/NOx Interaction.” *Nature* 315 (6016): 207–10. doi:10.1038/315207a0.

Gagliardi, RV, and C Andenna. 2020. “A Machine Learning Approach to Investigate the Surface Ozone Behavior.” *ATMOSPHERE* 11 (11). doi:10.3390/atmos11111173.

Gao, Da, Min Xie, Xing Chen, Tijian Wang, Chenchao Zhan, Junyu Ren, and Qian Liu. 2019. “Modeling the Effects of Climate Change on Surface Ozone during Summer in the Yangtze River Delta Region, China.” *INTERNATIONAL JOURNAL OF ENVIRONMENTAL RESEARCH AND PUBLIC HEALTH* 16 (9). doi:10.3390/ijerph16091528.

Gao, S, ZP Bai, S Liang, H Yu, L Chen, YL Sun, J Mao, et al. 2021. “Simulation of Surface Ozone over Hebei Province, China Using Kolmogorov-Zurbenko and Artificial Neural Network (KZ-ANN) Combined Model.” *ATMOSPHERIC ENVIRONMENT* 261 (September). doi:10.1016/j.atmosenv.2021.118599.

Gaudel, A., O. R. Cooper, G. Ancellet, B. Barret, A. Boynard, J. P. Burrows, C. Clerbaux, et al. 2018. “Tropospheric Ozone Assessment Report: Present-Day Distribution and Trends of Tropospheric Ozone Relevant to Climate and Global Atmospheric Chemistry Model Evaluation.” Edited by Detlev Helmig and Alastair Lewis. *Elementa: Science of the Anthropocene* 6 (January): 39. doi:10.1525/elementa.291.

Ghazali, Nurul Adyani, Nor Azam Ramli, Ahmad Shukri Yahaya, Noor Faizah Fitri Md Yusof, Nurulilyana Sansuddin, and Wesam Ahmed Al Madhoun. 2010. “Transformation of Nitrogen Dioxide into Ozone and Prediction of Ozone Concentrations Using Multiple Linear Regression Techniques.” *Environmental Monitoring and Assessment* 165 (1–4): 475–89. doi:10.1007/s10661-009-0960-3.

Ghozikali, MG, M Mosaferi, GH Safari, and J Jaafari. 2015. “Effect of Exposure to O3, NO2, and SO2 on Chronic Obstructive Pulmonary Disease Hospitalizations in Tabriz, Iran.” *ENVIRONMENTAL SCIENCE AND POLLUTION RESEARCH* 22 (4): 2817–23. doi:10.1007/s11356-014-3512-5.

Gilliland, AB, C Hogrefe, RW Pinder, JM Godowitch, KL Foley, and ST Rao. 2008. “Dynamic Evaluation of Regional Air Quality Models:: Assessing Changes in O3 Stemming from Changes in Emissions and Meteorology.” *ATMOSPHERIC ENVIRONMENT* 42 (20): 5110–23. doi:10.1016/j.atmosenv.2008.02.018.

Girach, Imran A., Narendra Ojha, Prabha R. Nair, Kandula V. Subrahmanyam, Neelakantan Koushik, Mohammed M. Nazeer, Nadimpally Kiran Kumar, Surendran Nair Suresh Babu, Jos Lelieveld, and Andrea Pozzer. 2023. “Influences of Downward Transport and Photochemistry on Surface Ozone over East Antarctica during Austral Summer: In Situ Observations and Model Simulations.” *EGUsphere*, August, 1–36. doi:10.5194/egusphere-2023-1524.

Glaze, W H. 1986. “Reaction Products of Ozone: A Review.” *Environmental Health Perspectives* 69 (November): 151–57. doi:10.1289/ehp.8669151.

Goodchild, Michael F. 1992. “Geographical Information Science.” *International Journal of Geographical Information Systems* 6 (1): 31–45. doi:10.1080/02693799208901893.

Goodchild, Michael F., May Yuan, and Thomas J. Cova. 2007. “Towards a General Theory of Geographic Representation in GIS.” *International Journal of Geographical Information Science* 21 (3): 239–60. doi:10.1080/13658810600965271.

Guan, YA, XJ Liu, ZY Zheng, YW Dai, GM Du, J Han, LA Hou, and ER Duan. 2023. “Summer O3 Pollution Cycle Characteristics and VOCs Sources in a Central City of Beijing-Tianjin-Hebei Area, China.” *ENVIRONMENTAL POLLUTION* 323 (April). doi:10.1016/j.envpol.2023.121293.

Hakim, Zainab Q., Scott Archer-Nicholls, Gufran Beig, Gerd A. Folberth, Kengo Sudo, Nathan Luke Abraham, Sachin Ghude, Daven K. Henze, and Alexander T. Archibald. 2019. “Evaluation of Tropospheric Ozone and Ozone Precursors in Simulations from the HTAPII and CCMI Model Intercomparisons – a Focus on the Indian Subcontinent.” *Atmospheric Chemistry and Physics* 19 (9). Copernicus GmbH: 6437–58. doi:10.5194/acp-19-6437-2019.

Han, X, LY Zhu, SL Wang, XY Meng, MG Zhang, and J Hu. 2018. “Modeling Study of Impacts on Surface Ozone of Regional Transport and Emissions Reductions over North China Plain in Summer 2015.” *ATMOSPHERIC CHEMISTRY AND PHYSICS* 18 (16): 12207–21. doi:10.5194/acp-18-12207-2018.

Hansen, J E. 2007. “Scientific Reticence and Sea Level Rise.” *Environmental Research Letters* 2 (2): 024002. doi:10.1088/1748-9326/2/2/024002.

He, Linchen, Zhiheng Hao, Charles J. Weschler, Feng Li, Yinping Zhang, and Junfeng Jim Zhang. 2024. “Indoor Ozone Reaction Products: Contributors to the Respiratory Health Effects Associated with Low-Level Outdoor Ozone.” *Atmospheric Environment* 340 (October): 120920. doi:10.1016/j.atmosenv.2024.120920.

He, Shan, and Gregory R. Carmichael. 1999. “Sensitivity of Photolysis Rates and Ozone Production in the Troposphere to Aerosol Properties.” *Journal of Geophysical Research: Atmospheres* 104 (D21): 26307–24. doi:10.1029/1999JD900789.

Heal, Mathew R., Clare Heaviside, Ruth M. Doherty, Massimo Vieno, David S. Stevenson, and Sotiris Vardoulakis. 2013. “Health Burdens of Surface Ozone in the UK for a Range of Future Scenarios.” *ENVIRONMENT INTERNATIONAL* 61 (November): 36–44. doi:10.1016/j.envint.2013.09.010.

Honrath, Richard E., Yaoxian Huang, Shiliang Wu, Louisa J. Kramer, and Detlev Helmig. 2017. “Surface Ozone and Its Precursors at Summit, Greenland: Comparison between Observations and Model Simulations.” *Atmospheric Chemistry and Physics* 17 (23): 14661–74. doi:10.5194/acp-17-14661-2017.

Hu, XM, J Zhang, WH Xue, LH Zhou, YF Che, and T Han. 2022. “Estimation of the Near-Surface Ozone Concentration with Full Spatiotemporal Coverage across the Beijing-Tianjin-Hebei Region Based on Extreme Gradient Boosting Combined with a WRF-Chem Model.” *ATMOSPHERE* 13 (4). doi:10.3390/atmos13040632.

Huang, Min, Gregory R. Carmichael, R. Bradley Pierce, Duseong S. Jo, Rokjin J. Park, Johannes Flemming, Louisa K. Emmons, et al. 2017. “Impact of Intercontinental Pollution Transport on North American Ozone Air Pollution: An HTAP Phase 2 Multi-Model Study.” *Atmospheric Chemistry and Physics* 17 (9): 5721–50. doi:10.5194/acp-17-5721-2017.

Im, U, SE Bauer, LM Frohn, C Geels, K Tsigaridis, and J Brandt. 2023. “Present-Day and Future PM2.5 and O3-Related Global and Regional Premature Mortality in the EVAv6.0 Health Impact Assessment Model.” *ENVIRONMENTAL RESEARCH* 216 (January). doi:10.1016/j.envres.2022.114702.

Javanmardi, Parviz, Pouran Morovati, Majid Farhadi, Sahar Geravandi, Yusef Omidi Khaniabadi, Kambiz Ahmadi Angali, Adewale Matthew Taiwo, et al. 2017. “Monitoring The Impact Of Ambient Ozone On Human Health Using Time Series Analysis And Air Quality Model Approaches.” *Fresenius Environmental Bulletin* 26 (November).

Jena, C, SD Ghude, G Beig, DM Chate, R Kumar, GG Pfister, DM Lal, DE Surendran, S Fadnavis, and RJ van der A. 2015. “Inter-Comparison of Different NOX Emission Inventories and Associated Variation in Simulated Surface Ozone in Indian Region.” *ATMOSPHERIC ENVIRONMENT* 117 (September): 61–73. doi:10.1016/j.atmosenv.2015.06.057.

Jenkin, Michael E., and Kevin C. Clemitshaw. 2000. “Ozone and Other Secondary Photochemical Pollutants: Chemical Processes Governing Their Formation in the Planetary Boundary Layer.” *Atmospheric Environment* 34 (16): 2499–2527. doi:10.1016/S1352-2310(99)00478-1.

Jerrett, Michael, Richard T. Burnett, C. Arden Pope, Kazuhiko Ito, George Thurston, Daniel Krewski, Yuanli Shi, Eugenia Calle, and Michael Thun. 2009. “Long-Term Ozone Exposure and Mortality.” *New England Journal of Medicine* 360 (11). Massachusetts Medical Society: 1085–95. doi:10.1056/NEJMoa0803894.

Jerrett, Michael, Sara Gale, and Caitlin Kontgis. 2010. “Spatial Modeling in Environmental and Public Health Research.” *International Journal of Environmental Research and Public Health* 7 (4): 1302–29. doi:10.3390/ijerph7041302.

Jiménez, P, and JM Baldasano. 2004. “Ozone Response to Precursor Controls in Very Complex Terrains:: Use of Photochemical Indicators to Assess O3-NOx-VOC Sensitivity in the Northeastern Iberian Peninsula -: Art. No. D20309.” *JOURNAL OF GEOPHYSICAL RESEARCH-ATMOSPHERES* 109 (D20). doi:10.1029/2004JD004985.

Kalabokas, PD, N Mihalopoulos, R Ellul, S Kleanthous, and CC Repapis. 2008. “An Investigation of the Meteorological and Photochemical Factors Influencing the Background Rural and Marine Surface Ozone Levels in the Central and Eastern Mediterranean.” *ATMOSPHERIC ENVIRONMENT* 42 (34): 7894–7906. doi:10.1016/j.atmosenv.2008.07.009.

Kang, Y, H Choi, J Im, S Park, M Shin, CK Song, and S Kim. 2021. “Estimation of Surface-Level NO2 and O3 Concentrations Using TROPOMI Data and Machine Learning over East Asia.” *ENVIRONMENTAL POLLUTION* 288 (November). doi:10.1016/j.envpol.2021.117711.

Karimi, A, M Shirmardi, M Hadei, YT Birgani, A Neisi, A Takdastan, and G Goudarzi. 2019. “Concentrations and Health Effects of Short- and Long-Term Exposure to PM2.5, NO2, and O3 in Ambient Air of Ahvaz City, Iran (2014-2017).” *ECOTOXICOLOGY AND ENVIRONMENTAL SAFETY* 180 (September): 542–48. doi:10.1016/j.ecoenv.2019.05.026.

Keller, Christoph A., Mathew J. Evans, J. Nathan Kutz, and Steven Pawson. 2017. “Machine Learning and Air Quality Modeling.” In *2017 IEEE International Conference on Big Data (Big Data)*, 4570–76. Boston, MA: IEEE. doi:10.1109/bigdata.2017.8258500.

Kim, SW, BC McDonald, S Baidar, SS Brown, B Dube, RA Ferrare, GJ Frost, et al. 2016. “Modeling the Weekly Cycle of NOx and CO Emissions and Their Impacts on O3 in the Los Angeles-South Coast Air Basin during the CalNex 2010 Field Campaign.” *JOURNAL OF GEOPHYSICAL RESEARCH-ATMOSPHERES* 121 (3): 1340–60. doi:10.1002/2015JD024292.

Kleinert, Felix, Lukas H. Leufen, and Martin G. Schultz. 2020. “IntelliO3-Ts v1.0: A Neural Network Approach to Predict near-Surface Ozone Concentrations in Germany.” *Geoscientific Model Development Discussions*, August. Copernicus Gesellschaft mbH, 1–69. doi:10.5194/gmd-2020-169.

Ko, K, S Cho, and RR Rao. 2022. “Machine-Learning-Based Near-Surface Ozone Forecasting Model with Planetary Boundary Layer Information.” *SENSORS* 22 (20). doi:10.3390/s22207864.

Kong, SJ, T Wang, F Li, JJ Yan, and ZG Qu. 2023. “Unraveling Spatiotemporal Patterns and Multiple Driving Factors of Surface Ozone across China and Its Urban Agglomerations Management Strategies.” *FRONTIERS IN ECOLOGY AND EVOLUTION* 11 (June). doi:10.3389/fevo.2023.1103503.

Konovalov, I. B., M. Beekmann, A. Richter, and J. P. Burrows. 2006. “Inverse Modelling of the Spatial Distribution of NOx Emissions on a Continental Scale Using Satellite Data.” *Atmospheric Chemistry and Physics* 6 (7). Copernicus GmbH: 1747–70. doi:10.5194/acp-6-1747-2006.

Kumari, S, A Lakhani, and KM Kumari. 2020. “Transport of Aerosols and Trace Gases during Dust and Crop-Residue Burning Events in Indo-Gangetic Plain: Influence on Surface Ozone Levels over Downwind Region.” *ATMOSPHERIC ENVIRONMENT* 241 (November). doi:10.1016/j.atmosenv.2020.117829.

Kuo, Cheng-Pin, and Joshua S. Fu. 2023. “Ozone Response Modeling to NOx and VOC Emissions: Examining Machine Learning Models.” *Environment International* 176 (June). Elsevier BV: 107969. doi:10.1016/j.envint.2023.107969.

Lee, EH, DT Tingey, RS Waschmann, DL Phillips, DM Olszyk, MG Johnson, and WE Hogsett. 2009. “Seasonal and Long-Term Effects of CO2 and O3 on Water Loss in Ponderosa Pine and Their Interaction with Climate and Soil Moisture.” *TREE PHYSIOLOGY* 29 (11): 1381–93. doi:10.1093/treephys/tpp071.

Li, MY, SC Yu, X Chen, Z Li, YB Zhang, LQ Wang, WP Liu, et al. 2021. “Large Scale Control of Surface Ozone by Relative Humidity Observed during Warm Seasons in China.” *ENVIRONMENTAL CHEMISTRY LETTERS* 19 (6): 3981–89. doi:10.1007/s10311-021-01265-0.

Li, TW, JG Wu, JJ Chen, and HF Shen. 2022. “An Enhanced Geographically and Temporally Weighted Neural Network for Remote Sensing Estimation of Surface Ozone.” *IEEE TRANSACTIONS ON GEOSCIENCE AND REMOTE SENSING* 60. doi:10.1109/TGRS.2022.3187095.

Li, Z, H Dong, ZL Zhang, L Luo, and SC He. 2023. “Estimation of Near-Ground Ozone With High Spatio-Temporal Resolution in the Yangtze River Delta Region of China Based on a Temporally Ensemble Model.” *IEEE JOURNAL OF SELECTED TOPICS IN APPLIED EARTH OBSERVATIONS AND REMOTE SENSING* 16: 7051–61. doi:10.1109/JSTARS.2023.3298996.

Lin, J.-T., Z. Liu, Q. Zhang, H. Liu, J. Mao, and G. Zhuang. 2012. “Modeling Uncertainties for Tropospheric Nitrogen Dioxide Columns Affecting Satellite-Based Inverse Modeling of Nitrogen Oxides Emissions.” *Atmospheric Chemistry and Physics* 12 (24). Copernicus GmbH: 12255–75. doi:10.5194/acp-12-12255-2012.

Liu, F, YG Zhu, and Y Zhao. 2008. “Contribution of Motor Vehicle Emissions to Surface Ozone in Urban Areas: A Case Study in Beijing.” *INTERNATIONAL JOURNAL OF SUSTAINABLE DEVELOPMENT AND WORLD ECOLOGY* 15 (4): 345–49. doi:10.3843/SusDev.15.4:9.

Liu, Qian, Yuan Gao, Weiwen Huang, Zhenhao Ling, Zhe Wang, and Xuemei Wang. 2022. “Carbonyl Compounds in the Atmosphere: A Review of Abundance, Source and Their Contributions to O3 and SOA Formation.” *Atmospheric Research* 274 (August). Elsevier B.V.: N.PAG-N.PAG. doi:10.1016/j.atmosres.2022.106184.

Long, M. S., R. Yantosca, J. Nielsen, J. C. Linford, C. A. Keller, M. Payer Sulprizio, and D. J. Jacob. 2014. “Development and Performance of the Modularized, High-Performance Computing and Hybrid-Architecture Capable GEOS-Chem Chemical Transport Model” 2014 (December): GC33A-0500.

Loughner, Christopher P., Melanie B. Follette-Cook, Bryan N. Duncan, Jennifer Hains, Kenneth E. Pickering, Justin Moy, and Maria Tzortziou. 2020. “The Benefits of Lower Ozone Due to Air Pollution Emission Reductions (2002–2011) in the Eastern United States during Extreme Heat.” *Journal of the Air & Waste Management Association* 70 (2): 193–205. doi:10.1080/10962247.2019.1694089.

Lu, Jiaying, and Ling Yao. 2023. “Observational Evidence for Detrimental Impact of Inhaled Ozone on Human Respiratory System.” *BMC Public Health* 23 (1): 929. doi:10.1186/s12889-023-15902-6.

Lu, X, L Zhang, X Yue, JC Zhang, DA Jaffe, A Stohl, YH Zhao, and JY Shao. 2016. “Wildfire Influences on the Variability and Trend of Summer Surface Ozone in the Mountainous Western United States.” *ATMOSPHERIC CHEMISTRY AND PHYSICS* 16 (22): 14687–702. doi:10.5194/acp-16-14687-2016.

Ma, HF, Q Zhang, W Liang, AJ Han, NH Xie, H Xiang, and X Wang. 2023. “Short-Term Exposure to PM2.5 and O3 Impairs Liver Function in HIV/AIDS Patients: Evidence from a Repeated Measurements Study.” *TOXICS* 11 (9). doi:10.3390/toxics11090729.

Ma, K, YS Lin, FM Fang, HR Tan, JW Li, L Ge, F Wang, and YR Yao. 2023. “Spatiotemporal Dynamics of Near-Surface Ozone Concentration and Potential Source Areas in Northern China during 2015-2020.” *ENVIRONMENTAL SCIENCE AND POLLUTION RESEARCH* 30 (38): 89123–39. doi:10.1007/s11356-023-28713-4.

Malley, Christopher S., Daven K. Henze, Johan C.I. Kuylenstierna, Harry W. Vallack, Yanko Davila, Susan C. Anenberg, Michelle C. Turner, and Mike R. Ashmore. 2017. “Updated Global Estimates of Respiratory Mortality in Adults ≥30Years of Age Attributable to Long-Term Ozone Exposure.” *Environmental Health Perspectives* 125 (8): 087021. doi:10.1289/EHP1390.

Mandal, S, S Boppani, V Dasari, and M Thakur. 2024. “A Bivariate Simultaneous Pollutant Forecasting Approach by Unified Spectro-Spatial Graph Neural Network (USSGNN) and Its Application in Prediction of O3 3 and NO2 2 for New Delhi, India.” *SUSTAINABLE CITIES AND SOCIETY* 114 (November). doi:10.1016/j.scs.2024.105741.

Manzini, J, Y Hoshika, P Sicard, A De Marco, F Ferrini, E Pallozzi, L Neri, R Baraldi, E Paoletti, and BB Moura. 2024. “Detection of Morphological and Eco-Physiological Traits of Ornamental Woody Species to Assess Their Potential Net O3 Uptake.” *ENVIRONMENTAL RESEARCH* 252 (July). doi:10.1016/j.envres.2024.118844.

Meo, SA, FJ Almutairi, AA Abukhalaf, and AM Usmani. 2021. “Effect of Green Space Environment on Air Pollutants PM2.5, PM10, CO, O3, and Incidence and Mortality of SARS-CoV-2 in Highly Green and Less-Green Countries.” *INTERNATIONAL JOURNAL OF ENVIRONMENTAL RESEARCH AND PUBLIC HEALTH* 18 (24). doi:10.3390/ijerph182413151.

Miñarro, MD, EG Ferradás, JB Rico, FD Alonso, FJM Martínez, and C Romero-Trigueros. 2011. “Study of the Uncertainty in NO2 Chemiluminescence Measurements Due to the NO-O3 Reaction in Sampling Lines.” *ENVIRONMENTAL SCIENCE AND POLLUTION RESEARCH* 18 (3): 436–45. doi:10.1007/s11356-010-0386-z.

Minghu Ding, Biao Tian, Michael C. B. Ashley, Davide Putero, Zhenxi Zhu, Lifan Wang, Shihai Yang, Chuanjin Li, and Cunde Xiao. 2020. “Year-Round Record of near-Surface Ozone and ‘O3 Enhancement Events’ (OEEs) at Dome A,East Antarctica.” *Earth System Science Data Discussions*, August. Copernicus Gesellschaft mbH, 1–31. doi:10.5194/essd-2020-130.

Mo, YQ, Q Li, H Karimian, ST Zhang, XY Kong, SW Fang, and BY Tang. 2021. “Daily Spatiotemporal Prediction of Surface Ozone at the National Level in China: An Improvement of CAMS Ozone Product.” *ATMOSPHERIC POLLUTION RESEARCH* 12 (1): 391–402. doi:10.1016/j.apr.2020.09.020.

Monks, P. S., A. T. Archibald, A. Colette, O. Cooper, M. Coyle, R. Derwent, D. Fowler, et al. 2015. “Tropospheric Ozone and Its Precursors from the Urban to the Global Scale from Air Quality to Short-Lived Climate Forcer.” *Atmospheric Chemistry and Physics* 15 (15): 8889–8973. doi:10.5194/acp-15-8889-2015.

Monteiro, A, I Ribeiro, O Tchepel, E Sá, J Ferreira, A Carvalho, V Martins, et al. 2013. “Bias Correction Techniques to Improve Air Quality Ensemble Predictions: Focus on O3 and PM Over Portugal.” *ENVIRONMENTAL MODELING & ASSESSMENT* 18 (5): 533–46. doi:10.1007/s10666-013-9358-2.

Mousavi, S. Mostafa, Weicliang Zhu, Yixiao Sheng, and Gregory C. Beroza. 2019. “CRED: A Deep Residual Network of Convolutional and Recurrent Units for Earthquake Signal Detection.” *SCIENTIFIC REPORTS* 9 (July). doi:10.1038/s41598-019-45748-1.

Mousavinezhad, S, M Ghahremanloo, Y Choi, A Pouyaei, N Khorshidian, and B Sadeghi. 2023. “Surface Ozone Trends and Related Mortality across the Climate Regions of the Contiguous United States during the Most Recent Climate Period, 1991-2020.” *ATMOSPHERIC ENVIRONMENT* 300 (May). doi:10.1016/j.atmosenv.2023.119693.

Moustris, K. P., P. T. Nastos, I. K. Larissi, and A. G. Paliatsos. 2012. “Application of Multiple Linear Regression Models and Artificial Neural Networks on the Surface Ozone Forecast in the Greater Athens Area, Greece.” *Advances in Meteorology* 2012: 1–8. doi:10.1155/2012/894714.

Mulholland, James A., André J. Butler, James G. Wilkinson, Armistead G. Russell, and Paige E. Tolbert. 1998. “Temporal and Spatial Distributions of Ozone in Atlanta: Regulatory and Epidemiologic Implications.” *Journal of the Air & Waste Management Association* 48 (5). Taylor & Francis: 418–26. doi:10.1080/10473289.1998.10463695.

Nadzir, MSM, MJ Ashfold, MF Khan, AD Robinson, C Bolas, MT Latif, BM Wallis, et al. 2018. “Spatial-Temporal Variations in Surface Ozone over Ushuaia and the Antarctic Region: Observations from in Situ Measurements, Satellite Data, and Global Models.” *ENVIRONMENTAL SCIENCE AND POLLUTION RESEARCH* 25 (3): 2194–2210. doi:10.1007/s11356-017-0521-1.

Nelson, D, Y Choi, B Sadeghi, AK Yeganeh, M Ghahremanloo, and J Park. 2023. “A Comprehensive Approach Combining Positive Matrix Factorization Modeling, Meteorology, and Machine Learning for Source Apportionment of Surface Ozone Precursors: Underlying Factors Contributing to Ozone Formation in Houston, Texas.” *ENVIRONMENTAL POLLUTION* 334 (October). doi:10.1016/j.envpol.2023.122223.

NIOSH, The National Institute for Occupational Safety and Health. 1994. “Ozone - IDLH | NIOSH | CDC.” *Ozone*. May. https://www.cdc.gov/niosh/idlh/10028156.html.

Niu, Yue, Huichu Li, Weidong Wang, Cuiping Wang, Cong Liu, Xihao Du, Qingli Zhang, et al. 2022. “Ozone Exposure and Prothrombosis: Mechanistic Insights from a Randomized Controlled Exposure Trial.” *Journal of Hazardous Materials* 429 (May): 128322. doi:10.1016/j.jhazmat.2022.128322.

Nuvolone, Daniela, Davide Petri, and Fabio Voller. 2018. “The Effects of Ozone on Human Health.” *Environmental Science and Pollution Research* 25 (9): 8074–88. doi:10.1007/s11356-017-9239-3.

Oltmans, SJ, and H Levy. 1992. “Seasonal Cycle Of Surface Ozone Over The Western North-Atlantic.” *Nature* 358 (6385): 392–94. doi:10.1038/358392a0.

Orellano, Pablo, Julieta Reynoso, Nancy Quaranta, Ariel Bardach, and Agustin Ciapponi. 2020. “Short-Term Exposure to Particulate Matter (PM10 and PM2.5), Nitrogen Dioxide (NO2), and Ozone (O3) and All-Cause and Cause-Specific Mortality: Systematic Review and Meta-Analysis.” *Environment International* 142 (September). Elsevier B.V.: N.PAG-N.PAG. doi:10.1016/j.envint.2020.105876.

Pan, JB, SY Chen, N Xu, MJ Cheng, X Wang, JW Lan, R Wang, and YJ Wang. 2024. “EFFECT OF SPATIAL DIFFERENTIATION OF PLANT COMMUNITIES ON PM2.5 AND O3 IN URBAN GREEN SPACES IN BEIJING, CHINA.” *JOURNAL OF ENVIRONMENTAL ENGINEERING AND LANDSCAPE MANAGEMENT* 32 (4): 372–80. doi:10.3846/jeelm.2024.22359.

Peng Liu, Christian Hogrefe, Ulas Im, Jesper H. Christensen, Johannes Bieser, Uarporn Nopmongcol, Greg Yarwood, Rohit Mathur, Shawn Rosselle, and Tanya Spero. 2018. “Multi-Model Comparison in the Impact of Lateral Boundary Conditions on Simulated Surface Ozone across the United States Using Chemically Inert Tracers.” *Atmospheric Chemistry & Physics Discussions*, March. Copernicus Gesellschaft mbH, 1–32. doi:10.5194/acp-2018-106.

Perera, GBS, MMID Manthilake, AGT Sugathapala, LN Huy, and SC Lee. 2019. “NOX-VOC-O3 Sensitivity in Urban Environments of Sri Lanka.” *ASIAN JOURNAL OF ATMOSPHERIC ENVIRONMENT* 13 (1): 62–72. doi:10.5572/ajae.2019.13.1.062.

Petetin, Hervé, Dene Bowdalo, Pierre-Antoine Bretonnière, Marc Guevara, Oriol Jorba, Jan Mateu Armengol, Margarida Samso Cabre, Kim Serradell, Albert Soret, and Carlos Pérez Garcia-Pando. 2021. “Model Output Statistics (MOS) Applied to CAMS O3 Forecasts: Trade-Offs between Continuous and Categorical Skill Scores.” *Atmospheric Chemistry & Physics Discussions*, December. Copernicus Gesellschaft mbH, 1–36. doi:10.5194/acp-2021-864.

Platikanov, S, M Terrado, MT Pay, A Soret, and R Tauler. 2022. “Understanding Temporal and Spatial Changes of O3 or NO2 Concentrations Combining Multivariate Data Analysis Methods and Air Quality Transport Models.” *SCIENCE OF THE TOTAL ENVIRONMENT* 806 (February). doi:10.1016/j.scitotenv.2021.150923.

Pozzer, A, MG Schultz, and D Helmig. 2020. “Impact of US Oil and Natural Gas Emission Increases on Surface Ozone Is Most Pronounced in the Central United States.” *ENVIRONMENTAL SCIENCE & TECHNOLOGY* 54 (19): 12423–33. doi:10.1021/acs.est.9b06983.

Rafael, CC, GG Javier, AB Ariza-Villaverde, EG de Ravé, and FJ Jiménez-Hornero. 2019. “Can Complex Networks Describe the Urban and Rural Tropospheric O3 Dynamics?” *CHEMOSPHERE* 230 (September): 59–66. doi:10.1016/j.chemosphere.2019.05.057.

Reddy, PJ, and GG Pfister. 2016. “Meteorological Factors Contributing to the Interannual Variability of Midsummer Surface Ozone in Colorado, Utah, and Other Western US States.” *JOURNAL OF GEOPHYSICAL RESEARCH-ATMOSPHERES* 121 (5): 2434–56. doi:10.1002/2015JD023840.

Reid, Colleen E., Jonathan M. Snowden, Caitlin Kontgis, and Ira B. Tager. 2012a. “The Role of Ambient Ozone in Epidemiologic Studies of Heat-Related Mortality.” *ENVIRONMENTAL HEALTH PERSPECTIVES* 120 (12): 1627–30. doi:10.1289/ehp.1205251.

Rojas, ALP, LE Venegas, and NA Mazzeo. 2016. “Uncertainty of Modelled Urban Peak O3 Concentrations and Its Sensitivity to Input Data Perturbations Based on the Monte Carlo Analysis.” *ATMOSPHERIC ENVIRONMENT* 141 (September): 422–29. doi:10.1016/j.atmosenv.2016.07.020.

Rui Zhu, Zhaojun Tang, Xiaokang Chen, Zhe Jiang, and Xiong Liu. 2023. “Rapid Assimilations of O3 Observations – Part 2: Tropospheric O3 Changes in 2 the United States and Europe in 2005-2020 .” *Atmospheric Chemistry & Physics Discussions*, April. Copernicus Gesellschaft mbH, 1–34. doi:10.5194/acp-2023-47.

Runmei Ma, Jie Ban, QingWang, Yayi Zhang, Yang Yang, Shenshen Li, Wenjiao Shi, and Tiantian Li. 2021. “Full-Coverage 1 Km Daily Ambient PM2.5 and O3 Concentrations of China in 2005-2017 Based on Multi-Variable Random Forest Model.” *Earth System Science Data Discussions*, September. Copernicus Gesellschaft mbH, 1–28. doi:10.5194/essd-2021-296.

Saeipourdizaj, Parisa, Saeed Musavi, Akbar Gholampour, and Parvin Sarbakhsh. 2022. “Correction to: Clustering the Concentrations of PM10 and O3: Application of Spatiotemporal Model–Based Clustering.” *Environmental Modeling & Assessment* 27 (1). Springer Nature: 55–55. doi:10.1007/s10666-021-09813-2.

Schlink, Uwe, Olf Herbarth, Matthias Richter, Stephen Dorling, Giuseppe Nunnari, Gavin Cawley, and Emil Pelikan. 2006. “Statistical Models to Assess the Health Effects and to Forecast Ground-Level Ozone.” *Environmental Modelling & Software* 21 (4): 547–58. doi:10.1016/j.envsoft.2004.12.002.

Schnell, JL, and MJ Prather. 2017. “Co-Occurrence of Extremes in Surface Ozone, Particulate Matter, and Temperature over Eastern North America.” *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA* 114 (11): 2854–59. doi:10.1073/pnas.1614453114.

Seo, Youngmin, Sungwon Kim, and Vijay P. Singh. 2015. “Estimating Spatial Precipitation Using Regression Kriging and Artificial Neural Network Residual Kriging (RKNNRK) Hybrid Approach.” *Water Resources Management* 29 (7): 2189–2204. doi:10.1007/s11269-015-0935-9.

Serra, Maria Emilia Gadelha, José Baeza-Noci, Carmen Verônica Mendes Abdala, Marilia Moura Luvisotto, Charise Dallazem Bertol, and Ana Paula Anzolin. 2022. “The Role of Ozone Treatment as Integrative Medicine. An Evidence and Gap Map.” *Frontiers in Public Health* 10: 1112296. doi:10.3389/fpubh.2022.1112296.

Shin, HH, WS Burr, D Stieb, L Haque, H Kalayci, B Jovic, and M Smith-Doiron. 2018. “Air Health Trend Indicator: Association between Short-Term Exposure to Ground Ozone and Circulatory Hospitalizations in Canada for 17 Years, 1996-2012.” *INTERNATIONAL JOURNAL OF ENVIRONMENTAL RESEARCH AND PUBLIC HEALTH* 15 (8). doi:10.3390/ijerph15081566.

Smith, Kate R., Peter M. Edwards, Peter D. Ivatt, James D. Lee, Freya Squires, Chengliang Dai, Richard E. Peltier, Mat J. Evans, and Alastair C. Lewis. 2018. “An Improved Low Power Measurement of Ambient NO2 and O3 Combining Electrochemical Sensor Clusters and Machine Learning.” *Atmospheric Measurement Techniques Discussions*, September. Copernicus Gesellschaft mbH, 1–21. doi:10.5194/amt-2018-285.

Sousa, S, F Martins, M Alvimferraz, and M Pereira. 2007. “Multiple Linear Regression and Artificial Neural Networks Based on Principal Components to Predict Ozone Concentrations.” *Environmental Modelling & Software* 22 (1): 97–103. doi:10.1016/j.envsoft.2005.12.002.

Staehle, Christoph, Harald E. Rieder, and Arlene M. Fiore. 2023. “Technical Note: An Assessment of the Performance of Statistical Bias Correction Techniques for Global Chemistry-Climate Model Surface Ozone Fields.” *EGUsphere*, November, 1–21. doi:10.5194/egusphere-2023-2743.

Starbuck, Craig. 2023. “Linear Regression.” In *The Fundamentals of People Analytics*, 181–206. Cham: Springer International Publishing. doi:10.1007/978-3-031-28674-2\_10.

Sun, HC, JCH Fung, Y Chen, WY Chen, ZN Li, YQ Huang, CQ Lin, MY Hu, and XC Lu. 2021. “Improvement of PM2.5 and O3 Forecasting by Integration of 3D Numerical Simulation with Deep Learning Techniques.” *SUSTAINABLE CITIES AND SOCIETY* 75 (December). doi:10.1016/j.scs.2021.103372.

Sun, HT, YM Shin, MT Xia, SX Ke, M Wan, L Yuan, YM Guo, and AT Archibald. 2022. “Spatial Resolved Surface Ozone with Urban and Rural Differentiation during 1990-2019: A Space-Time Bayesian Neural Network Downscaler.” *ENVIRONMENTAL SCIENCE & TECHNOLOGY* 56 (11): 7337–49. doi:10.1021/acs.est.1c04797.

Sun, W, A Palazoglu, A Singh, H Zhang, Q Wang, ZM Zhao, and D Cao. 2015. “Prediction of Surface Ozone Episodes Using Clusters Based Generalized Linear Mixed Effects Models in Houston-Galveston-Brazoria Area, Texas.” *ATMOSPHERIC POLLUTION RESEARCH* 6 (2): 245–53. doi:10.5094/APR.2015.029.

Tang, ZQ, JH Guo, JY Zhou, H Yu, YQ Wang, XY Lian, J Ye, et al. 2024. “The Impact of Short-Term Exposures to Ambient NO2, O3, and Their Combined Oxidative Potential on Daily Mortality.” *ENVIRONMENTAL RESEARCH* 241 (January). doi:10.1016/j.envres.2023.117634.

Tian, XY, J Zeng, XL Li, S Li, T Zhang, Y Deng, F Yin, and Y Ma. 2024. “Assessing the Short-Term Effects of PM2.5 and O3 on Cardiovascular Mortality Using High-Resolution Exposure: A Time-Stratified Case Cross-over Study in Southwestern China.” *ENVIRONMENTAL SCIENCE AND POLLUTION RESEARCH* 31 (3): 3775–85. doi:10.1007/s11356-023-31276-z.

Tobler, W. R. 1970. “A Computer Movie Simulating Urban Growth in the Detroit Region.” *Economic Geography* 46 (June): 234. doi:10.2307/143141.

Tondini, S, R Scilla, and P Casari. 2024. “Minimized Training of Machine Learning-Based Calibration Methods for Low-Cost O3 Sensors.” *IEEE SENSORS JOURNAL* 24 (3): 3973–87. doi:10.1109/JSEN.2023.3339202.

Tong, L, HL Zhang, J Yu, MM He, NB Xu, JJ Zhang, FZ Qian, JY Feng, and H Xiao. 2017. “Characteristics of Surface Ozone and Nitrogen Oxides at Urban, Suburban and Rural Sites in Ningbo, China.” *ATMOSPHERIC RESEARCH* 187 (May): 57–68. doi:10.1016/j.atmosres.2016.12.006.

Travis, Katherine R., and Daniel J. Jacob. 2019. “Systematic Bias in Evaluating Chemical Transport Models with Maximum Daily 8 h Average (MDA8) Surface Ozone for Air Quality Applications: A Case Study with GEOS-Chem v9.02.” *Geoscientific Model Development* 12 (8): 3641–48. doi:10.5194/gmd-12-3641-2019.

Tucker, Compton J. 1979. “Red and Photographic Infrared Linear Combinations for Monitoring Vegetation.” *Remote Sensing of Environment* 8 (2): 127–50. doi:10.1016/0034-4257(79)90013-0.

Turner, Michelle C., Michael Jerrett, C. Arden Pope, Daniel Krewski, Susan M. Gapstur, W. Ryan Diver, Bernardo S. Beckerman, et al. 2016. “Long-Term Ozone Exposure and Mortality in a Large Prospective Study.” *American Journal of Respiratory and Critical Care Medicine* 193 (10): 1134–42. doi:10.1164/rccm.201508-1633OC.

Wang, JY, J Qian, JY Chen, S Li, MH Yao, QQ Du, N Yang, et al. 2024. “High-Resolution Full-Coverage Ozone (O3) Estimates Using a Data-Driven Spatial Random Forest Model in Beijing-Tianjin-Hebei Region, China.” *JOURNAL OF HAZARDOUS MATERIALS* 480 (December). doi:10.1016/j.jhazmat.2024.136047.

Wang, Meng, Paul D. Sampson, Jianlin Hu, Michael Kleeman, Joshua P. Keller, Casey Olives, Adam A. Szpiro, Sverre Vedal, and Joel D. Kaufman. 2016. “Combining Land-Use Regression and Chemical Transport Modeling in a Spatiotemporal Geostatistical Model for Ozone and PM2.5.” *Environmental Science & Technology* 50 (10). American Chemical Society (ACS): 5111–18. doi:10.1021/acs.est.5b06001.

Wang, Q, XH Wang, RZ Huang, JB Wu, Y Xiao, M Hu, QY Fu, YS Duan, and JM Chen. 2022. “Regional Transport of PM2.5 and O3 Based on Complex Network Method and Chemical Transport Model in the Yangtze River Delta, China.” *JOURNAL OF GEOPHYSICAL RESEARCH-ATMOSPHERES* 127 (5). doi:10.1029/2021JD034807.

Wang, RP, WJ Duan, SY Cheng, and XQ Wang. 2023. “Nonlinear and Lagged Effects of VOCs on SOA and O3 and Multi-Model Validated Control Strategy for VOC Sources.” *SCIENCE OF THE TOTAL ENVIRONMENT* 887 (August). doi:10.1016/j.scitotenv.2023.164113.

Wang, Y, QQ Yuan, TW Li, LY Zhu, and LP Zhang. 2021. “Estimating Daily Full-Coverage near Surface O3, CO, and NO2 Concentrations at a High Spatial Resolution over China Based on S5P-TROPOMI and GEOS-FP.” *ISPRS JOURNAL OF PHOTOGRAMMETRY AND REMOTE SENSING* 175 (May): 311–25. doi:10.1016/j.isprsjprs.2021.03.018.

Wang, Yuting, Guy P. Brasseur, Yong‐Feng Ma, Vincent‐Henri Peuch, and Tao Wang. 2023. “Does Downscaling Improve the Performance of Urban Ozone Modeling?” *Geophysical Research Letters* 50 (23): e2023GL104761. doi:10.1029/2023GL104761.

Watson, Gregory L., Donatello Telesca, Colleen E. Reid, Gabriele G. Pfister, and Michael Jerrett. 2019. “Machine Learning Models Accurately Predict Ozone Exposure during Wildfire Events.” *Environmental Pollution* 254 (November): 112792. doi:10.1016/j.envpol.2019.06.088.

Webster, C. R., R. D. May, D. W. Toohey, L. M. Avallone, J. G. Anderson, P. Newman, L. Lait, M. R. Schoeberl, J. W. Elkins, and K. R. Chan. 1993. “Chlorine Chemistry on Polar Stratospheric Cloud Particles in the Arctic Winter.” *Science* 261 (5125). American Association for the Advancement of Science (AAAS): 1130–34. doi:10.1126/science.261.5125.1130.

Wen, W, S Shen, L Liu, X Ma, Y Wei, JK Wang, Y Xing, and W Su. 2021. “Comparative Analysis of PM2.5 and O3 Source in Beijing Using a Chemical Transport Model.” *REMOTE SENSING* 13 (17). doi:10.3390/rs13173457.

Wie, J, and BK Moon. 2016. “Seasonal Relationship between Meteorological Conditions and Surface Ozone in Korea Based on an Offline Chemistry-Climate Model.” *ATMOSPHERIC POLLUTION RESEARCH* 7 (3): 385–92. doi:10.1016/j.apr.2015.10.020.

Wright, Marvin N., and Andreas Ziegler. 2017. “**Ranger** : A Fast Implementation of Random Forests for High Dimensional Data in *C++* and *R*.” *Journal of Statistical Software* 77 (1). doi:10.18637/jss.v077.i01.

Wu, TH, ZC Tseng, and CY Huang. 2024. “Recognition of NO2 and O3 Gases Using Patterned Cu2O Nanoparticles on IGZO Thin Films through Machine Learning.” *JOURNAL OF MATERIALS CHEMISTRY C* 12 (45): 18427–34. doi:10.1039/d4tc03451a.

Xiong, KL, XD Xie, L Huang, and JL Hu. 2024. “Improved O3 Predictions in China by Combining Chemical Transport Model and Multi-Source Data with Machining Learning Techniques.” *ATMOSPHERIC ENVIRONMENT* 318 (February). doi:10.1016/j.atmosenv.2023.120269.

Yang, Z, J Yang, MM Li, JJ Chen, and CQ Ou. 2021. “Nonlinear and Lagged Meteorological Effects on Daily Levels of Ambient PM2.5 and O3: Evidence from 284 Chinese Cities.” *JOURNAL OF CLEANER PRODUCTION* 278 (January). doi:10.1016/j.jclepro.2020.123931.

You, Zhiqiang, Yun Zhu, Carey Jang, Shuxiao Wang, Jian Gao, Che-Jen Lin, Minhui Li, Zhenghua Zhu, Hao Wei, and Wenwei Yang. 2017. “Response Surface Modeling-Based Source Contribution Analysis and VOC Emission Control Policy Assessment in a Typical Ozone-Polluted Urban Shunde, China.” *JOURNAL OF ENVIRONMENTAL SCIENCES* 51 (January): 294–304. doi:10.1016/j.jes.2016.05.034.

Yu, Karen, Christoph A. Keller, Daniel J. Jacob, Andrea M. Molod, Sebastian D. Eastham, and Michael S. Long. 2018a. “Errors and Improvements in the Use of Archived Meteorological Data for Chemical Transport Modeling: An Analysis Using GEOS-Chem V11-01 Driven by GEOS-5 Meteorology.” *Geoscientific Model Development* 11 (1). Copernicus GmbH: 305–19. doi:10.5194/gmd-11-305-2018.

Zhao, N, HY Zhang, and G Wang. 2025. “Revealing the Nonlinear Responses of PM2.5 and O3 to VOC and NOx Emissions from Various Sources in Shandong, China.” *JOURNAL OF HAZARDOUS MATERIALS* 489 (June). doi:10.1016/j.jhazmat.2025.137655.

Zhao, XX, M Song, XJ Zhao, CY Xue, PF Liu, C Ye, XW He, YJ Mu, and B Hu. 2024. “Improvement of Model Simulation for Summer PM2.5 and O3 through Coupling with Two New Potential HONO Sources in the North China Plain.” *SCIENCE OF THE TOTAL ENVIRONMENT* 950 (November). doi:10.1016/j.scitotenv.2024.175168.

Zhou, Shan S., Amos P. K. Tai, Shihan Sun, Mehliyar Sadiq, Colette L. Heald, and Jeffrey A. Geddes. 2018. “Coupling between Surface Ozone and Leaf Area Index in a Chemical Transport Model: Strength of Feedback and Implications for Ozone Air Quality and Vegetation Health.” *ATMOSPHERIC CHEMISTRY AND PHYSICS* 18 (19): 14133–48. doi:10.5194/acp-18-14133-2018.

Ziemke, J. R., S. Chandra, G. J. Labow, P. K. Bhartia, L. Froidevaux, and J. C. Witte. 2011. “A Global Climatology of Tropospheric and Stratospheric Ozone Derived from Aura OMI and MLS Measurements.” *Atmospheric Chemistry and Physics* 11 (17): 9237–51. doi:10.5194/acp-11-9237-2011.

Zvyagintsev, AM, OA Tarasova, and GI Kuznetsov. 2008. “Seasonal and Daily Cycles of Surface Ozone in the Extratropical Latitudes.” *IZVESTIYA ATMOSPHERIC AND OCEANIC PHYSICS* 44 (4): 474–85. doi:10.1134/S0001433808040087.