CHAPTER I

INTRODUCTION

Historical analysis of atmospheric chemistry shows global ozone (O₃) concentrations are heavily influenced by multiple catalytic cycles involving halogen, nitrogen, hydrogen, and oxygen species (Caffrey et al. 2001; Dobson 1923; He and Carmichael 1999; Lyons, Reinhard, and Planavsky 2014; WMO 2022). The global movement of carbon among the atmosphere, biosphere, oceans, and geosphere, indirectly yet significantly influence O3 concentrations, in the troposphere through greenhouse gas effects and atmospheric chemistry interactions (Danyang Ma et al. 2023; Hata et al. 2023; Q. Liu et al. 2022). Continued regulation, monitoring, and development of air pollution control initiatives are essential for continued maintenance of ozone depleting substances (US EPA 2015a; WMO 2022) which can impact the evolutionary potential of biological mechanisms on Earth (Grenfell et al. 2010; Kasting and Siefert 2002). The source of atmospheric cycles seems to be this highly reactive, unstable, triatomic molecule; providing a canvas for dioxide cycles necessary for organic systems (Caffrey et al. 2001; Lyons, Reinhard, and Planavsky 2014). Varying degrees of O3 allow for redox reactions, forming as both a product and constituent of the natural environment (Chapleski et al. 2016; Xing et al. 2016; Zoran et al. 2014).

Anthropogenic sources have deeply affected these necessary cycles by shifting natural concentrations of O3 in unnatural manners (Chauhan, Gupta, and Liou 2023; Cheadle et al. 2017; Danyang Ma et al. 2023; Flynn et al. 2021). As climate change continues to abet abnormal temperatures and weather cycles, the development of high-resolution predictive models such as those shown by this thesis are even more necessary to combat the exponential rate of urbanization (Balk et al. 2018; EPA 2021; Iglesias et al. 2021). This thesis seeks to provide a novel methodology which better incorporates geospatial relationships into modern statistical methods via residual kriging to three of the most populous counties in Arizona. The Statistical Model and Residual Krige (SMaRK) methodology is overlayed with statistical representations of census data in Maricopa, Pima, and Pinal Counties to show that leveraging the advantages of both techniques can better depict complex systems like O3. Similar methods have already shown great promise in modeling PM2.5, NOx, and similar air pollutants as complex as O3 (Y. Liu et al. 2018).

I.1. Machine Learning/Artificial Intelligence Predictions Require Proper Incorporation of Geospatial Data

Policies set by world governments can help reduce overall surface ozone pollution, but this is only as effective as the models used in gauging vulnerable areas. Current numerical modeling approaches, such as WRF-Chem, GEOS-Chem, and GODfit-Algorithms (Flandorfer 2019; Lerot et al. 2010; C. Lin et al. 2016; Yu et al. 2018), are computationally expensive, restricting the output of surface O3 maps to coarse spatial resolutions that are not suitable for public health studies. Health experts build their own datasets, resulting in highly accurate, but non-rasterized depictions of surface O3. Most ozone representations of the surface take numerous days to produce their final products (Kwok et al. 2015; C. Lin et al. 2016; Travis and Jacob 2019; Wu et al. 2021) and modelling efforts based on remote sensing measurements still have trouble capturing the complexity of surface ozone in urban settings without further improvements made by the researcher (Balamurugan, Balamurugan, and Chen 2022; Wang et al. 2023). When predictions from modelled O3 reactions are compared against surface observations from monitors, they tend to have difficulty simulating O3 concentrations at high-temporal resolutions. This suggests that the underlying geospatial patterns used during observation may not fully characterize regions accurately and/or that the resolution of the models is not adequate to simulate the photo-chemical environment of these finer observations. There is a compelling need in recent literature to improve high resolution surface O3 concentrations by incorporating simple spatial patterns into complex models.

Machine learning methods like Random forests can account for complex relationships between ozone and other covariates but tend to ignore spatial correlations of remote sensing (Niu et al. 2022; Telesca et al., n.d.; Wright and Ziegler 2017). With large data, linear and weighted regression tends to be exponentially faster, at the cost of egregious error (Feng et al. 2016; Huang et al. 2017; Watson et al. 2019). Combining an advanced model with its corresponding geospatial residuals helps account for the spatial correlation between modeled values while simultaneously accounting for complex relationships. Regression kriging is a commonly used kriging method based on multiple linear regressions and variograms (Yakowitz and Szidarovszky 1985; Q. Meng, Liu, and Borders 2013; Kleijnen 2017). In application to surface O3 values, this helps in incorporating co-funding covariates from a non-geospatial perspective. Five ensemble learning models were compared: Adaptive boosting, Stochastic Gradient Boosting, Extreme Gradient Boosting, Random Forest bagging, and a 2D recursive convolutional neural network (RCNN). These were created over a study area containing Arizona’s most populous counties of Maricopa, Pinal, and Pima from 1980-2023. Each model was created using a hyper-parameter tuner available through sci-kit learn in python (Raschka and Mirjalili 2019).

I.2. Why Surface Ozone? – Relations to Urban Air Quality

O3 has been detected in Earth’s stratosphere, troposphere, and more recently, on its surface (Claeyman et al. 2011; Davies and Schuepbach 1994; He and Carmichael 1999; M. Lin et al. 2012; Richter 2009; Xing et al. 2016). In 1955, the United States of North America (USNA) issued the Air Quality Control Act which dedicated the nation’s vast resources to additional monitoring, addressing air pollution concerns post-scientific revolution enticed by the Space Race of 1950. The acting President of the United States (POTUS) at the time; Richard Nixon, aided in the establishment of an Environmental Protection Agency (EPA) and National Oceanic and Atmospheric Administration (NOAA) to combat this newfound enemy with extreme prejudice (Nixon 1970). In doing so, new environmental movements emerged due to unprecedented economic growth at the time; regulation policies which initially slowed some sectors, later exhibited long-term beneficial human and economic trends, as was theorized in the early 90s by Dr. Micheal E. Porter (Ambec and Barla 2002). Geographic Informational Science (GIS) has been dedicated to the proper implementation of these goals set forth in the early 1970s. With it came a new way to write Earth’s history via digital transformation of newfound resources; relating to trends near and far to answer difficult questions associated with life. From micro- to macro-scales, a geographer specializes in observations and predictions from planetary to microbial systems, inadvertently weaving complex knowledge of space and time beyond the scope it represents (Goodchild 1992).

Many communities at risk of high surface ozone concentrations are further threatened by urban heat island effects, vehicle emissions and industrial processes attributing to a variety of pollutants due to the mechanism which drives O3. It’s a precursor to many things due to its highly degenerative state (Afonso and Pires 2017; Bojkov and Fioletov 1995; Harithasree et al. 2024; J. Li et al. 2014). After zooming-in, ground-level O3 has been found to have a lasting impact on human health via reductions in life expectancy, abrupt changes to normalized Earthly air chemistries, and related oxo-based cycles for its development (Barzeghar et al. 2020; Ding, He, and Liu 2021; C. Lin et al. 2016; Manisalidis et al. 2020; Schlink et al. 2006; WHO 2013; Zhang, Wei, and Fang 2019). Surface O3 exposure has been found to contribute to several adverse respiratory symptoms, childhood cancers, adverse birth outcomes, overall mortality, and neurological disorders (Ni et al. 2024; Ghozikali et al. 2015; Tang et al. 2024; Turner et al. 2016). In addition, atmospheric studies have found the most significant constituents of ground-level O3 reactions to be nitrogen-oxides (NOx) and volatile organic compounds (VoCs) (Brown-Steiner and Hess 2011; Cheng et al. 2018; Girach et al. 2012). When these are combined with large amounts of UV radiation, O3 begins to form and can have numerous effects on organic and in-organic material. Surface ozone has been found to be one of the leading pollutants on the Global Burden of Disease (GBD) (Anenberg et al. 2018; Brauer et al. 2024; Sun et al. 2024), harboring stealthy consequences that can only be seen with appropriate consideration of both formation and exposure to fully understand its impacts. Varying concentrations of O3 have been found to have numerous beneficial and adverse effects on various systems in a myriad of ways due to interactions with surrounding ecosystems (US EPA 2015b). This thesis applies the three laws of Geography to create a high-resolution representation of surface O3 at tiled resolutions ranging from 300m down to 25m. While the starting area is a small section of three counties within the United States, the framework applied here can be utilized for representations of O3 across the world as the incorporation of GIS and improvement of computational systems continue to progress in this era of Big Data (Cao 2022; Tamiminia et al. 2020; Bughin 2016; Curry 2016; Xu et al. 2023).

I.3. A Tale of Two Layers

Two layers in Earth’s atmosphere are known to house this reaction. It is generally beneficial to the environment and can act as a catalyst for certain biological and chemical systems whose main constituent is oxygen. Therefore, the patterns observed by researchers of specifically surface O3 (i.e 2m above the ground), have been difficult to follow. Generally, O3 is highly reactive and decomposes quickly, therefore increasing the probability for a reactive oxygen species (ROS) to “unnaturally” exist in any environment/system which it’s found to be a part of. Highly concentrated O3 areas near Earth’s surface typically affect populations outside highly industrialized zones with high vegetation, as the byproduct of plants is mainly CO2. Studies interested in surface ozone exposure within one’s activity space have noted severe differences in health outcomes among varying populations. To better understand the harmful cycles of surface O3, the beneficial aspects of O3 are worth mentioning in detail.

In the Stratosphere, O3 protects the surface of Earth by absorbing UV rays. Due to the chemical composition of this layer, stratospheric O3 naturally follows seasonal cycles, as these correlate to the distance from the sun and positioning of Earth’s tilt in its rotational pattern. However, due to rising temperatures, this beneficial, and natural cycle is threatened, potentially mixing with surface air quality and chemistries. As the Ozone Layer doesn’t absorb all UV radiation, what’s left over reflects off the surface of the Earth. Remote sensing is a field dedicated to measuring these reflections, correcting for the numerous atmospheric and geographic distortions provided by optical, electrical, and human error.

Ground-level ozone combined with other reactive gases will tend to correlate to the quality of air encompassing human communities (Bojkov and Fioletov 1995; Díaz et al. 2018; Gaudel et al. 2018; Schultz et al. 2017). As this dual formation involves titrations with varying chemicals, complex, non-linear associations begin closer to the source of common pollutants; later being reincorporated into the environment at some distance away. This makes it difficult for these O3 reactions to be identifiable and effectively modelled for decision making and regulatory entities. (Abdullah et al. 2019; Balamurugan, Balamurugan, and Chen 2022; Gaudel et al. 2018; Huang et al. 2017; Yamashita et al. 2010). In addition, concentrations of stratospheric ozone in the future will depend on the decrease of O3-depleting substances (ODS)s found near the surface due to reducing the frequency and hence; likelihood of these interactions (Huang et al. 2017; Manisalidis et al. 2020; Zhao et al. 2021).

I.4 Surface O3 Exposure and Transport

While most hazardous pollutants are emitted directly, complex pollutants such as surface O3 form as byproduct, later becoming a constituent for other chemicals. O3 is known as a secondary pollutant (J.-T. Lin et al. 2012; Watson et al. 2019; Venkanna et al. 2015) wherein it can act as an ingredient and result of chemical processes. The slightest change in wind speeds, environmental conditions (coastal to arid), and ecological elements (available greenspace vs. concrete) can influence O3 formation and degradation (Badia et al. 2023; K. Meng et al. 2022; Xing et al. 2016). The data provided by these, and numerous other works gives insights into historical transport of O3 due to urban, suburban, and rural development which were incorporated during development. Studies which gathered similar data products have found a link between urbanization and the populations which are exposed to unhealthy levels of air pollution; typically well above those of current standards set by the Environmental Protection Agency and World Health Organization (EPA 2021; Kumar et al. 2015; X. Liu et al. 2022; WHO 2013) set at 70 ppb (EPA 2013).

The trajectory of these emissions has a direct impact on policy decisions affecting numerous socio-economic statuses (SES) due to inherent constituents. Sand, smoke, volcanic plumes, dust, other gaseous components like clouds can affect the overarching operations of O3 cycles and complexity as seen in many studies (Harithasree et al. 2024; Venkanna et al. 2015; Tong et al. 2017). The precursors for its existence are risks to human health, as indicated by informed policies limiting exposures to other pollutants (e.g. Particulate matter (PM), Carbon monoxide (CO), Nitrogen dioxide (NO2), and more) per the CDC, EPA, and WHO (CDC 2024; US EPA 2015a; WHO 2013). Policies which limit the general reduction of emissions; like carbon dioxide (CO2), formaldehyde (HCHO or CH2O), methane (CH4) and nitrous oxides (NOx), tend to reduce surface O3 reactions as well, decreasing the probability for a reaction to occur in populated areas. Current representations and remote sensing methods used for surface ozone can be too coarse for urban analysis, and might not highlight key details known to interact with urbanization and natural disasters in communities at finer spatial scales (Nawaz 2023; Zhang, Wei, and Fang 2019; Abdullah et al. 2019). These instruments often rely on novel approaches to aerosol forecasting and implement a slew of corrective algorithms for proper representation of meteorological variables. A Statistical Model and Residual Kriging methodology is proposed to refine S5P’s tropospheric O3 representation into a surface O3 estimates with a spatial resolution of 250m, a resolution suited for urban analysis (Wang et al. 2023)

I.5. Structure of Thesis

This thesis seeks to compare the performance of common machine learning (ML) and artificial intelligence (AI) methods with the enhancements made by the Residual Kriging method on forecasted O3 values for further development into a python-based air pollution modelling library. Beginning with a substantial literature review on the formation of O3, it’s found that almost every aspect of it can impact local ecologies, health, and people. These are heavily discussed to provide a high-quality basis for feature creation and model tuning based on scientific evidence. Some drivers included in the initial dataset were not utilized in the final model, albeit all data initially gathered was due to the synthesis of literature. A section dedicated to data sources and materials delves into further reasoning for the features best suited for ML/AI ensembles and integration with the RK method. After understanding the fundamental drivers, constituents, and numerical model tuning methods, a geospatial regression krige is applied to the resulting uncertainty left by the estimated trend. The full combination of these techniques creates daily high spatial resolution rasters for the urban cities of Phoenix and Tucson in Arizona. These cities are encompassed in two counties, with a third sitting in between them. An extremely brief demographic analysis depicting income, total population, and occupied households is conducted via census data provided by the U.S. Census Bureau followed by an assessment of possible health outcomes due to excessive exposure to surface O3 above concentrations of 70 ppb. The main portion of the thesis is concluded with a detailed description of future directions, model improvements, and further reasonings for why high-spatial resolution surface O3 models are needed, especially within the contiguous United States. A small portion on the use of Geographical laws and theory in historical scientific literature is presented as the final notes to this thesis to depict a proposed economic solution garnered from the betterment of air pollution modelling. Methodology used in this thesis can be best described as a common case-study using the Scientific Method, Geo-spatial statistical analysis, and application of the three main laws of geography to modern ML/AI modelling methodologies.

*Citations*

Abdullah, Samsuri, Najihah Husna Ahmad Nasir, Marzuki Ismail, Ali Najah Ahmed, and Mohamad Nor Khasbi Jarkoni. 2019. “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.

Afonso, NF, and JCM Pires. 2017. “Characterization of Surface Ozone Behavior at Different Regimes.” *APPLIED SCIENCES-BASEL* 7 (9). doi:10.3390/app7090944.

Ambec, Stefan, and Philippe Barla. 2002. “A Theoretical Foundation of the Porter Hypothesis.” *Economics Letters* 75 (3): 355–60. doi:10.1016/S0165-1765(02)00005-8.

Anenberg, Susan C., Daven K. Henze, Veronica Tinney, Patrick L. Kinney, William Raich, Neal Fann, Chris S. Malley, et al. 2018. “Estimates of the Global Burden of Ambient PM2.5, Ozone, and NO2 on Asthma Incidence and Emergency Room Visits.” *Environmental Health Perspectives* 126 (10). Environmental Health Perspectives: 107004. doi:10.1289/EHP3766.

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.

Balk, Deborah, Stefan Leyk, Bryan Jones, Mark R. Montgomery, and Anastasia Clark. 2018. “Understanding Urbanization: A Study of Census and Satellite-Derived Urban Classes in the United States, 1990-2010.” *PloS One* 13 (12): e0208487. doi:10.1371/journal.pone.0208487.

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.

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.

Brauer, Michael, Gregory A Roth, Aleksandr Y Aravkin, Peng Zheng, Kalkidan Hassen Abate, Yohannes Habtegiorgis Abate, Cristiana Abbafati, et al. 2024. “Global Burden and Strength of Evidence for 88 Risk Factors in 204 Countries and 811 Subnational Locations, 1990–2021: A Systematic Analysis for the Global Burden of Disease Study 2021.” *The Lancet* 403 (10440). Elsevier BV: 2162–2203. doi:10.1016/s0140-6736(24)00933-4.

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.

Bughin, Jacques. 2016. “Big Data, Big Bang?” *Journal of Big Data* 3 (1). Springer Science and Business Media LLC. doi:10.1186/s40537-015-0014-3.

Caffrey, P, W Hoppel, G Frick, L Pasternack, J Fitzgerald, D Hegg, S Gao, et al. 2001. “In-Cloud Oxidation of SO2 by O3 and H2O2:: Cloud Chamber Measurements and Modeling of Particle Growth.” *JOURNAL OF GEOPHYSICAL RESEARCH-ATMOSPHERES* 106 (D21): 27587–601. doi:10.1029/2000JD900844.

Cao, Guofeng. 2022. “Deep Learning of Big Geospatial Data: Challenges and Opportunities.” In *New Thinking in GIScience*, by Bin Li, A-Xing Zhu, Hui Lin, Xun Shi, and Cuizhen Wang, 159–69. Singapore: Springer Nature Singapore. doi:10.1007/978-981-19-3816-0\_18.

CDC, U.S Centers for Disease Control. 2024. “Air Pollutants.” Information. *Air Quality*. February 16. https://www.cdc.gov/air-quality/pollutants/index.html.

Chapleski, Robert C., Yafen Zhang, Diego Troya, and John R. Morris. 2016. “Heterogeneous Chemistry and Reaction Dynamics of the Atmospheric Oxidants, O3, NO3, and OH, on Organic Surfaces.” *Chemical Society Reviews* 45 (13). Royal Society of Chemistry: 3731–46. doi:10.1039/c5cs00375j.

Chauhan, A, SK Gupta, and YA Liou. 2023. “Rising Surface Ozone Due to Anthropogenic Activities and Its Impact on COVID-19 Related Deaths in Delhi, India.” *HELIYON* 9 (4). doi:10.1016/j.heliyon.2023.e14975.

Cheadle, LC, SJ Oltmans, G Pétron, RC Schnell, EJ Mattson, SC Herndon, AM Thompson, DR Blake, and A McClure-Begley. 2017. “Surface Ozone in the Colorado Northern Front Range and the Influence of Oil and Gas Development during FRAPPE/DISCOVER-AQ in Summer 2014.” *ELEMENTA-SCIENCE OF THE ANTHROPOCENE* 5 (November). doi:10.1525/elementa.254.

Cheng, Y, YH Wang, YZ Zhang, JH Crawford, GS Diskin, AJ Weinheimer, and A Fried. 2018. “Estimator of Surface Ozone Using Formaldehyde and Carbon Monoxide Concentrations Over the Eastern United States in Summer.” *JOURNAL OF GEOPHYSICAL RESEARCH-ATMOSPHERES* 123 (14): 7642–55. doi:10.1029/2018JD028452.

Claeyman, M, JL Attié, VH Peuch, L El Amraoui, WA Lahoz, B Josse, P Ricaud, et al. 2011. “A Geostationary Thermal Infrared Sensor to Monitor the Lowermost Troposphere: O3 and CO Retrieval Studies.” *ATMOSPHERIC MEASUREMENT TECHNIQUES* 4 (2): 297–317. doi:10.5194/amt-4-297-2011.

Curry, Edward. 2016. “The Big Data Value Chain: Definitions, Concepts, and Theoretical Approaches.” In *New Horizons for a Data-Driven Economy*, 29–37. Cham: Springer International Publishing. doi:10.1007/978-3-319-21569-3\_3.

Danyang Ma, Tijian Wang, Hao Wu, Yawei Qu, Jian Liu, Jane Liu, Shu Li, Bingliang Zhuang, Mengmeng Li, and Min Xie. 2023. “The Effect of Anthropogenic Emission, Meteorological Factors, 2 and Carbon Dioxide on the Surface Ozone Increase in China from 3 2008 to 2018 during the East Asia Summer Monsoon Season.” *Atmospheric Chemistry & Physics Discussions*, February. Copernicus Gesellschaft mbH, 1–24. doi:10.5194/acp-2022-850.

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.

Díaz, Julio, Cristina Ortiz, Isabel Falcón, Coral Salvador, and Cristina Linares. 2018. “Short-Term Effect of Tropospheric Ozone on Daily Mortality in Spain.” *Atmospheric Environment* 187 (August): 107–16. doi:10.1016/j.atmosenv.2018.05.059.

Ding, S, JH He, and DF Liu. 2021. “Investigating the Biophysical and Socioeconomic Determinants of China Tropospheric O3 Pollution Based on a Multilevel Analysis Approach.” *ENVIRONMENTAL GEOCHEMISTRY AND HEALTH* 43 (8): 2835–49. doi:10.1007/s10653-020-00797-8.

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.

EPA. 2021. “Climate Change And Social Vulnerability in the United States - A Focus on Six Impacts.” doi:10.1163/9789004322714\_cclc\_2021-0166-513.

EPA, US. 2013. “Final Report: Integrated Science Assessment of Ozone and Related Photochemical Oxidants.” *US Environmental Protection Agency, Washington, DC*.

Feng, Sha, Thomas Lauvaux, Sally Newman, Preeti Rao, Ravan Ahmadov, Aijun Deng, Liza I. Díaz-Isaac, et al. 2016. “Los Angeles Megacity: A High-Resolution Land–Atmosphere Modelling System for Urban CO2.” *Atmospheric Chemistry and Physics* 16 (14): 9019–45. doi:10.5194/acp-16-9019-2016.

Flandorfer, Claudia. 2019. “Evaluation and Comparison of O3 and PM10 Forecasts of ALARO-CAMx and WRF-Chem.” *Geophysical Research Abstracts* 21 (January). Copernicus Gesellschaft mbH: 1–1.

Flynn, MT, EJ Mattson, DA Jaffe, and LE Gratz. 2021. “Spatial Patterns in Summertime Surface Ozone in the Southern Front Range of the US Rocky Mountains.” *ELEMENTA-SCIENCE OF THE ANTHROPOCENE* 9 (1). doi:10.1525/elementa.2020.00104.

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.

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.

Girach, IA, PR Nair, LM David, P Hegde, MK Mishra, GM Kumar, SM Das, N Ojha, and M Naja. 2012. “The Changes in Near-Surface Ozone and Precursors at Two Nearby Tropical Sites during Annular Solar Eclipse of 15 January 2010.” *JOURNAL OF GEOPHYSICAL RESEARCH-ATMOSPHERES* 117 (January). doi:10.1029/2011JD016521.

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

Grenfell, John Lee, Heike Rauer, Franck Selsis, Lisa Kaltenegger, Charles Beichman, William Danchi, Carlos Eiroa, et al. 2010. “Co-Evolution of Atmospheres, Life, and Climate.” *Astrobiology* 10 (1): 77–88. doi:10.1089/ast.2009.0375.

Harithasree, S, K Sharma, IA Girach, LK Sahu, PR Nair, N Singh, J Flemming, SS Babu, and N Ojha. 2024. “Surface Ozone over Doon Valley of the Indian Himalaya: Characteristics, Impact Assessment, and Model Results.” *ATMOSPHERIC ENVIRONMENT-X* 21 (January). doi:10.1016/j.aeaoa.2024.100247.

Hata, H, K Inoue, H Yoshikado, Y Genchi, and K Tsunemi. 2023. “Impact of Introducing Net-Zero Carbon Strategies on Tropospheric Ozone (O3) and Fine Particulate Matter (PM2.5) Concentrations in Japanese Region in 2050.” *SCIENCE OF THE TOTAL ENVIRONMENT* 891 (September). doi:10.1016/j.scitotenv.2023.164442.

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.

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.

Iglesias, Virginia, Anna E. Braswell, Matthew W. Rossi, Maxwell B. Joseph, Caitlin McShane, Megan Cattau, Michael J. Koontz, et al. 2021. “Risky Development: Increasing Exposure to Natural Hazards in the United States.” *Earth’s Future* 9 (7): e2020EF001795. doi:10.1029/2020EF001795.

Kasting, James F., and Janet L. Siefert. 2002. “Life and the Evolution of Earth’s Atmosphere.” *Science* 296 (5570): 1066–68. doi:10.1126/science.1071184.

Kleijnen, Jack P.C. 2017. “Regression and Kriging Metamodels with Their Experimental Designs in Simulation: A Review.” *European Journal of Operational Research* 256 (1): 1–16. doi:10.1016/j.ejor.2016.06.041.

Kumar, Amit, Deepak Singh, Bhupendra Pratap Singh, Manoj Singh, Kumar Anandam, Krishan Kumar, and V. K. Jain. 2015. “Spatial and Temporal Variability of Surface Ozone and Nitrogen Oxides in Urban and Rural Ambient Air of Delhi-NCR, India.” *AIR QUALITY ATMOSPHERE AND HEALTH* 8 (4): 391–99. doi:10.1007/s11869-014-0309-0.

Kwok, RHF, KR Baker, SL Napelenok, and GS Tonnesen. 2015. “Photochemical Grid Model Implementation and Application of VOC, NOx, and O3 Source Apportionment.” *GEOSCIENTIFIC MODEL DEVELOPMENT* 8 (1): 99–114. doi:10.5194/gmd-8-99-2015.

Lerot, C., M. Van Roozendael, J.-C. Lambert, J. Granville, J. Van Gent, D. Loyola, and R. Spurr. 2010. “The GODFIT Algorithm: A Direct Fitting Approach to Improve the Accuracy of Total Ozone Measurements from GOME.” *International Journal of Remote Sensing* 31 (2). Informa UK Limited: 543–50. doi:10.1080/01431160902893576.

Li, JF, KD Lu, W Lv, J Li, LJ Zhong, YB Ou, DH Chen, X Huang, and YH Zhang. 2014. “Fast Increasing of Surface Ozone Concentrations in Pearl River Delta Characterized by a Regional Air Quality Monitoring Network during 2006-2011.” *JOURNAL OF ENVIRONMENTAL SCIENCES* 26 (1): 23–36. doi:10.1016/S1001-0742(13)60377-0.

Lin, C., M. R. Heal, M. Vieno, I. A. MacKenzie, B. G. Armstrong, B. K. Butland, A. Milojevic, et al. 2016. “Spatiotemporal Evaluation of EMEP4UK-WRF v4.3 Atmospheric Chemistry Transport Simulations of Health-Related Metrics for NO2, O3, PM10 and PM2.5 for 2001–2010.” *Geoscientific Model Development Discussions*, July. Copernicus Gesellschaft mbH, 1–28. doi:10.5194/gmd-2016-183.

Lin, J.-T., Z. Liu, Q. Zhang, H. Liu, J. Mao, and G. Zhuang. 2012. “Model Uncertainties Affecting Satellite-Based Inverse Modeling of Nitrogen Oxides Emissions and Implications for Surface Ozone Simulation.” *Atmospheric Chemistry & Physics Discussions* 12 (6). Copernicus Gesellschaft mbH: 14269–327. doi:10.5194/acpd-12-14269-2012.

Lin, MY, AM Fiore, OR Cooper, LW Horowitz, AO Langford, H Levy, BJ Johnson, V Naik, SJ Oltmans, and CJ Senff. 2012. “Springtime High Surface Ozone Events over the Western United States: Quantifying the Role of Stratospheric Intrusions.” *JOURNAL OF GEOPHYSICAL RESEARCH-ATMOSPHERES* 117 (October). doi:10.1029/2012JD018151.

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.

Liu, Xiaoyong, Jiqiang Niu, Jun Yan, Junhui Yan, Chengmei Zhao, Feng Xu, Yidan Zhang, and Bingbing Zhang. 2022. “Surface Ozone in the Central Plains Urban Agglomeration, China: Spatial-Temporal Variations and Health Impacts.” *POLISH JOURNAL OF ENVIRONMENTAL STUDIES* 31 (5): 4767–77. doi:10.15244/pjoes/150460.

Liu, Ying, Guofeng Cao, Naizhuo Zhao, Kevin Mulligan, and Xinyue Ye. 2018. “Improve Ground-Level PM2.5 Concentration Mapping Using a Random Forests-Based Geostatistical Approach.” *Environmental Pollution* 235 (April): 272–82. doi:10.1016/j.envpol.2017.12.070.

Lyons, Timothy W., Christopher T. Reinhard, and Noah J. Planavsky. 2014. “The Rise of Oxygen in Earth’s Early Ocean and Atmosphere.” *Nature* 506 (7488): 307–15. doi:10.1038/nature13068.

Manisalidis, Ioannis, Elisavet Stavropoulou, Agathangelos Stavropoulos, and Eugenia Bezirtzoglou. 2020. “Environmental and Health Impacts of Air Pollution: A Review.” *Frontiers in Public Health* 8 (February): 14. doi:10.3389/fpubh.2020.00014.

Meng, Kai, Tianliang Zhao, Xiangde Xu, Zhongjie Zhang, Yongqing Bai, Yannan Hu, Yang Zhao, Xiao Zhang, and Yushan Xin. 2022. “Influence of Stratosphere-to-Troposphere Transport on Summertime Surface O3 Changes in North China Plain in 2019.” *Atmospheric Research* 276 (October). Elsevier B.V.: N.PAG-N.PAG. doi:10.1016/j.atmosres.2022.106271.

Meng, Qingmin, Zhijun Liu, and Bruce E. Borders. 2013. “Assessment of Regression Kriging for Spatial Interpolation – Comparisons of Seven GIS Interpolation Methods.” *Cartography and Geographic Information Science* 40 (1): 28–39. doi:10.1080/15230406.2013.762138.

Nawaz, M. Omar. 2023. “An Adjoint Sensitivity Framework for Public Health: The Sources of Air Pollution and Their Current and Future Impacts at Both the Urban and National Scale.” Dissertation, University of Colorado, Boulder. https://scholar.colorado.edu/concern/graduate\_thesis\_or\_dissertations/q237ht48v.

Ni, JM, JM Jin, YW Wang, B Li, Q Wu, YF Chen, SW Du, YL Li, and C He. 2024. “Surface Ozone in Global Cities: A Synthesis of Basic Features, Exposure Risk, and Factors.” *GEOGRAPHY AND SUSTAINABILITY* 5 (1): 64–76. doi:10.1016/j.geosus.2023.09.008.

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.

Nixon, Richard. 1970. *Reorganization Plan No. 3 of 1970*. *5 U.S.C. App.* Vol. 84 Stat. 2086. https://www.ecfr.gov/current/title-40/part-1.

Raschka, Sebastian, and Vahid Mirjalili. 2019. *Python Machine Learning: Machine Learning and Deep Learning with Python, Scikit-Learn, and TensorFlow 2*. Third edition. Expert Insight. Birmingham Mumbai: Packt.

Richter, A. 2009. “Nitrogen Oxides in the Troposphere – What Have We Learned from Satellite Measurements?” *The European Physical Journal Conferences* 1: 149–56. doi:10.1140/epjconf/e2009-00916-9.

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.

Schultz, Martin G., Sabine Schröder, Olga Lyapina, Owen R. Cooper, Ian Galbally, Irina Petropavlovskikh, Erika Von Schneidemesser, et al. 2017. “Tropospheric Ozone Assessment Report: Database and Metrics Data of Global Surface Ozone Observations.” Edited by Michael E. Chang and Alastair Lewis. *Elementa: Science of the Anthropocene* 5 (January): 58. doi:10.1525/elementa.244.

Sun, Haitong Zhe, Kim Robin Van Daalen, Lidia Morawska, Serge Guillas, Chiara Giorio, Qian Di, Haidong Kan, et al. 2024. “An Estimate of Global Cardiovascular Mortality Burden Attributable to Ambient Ozone Exposure Reveals Urban-Rural Environmental Injustice.” *One Earth* 7 (10): 1803–19. doi:10.1016/j.oneear.2024.08.018.

Tamiminia, Haifa, Bahram Salehi, Masoud Mahdianpari, Lindi Quackenbush, Sarina Adeli, and Brian Brisco. 2020. “Google Earth Engine for Geo-Big Data Applications: A Meta-Analysis and Systematic Review.” *ISPRS Journal of Photogrammetry and Remote Sensing* 164 (June): 152–70. doi:10.1016/j.isprsjprs.2020.04.001.

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.

Telesca, Donatello, Gregory L. Watson, Michael Jerrett, Colleen Elizabeth Reid, and Gabriele G. Pfister. n.d. “Machine Learning Models Accurately Model Ozone Exposure during Wildfire Events.”

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.

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.

US EPA. 2015a. *The Benefits and Costs of the Clean Air Act from 1990 to 2020, Final Report, Revision A, April 2011*. The Benefits and Costs of the Clean Air Act from 1990 to 2020. U.S. Environmental Protection Agency Office of Air and Radiation.

US EPA, OAR. 2015b. “Health Effects of Ozone Pollution.” Overviews and Factsheets. June 5. https://www.epa.gov/ground-level-ozone-pollution/health-effects-ozone-pollution.

Venkanna, R, GN Nikhil, TS Rao, PR Sinha, and YV Swamy. 2015. “Environmental Monitoring of Surface Ozone and Other Trace Gases over Different Time Scales: Chemistry, Transport and Modeling.” *INTERNATIONAL JOURNAL OF ENVIRONMENTAL SCIENCE AND TECHNOLOGY* 12 (5): 1749–58. doi:10.1007/s13762-014-0537-8.

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.

WHO, Regional Office for Europe. 2013. “Health Effects of Ozone.” In *Review of Evidence on Health Aspects of Air Pollution – REVIHAAP Project: Technical Report*. WHO Regional Office for Europe. https://www.ncbi.nlm.nih.gov/books/NBK361809/.

WMO, World Meteorlogical Organization. 2022. *Scientific Assessment of Ozone Depletion: 2022*. GAW Report No. 278. Geneva: WMO.

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

Wu, LL, J Hang, XM Wang, M Shao, and C Gong. 2021. “APFoam 1.0: Integrated Computational Fluid Dynamics Simulation of O3-NO x -Volatile Organic Compound Chemistry and Pollutant Dispersion in a Typical Street Canyon.” *GEOSCIENTIFIC MODEL DEVELOPMENT* 14 (7): 4655–81. doi:10.5194/gmd-14-4655-2021.

Xing, J, R Mathur, J Pleim, C Hogrefe, JD Wang, CM Gan, G Sarwar, DC Wong, and S McKeen. 2016. “Representing the Effects of Stratosphere-Troposphere Exchange on 3-D O3 Distributions in Chemistry Transport Models Using a Potential Vorticity-Based Parameterization.” *ATMOSPHERIC CHEMISTRY AND PHYSICS* 16 (17): 10865–77. doi:10.5194/acp-16-10865-2016.

Xu, Jiang, Aidong Li, Calvin King Lam Chung, and Yang Yue. 2023. “Mapping the Unmapped: Investigating Big Data Companies via Online Sources.” *The Professional Geographer* 75 (5). Informa UK Limited: 816–26. doi:10.1080/00330124.2023.2169175.

Yakowitz, S.J., and F. Szidarovszky. 1985. “A Comparison of Kriging with Nonparametric Regression Methods.” *Journal of Multivariate Analysis* 16 (1): 21–53. doi:10.1016/0047-259X(85)90050-8.

Yamashita, Yousuke, Kei Sakamoto, Hideharu Akiyoshi, Masaaki Takahashi, Tatsuya Nagashima, and L. B. Zhou. 2010. “Ozone and Temperature Response of a Chemistry Climate Model to the Solar Cycle and Sea Surface Temperature.” *JOURNAL OF GEOPHYSICAL RESEARCH-ATMOSPHERES* 115 (September). doi:10.1029/2009JD013436.

Yu, Karen, Christoph A. Keller, Daniel J. Jacob, Andrea M. Molod, Sebastian D. Eastham, and Michael S. Long. 2018. “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): 305–19. doi:10.5194/gmd-11-305-2018.

Zhang, Junfeng, Yongjie Wei, and Zhangfu Fang. 2019. “Ozone Pollution: A Major Health Hazard Worldwide.” *Frontiers in Immunology* 10 (October). Frontiers. doi:10.3389/fimmu.2019.02518.

Zhao, Na, Xinyi Dong, Kan Huang, Joshua S. Fu, Marianne Tronstad Lund, Kengo Sudo, Daven Henze, et al. 2021. “Responses of Arctic Black Carbon and Surface Temperature to Multi-Region Emission Reductions: A Hemispheric Transport of Air Pollution Phase 2 (HTAP2) Ensemble Modeling Study.” *Atmospheric Chemistry and Physics* 21 (11). Copernicus GmbH: 8637–54. doi:10.5194/acp-21-8637-2021.

Zoran, M, MR Dida, R Savastru, D Savastru, A Dida, and O Ionescu. 2014. “Ground Level Ozone (O3) Associated with Radon (222Rn) and Particulate Matter (PM) Concentrations in Bucharest Metropolitan Area and Adverse Health Effects.” *JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY* 300 (2): 729–46. doi:10.1007/s10967-014-3041-1.