CHAPTER VII

Conclusion

This project yielded low errors with to minimal incorporation of training values for each quantum mechanical geo-field representing surface O3 at each pixel. If completed properly, the new-found achievements of modern GIS can be further enhanced with in-situ measurements at consistent points. Errors seen in the models can be attributed to the filling of missing values via interpolation and imputation, and missing satellite data. While these values can be either gathered or better interpolated with GEE by adding the surrounding counties outside of the AOI, the pre-processing portion of this project was meant to establish the framework for continued research. The light work required to properly fill NA values should simply be done as part of a larger dissertation creating a model which effectively spans the US. Advanced applications of pre-processing methods would be significantly better for ensuring proper continuity in the initial time-series for variables such as NDVI and formaldehyde. While especially effective for datasets with only a few days missing (e.g TOM/OMI and GRIDmet collections), the interpolation and imputation methods are likely not suitable for long spans of missing data unless given proper consideration into historical available data. In addition, much of the display pre-processing a was complete in python and ArcPRO before final importations into GIMP 3.0 for final touch ups and color corrections. Despite the power of ArcPRO and its contributions to the GIS community, long series mapping such as this thesis did not seem worth the extra time associated with processing each final raster through a toolbox for display. Rather, the creation of such a toolbox which automatically corrects satellite imagery given its monitored value should be implemented as a further project and not as the result of an MA thesis.

This project also required the assumption that monitors were not moved, removing such monitors from the AOI. When a monitor is moved, it no longer offers the potential for future trends unless the original point location and measurements are properly combined prior to being initialized within an ensemble. SMaRK improvements would allow for the proper tuning of monitor locations and their location in reference to the overall geo-field driving process. Further work and incorporation of this method into spatial programs is necessary to unleash the full capacity of GIS into the modern world. The establishment of complex trend analysis from GeoAI and Big Data has finally enabled for the proper quantification of surface O3 estimations. Further applications of RK could advance optical technologies of numerous disciplines which utilize similar observations and correctional schema, e.g. correlating satellite imagery to rovers or stations on Mars.

Remote sensing engineers are constantly finding adaptations to algorithms and noisy data to reduce the error of its coarse results. Utilizing monitoring points as geo-atoms associated with the process they are meant to depict incorporates the concept of GCPs seen in extremely high-resolution remote sensing via remote piloting of drone technology. GCPs in this field are stagnant points which the drone can always see to relate a constant point to all images which need to be tiles. High-resolution satellite retrievals are stored and shared via similar tiling of data, requiring interpolation and resampling techniques like the ones in this thesis. If imagery can be associated with a monitored location during the resampling methods, the concept of an uncertain geo-atom can be accounted for and further reduce the error of the image. This project showed that the application of spatial thought with ML/AI ensembles can better depict geographic patterns and trends noted by analyses of known observations. With better high-resolution surface O3 representations, many communities can be protected from risks associated with it and its constituents.

VII.1. Interpolation vs. Imputation Strategies

The results of the employed K-nearest neighbors (KNN) imputation on the dependent variable achieved a high degree of accuracy due to the available data in this study’s timeframe. Interpolation can be expanded among the entirety of the dataset older measurements from dismantled monitors wish to be utilized. Imputation was crucial for achieving consistency across the available monitors and ensured reliable data for final model training and evaluation. The Linear and Modified Akima interpolation strategies used on the maximum value may not be the best predictive measure if given a larger temporal resolution or reactive feature such as an aerosol. When imputation was conducted on data from 2000-2024, numerous aerosols benefited from 2nd and 3rd degree polynomial interpolation strategies. In addition, interpolation may not be as effective for highly responsive variables such as CO, NO, and Formaldehyde, as these constituents typically show high variability at fine temporal scales. Imputation can be further utilized to accurately predict these features; however, the overall estimation of unknown values leads to increased spreads of error in the final model. This project focused on interpolation of unknown values with the methodology for imputations provided in case it’s needed.

VII.2. Feature Evaluation, Importance and Development

Most of the satellite data launched in late 2018 were highly correlated with surface ozone. Individual features known to be precursors for surface ozone reactions from prior models and simulations (Ahmadov et al. 2015; Akimoto et al. 2019; Bowdalo, Evans, and Sofen 2016; Engardt 2008; Hakim et al. 2019; Jacob 2000) were among the top features. The distribution of latitudes, longitudes and elevation were heavily skewed as per Table X; while a more normal distribution of these features may provide higher correlation areas spanning numerous elevations, two main caveats still come to light from using latitudes and longitudes as a numerical feature in geospatial models:

1. They are essentially properties of a geo-atom, such as time, elevation, site-id, etc.; incorporating a property as a feature is like incorporating a tuning metric into the model as a feature.
2. The spatial dependency of a monitor’s metrological depiction is provided by a transformation based on its remotely sensed source, numerical representations of spatial data artificially group these transformations and adds bias to models

ML/AI ensembles utilizing geospatial data are estimating trends based on geo-atoms gathered over the estimated AOI in the way of pixels. When latitudes and longitudes are incorporated into prediction, the distribution must be assumed normal, hence why these may not yield significant results in AOIs whose spatial properties don’t vary via the typical normal bell-curve.

Residual Kriging offers a more stable solution to incorporate geospatial data into ML/AI by integrating geo-atoms as separate, predictive measures. They become a feature of the model without acting as a feature withing the ensemble itself, better depicting spatial dependance and improving overall accuracy as seen in this study. RK is written to model spatial drift, which is difficult to capture for ML/AI models as a dependent variable; RK enhancements to the final models account for drift while separating the prediction from group bias. As per the literature review, finely tuned models such as WRFC-XGB and MATCH[[1]](#footnote-1) (Engardt 2008; Hu et al. 2022) mainly utilize chemical transport models in addition to satellite imagery to account for spatial error by integrating atmospheric dynamics and emission inventories, enhancing the accuracy of pollutant dispersion estimates across available resolutions. Studies like (Becker 2021; Centoni 2017; G. Chen et al. 2021; X. Chen et al. 2023; Hu et al. 2022) incorporate more data; such as fine resolution land-use data, evaluations of tropospheric/ground level ozone measurements, and higher quality data from the source[[2]](#footnote-2), yielding extremely accurate results without the correction of monitor values.

Remote sensing is simply the analysis of measured, reflected light. After numerous optical corrections and mathematical transforms rooted in sibling-sciences, astronomy-based processes and biological activity can be detected with great accuracy and precision. For example, the normalized differential vegetation index (NDVI) is a great depiction of plant health stemming in differences between red and shortwave UV light. Remote Sensing can be a geographer’s best tool in this modern day of spatial computing. Studies utilizing this analysis of geospatial correction to reflected light are attempting to incorporate geospatial corrections into these models as hardcoded feature transformations. As imagery gets more advanced, technology begins to better account for the errors recorded among satellite imagery, models which don’t incorporate spatial error via residual kriging are slightly incorporating this error by way of complex physics and optics. The estimated kinetic energy depicted on the day and time that the ozone concentration was gathered may offer key insights into a new, highly correlated feature with minimal collinearity

VII.3. An Advanced Adaptation of Lagrangian Mechanics

The basics of Lagrangian field theory were initially known to the research and used to construct two features for prediction, one of which does not exist for gaseous states: KE and UE. Using a series of transformations, an entire system can be explained as an integral of internal energies over time: The general scope of this theory is if a system's motion is subject to any form of constraint, then there exists a set of generalized coordinates which are compatible with those constraints and hence, simplify the analysis of the system's motion. It was initially believed that a system carried out motions that minimize its actions. This was called the Principle of Least Action, but later, it was realized that an infinitesimal variation in the path yielded no effect on the action of the system. In the world of physics, the difference between minimal and 0 drastically changes the theory. With this new assumption that actions are assumed to be stationary with respect to small variations in their motion, a set of equations known as Euler-Lagrange equations can be implemented and utilized as a feature known as the Action Potential.

These equations represent general coordinates that are replaced by Lagrangian densities (Lρ). Like replacing loss functions within a statistical model to change outcomes, LFT allows for numerous representations of Lρ to account for the numerous mechanics discovered in thermodynamical and chemical-based features mentioned in Chapter III. The history of these developing theories and their core, the Principle of Least Action (PLA), offers exciting new relationships to modern satellite technology which can be further developed into features of many molecular and mechanical surface measurements.

VII.3.1. The Principle of Least Action

PLA was initially established under the theory that a system always moves in regard to the minimal number of actions allowable from the degrees of freedom defining the system. Later, PLA established that an infinitesimal variation within the path yielded no effects on the overall actions a system can have. In the world of physics, the difference between minimal and 0 drastically changes the theory; actions now are assumed to be stationary with respect to small variations in motion. A set of equations known as Euler-Lagrange equations can be implemented and utilized as a feature known as the Action Potential (AP). These represent a function of general coordinates that are replaced by Lagrangian densities (Lρ). Like replacing loss functions within a statistical model to change outcomes, LFT allows for numerous representations of Lρ to account for the numerous sub-fields in physics.

The proposed kinetic energy calculations for the properties of geo-atoms in this thesis are precursors to a much broader set of terms stemming from these Lagrangian mechanics. In its most general form, any independent variable in LFT can be represented as some theoretical event in space-time S(x, y, z, t) similar to the geo-atom established in 2007 by Dr Goodchild. Dependent variables can be represented as a quantifiable action attributing to the independent event occurring at that time, φ(x,y,z,t). If these actions can be properly defined as properties establishing values for a geo-atom and in a geo-field, then implementation of LFT via modern complex ensembles would assume that once an event has happened, it does not happen again until the same number of actions are present in the system. While underlying complex mathematics like this are included in CTMs by way of features representing emissions, the accuracy offered by RK shows there are potential missing transport mechanisms that can be further improved.

In general, this thesis used three main takeaways from LFT which are also used in the bases of CTM models to establish the core concepts of KE depictions in Chapter III:

* + A system wants to be stationarity unless actions cause it to be otherwise. Stationarity ensues an energy state of 0, or a systems ground state.
  + Where a system's motion is subject to constraints, there exists a set of generalized coordinates that are compatible with those constraints
  + The analysis of the system's motion can be represented as an equivalency of energy such that:

Where i represents any number of actions in the system at any point in time t. Some systems do not contain potential energy given their state, such as chemical systems. Chemical potential energy and thermodynamic relationships drastically change the representation of Lagrangian densities; vast fields dedicated to this concept have yet to fully reach the world of GIS transformations. If given a continuous set of maximum and minimums over time, the property of a geo-atom can be a representation of Lρ using Euler–Lagrange transformations of available imagery. These equations are a system of second-order ordinary differential equations whose solutions are stationary points of a given action. They can be related to entropy and thermodynamics to describe the geodesic flow of any field, φ, for some set of time:

Taking the variation with respect to φ, one obtains the typical states of systematic entropy:

Given the space and time features produced in pre-processing, variables ds/dt, dp/dt, dv/dt, etc., geo-atoms representing the PLA of any states can be implemented via proper consideration of these transformations. The final representation of surface ozone actions via Euler-LaGrange Mechanics then can be further implemented into a multidisciplinary approach known as the Supersymmetric Theory of Stochastic Dynamics (SSD).

VII.3.2. Spontaneous Symmetric Breaking

The estimated kinetic energy depicted on the day and time that the ozone concentration was gathered may offer key insights into a new, highly correlated feature with minimal collinearity. The estimated kinetic energy must be representative of the chemical and physical properties just mentioned. Further analysis of Lagrangian Field Thery applied to surface ozone densities is mentioned in Chapter 6. The basic take away from this is the construction of the theoretical kinetic energy of the reaction at a given state, in some space at some time it is given as a combination of chemical-thermodynamics and LFT, for later use with a scaled field correlating to the predictor variable:

If one delves deep enough into the darkness of condensed matter physics, field theory and applications of Feynman mechanics; the act of “spontaneous symmetry breaking” seems oddly familiar to the spontaneity of ozone reactions. Spontaneous symmetry breaking (SSB) refers to a special case where the lowest energy state (a vacuum), may not be invariant under all symmetries. In other words, several vacuums are possible, and the overall field may not change with respect to a singular process. SSB states that a spontaneous process of symmetry breaking, by which a physical system in a symmetric state may spontaneously end up in an asymmetric state. In the case of surface ozone, light, NO2, and other atmospheric processes which drive ozone, depict the symmetric states required to produce the asymmetric state of surface ozone. Proper implementation of this theory with regards to remote sensing, geospatial transformations, and spatial-temporal analytics may be a novel missing link in modeling chemical transport systems.

VII.4. Advancing Surface O3 Mapping with RK Regression

The RK method emerged as a standout approach, offering robust spatial refinement to all baseline models by accounting for residual spatial dependencies. While some base ensembles out predicted SMaRK based estimations due to a stronger complex property, the overall SMaRK version of that ensemble still shows stronger associations with the in-situ value at each location. This approach successfully captured O3 concentrations across diverse anthropogenic environments with similar meteorological conditions as well as if not better than current ensemble approaches to correcting imagery.

If the associated instrument can be correlated to a monitor of the same type which is properly gathered (e.g. Dobson Monitors and TOMS/OMI imagery or high-resolution drone imagery corrected with GCPs and NDVI imagery from Landsat in-between retrievals), then predictive ensembles using remotely sensed data would inherently benefit from the reduced error in imagery. SMaRK’s low error rates and enhanced spatial precision offers novel solutions to correcting high-resolution imagery beneficial for numerous sectors; like public health research, urban chemical transport studies, and local weather mapping, where fine-scale exposure assessments are critical (Kong et al. 2023; Lo et al. 2024; Northeim, Tiwari, and Oppong 2021; Yin et al. 2019).

RK can be used to mitigate the Modifiable Areal Unit Problem (MAUP) and a unique advantage for remotely sensed imagery, providing more accurate, localized predictions of retrieval from current and historical technologies. By modelling the relative distance an observation is from its predicted value, the SMaRK approach can be thought of a mathematical implementation of Tobler’s Law in ML/AI models. Each residual geo-atom, a representation of a complex trend based on geo-atoms within a set field, dictates the amount of similarity between the source and estimated value. By including this in modern imagery, large sets of geo-spatial uncertainty can be accounted for.

VII.5. Implications For Public Health and Policy

Enhanced ozone modeling has significant implications for public health. By addressing spatial and temporal variability more effectively, RK and ensemble methods can support targeted interventions to reduce ozone exposure, particularly in vulnerable populations. Policies informed by high-resolution ozone models can prioritize areas with high exposure, guiding infrastructure development and resource allocation for air quality improvement initiatives. Furthermore, the capacity of RK to capture fine-scale ozone variations holds potential for advancing urban planning, where localized emission control measures could significantly impact public health (Jerrett et al., 2009; Bell et al., 2014).

This study’s findings underscore the need for high-resolution models to achieve accurate exposure assessments that inform public health strategies and urban expansion plans. The RK method provides an advanced tool for mapping not only surface O3 concentrations, but many air pollutants and aerosols at resolutions finer than 300m in need be. If the dataset for surface O3 is expanded upon, it can offer the ability to rapidly estimate exposure risks for participants in exposure studies, especially in densely populated urban centers. Public health officials and policymakers could leverage this to implement localized interventions and standards, such as regulating vehicular emissions and industrial pollutants via emission credits, ultimately reducing health burdens associated with ozone and air pollution exposures.

VII.6. Insights Into Historical Exposures and Concentrations

The historical feasibility of high-resolution ozone modeling, particularly from 1980 to 2000, relies heavily on the RK method’s ability to accurately capture residual spatial dependencies. With RK, historical data from sources like TOMS can be spatially refined to produce monthly average ozone concentrations, filling a critical gap in historical ozone exposure records. This capability is invaluable for public health research, as it allows for the retrospective analysis of exposure patterns over time, linking long-term ozone trends with health outcomes in different populations. The RK method’s refinement of historical datasets can thus support an unprecedented level of detail in exposure mapping, fostering a new understanding of how ozone exposure has evolved in response to environmental and socio-economic changes. From 2000 onwards, with the advent of advanced satellite data from instruments like Sentinel-5P, the RK method can facilitate daily average ozone models by enabling granular spatial predictions, making high-resolution daily models feasible for the first time.

One of the most promising aspects of the RK method lies in its potential to improve existing statistical models, estimating predictions before 2005. By predicting geospatial error within a larger temporal range, RK can enhance the predictive accuracy of ML/AI corrections used for understanding trends over large decades if collected imagery. Statistical models, when combined with residual kriging, are empowered to deliver predictions that reflect both large-scale trends and localized variations. This integration enables a new generation of high-resolution spatial datasets that offer valuable insights for epidemiological studies, allowing for a more precise estimation of the impacts associated with different O3 exposure levels and more. The RK method provides a structured means of adjusting for the inherent variability in ozone concentrations that traditional statistical models cannot easily account for. This adjustment is critical in capturing the ozone’s complex behavior across diverse landscapes, which is essential for accurate long-term health impact assessments.

In tandem, the enhancement of remote sensing monitoring systems through RK underscores the potential for a more comprehensive air pollution monitoring network that combines satellite data with ground-level measurements. This approach addresses a key limitation of remote sensing: the lack of fine-scale spatial detail required for accurate exposure predictions in urban and rural microenvironments. RK can improve the spatial accuracy of satellite data by integrating it with in-situ measurements, thereby creating a more precise depiction of ozone concentrations near densely populated areas. Such high spatial resolution is essential for not only quicky estimating exposures, it showed populations in this thesis are disproportionately affected by O3 due to their geographic location, socio-economic status, or underlying health vulnerabilities given their surroundings. By refining satellite-based O3 estimates, RK can also facilitate more responsive public health interventions, allowing for the timely identification and mitigation of high-exposure areas.

Multi-disciplinary GIS modeling techniques such as SMaRK have become more widespread because of this most recent data revolution (Goodchild 2018). Brought about by the exponential growth in data storage and processing capacities via advancements in Big Data, new-found spatial and temporal analysis of both micro- and macro- ecologies have spurred the need for simplified, sound methodologies. The pursuit of high spatial resolution O3 models may represent a landmark methodology for GIS users. This ambition, driven by the imperative need for readily available, accurate, spatial-temporal based data has only become attainable due to advances in technology. Particularly, the availability of Big Data like TOAR/Google Earth Engine, application of spatial uncertainty into ML/AI representations of satellite data, and overall improvement of programming language syntaxes (Python 3.12.x, Java 8.x, R 4.x, SQL Server 2022, etc.). The SMaRK approach significantly enhanced the predictive accuracy of traditional ML/AI models by spatially interpolating residuals from features at a given point and adding the predicted error back into the model. Satellite imagery in the PHOTUC region via SMaRK provides transformative capabilities for surface O3 mapping, CTMs, and exposure studies by including known values detected at the surface. The incorporation of spatial uncertainty into ML/AI methods for the proper display of geospatial information is critical to the progression of GIS programs. It enables finer, more nuanced depictions of any independent variable of interest across any temporal and geographic scale with the appropriate coverage of monitors. These fine-grained enhancements are critical for uncovering the full spectrum of micro- and macro-effects of the many pollutants threatening human health, ecosystems, and air quality.

VII.7. Final Comments on the SMaRK Method

In general, utilizing the RK method allowed for capturing complex error trends associated with predicted and actual values of surface O3. SMaRK displayed high variability and complexity of O3 concentrations due to emissions (Staehle, Rieder, and Fiore 2023) while accounting for minute associations due to metrological factors (Hou et al. 2024; Liang et al. 2018; Liu et al. 2023; Meng et al. 2022; Venkanna et al. 2015). While kriging has been known about for some time, it’s frequency and applications to geospatial representation in ML/AI ensembles and corrective measures remain extinct. In addition, a high-spatial resolution less than 300m of surface O3 does not yet exist for the USNA as it does for other nations. Models have been utilized via atmospheric monitoring networks provided by large institutions and networks such as tropospheric ozone assessment report (TOAR), EPA, and NASA.

The RK method’s innovations addressed explicit limitations inherent in traditional geo-statistical models, particularly with respect to handling complex spatial dependencies and improving spatial resolution. Statistical models, such as linear and ridge regression, have long served as foundational tools for geographic and environmental predictions due to their simplicity and interpretability. However, their effectiveness in ozone modeling has been restricted by an inability to handle non-linear and spatially heterogeneous relationships, which are fundamental characteristics of ozone transport and transformation in the atmosphere. Atmospheric chemistry models, like geos-chem, offer the non-linear predictive power required to understand ozone formation processes at large scales but often lack the spatial granularity necessary for detailed exposure assessments. These models, though informative for understanding ozone formation mechanisms, typically provide results that are too coarse to capture the spatial variations crucial to localized public health research. The RK method, by interpolating spatial residuals from baseline models, introduces a critical enhancement that addresses these deficiencies, providing a more refined spatial resolution that is suitable for high-resolution monthly and daily historical modeling.

VII.8. Necessity of Residual Kriging

The advent of satellite monitoring systems has also contributed significantly to ozone modeling by supplying remote sensing data that is crucial for large-scale atmospheric studies. Instruments like the total ozone mapping spectrometer (toms) and the more recent Sentinel-5P satellite offer invaluable datasets that track ozone and its precursors at a global level. These data, however, are subject to spatial limitations and are constrained by their resolution, particularly in densely populated or topographically diverse regions where ozone variability can be substantial. Satellite data alone cannot achieve the spatial and temporal precision needed for accurate, localized exposure assessments. However, the integration of satellite data with the RK method opens new possibilities. By applying residual kriging to the baseline satellite data, we can account for local variability and improve upon the spatial resolution, rendering the dataset much more useful for high-resolution historical and current-day models. This enhancement is particularly promising for bridging the gap in ozone data quality from 1980 to the present, enabling continuous historical models that track monthly and daily ozone variations across decades.

VII.9. SMaRK Developments and Future Directions

The deployment of advanced ozone models, however, particularly regarding funding and the willingness of research institutions and governmental bodies to sustain long-term efforts in ozone exposure modeling. High spatial resolution ozone models require substantial computational resources and ongoing support for data collection and analysis. In particular, the production of continuous historical models from 1980 to 2000 necessitates significant funding for the acquisition and processing of archival data, as well as the refinement of modeling techniques to ensure accuracy. Moreover, the establishment of daily average models from 2000 to the present will require robust investment in both hardware and software infrastructure capable of handling the high-resolution demands of RK-enhanced datasets. This sustained funding is essential not only for the generation of accurate ozone models but also for fostering public health research that can meaningfully impact policy and environmental regulations.

A commitment to understanding the full scope of ozone’s impact on human health extends beyond the scientific community and requires collaborative action from public health officials, environmental agencies, and policymakers. The development of high-resolution ozone models could reveal the toxicology of surface ozone with unprecedented clarity, illustrating the exposure risks associated with both indoor and outdoor environments. This knowledge is critical for protecting vulnerable populations, especially those who live in regions with frequent ozone pollution events or who work in industries where indoor ozone exposure may be elevated. Ozone modeling those accounts for both indoor and outdoor exposure is crucial for accurately estimating the true burden of ozone-related diseases, as indoor exposure can vary significantly depending on building ventilation, material interactions, and proximity to outdoor pollution sources. A comprehensive understanding of ozone exposure patterns could facilitate policies aimed at reducing indoor ozone levels in Workplaces, schools, and homes, further protecting public health.

Accurate ozone models have the potential to reduce mortality rates associated with air pollution by informing more targeted and effective interventions. By providing a clearer picture of where and when high ozone concentrations occur, these models empower public health officials to issue more accurate advisories and allocate resources to areas in need. This can lead to reduced hospital admissions, fewer cases of respiratory distress, and ultimately a decrease in the mortality rate associated with ozone-related health issues. The knowledge gained from high-resolution ozone models can also serve as a foundation for preventative measures, such as urban planning initiatives that reduce vehicle emissions in densely populated areas, minimizing the risk of acute ozone exposure. Such measures not only improve air quality but also contribute to sustainable urban environments, promoting public health and well-being over the long term.

VII.9.1 Accessing Code and Data

All raster data is freely available on GitHub. Scripts for downloading the necessary data are based in python. While the full project is privately available on GitHub, a public version with access to scripts and sample data can be accessed via the following link: The full scope of this project is in its infancy, and while discerning the available code now may be difficult; developments and improvements are being made daily to make this an easily distributable package via python to facilitate development of high spatial resolution imagery.

VII.10. Closing Remarks

The insights gained from these models can aid the development of high-resolution surface ozone metrics for numerous areas. To reduce ozone-related health risks, support sustainable urban environments, and restore the Earth’s natural ozone cycles, the SMaRK method enables a more accurate representation of ozone concentrations across diverse settings. This has the potential to reshape current understandings of ozone exposure, impacts to general air pollution, and could pave the way for a future where scientifically informed air quality management and deeply attuned to the needs of human health and environmental sustainability.

There are many worries associated with semi-known/fully known health outcomes. Developing theories on health associations from surface ozone exposure on pediatric/elderly populations call for more detailed ozone models to quickly assign accurate exposures to aid air quality, public health, and urban ecology studies. Given that data for these studies are typically small in total area (compared to that of an entire nation or state), there is a need for methodology that can incorporate machine learning and geographic information, when necessary, fully leveraging advantages of both sides for use in high-resolution geographic modelling.

Atmospheric chemistry plays a foundational role in the history of life on Earth (Barzeghar et al. 2020; Chapleski et al. 2016; Flynn et al. 2021; Tanimoto et al. 2008). Abiogenetic processes on Earth nearly 4 billion years ago were attributed to the emergence of oxygen during the Great Oxidation Event (GOE); enabling the formation of the ozone (O3) layer and promoting photosynthetic processes (Schell, Ackemann, and Hass 2002; Lyons, Reinhard, and Planavsky 2014). As O3 and organisms respectively grew in abundance and complexity, atmospheric composition began to stabilize, eventually resulting in the Earth as we know it today. For eons, the niche composition of chemicals on Earth has allowed life to further evolve by maintaining hypoxia tolerances through the variance in energy levels reaching the surface (Sperling et al. 2022). In this sense, atmospheric chemistry is both guardian and shepherd to biological evolution.

The safety and well-being of past, present, and future generations is essential work of many in geography. Applications of spatial analytics are being utilized in numerous fields to refine and theorize the complexities of the human health and cognition to better understand environmental impacts on daily life (Jerrett, Gale, and Kontgis 2010; Greenough and Nelson 2019; Nawaz 2023; Fuller et al. 2022; Schlink et al. 2006; Cakaj et al. 2023; Borchert et al. 2023). Decades of geospatial computer science implementations with statistical modeling have paved the way for unique, multi-disciplinary specializations to investigate these topics. As computer science grows in availability, quality, and most importantly, ease of access, geographers continue to weave complex spatial thought into “sibling-sciences”, creating innovative solutions to known and unknown problems (Goodchild 2009; Blaschke and Merschdorf 2014).

VII.10.1 A Note from the Researcher

This thesis seeks to genesis a new initiative with available satellite imagery; stemming from its final product, the high-resolution imagery proposed has potential to further reduce emissions beyond their current trajectory, bolster American economy, and induce harmony between environmental activists and private cooperate entities. The SMaRK method can be further improved with additional coding enhancements and appropriate tuning. Between the ease of access of current/future satellite technologies, incorporation of geospatial thought ML/AI methods, and resulting enhancements to depictions of molecular systems; this thesis can be further used to develop highly accurate, historical, and future predictions of molecular imagery to aid in the establishment of a new molecular credit, rewarding businesses for maintaining a certain standard.

SMaRK operates with correlations to in-situ measurements; when monitors are properly placed as they currently are for some urban areas, the resulting change in environmental patterns due to Anthropogenic sources can be properly translated into monetary units of maintenance the proposed pollutant per area. Like a Carbon Credit (Shah et al. 2024; Trouwloon et al. 2023), the resulting system would be significantly more reliable due to in-arguable comparisons to monitoring systems. Unlike some forms of carbon credit (e.g. mentioned in (Probst et al. 2024; Lokuge and Anders 2022); the newly established credit from a final can be offered with more confidence and reliability in the modeled outcomes.

Citations

Ahmadov, R., S. McKeen, M. Trainer, R. Banta, A. Brewer, S. Brown, P. M. Edwards, et al. 2015. “Understanding High Wintertime Ozone Pollution Events in an Oil- and Natural Gas-Producing Region of the Western US.” *Atmospheric Chemistry and Physics* 15 (1): 411–29. doi:10.5194/acp-15-411-2015.

Akimoto, Hajime, Tatsuya Nagashima, Jie Li, Joshua S. Fu, Dongsheng Ji, Jiani Tan, and Zifa Wang. 2019. “Comparison of Surface Ozone Simulation among Selected Regional Models in MICS-Asia III - Effects of Chemistry and Vertical Transport for the Causes of Difference.” *ATMOSPHERIC CHEMISTRY AND PHYSICS* 19 (1): 603–15. doi:10.5194/acp-19-603-2019.

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.

Becker, Jacob Sugar. 2021. *Using Regionalized Air Quality Model Performance and Bayesian Maximum Entropy Data Fusion to Map Global Surface Ozone Concentration and Associated Uncertainty*.

Blaschke, Thomas, and Helena Merschdorf. 2014. “Geographic Information Science as a Multidisciplinary and Multiparadigmatic Field.” *Cartography and Geographic Information Science* 41 (3): 196–213. doi:10.1080/15230406.2014.905755.

Borchert, William, Stephanie T. Grady, Jie Chen, Nicole V. Deville, Charlotte Roscoe, Futu Chen, Carol Mita, et al. 2023. “Air Pollution and Temperature: A Systematic Review of Ubiquitous Environmental Exposures and Sudden Cardiac Death.” *CURRENT ENVIRONMENTAL HEALTH REPORTS* 10 (4): 490–500. doi:10.1007/s40572-023-00414-7.

Bowdalo, Dene R., Mathew J. Evans, and Eric D. Sofen. 2016. “Spectral Analysis of Atmospheric Composition: Application to Surface Ozone Model-Measurement Comparisons.” *ATMOSPHERIC CHEMISTRY AND PHYSICS* 16 (13): 8295–8308. doi:10.5194/acp-16-8295-2016.

Cakaj, Arlinda, Erjon Qorri, Fatimatou Coulibaly, Alessandra De Marco, Evgenios Agathokleous, Stefan Leca, and Pierre Sicard. 2023. “Assessing Surface Ozone Risk to Human Health and Forests over Time in Poland.” *ATMOSPHERIC ENVIRONMENT* 309 (September). doi:10.1016/j.atmosenv.2023.119926.

Centoni, Federico. 2017. “Global Scale Modelling of Ozone Deposition Processes and Interaction between Surface Ozone and Climate Change.”

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.

Chen, Gongbo, Jiang Chen, Guang-hui Dong, Bo-yi Yang, Yisi Liu, Tianjun Lu, Pei Yu, Yuming Guo, and Shanshan Li. 2021. “Improving Satellite-Based Estimation of Surface Ozone across China during 2008-2019 Using Iterative Random Forest Model and High-Resolution Grid Meteorological Data.” *SUSTAINABLE CITIES AND SOCIETY* 69 (June). doi:10.1016/j.scs.2021.102807.

Chen, Xueyao, Zhige Wang, Yulin Shangguan, Jie Yu, Bifeng Hu, Qiaohui Shen, Jie Xue, Xianglin Zhang, and Zhou Shi. 2023. “Estimating Monthly Surface Ozone Using Multi-Source Satellite Products in China Based on Deep Forest Model.” *ATMOSPHERIC ENVIRONMENT* 307 (August). doi:10.1016/j.atmosenv.2023.119819.

Engardt, Magnuz. 2008. “Modelling of Near-Surface Ozone over South Asia.” *JOURNAL OF ATMOSPHERIC CHEMISTRY* 59 (1): 61–80. doi:10.1007/s10874-008-9096-z.

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.

Fuller, Richard, Philip J Landrigan, Kalpana Balakrishnan, Glynda Bathan, Stephan Bose-O’Reilly, Michael Brauer, Jack Caravanos, et al. 2022. “Pollution and Health: A Progress Update.” *The Lancet Planetary Health* 6 (6): e535–47. doi:10.1016/S2542-5196(22)00090-0.

Goodchild, Michael F. 2009. “Geographic Information Systems and Science: Today and Tomorrow.” *Annals of GIS* 15 (1): 3–9. doi:10.1080/19475680903250715.

———. 2018. “Mapping Across Academia.” *The AAG Review of Books* 6 (2). Informa UK Limited: 115–17. doi:10.1080/2325548x.2018.1402278.

Greenough, P. Gregg, and Erica L. Nelson. 2019. “Beyond Mapping: A Case for Geospatial Analytics in Humanitarian Health.” *Conflict and Health* 13 (1): 50. doi:10.1186/s13031-019-0234-9.

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.

Hou, XS, XQ Wang, SY Cheng, HY Qi, CD Wang, and ZJ Huang. 2024. “Elucidating Transport Dynamics and Regional Division of PM2.5 and O3 in China Using an Advanced Network Model.” *ENVIRONMENT INTERNATIONAL* 188 (June). doi:10.1016/j.envint.2024.108731.

Hu, Xiaomin, Jing Zhang, Wenhao Xue, Lihua Zhou, Yunfei Che, and Tian 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.

Jacob, D. 2000. “Heterogeneous Chemistry and Tropospheric Ozone.” *Atmospheric Environment* 34 (12–14): 2131–59. doi:10.1016/S1352-2310(99)00462-8.

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.

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.

Liang, Ciao-Kai, J. Jason West, Raquel A. Silva, Huisheng Bian, Mian Chin, Yanko Davila, Frank J. Dentener, et al. 2018. “HTAP2 Multi-Model Estimates of Premature Human Mortality Due to Intercontinental Transport of Air Pollution and Emission Sectors.” *Atmospheric Chemistry and Physics* 18 (14). Copernicus GmbH: 10497–520. doi:10.5194/acp-18-10497-2018.

Liu, S, WH Zhao, LJ Li, JN Jin, TZ Li, HT Xu, and WJ Zhao. 2023. “Meteorological Mechanisms of Regional PM2.5 and O3 Transport in the North China Plain Driven by the East Asian Monsoon.” *ATMOSPHERIC POLLUTION RESEARCH* 14 (1). doi:10.1016/j.apr.2022.101638.

Lo, KC, WH Cheng, C Lin, CH Hung, CS Yuan, and YL Tseng. 2024. “Elevated Surface Ozone Concentration Caused by Subtropical Cyclones and Topographical Effect: Model Simulation and Field Measurement.” *URBAN CLIMATE* 57 (September). doi:10.1016/j.uclim.2024.102093.

Lokuge, Nimanthika, and Sven Anders. 2022. “Carbon Credit Systems in Agriculture: A Review of Literature.” *The School of Public Policy Publications*, April. The School of Public Policy Publications, Vol. 15 No. 1 (2022). doi:10.11575/SPPP.V15I1.74591.

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.

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.

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.

Northeim, K, C Tiwari, and J Oppong. 2021. “Surface Ozone Monitoring and Policy: A Geospatial Decision Support Tool for Suitable Location of Monitoring Stations in Urban Areas.” *ENVIRONMENTAL SCIENCE & POLICY* 126 (December): 48–59. doi:10.1016/j.envsci.2021.09.011.

Probst, Benedict S., Malte Toetzke, Andreas Kontoleon, Laura Díaz Anadón, Jan C. Minx, Barbara K. Haya, Lambert Schneider, et al. 2024. “Systematic Assessment of the Achieved Emission Reductions of Carbon Crediting Projects.” *Nature Communications* 15 (1). Springer Science and Business Media LLC. doi:10.1038/s41467-024-53645-z.

Schell, B, IJ Ackemann, and H Hass. 2002. “Reformulated and Alternative Fuels: Modeled Impacts on Regional Air Quality with Special Emphasis on Surface Ozone Concentration.” *ENVIRONMENTAL SCIENCE & TECHNOLOGY* 36 (14): 3147–56. doi:10.1021/es015817m.

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.

Shah, Sachi, Tvisha Modi, Janki Kanakia, Esha Shah, Kayvan Shah, and Archana Nanade. 2024. “A Comprehensive Approach to Unify Carbon Registries Data Access.” In *2024 OITS International Conference on Information Technology (OCIT)*, 525–29. Vijayawada, India: IEEE. doi:10.1109/ocit65031.2024.00097.

Sperling, Erik A., Thomas H. Boag, Murray I. Duncan, Cecilia R. Endriga, J. Andres Marquez, Daniel B. Mills, Pedro M. Monarrez, Judith A. Sclafani, Richard G. Stockey, and Jonathan L. Payne. 2022. “Breathless through Time: Oxygen and Animals across Earth’s History.” *The Biological Bulletin* 243 (2): 184–206. doi:10.1086/721754.

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.

Tanimoto, H., Y. Sawa, S. Yonemura, K. Yumimoto, H. Matsueda, I. Uno, T. Hayasaka, et al. 2008. “Diagnosing Recent CO Emissions and Springtime O3 Evolution in East Asia Using Coordinated Ground-Based Observations of O3 and CO during the East Asian Regional Experiment (EAREX) 2005 Campaign.” *Atmospheric Chemistry & Physics Discussions* 8 (1). Copernicus Gesellschaft mbH: 3525–61. doi:10.5194/acpd-8-3525-2008.

Trouwloon, Danick, Charlotte Streck, Thiago Chagas, and Glenpherd Martinus. 2023. “Understanding the Use of Carbon Credits by Companies: A Review of the Defining Elements of Corporate Climate Claims.” *Global Challenges (Hoboken, NJ)* 7 (4): 2200158. doi:10.1002/gch2.202200158.

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.

Yin, CQ, XJ Deng, Y Zou, F Solmon, F Li, and T Deng. 2019. “Trend Analysis of Surface Ozone at Suburban Guangzhou, China.” *SCIENCE OF THE TOTAL ENVIRONMENT* 695 (December). doi:10.1016/j.scitotenv.2019.133880.

1. Multiple-scale Atmospheric Transport and Chemistry modelling system, in this case, version 4.4.0 [↑](#footnote-ref-1)
2. I.e not pre-processed via methods mentioned in Google Earth Engine in chapter 3 [↑](#footnote-ref-2)