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Scenarios Analysis of Stratospheric Ozone Concentrations – Box Modeling and Statistical Inference

Jiang Chen

Shanghai Foreign Language School Affiliated to SISU Hangzhou, China
jefferson_jiang@outlook.com

ABSTRACT

This study uses a method that combines box models and statistical inference to deeply explore the interaction between stratospheric ozone concentration and nitrogen oxides (NOx) and chlorine compounds (ClOx). Ordinary differential equations written in MATLAB were used to simulate chemical reactions in the atmosphere. Based on these results, evaluate qualitatively the effects of NOx and ClOx on ozone concentration by further multiple linear regression analysis using VIF for multicollinearity detection and AIC for model selection. Results show that NO2 and N2O5 have significant effects on the variations of O3, while Cl is related to the content of another species. The developed fast simulator can quickly process complex chemical reaction equations and meteorological data to predict future ozone concentration changes. The research not only enhances understanding of atmospheric chemical dynamics but also helps inform environmental policy.

KEYWORDS

Stratospheric Ozone; Nitrogen Oxides (NOx); Chlorine Compounds (ClOx); Box Modeling; Statistical Inference

1. INTRODUCTION

1.1. Research Background and Importance

It is through the atmospheric ozone layer that the Earth is protected from much of the ultraviolet radiation that proves to be so dangerous to plants, animals, and human beings. Since 1960, anthropogenic emissions of ozone-depleting substances (ODS) have dramatically reduced ozone concentrations. However, due to the control of ODS usage by the 1987 Montreal Protocol and subsequent adjustments, ODS concentrations began to decrease in the mid-1990s, and as such, it is projected that the total ozone layer will revert back to pre-1980 values at some point in time [1]. Still, changes in the ozone layer do not arise solely based on ODS concentration reductions but are modulated also by changes in atmospheric composition and circulation [2]. Changes in the ozone layer are particularly significant in the Antarctic Peninsula, where changes in ozone concentration affect air temperature distribution and lead to significant regional climate changes [3]. Recent studies have shown that ozone reduction is closely associated with increased greenhouse gas emissions, leading to enhanced tropical upwelling and accelerated transport of atmospheric components [4]. Furthermore, changes in the ozone layer have profound effects on the global climate system, including effects on the dynamic exchanges between the stratosphere and troposphere [5].

This study provides an in-depth exploration of the interaction between stratospheric ozone concentration and nitrogen oxides (NO_x) and chlorine compounds (ClO_x) by combining box models and statistical inference methods. This not only helps improve the understanding of atmospheric chemical dynamics but also helps provide a scientific basis for environmental policy [6]. By studying the impact of NO_x and ClO_x on ozone concentration, we can better predict the future change trend of the ozone layer and formulate more effective environmental protection measures.

1.2. Research Objectives

This is meant to provide insight into how the stratospheric ozone concentration interacts with NO_x and ClO_x through simple box models and statistical inference techniques. Ordinary differential equations written in MATLAB are run for simulations of the chemical reactions occurring in the atmosphere to obtain results on the different impacts of NO_x and ClO_x on ozone concentration. In the course of research, the variance inflation factor was used for multicollinearity detection, whereas Akaike information criterion was used in the selection of models. Finally, multiple linear regression analysis was done. This study has developed not only a fast simulator able to quickly dispose of complex chemical reaction equations and meteorological data but also forecasts future changes in ozone concentration. It will improve the understanding of the dynamics of atmospheric chemicals and help in formulating more scientific environmental policies.

2. LITERATURE REVIEW

2.1. Historical Review of Stratospheric Ozone Research

Research into stratospheric ozone began in the early twentieth century. As scientists realized gradually the significance that the ozone layer played in absorbing ultraviolet radiation, related research has developed very fast. In the 1930s, Gordon Dobson invented an ozone meter that first measured the vertical distribution of ozone, furnishing a foundation for follow-up research [7]. In the 1970s, it was realized that, among the anthropogenic compounds containing chlorine, chlorofluorocarbons have a destructive effect on the ozone layer. Wide attention from the international community was quickly received, leading finally to the signing of the Montreal Protocol in 1987 [8]. It has reduced global emissions of ozone-depleting substances, and changes in the ozone layer were continuously monitored by scientists through satellite observations and model simulations. Gradually, research shifted in the recent years to an understanding of complicated interactions between climate change and ozone-layer processes [9]. For example, how rising greenhouse gas concentrations affect the ozone layer and regional differences during the recovery of the ozone layer have become prominent research directions [10].

2.2. Effects of Nitrogen Oxides (NO_x) and Chlorine Compounds (ClO_x) on Ozone Depletion

Nitrogen oxides (NO_x) and chlorine compounds (ClO_x) are the main catalysts for stratospheric ozone depletion. NO_x enters the stratosphere mainly through lightning and aircraft emissions, while ClO_x mainly comes from the decomposition products of anthropogenic compounds such as CFCs [11]. NO_x destroys ozone through a catalytic cycle, in which the mutual conversion of NO and NO_2 and the reaction with ozone are the main mechanisms [12]. ClO_x significantly reduces ozone concentration through the cycle reaction of Cl and ClO, especially in the polar stratosphere [13]. Recent studies have shown that although the Montreal Protocol has significantly reduced ClO_x emissions, NO_x still poses a threat to the ozone layer at certain altitudes and regions [14]. In addition, the interaction between NO_x and ClO_x has also been found to have a compound effect on ozone depletion, which increases the complexity of predicting ozone recovery [15].

2.3. Advances in Box Models and Statistical Methods in Atmospheric Chemistry

Box models are widely used in atmospheric chemistry research. They simplify complex chemical kinetic systems by partitioning the chemical reaction processes in the atmosphere [16]. These models can effectively simulate the spatial distribution and temporal variation of chemical substances in the atmosphere by setting different initial conditions and boundary conditions [17]. Therefore, in the last few years, statistical inference methods have increased in computing power and data acquisition has become easier and has had wide applications in atmospheric chemistry research [18]. For example, Akaike Information Criterion is applied to model selection and variance inflation factor can detect multicollinearity problems [19]. These methods increase not only the model accuracy but they also give insight into the atmospheric chemical processes. Box models can thus be combined with statistical methods to make more precise predictions of changes in ozone concentrations provided perturbations to different factors are applied.

3. METHODOLOGY

3.1. Box Model / Ordinary Differential Equation Model

In our comprehensive investigation of the stratospheric ozone concentrations, a box modeling approach is employed to simulate the impacts of nitrogen oxides (NO_x) and chlorine com-pounds (ClO_x) on ozone levels. The study encompasses varying initial concentrations of these substances to examine their effects on the steady-state concentration of ozone. This method provides an insightful analysis into the complex interplay of chemical constituents within the stratosphere.

In this study, MATLAB was utilized for numerical simulations and data analysis to investigate the impact of various chemical substances on ozone concentration. We developed a custom ordinary differential equation (ODE) solver 'New Mysolver'(Appendix 1), which models a series of complex atmospheric chemical reactions.

Our model is based on a set of chemical reaction equations that describe the interactions of ozone (O_3) with NO_x and ClO_x, and other substances.

Table 1. Chemical reactions simulated in the box model in this study.

O_2+hv=2O	O+O2=O_3	O_3+hv=O+O_2	O+O_3=2O_2
O_3+hv=O1D+O_2	NO_2+hv=NO+O	O1D+O_3=2O_2	NO+O_3=NO_2+O_2
NO_2+O=NO+O_2	O1D+M=O+M	NO_3+NO=2NO_2	NO_3+hv=0.89NO_2+0.11 NO+0.89O_3
N_2O_5=NO_2+NO_3	NO_3+O=NO_2 +O_2	NO_2+O_3=NO_3+O_2	NO_2+NO_3+M=N_2O_5+M
NO_2+O+M=NO_3+M	Cl+O_3=ClO+O_2	OH+O_3=HO_2+O_2	ClO+HO_2 =HOCl+O_2
HOCl+hv=OH+Cl	ClO+O=Cl+O_2	$ClONO_2$+hv=Cl+NO_3	ClO+NO_2 +M=$ClONO_2$+M
H+O_3=OH+O_2	OH+O=H+O_2	HO_2+O=OH+O_2	$ClONO_2$+hv=ClO+NO_2

Our model, based on box model code in the appendix, simulates the dynamics of reactions depicting temporal changes in the concentrations of atmospheric substances. Calculating molecular concentration based on atmospheric pressure and determining variations in solar radiation, it reflects diurnal variations different substances undergo. Considering various reaction pathways of nitrogen oxides and chlorine compounds, including their interactions with ozone, the model outputs changes in ozone concentration under different environmental conditions. The data, showing final steady-state ozone concentration under different initial concentrations, is extracted and organized into a table.

3.2. Akaike Information Criterion (AIC) Model

The stepwise model selection procedure is a well-established method for choosing the most appropriate predictors for a multiple regression model. This method involves sequentially comparing multiple linear regression models with different predictors, with the goal of improving a performance measure through a greedy search. The performance measure used by stepwise model selection is typically an information criterion, which balances the fitness of a model with the number of predictors employed. The Akaike Information Criterion (AIC) is one common information criterion used to determine the best model, which is the one that minimizes the considered information criterion. It is based on balancing the model fitness and its complexity:

$$AIC = e^{\left(\frac{2k}{T}\right)} \frac{\sum_{t=1}^{T} e_t^2}{T} = 2k - 2\ln(L) \tag{1}$$

Where $e^{\left(\frac{2k}{T}\right)}$ is penalty factor, k is the number model parameters, L is the likelihood of model.

After identifying the most suitable predictors by comparing the AIC, we will conduct a multivariate linear regression analysis. This approach will enable us to fit a multivariate function that best explains the relationships and interactions among the variables selected.

3.3. Multiple Linear Regression Analysis

During the variable selection process, we also use variance inflation factor (VIF) to detect multicollinearity problems. VIF is a statistical method to measure the linear relationship between an independent variable and all other independent variables. The higher the VIF value, the stronger the multicollinearity between the variable and other variables. If the VIF value exceeds 10, it is generally considered that the variable has high collinearity and should be considered for removal from the model. In this way, we can improve the robustness and interpretability of the model and ensure that the results are more reliable.

The analysis of the data obtained from these simulations is performed through a multiple linear regression approach. Multiple linear regression is a statistical technique that examines the linear relationship between a dependent variable (Y) and two or more independent variables (X_1, X_2, ... X_k). The mathematical formulation of the model is:

$$Y = \beta 0 + \beta 1X1 + \beta 2X2 + ... + \beta kXk + \varepsilon \tag{2}$$

Here, Y represents the dependent variable (steady-state ozone concentration in this study),

X_1, X_2, ...X_k are the independent variables (concentrations of other substances), β0, β1, β2, ..., βk are the model parameters including the intercept β0 and slopes β1, β2, ..., βk, and ε is the error term. This regression model enables a comprehensive quantification of the sensitivity of ozone concentration to variations in NO_x and ClO_x levels.

3.4. Fast Simulator

The use of an integrative approach, combining advanced box modeling with statistical analysis, helps in understanding the dynamics of stratospheric ozone and the impact of atmospheric constituents' changes on ozone concentration. This approach aims to create a fast simulator that can process complex chemical reaction equations and meteorological data. This simulator will aid in predicting future changes in ozone concentrations and understanding the influence of variations in NO_x and ClO_x levels on ozone concentration. These findings will significantly contribute to environmental policy formulation and the global effort to preserve the ozone layer.

4. RESULT AND ANALYSIS

4.1. Dataset

Initially, we established the initial concentrations of fourteen substances within the box model. The units for these concentrations are molecules per cubic centimeter.

Table 2. Initial concentration

O1D	O	O_3	NO	NO_2	NO_3	N_2O_5
187	1.24E9	2.0E12	1	9.22E8	2.2E6	7.86E8
Cl	ClO	HOCl	$ClONO_2$	OH	OH2	H
1.0E8	1	1	1	1.0E8	0	0

In our study, we employ a periodic function to simulate the diurnal variation of solar radiation, thereby graphically illustrating its fluctuation.

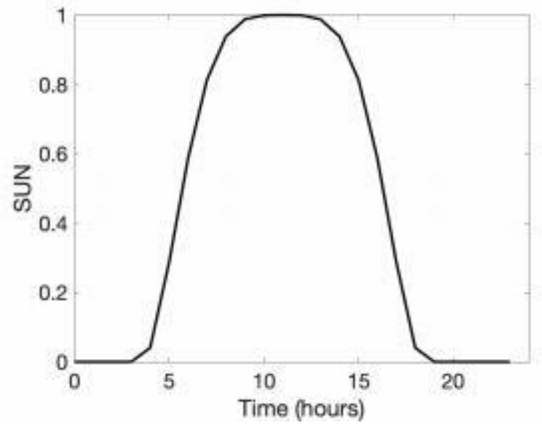
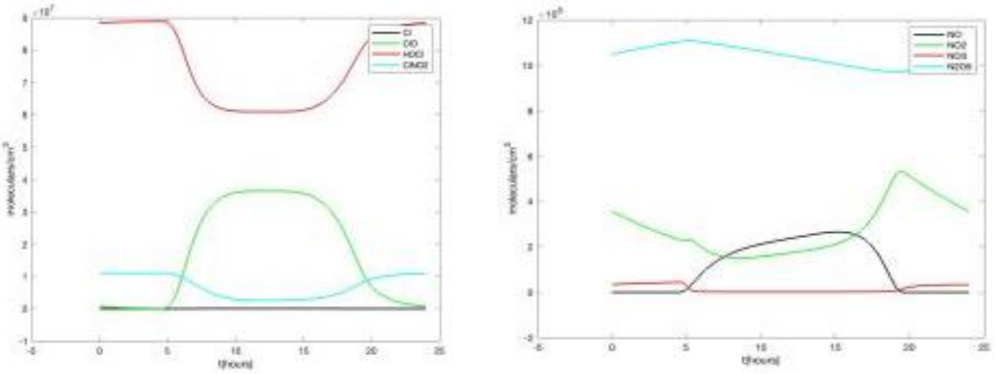


Figure 1. Solar radiation

This approach enables us to ascertain the daily variation trends of nitrogen oxides (NO_x) and chlorine compounds (ClO_x), critical to understanding their atmospheric behavior.



(a) chlorine compounds (b) nitrogen oxides

Figure 2. NO_x and Cl_x daily variation trends

4.2. [O3] In Different Initial Field

In our study, we adjusted the initial concentrations of each nitrogen oxide and chlorine compound. We varied the initial concentrations of each substance from 80 percents to 120 percents of their original values, in increments of 2 percents. We then recorded the average concentration of ozone in its steady state over a duration of 500,000 seconds (the last 6 days) for each of these initial conditions. This approach allowed us to systematically analyze how variations in the initial concentrations of these substances influence the equilibriumconcentration of ozone.

4.3. AIC and Multiple Linear Regression Analysis

Our approach involves employing backward, forward, and stepwise (both) selection methods within the code to examine the relationship between ozone concentrations and the initial concentrations of various substances. Ultimately, we aim to identify the combination with the smallest Akaike Information Criterion (AIC) value and subject it to multivariate regression analysis.

The outputs of the code were organized to yield the optimal combination for multivariate linear regression, as illustrated below:

$$O_3 \sim NO_2 + N_2O_5 + Cl, \text{ data = allozone} \quad (3)$$

Table 2. Optimal combination

Coefficients:			
(Intercept)	NO_2	N_2O_5	Cl
3.728e+12	-1 .635e+02	-3 .271e+02	8.344e+02

The coefficients obtained from the linear regression model, as shown in the output above, play a crucial role in understanding the relationships between the dependent variable (ozone concentration, $[O_3]$) and the independent variables (NO_2, N_2O_5, and Cl concentrations).

NO_2 Coefficient (-1.635e+02): The negative coefficient for NO_2 indicates that it serves as a sink for ozone. This means that an increase in the concentration of NO_2 is associated with a decrease in the concentration of ozone. Nitrogen oxides (NO_x), which include NO_2, are known to participate in catalytic cycles that destroy ozone molecules in the stratosphere.

N_2O_5 Coefficient (-3.271e+02): Similar to NO_2, the negative coefficient for N_2O_5 suggests that it also acts as a sink for ozone. N_2O_5 is involved in the nighttime chemistry of the atmosphere and can lead to the formation of NO_x, which in turn depletes ozone.

Cl Coefficient (8.344e+02): The positive coefficient for Cl implies that it acts as a source for ozone, meaning that an increase in Cl concentration is associated with an increase in ozone concentration. This positive relationship could be indicative of complex chemical interactions in the atmosphere where chlorine compounds, under certain conditions, may lead to ozone formation or be involved in reactions that do not deplete ozone.

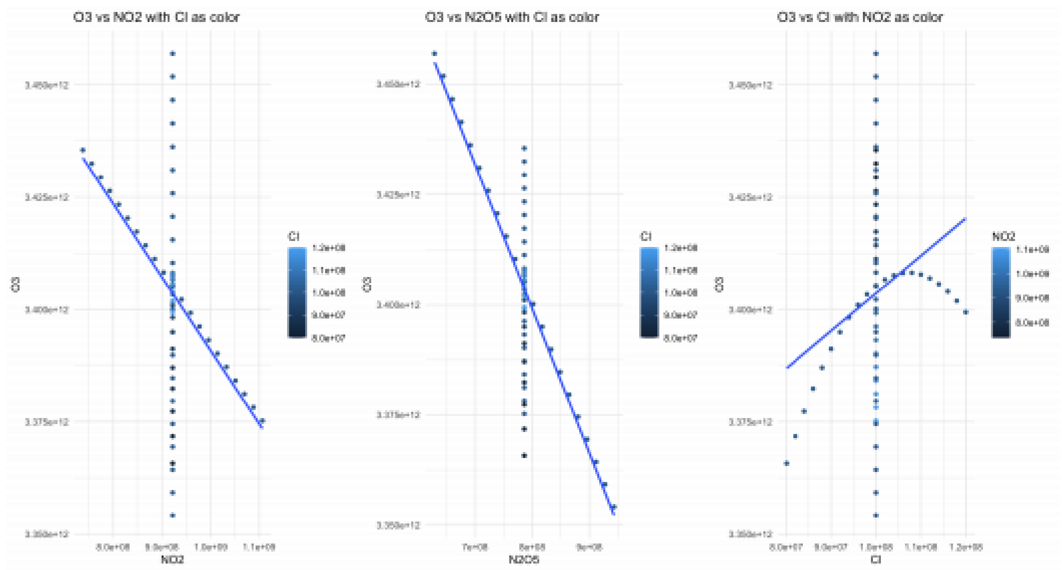


Figure 3. linear regression for each predictor

Our findings have culminated in a precise formulation that delineates the relationship be- tween the steady-state concentrations of stratospheric ozone and the initial concentrations of stratospheric NO_x, ClO_x, and Cl, which can be considered as a fast simulator to predict the concentration of ozone:

$$[O_3] = -1.635 \times 102\ [NO_2] + -3.271 \times 102\ [N_2O_5] + 8.344 \times 102\ [Cl] + 3.728 \times 1012$$

5. DISCUSSION

This study, through the integration of box modeling and statistical analysis, offers a comprehensive understanding of the interactions between ozone and various atmospheric elements. Utilizing MATLAB’s complex Ordinary Differential Equations (ODEs) ensures an authentic simulation of atmospheric chemical reactions, accurately portraying the chemical dynamics of the stratosphere. The employment of multivariate linear regression analysis and the Akaike Information Criterion (AIC) for model selection solidifies the research’s statistical credibility, rendering the results both scientifically and statistically robust. The development of a rapid simulator aids in forecasting ozone concentration scenarios, assisting policymakers and researchers in addressing ozone depletion. This interdisciplinary endeavor significantly advances understanding in atmospheric chemistry, environmental science, and statistical modeling. However, the study faces limitations such as the potential oversimplification of certain atmospheric interactions, inaccuracies in predicted ozone levels, and the overlook of other atmospheric components' influence on ozone concentration. While multiple linear regression and AIC are effective, they may falter in addressing complex nonlinear relationships and variable interactions. Future research should aim to overcome these constraints to enhance our understanding of the ozone layer's dynamics.

6. CONCLUSION

This study engaged in an in-depth investigation of stratospheric ozone dynamics, providing key insights into interactions between ozone and atmospheric constituents such as nitrogen oxides and chlorine compounds. By employing an innovative box modeling approach that combined advanced statistical methods with box modeling techniques, our research not only illuminated complex chemical processes occurring within the stratosphere but also provided a robust framework for simulating and predicting future concentration scenarios of ozone concentration.

Applying ordinary differential equations in MATLAB enabled accurate simulations of atmospheric chemical reactions, improving our understanding of ozone layer dynamics. Our findings highlight the critical roles played by NO_x and ClO_x in depleting ozone, thus underscoring their importance as substances to monitor to reduce their impact. Furthermore, developing a fast simulator represents an immense advance towards forecasting future ozone concentration levels. Change analysis provides researchers and policymakers with a powerful tool.

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