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Complexity Analysis of Atmospheric Pollutants: Taj Mahal

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ABSTRACT

This paper deals with the mathematical modelling of environment cycle where atmospheric elements are competing for naturally available oxygen. The nonlinear kinematic reactions between the atmospheric components have been studied through differential rate equations which form a nonlinear six dimensional system. Through numerical simulation of this model the reaction dynamics of atmospheric pollutants in atmosphere of Agra city has been simulated. The trend for levels of Nitrogen Oxide, Nitrogen Dioxide and Ozone are observed in sync with the actual trend observed. The level of Carbon Dioxide is observed to be very high through simulation indication a need of massive afforestation to absorb it from air in order to reduce the corrosion of Taj Mahal.

Keywords: nonlinear interactions, intermediate reaction, reaction network, reaction dynamics, simulation.

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Introduction

In the past one decade environmental pollution has become the matter of serious concern which is affecting the nature and the ecological species by disturbing the food chains and the environmental cycles. The industrial growth and exploitation of natural resources at massive scale has led to pollution of air, water and soil. As a result the levels of primary pollutants like oxides of nitrogen, sulphur dioxide and carbon oxides have increased by a greater extent leading to hike in concentration of secondary pollutants like nitric acid, sulphuric acid, sulphide and ozone.

These secondary pollutants along with primary pollutants are not only affecting the air quality in atmosphere but also hazardous to human world. Especially in developing countries like India the problem is severe as due to uncontrolled emission of the pollutants from industries and vehicles on roads the level of pollutants are very high [1, 4, 6]. With enforcement of new guidelines on emissions to protect environment some control has been observed but still the problem persists due to lack of afforestation. Even after attempts being made due to growing urbanization there effect is getting nullified as forest cover in several cities are shrinking faster. As a result the biological control which trees provide as massive biological absorber of carbon dioxide and nitrites are getting eliminated under deforestation.

In India the extent of hazards caused by high atmospheric pollution is not restricted to human health only but extends to corrosion of its heritage monuments. The worst affected among these heritage monuments has been Taj Mahal one of the seven wonders and pride of Indian heritage. The corrosion caused by acid rain and high content of acid components in the atmosphere has been highlighted in several reports by Indian news media. Due to awareness a lot of strict regulations have been implemented nearby the monument sight but still the pollutant level and small forest cover of Agra is not letting the danger caused pollution be eliminated.

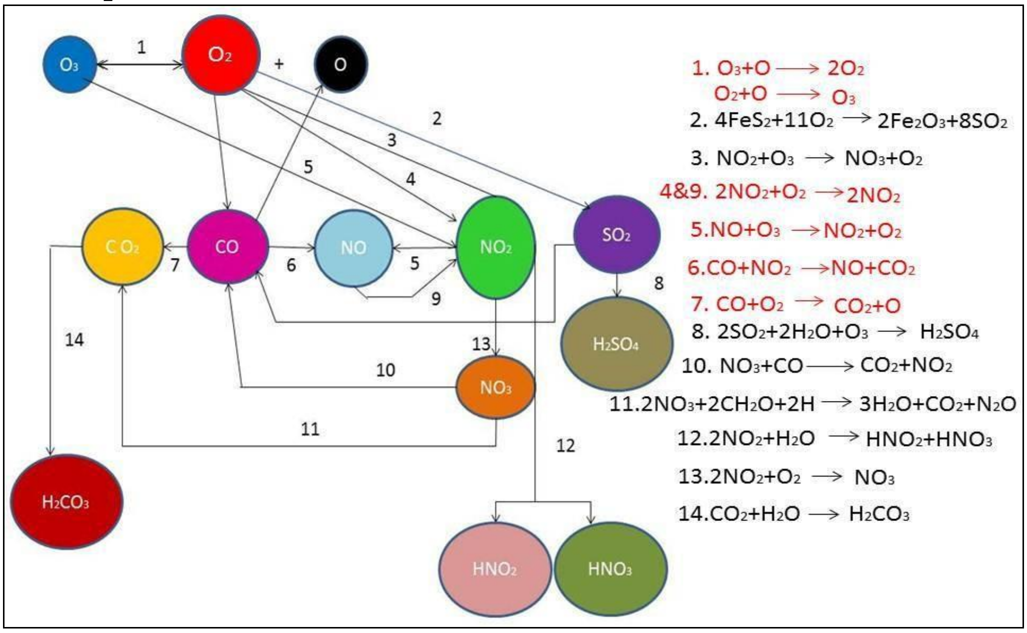
Nature comprises of several environmental cycles like Ozone cycle, Nitrogen cycle, Oxygen cycle and Carbon cycle. These cycles are interconnected by intermediate reactions which gives feedback of intermediate components in the individual. This intermediate reaction network is crucial as it is the dynamics of these reaction which plays crucial role in effective functioning of the cycles. The core of the problem is high level of primary pollutants which lead to the generation of secondary pollutants like nitric acid, sulphuric acid and carbonic acid in atmosphere causing the high level of corrosion of white marble surface of Taj Mahal turning it yellow [8, 9]. Thus it is important to study the dynamics of these pollutants in the atmosphere.

In this paper mathematical modelling of dynamics of atmospheric elements have been done and analysed. The atmospheric components include the oxides of nitrogen, carbon and ozone with supplies from emissions from industries and vehicles causing their concentration in atmosphere to rise beyond the threshold level making them pollutants. Oxygen is the common element in these reactions. From the reaction network the intermediate reaction network is obtained. A six dimensional differential equation system is determined from the intermediate reaction network whose simulation predicts the future concentration level of these primary pollutants in atmosphere.

Mathematical Model

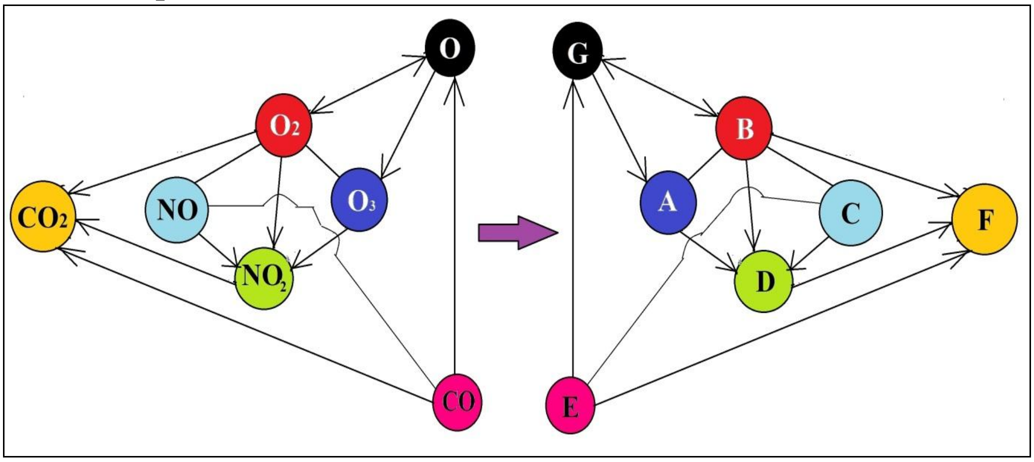
In this paper the reaction dynamics of intermediate reactions between primary pollutant components in air have been mathematically modelled and analysed through simulation. The reaction network between these primary pollutants is as follows:

Figure 1. *The Reaction Network between Primary Pollutants O_3, NO, NO_2, CO and CO_2*



From the above mentioned reaction network we obtain the following intermediate reaction network shown as follows:

Figure 2. *Intermediate Reaction Network of Primary Pollutants O_3, NO, NO_2, CO and CO_2*



The chemical reactions for the intermediate reaction network are as follows:

$$1.\ NO + O_3 \xrightarrow{k_1} NO_2 + O_2, \qquad k_1 = 1.08\times10^{10}\, cm^3 mol^{-1}\sec^{-1}$$

$$2.\ 2NO + O_2 \xrightarrow{k_2} 2NO_2, \qquad k_2 = 2.80\times10^{12}\, cm^6 mol^{-2}\sec^{-1}$$

$$3.\ CO + O_2 \xrightarrow{k_3} CO_2 + O, \qquad k_3 = 2.20\times10^{11}\, cm^3 mol^{-1}\sec^{-1}$$

$$4.\ NO_2 + CO \xrightarrow{k_4} CO_2 + NO, \qquad k_4 = 4.32\times10^{14}\, cm^3 mol^{-1}\sec^{-1}$$

$$5.\ O_3 + O \xrightarrow{k_5} 2O_2, \qquad k_5 = 6.022\times10^{8}\, cm^3 mol^{-1}\sec^{-1}$$

$$6.\ O_2 + O \xrightarrow{k_6} O_3, \qquad k_6 = 9.3\times10^{9}\, cm^3 mol^{-1}\sec^{-1}$$

This leads to a six dimensional ordinary differential equation system given by following equations:

$$\dot{x}_A = -k_1 x_A x_C - k_5 x_A x_G + k_6 x_B x_G + s_A - d_A x_A$$

$$\dot{x}_B = -k_2 x_B x_C{}^2 - k_3 x_B x_E + k_1 x_A x_C + k_6 x_B x_G + s_B - d_B x_B$$

$$\dot{x}_C = -2k_2 x_B x_C{}^2 - k_1 x_A x_C + k_4 x_D x_E + s_C - d_C x_C$$

$$\dot{x}_D = -k_4 x_D x_E - 2k_2 x_B x_C{}^2 + k_1 x_A x_C + s_D - d_D x_D$$

$$\dot{x}_E = -k_4 x_D x_E - k_3 x_B x_E + s_E - d_E x_E$$

$$\dot{x}_F = k_4 x_D x_E + k_3 x_B x_E + s_F - d_F x_F$$

$$\dot{x}_G = -k_5 x_A x_G - k_6 x_B x_G + k_3 x_B x_E + s_G - d_G x_G$$

where

$x_A = \text{concentration}; s_A = \text{supply}; d_A = \textit{decay rate for } O_3$

$x_B = \textit{concentration}; s_B = \text{supply}; d_B = \textit{decay rate for } O_2$

$x_C = \textit{concentration}; s_C = \text{supply}; d_C = \textit{decay rate for } NO$

$x_D = \textit{concentration}; s_D = \text{supply}; d_D = \textit{decay rate for } NO_2$

$x_E = \textit{concentration}; s_E = \text{supply}; d_E = \textit{decay rate for } CO$

$x_F = \textit{concentration}; s_F = \text{supply}; d_F = \textit{decay rate for } CO_2$

$x_G = \textit{concentration}; s_G = \text{supply}; d_G = \textit{decay rate for } O$

Results and Discussion

After obtaining the differential equation using MATLAB for the following input the simulation is carried out:

Element/*Quantity*	O_3	O_2	NO	NO_2	CO	CO_2	O
$Supply(\mu mol / m^3)$	2.378	0.39	0.552	2.376	43.41	22138.12	1.0
$Decay\ rate(per\ \text{sec})$	0	0	0.0011	0.0002	0	0	0

Taking data obtained from online monitoring site of Central Pollution Control Board of India for Agra city [3, 5, 7] as input the simulation is performed. The following time series is obtained for concentration levels of the primary pollutants as shown:

Figure 3. *Time Series of Pollutants O_3, NO, NO_2, CO and CO_2 from January 2016 to May 2016*

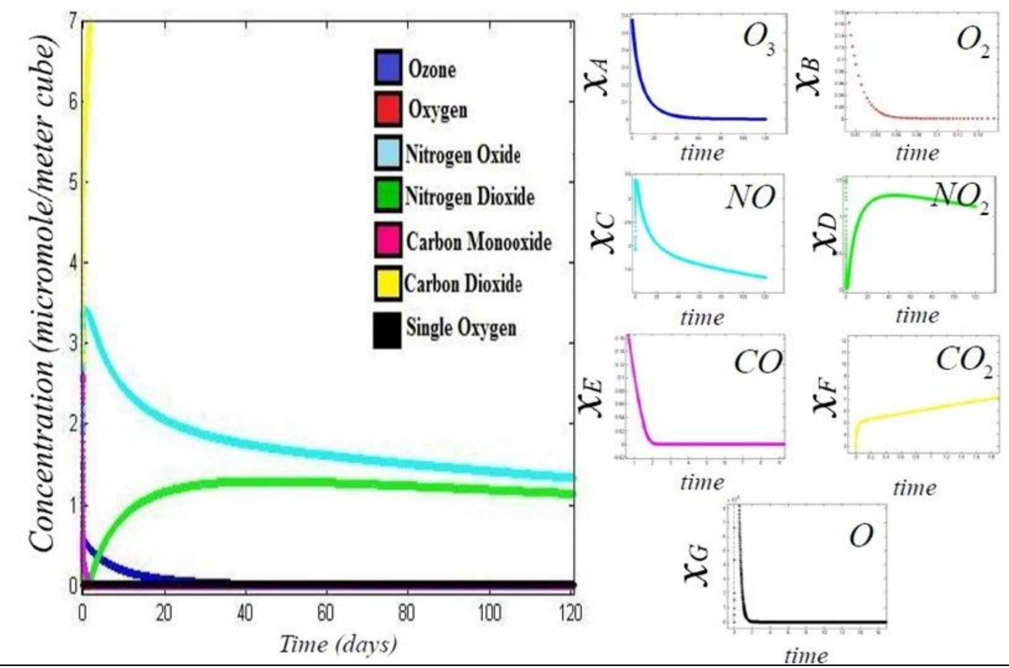
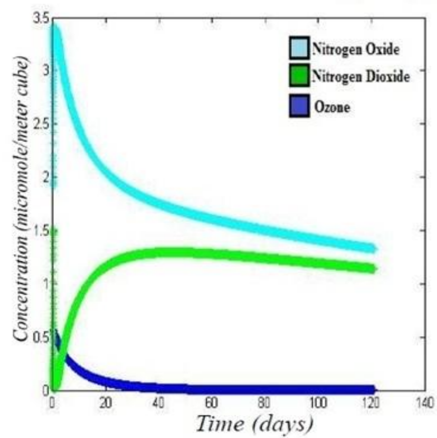
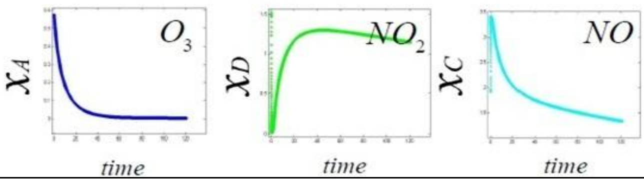


Figure 4. *Time Series of Pollutants O_3, NO and NO_2 from January 2016 to May 2016*

Pollutant	Actual (Micromoles /meter cube) 01/01/16	Actual (Micromoles/meter cube) 01/05/16	Observed (Micromoles/meter cube)
O_3	0.578	0.37	0.02
NO_2	1.517	1.26	1.13
NO	1.908	1.45	1.33





It is observed that the actual values of Nitrogen Oxide and Nitrogen Dioxide obtained from CPCB data match almost with the value obtained from our simulation. However the value of ozone concentration doesn't match with the predicted values. The reason behind the matching of results for Nitrogen Oxide and Nitrogen Dioxide is due to the inclusion of complete chain of reactions between both of them. As all the reactions for ozone are not included thus the mismatch between the values for ozone is observed.

Conclusions

From the Simulation the trends obtained are similar though the values obtained from CPCB open data source and the values obtained from our simulation are found matching for Nitrogen oxide and Nitrogen Dioxide unlike ozone. The trend of hike in Carbon Dioxide concentration is alarming as it will lead to more carbonic acid concentration and increase in threats to Taj Mahal from Acid Rain. The high concentration levels of Carbon Dioxide need to be controlled by Afforestation and controlling the vehicle emission by controlling the fuel quality.

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