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Dynamic Indicator for the Prediction of Atmospheric Pollutants

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Abstract: This paper deals with the study of the co-existence of the chemical compounds CO_2 and NO_3 in substantial amounts over a long period of time for a wide range of atmospheric conditions. Using the presence of chemical compounds in the nature, the mathematical model for the behaviour is modelled. Lyapunov Characteristic Exponents (LCE) along with the indicators i.e., Small Alignment Index (SALI), Fast Lyapunov Indicator (FLI) and Dynamic Lyapunov Indicator (DLI) are applied to make a distinction concerning ordered/unordered trajectories of the dynamics for these chemical compounds. DLI indicator gives the largest of the eigenvalues of the Jacobian matrix and correct conclusions when applied to models of dynamical systems. FLI method is used to differentiate between regular motion and chaos in the intricate systems. SALI is a competent indicator of predictability which could discriminate amid different steady as well as randomness levels. FLI as well as SALI advance eigenvectors via iterating the progressing Jacobian matrix at every iteration for the set-up. Entropy, on the other hand, is the measure of randomness that would be generated as the system changes its state from consistency to chaos. It is observed that for stable environment the mutual sustenance of NO_3 and CO_2 should be maintained in a balanced manner, otherwise the environmental cycles get disrupted which results in rise in pollution levels.

Key words: Fast Lyapunov Indicator-(FLI), Dynamic Lyapunov Indicator-(DLI), Small Alignment Index-(SALI), non-linear predictive model, Lyapunov Exponents, entropy.

Introduction

The key constituents for air are nitrogen (78.1%), oxygen (20.93%), carbon-dioxide (0.03%), presence of water-vapour along with suspended particles. NO_3 and CO_2 are major oxygen consuming chemical compounds in the atmosphere, for a long period of time to maintain the widespread atmospheric surroundings in substantial amounts. In general, NO_3 reacts promptly with a lot of unsaturated hydrocarbons in the atmosphere which further impacts the resources of the species and the associated deprivation produces. NO_3 mainly compounded via the reaction of nitrogen dioxide (NO_2) and oxygen present in radical, elemental and compound forms. CO_2 is referred as a greenhouse gas. Deforestation, burning-of-coal, oil etc. increase the atmospheric CO_2 causing greenhouse effect. Atmospheric oxygen depletes almost at the similar rate as there is increase in atmospheric CO_2, that explains that source of the alteration is through the discharge of carbon intermingling with the atmospheric-oxygen instead of the usual discharge of CO_2. Bhardwaj (2017) studied the interaction dynamics of chemical pollutants and discussed about their interactions in the environment as can be seen in Figure 1.

The amount of oxygen is limited in atmosphere but is uniformly available to all the elements in an adequate manner. With passage of time the concentration of

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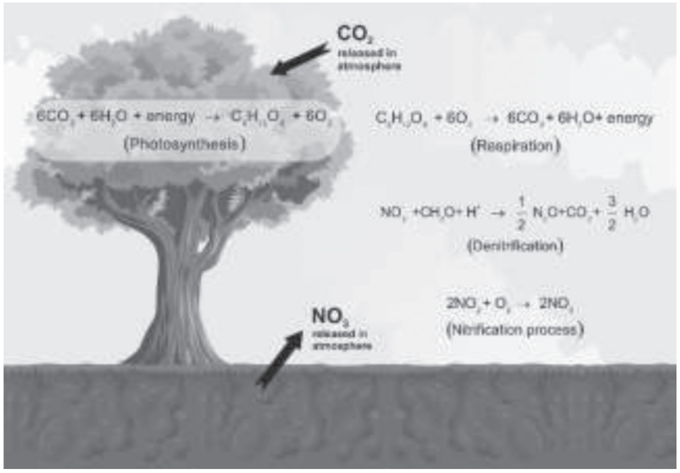

Figure 1: Interaction of pollutant species in the environment.

elements grows which produces new compounds, leading to load generation on the resource as consumption becomes faster. The statistics available for fossil fuel usage states that there has been that particular long-term reduction into the atmospheric O_2 concentration, as O_2 is conveyed to CO_2 during combustion. This is although a very unhurried procedure, in comparison towards total quantity of O_2 but prevalent on Earth's atmosphere for a noticeable time period. Thus, demand grows over supply which leads to increase in the encounters between these elements. Elements may interact through linear or non-linear interactions in nature depending on simple or complex environmental cycle respectively.

Chaotic notion is defined as the sub-branch of dynamical theory concentrated on the behaviour for nonlinear dynamics of structures which would be extremely delicate towards preliminary conditions. Environmental situations like weather and climate are frequently non-linear; therefore, presence of randomness is quite normal. The different tools exist towards classifying various orbits which can be listed are time series analysis, phase-diagrams, Poincaré maps, power spectra, etc. These introduced procedures prove to be powerful but they are not sufficient to segregate stable/unstable orbits if the set-ups endure greater degrees of freedom. Lyapunov characteristic exponents (LCEs), have proven to be highly useful in terms of separating consistent and frenzied orbits. Also, offer to measure the degree of chaos. Recently, advances among non-linear dynamics deliver various novel implements i.e., FLI, SALI, DLI etc. so as to understand chaotic behaviour.

Anna et al. (2018) focused on methods of removal of pollutants from polluted water. Antonopoulos et al. (2004) studied the efficient indicator SALI for Hamiltonian Systems. Bhardwaj (2016) discussed the environmental scenarios through wavelet and fractal methods. Interaction of atmospheric components in the environmental cycle was modelled by Bhardwaj (2017). Bhardwaj and Bangia (2016) developed the model for meditating body. Bhardwaj and Bangia (2018) studied the spread of Human-Immunodeficiency-Virus. Bhardwaj et al. (2007) studied various environmental issues with the help of various existing techniques like fractal and wavelet methods. Bhardwaj et al. (2014) studied the dynamical impact of pollutants on health assessment. In addition, Bhardwaj et al. (2014) discussed the different methodologies, forecasting techniques to predict air pollution, water pollution and weather forecasting. Choudhury et al. (2017) implemented the model for optimization of decision-making statistics in water treatment in India. Deleanu (2011) explained in detail the Lyapunov indicator tool for distinction of various orbits.

Durai and Bhardwaj (2014) estimated qualitative rainfall using an innovative multi-model technique. The concept of FLI was proposed by Froeschle (2001). Hassan et al. (2017) described the impact of Ecotourism in Malaysia. Kumar (2017) contributed towards the environment via recycling waste and recycled papers. Parmar and Bhardwaj (2013) discussed in detail numerous methods including statistical, time-series, variability, and predictability index and fractality analysis on water quality dynamics. Saha et al. (2006) measured chaos with the help of SALI indicator. Skokos et al. (2001) discussed an alignment indices methodology for different nature of orbits. Teka et al. (2018) explained in their study different patterns of the Izhikevich model.

In this paper the following section gives the Methodology which includes definitions of the Lyapunov Characteristic Exponents (LCE), DLI, FLI and SALI. Routh-Hurwitz stability analysis is performed to observe the regular and chaotic behaviour of the model. In next section, the mathematical model of 2-dimensional system of logistic dynamic interaction between environmental components in atmosphere is discussed when two or more elements are competing for oxygen available in nature. Lyapunov Exponents along with some regular and chaotic orbits of the 2-dimensional system by changing the constant values of system parameters is numerically simulated and discussion of the results so obtained is given in penultimate section. Conclusions are discussed in the last section.

Methodology

Lyapunov Characteristic Exponents (LCE)

Lyapunov exponent deals with the relative stability of the equations of system which are the most direct indicators and quantifiers of deterministic chaos. The dimension of the phase space defines the number of LCEs that the dynamical system can have. When the exponents are ≤ 0, the neighbourhood preliminaries implies towards converging to each other further, initial epsilon inaccuracies reduce with respect to time. Whereas when they are positive, infinitesimally nearby preliminaries deviate from each other exponentially, wherein accuracies in initial conditions propagate with respect to time. Thus, this scenario is defined as intricate dependency upon initial conditions that explains randomness.

The eigenvalues of the limit-cycle illustrate the degree of convergence/divergence of trajectories of the orbit. LCEs are considered to be normalizations of eigen values of stable or limit-cycle orbits. Determination of LCEs for non-linearity involves simulation for the differential-equalities along with the attached equalities of variation. Largest eigen value of the multifaceted dynamics serves as the indicator for randomness. Of one-dimensional mapping, the parting at n^{th} iteration can be known through:

$$|x_n - y_n| \approx \left(\prod_{t=0}^{n-1} |f'(t)|\,|x_0 - y_0|\right) \tag{1}$$

where $|x_0 - y_0| \ll 1, |x_n - y_n| \ll 1,$ and $x_n = f_n(x_0)$, $y_n = f_n(y_n)$ correspondingly at the n^{th} iteration of cycles for x_0 and y_0 under f. Then, the exponential separation rate $\log |f'(x)|$ of two proximate primary conditions, be an average of the complete trail, could be given by

$$\lambda(x_0) = \lim_{n\to\infty} \frac{1}{n} \log\left(\prod_{t=0}^{n-1} |f'(x_t)|\right) \tag{2}$$

where $\prod_{t-0}^{n-1} |f'(x_t)| \approx e^{\lambda(x_0)n}$ for, $n >> 1$. The $\lambda(x_0)$ modified in (2) is LCE of trajectory for x_0. Quantitatively, two curves in phase-space via early separation δx_0 deviate

$$|\delta x(t)| \approx e^{\lambda t} |\delta x(0)| \tag{3}$$

where $\lambda>0$ is the Lyapunov exponent. Lyapunov exponents are equal to the real parts of the eigen-values at the critical points.

Some of the indicator tools of Lyapunov exponents which can be applied to real-life systems are defined as follows.

Dynamic Lyapunov Indicator (DLI)

Let J be the Jacobian matrix of the system. The eigenvalues, λ_j of the matrix J are calculated as:

$$J - \lambda_j I = 0 \tag{4}$$

as I is the identity matrix and J is the Jacobian matrix. Then, the largest eigenvalues are plotted. When the eigenvalues form a definite pattern, then the motion is regular and if they are distributed randomly (with no definite pattern), then the motion is chaotic.

Fast Lyapunov Indicator (FLI)

This indicator is defined as follows:
Starting with m-dimensional basis:

$$V_m(0) = (v_1(0), v_2(0),\ldots,v_m(0))$$

Rooted in an n-dimensional space with the primary condition:

$$(x_1(0), x_2(0),\ldots,x_m(0)),$$

then consider for every iteration, largest eigenvectors amid vectors of the evolving basis. Consequently, FLI gets based on:

$$FLI = \sup \|v_j\|, \; j = 1,2,\ldots,m \tag{5}$$

Hence, norm of the deviancy vector spreads rapidly towards totally diverse values for unvarying and disordered paths that may vary via many orders of scale. The performance offers towards classifying steady state, at which FLI contains comparatively small-values, and frenzied state, at which FLI simulates larger values. Froeschle shows either FLI upsurges exponentially depicting chaos or linear to indicate consistency. FLI lists the instantaneous value of norm of the deviance vector and do not attempt towards simulating limit values, as $t \to \infty$.

Small Alignment Index (SALI)

Contemplate the n-dimensional phase diagram for the dynamical structure. Further, let the trajectory in the space having preliminary condition:

$$P(0) = (x_1(0), x_2(0),\ldots,x_m(0))$$

along with the deviance-vector $\xi(0) = (dx_1(0), dx_2(0), \ldots, dx_n(0))$ through initial point $P(0)$. So as towards calculate the SALI for any known path, ensue time advancement with the path along with the primary condition, $P(0)$ itself plus the of two deviance vectors $(\xi_1(t), (\xi_2(t))$ that in the beginning are directed in two various directions. Progress of these deviance vectors gets specified through variational equalities for the stream and through a tangent-map of the discrete-time structure. Two separation vectors $\xi_1(t)$ and $\xi_2(t)$ have to be normalized at each time step for SALI to be simulated as:

$$SALI(t) = \min\left\{\left\|\frac{\xi_1(t)}{\|\xi_1(t)\|} + \frac{\xi_2(t)}{\|\xi_2(t)\|}\right\|, \left\|\frac{\xi_1(t)}{\|\xi_1(t)\|} - \frac{\xi_2(t)}{\|\xi_2(t)\|}\right\|\right\} \quad (6)$$

The n-dimensional environment where $n \geq 2$, SALI oscillates in the neighbourhood of non-zero values indicating systematic paths, whereas the values converges towards zero signifying chaotic paths. However, for 2D maps the SALI inclines towards zero for both the orbits, but follow entirely diverse rate of change of time, that allows discrimination amid the cases.

Entropy

The entropy is basically the amount of randomness in any event taking place in the system. In general, entropy is the measure-of-probability for the disarrangement of system at macroscopic level. In a system that can be described by variables, there are a certain number of configurations those variables may assume. In mathematics, a more abstract definition is used.

Algorithm for the Simulation of Entropy

1. Let n be the size of the sample space for the events that may be functions as: $F_1, F_2, \ldots, F_n$.
2. Contemplate that $p_1, p_2, \ldots, p_n$ are the probabilities that the functions (events) are in the states $f_1, f_2, \ldots, f_n$.
3. Equivalently, consider the probability mass functions (pmfs) are $p(f_1), p(f_2), \ldots, p(f_n)$.
4. So, combined entropy of $F_1, \ldots, F_n$ which can be derived from the summation of product of the *pmfs* and the negative logarithm of *pmfs* is termed as:

$$\hbar(F_1, \ldots, F_n) \equiv -\sum_{x_1}\ldots\sum_{x_n} p(f_1,\ldots,f_n)\log_2\left[p(f_1,\ldots,f_n)\right].$$

As $p(f)$ denotes probability with which $\hbar$ is in the state f; $p \log_2 p$ termed to be zero if p equals zero.

Figure 2 depicts the role entropy plays in changing the state of the system.

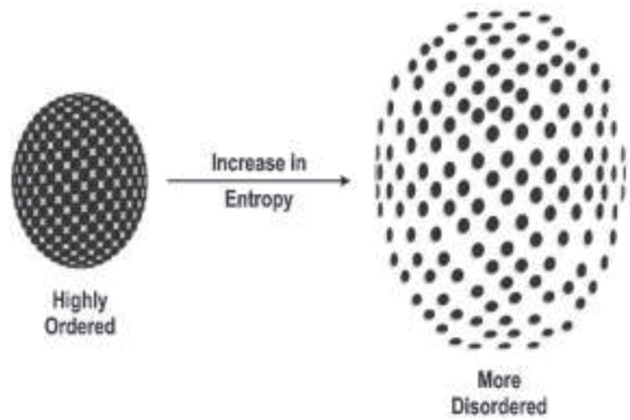

Figure 2: Increase in entropy changes the state of the system.

Routh-Hurwitz Stability Analysis

The point $u^* \in R^n$ where $f(u^*) = 0$ is referred to as an equilibrium point of the structure defined by $du/dt = f(u)$. Let the set-up be: $x'(t) = f(x, y)$, $y'(t) = g(x, y)$, having f, g and h as differentiable and continuous partial derivatives that vanish at the equilibrium point (x_0, y_0).

Theorem 1: If $f: R^n \to R^n$ considered to be differentiable at x_0, then, partial derivatives $\frac{\partial f_i}{\partial x_j}$, $i, j = 1, 2, \ldots, n$ all exist at x_0, for all $x \in R^n$, $Df(x_0)x = \sum_{j=1}^{n} \frac{\partial f}{\partial x_j}(x_0)x_j$

Thus, if f is a differentiable function, derivative Df is given by the $n \times n$ Jacobian matrix

$$J = Df = \left[\frac{\partial f_i}{\partial x_i}\right]$$

Assume that J denotes Jacobian-matrix at the equilibrium point, then

$$J = \begin{bmatrix} f_x(x_0, y_0) & f_y(x_0, y_0) \\ g_x(x_0, y_0) & g_y(x_0, y_0) \end{bmatrix} \quad (7)$$

By the Hurwitz and Routh tests, for a characteristic polynomial

$$d_1\lambda^2 + d_2\lambda + d_3 = 0 \quad (8)$$

is obtained from Jacobian at a particular fixed point. For second order polynomial, Routh's stability criterion states that for all d_i to be positive, i.e. $d_1 > 0$, $d_2 > 0$ and $d_3 > 0$, then, that equilibrium point is a stable point.

The behaviour of the attractor as per the value of the Lyapunov exponent is defined as:

1. Equilibrium: $0 > \lambda_1 \geq \lambda_2 \ldots \geq \lambda_n$;
2. Strange chaotic: $\lambda_1 > 0$, $\sum_{i=1}^{n} \lambda_i < 0$.

Mathematical Modelling

The mathematical model of logistic dynamic interaction between environmental components in atmosphere is discussed when two or more elements are competing for oxygen available in nature. In the present scenario, two kinds of possibilities take place. First, either one of the chemical compounds consumes more than other compounds. Second, simultaneous oxygen intake i.e. oxidation by both the pollutants occur. This results in resource crunch and as a result the rate of change of the concentration becomes negative. No chemical compound is dominant and both begin to decay. Thus, resources begin to replenish again. Diffusion also takes place which leads to growth of both the components in other locations. Thus, sustenance and dominance both transfer from one chemical compound to other in a cyclic pattern ensuring mutual sustenance. As dependence grows, the limit cycles begin to shrink in size and finally a stage comes where replenishment of resources does not take place efficiently enough and there arises a situation of catastrophe in the environmental cycle.

The chemical species NO_3 and CO_2 are assumed that they are present in the same environment and compete for the available amount of oxygen in all forms whether oxygen compound or radical form in the system. The production rate of one affects the production rate of the other. This means that if one is produced it uses more of oxygen and hence, less availability of oxygen for the other chemical pollutant. Also, in the absence of one pollutant, assume that the other is produced logistically. Thus, the model is defined as follows:

$$x'[t] = (a_1 - x - b_1 y)x \tag{9}$$

$$y'[t] = (a_2 - b_2 x - y)y \tag{10}$$

where $x[t]$ is concentration for NO_3, $y[t]$ is concentration for CO_2, a_1 is the rate of NO_3 production, a_2 is rate of CO_2 production, b_1 is the dependence of NO_3 on CO_2 production and b_2 is dependence of CO_2 on NO_3 production. The x^2 and y^2 terms are added so that in the absence of production of one pollutant, the other does not get produced exponentially. Also, a_1 and a_2 are production rates of NO_3 and CO_2 respectively so, they will always have positive values as they will be produced continually in the environment through one or the other source. b_1 and b_2 are assumed to have negative effect as they report the dependence rates of NO_3 on CO_2 production and CO_2 on NO_3 production respectively.

Fixed points of the system are obtained from equations of system (9) and (10), $x'[t] = 0$ and $y'[t] = 0$

$$(a_1 - x - b_1 y) = 0 \tag{11}$$

or

$$x = 0 \tag{12}$$

$$(a_2 - b_2 x - y) = 0 \tag{13}$$

or

$$y = 0 \tag{14}$$

Jacobian for system of equations (9) and (10) can be given as:

$$J = \begin{bmatrix} a_1 - 2x - b_1 y & -b_1 x \\ -b_2 y & a_2 - 2y - b_2 x \end{bmatrix}$$

Characteristic Polynomial of system of equations (9) and (10) are given as:

$$\lambda^2 + \lambda(-a_1 - a_2 + 2x[t] + b_2 x[t] + 2y[t] + b_1 y[t]) + a_1 a_2 - 2a_2 x[t] - a_1 b_2 x[t] + 2b_2 x[t]^2 - 2a_1 y[t] - b_1 a_2 y[t] + 4x[t]y[t] + 2b_1 y[t]^2 = 0$$

For the given system, as per variation in system parameters the fixed point is calculated. Using Hurwitz and Routh stability analysis, the stability conditions for system parameters is discussed in the next section.

Results and Discussions

The fixed point of the system of the atmospheric pollutants NO_3 and CO_2 interaction are obtained by solving the equations (11), (12), (13) and (14), which are given as follows:

$$\left(\frac{a_1 - a_2 b_1}{1 - b_1 b_2}, \frac{a_2 - a_1 b_2}{1 - b_1 b_2}\right); (a, 0); (0, c); (0, 0)$$

Case 1: For the fixed point $\left(\frac{a_1 - a_2 b_1}{1 - b_1 b_2}, \frac{a_2 - a_1 b_2}{1 - b_1 b_2}\right)$:

At this point, both the components coexist in the system and the balance is maintained. The Jacobian and Characteristic Polynomial is given as:

$$J = \left(a_1 - 2\left(\frac{a_1 - b_1 a_2}{1 - b_1 b_2}\right) - b_1\left(\frac{a_2 - a_1 b_2}{1 - b_1 b_2}\right) - b_1\left(\frac{a_1 - b_1 a_2}{1 - b_1 b_2}\right) - b_2\left(\frac{a_2 - a_1 b_2}{1 - b_1 b_2}\right) a_2 - b_2\left(\frac{a_1 - b_1 a_2}{1 - b_1 b_2}\right) - 2\left(\frac{a_2 - a_1 b_2}{1 - b_1 b_2}\right)\right)$$

$$\lambda^2 + \frac{(-a_1 - a_2 + b_1 a_2 + a_1 b_2)}{1 - b_1 b_2}\lambda + \frac{(-a_1 a_2 + b_1 a_2^2 + a_1^2 b_2 - a_1 b_1 a_2 b_2)}{1 - b_1 b_2} = 0$$

Comparing with equation (8), we get

$$d_1 = 1 > 0,$$

$$d_2 = \frac{(-a_1 - a_2 + b_1 a_2 + a_1 b_2)}{1 - b_1 b_2} > 0$$

$\Rightarrow$ Either $(-a_1 - a_2 + b_1a_2 + a_1b_2) > 0$ and $(1 - b_1b_2) > 0$

or $(-a_1 - a_2 + b_1a_2 + a_1b_2) < 0$

and $(1 - b_1b_2) < 0$ (Condition 1)

$$d_3 = \frac{-a_1a_2 + b_1a_2^2 + a_1^2b_2 - a_1b_1a_2b_2}{1 - b_1b_2} > 0$$

$\Rightarrow$ Either $(-a_1a_2 + b_1a_2^2 + a_1^2b_2 - a_1b_1a_2b_2) > 0$ and

$(1 - b_1b_2) > 0$ or $(-a_1a_2 + b_1a_2^2 + a_1^2b_2 - a_1b_1a_2b_2) < 0$

and $(1 - b_1b_2) < 0$ (Condition 2)

Case 2: For the fixed point (a_1, 0):

At this point, NO_3 is present and CO_2 vanishes i.e. cannot exist in the system. The Jacobian and Characteristic Polynomial is given as:

$$J = \begin{bmatrix} -a_1 & -b_1a_1 \\ 0 & a_2 - a_1b_2 \end{bmatrix}$$

$$\lambda^2 + (-(-a_1 + a_2 - a_1b_2))\lambda + a_1^2b_2 - a_1a_2 = 0$$

Comparing with Routh's equation (8), we get

$d_1 = 1$ (> 0),

$d_2 = (-a_2 + a_1(1 + b_2)) > 0$

$\Rightarrow a_1(1 + b_2) > a_2$ (Condition 3)

$d_3 = a_1(a_1b_2 - a_2) > 0$ as $a_1 > 0$,

thus $a_1 > a_2/b_2$ (Condition 4)

Case 3: For the fixed point (0, a_2):

At this point, CO_2 is present and NO_3 vanishes i.e. cannot exist in the system. The Jacobian and Characteristic Polynomial is given as:

$$J = \begin{bmatrix} a_1 - a_2b_1 & 0 \\ -a_2b_2 & -a_2 \end{bmatrix}$$

$$\lambda^2 + (-(a_1 - a_2b_1 - a_2))\lambda - a_1a_2 + b_1a_2^2 = 0$$

Comparing with Routh's equation (8), we get

$d_1 = 1$ (> 0),

$d_2 = (-a_1 + a_2(1 + b_1)) > 0$

$\Rightarrow a_1 < a_2(1 + b_1)$ (Condition 5)

$d_3 = a_2(a_2b_1 - a_1) > 0$ as $a_2 > 0$,

thus $a_1 > a_2/b_2$ (Condition 6)

Case 4: For the fixed point (0, 0):

At this point, both the pollutants tend to diminish from the environmental system considered and the chemical compounds cease to exist in the nature which creates a situation of catastrophe. So, to prevent this situation from happening in the atmosphere over large regions, we need to control the other affecting factors. This case is studied in detail for two sets of parameters. The Jacobian and Characteristic Polynomial is given as:

$$J = \begin{bmatrix} a_1 & 0 \\ 0 & a_2 \end{bmatrix}$$

$$\lambda^2 + (-(a_1 + a_2))\lambda + a_1a_2 = 0$$

Comparing with Routh's equation (8), we get

$d_1 = 1$ (> 0),

$d_2 = (-(a_1 + a_2)) > 0$ (Not possible as $a_1 > 0$, $a_2 > 0$)

$d_3 = a_1a_2 > 0 \Rightarrow a_1 > 0, a_2 > 0$ (Condition 7)

For each fixed point, different conditions are obtained which are numerically simulated for different values of the parameters. Let us assume that $a_1 = 3.5$, $b_1 = -0.1$, $a_2 = 3.5$, $b_2 = -0.15$. The details of each fixed point with stability conditions and the behaviour of fixed point is tabulated in Table 1, Table 2, Table 3 and Table 4 respectively.

Table 1 gives details of the point $\left(\frac{a_1 - a_2b_1}{1 - b_1b_2}, \frac{a_2 - a_1b_2}{1 - b_1b_2}\right)$ = (3.91, 3.91). From Table 1, it is observed that the point does not satisfy Routh's stability condition and thus, not a stable point. Table 2 gives the details of the point (a_1, 0) = (3.5, 0). From Table 2, it is observed that the point (3.5, 0) satisfies Routh's stability condition thus, a stable point and also the eigenvalues obtained are real and negative. Therefore (3.5, 0) is a stable point. Table 3 gives the details of the point (0, a_2) = (0, 3.5). From Table 3, it is observed that the point (0, 3.5) satisfies Routh's stability condition; thus, a stable point and also the eigenvalues obtained are real and negative. Therefore, (0, 3.5) is a stable point. Table 4 gives the details of the point (0, 0). From Table 4, it is observed that the point (0, 0) does not satisfy Routh's stability condition and thus, it is unstable point. Also, the eigenvalues are positive (>0). Therefore, this is an unstable point.

It is observed that the point (0, 0) is an unstable point. Thus, in the neighbourhood of (0, 0) i.e. at a point (0.1, 0.1) the time series behaviour is simulated numerically for the two sets of parameters which are defined as follows:

Table 1: Stability of fixed point at a_1 = 3.5, b_1 = –0.1, a_2 = 3.5, b_2 = –0.15, for $\left(\frac{a_1 - a_2 b_1}{1 - b_1 b_2}, \frac{a_2 - a_1 b_2}{1 - b_1 b_2}\right) = (3.91, 3.91)$

Condition	*Value*	*Behaviour*
$d_1 > 0$	$1 > 0$	Satisfied
Condition 1 $d_2 = \frac{(-a_1 - a_2 + b_1 a_2 + a_1 b_2)}{1 - b_1 b_2} > 0$ $\Rightarrow$ either $(-a_1 - a_2 + b_1 a_2 + a_1 b_2) > 0$ and $(1 - b_1 b_2) > 0$ or $(-a_1 - a_2 + b_1 a_2 + a_1 b_2) < 0$ and $(1 - b_1 b_2) < 0$	$(1 - b_1 b_2) > 0$ and $(-a_1 - a_2 + b_1 a_2 + a_1 b_2) > 0$ $\Rightarrow 0.985 > 0$ and $-7.875 > 0$ (False) $(-a_1 - a_2 + b_1 a_2 + a_1 b_2) < 0$ and $(1 - b_1 b_2) < 0$ $\Rightarrow -7.875 > 0$ and $0.985 > 0$ (False)	Not satisfied
Condition 2 $d_3 = \frac{-a_1 a_2 + b_1 a_2^2 + a_1^2 b_2 - a_1 b_1 a_2 b_2}{1 - b_1 b_2} > 0$ $\Rightarrow$ Either $(-a_1 a_2 + b_1 a_2^2 + a_1^2 b_2 - a_1 b_1 a_2 b_2) > 0$ and $(1 - b_1 b_2) > 0$ or $(-a_1 a_2 + b_1 a_2^2 + a_1^2 b_2 - a_1 b_1 a_2 b_2) < 0$ and $(1 - b_1 b_2) < 0$	$(1 - b_1 b_2) > 0$ and $(-a_1 a_2 + b_1 a_2^2 + a_1^2 b_2 - a_1 b_1 a_2 b_2) > 0$ $\Rightarrow (0.985) > 0$ and $(-15.49625) > 0$ (False) or $(-a_1 a_2 + b_1 a_2^2 + a_1^2 b_2 - a_1 b_1 a_2 b_2) < 0$ and $(1 - b_1 b_2) < 0$ $\Rightarrow ((-15.49625) < 0$ and $0.985) > 0$ (False)	Not satisfied

Table 2: Stability of fixed point at a_1 = 3.5, b_1 = –0.1, a_2 = 3.5, b_2 = –0.15, for (a_1, 0) = (3.5, 0)

Condition	*Value*	*Behaviour*
$d_1 > 0$	$1 > 0$	Satisfied
Condition 3: $d_2 > 0$: = > a_1 (1 + b_2) < a_2	a_1 (1+ b_2) < $a_2 \Rightarrow$ 4.0365 < 3.5	Satisfied
Condition 4: $d_3 > 0$: = > $a_1 > a_2/b_2$	$a_1 > a_2/b_2$ = 3.5>(3.5/–0.15)	Satisfied

Table 3: Stability of fixed point at a_1 = 3.5, b_1 = –0.1, a_2 = 3.5, b_2 = –0.15, for (0, a_0) = (0, 3.5)

Condition	*Value*	*Behaviour*
$d_1 > 0$	$1 > 0$	Satisfied
Condition 5: $d_2 > 0$: => $a_1 < a_2$ (1+b)	3.5 < 3.5(1-0.1)	Satisfied
Condition 6: $d_3 > 0$: => $a_2 > a_1/b_1$	$a_2 > a_1/b_1 \Rightarrow$ 3.5 > (3.5/–0.1)	Satisfied

Table 4: Stability of fixed point at a_1 = 3.5, b_1 = –0.1, a_2 = 3.5, b_2 = –0.15, for (0, 0)

Condition	*Value*	*Behaviour*
$d_1 > 0$	$1 > 0$	Satisfied
$d_2 > 0$: => $a_1 < a_2$ (Not possible as $a_1 = a_2$)	$a_1 = a_2$ = 3.5, thus this condition is not possible.	Unsatisfied
$d_3 > 0$: a_1 $a_2 > 0$ => $a_1 > 0$; $a_2 > 0$	a_1 = 3.5 > 0; a_2 = 3.5 > 0	Satisfied

(i) Set I: $a_1 = 3.5$, $b_1 = -0.1$, $a_2 = 3.5$, $b_2 = -0.15$
(ii) Set II: $a_1 = 3.8$, $b_1 = -0.1$, $a_2 = 3.8$, $b_2 = -0.15$

Time series behaviour of the chemical pollutants NO_3 and CO_2 are simulated in Figure 1(a), (b) for the parameter set I and II respectively. Lyapunov Exponents depict the behaviour of the system over a period of time and the transition from regular to chaotic state which are tabulated in Table 5 and is plotted in Figure 2(a), (b) for the parameter Set I and Set II respectively. The behaviour of the Lyapunov indicators DLI, FLI and SALI is tabulated in Table 6 and it is observed that the values of FLI and DLI fluctuates very vastly between regular and chaotic orbit. In chaotic state, values of SALI vary differently for the number of iterations with simultaneous increase and decrease. The system exhibits regular and chaotic behaviour as the system parameters varies. The parameters considered in the system govern the direction in which environmental cycle evolves. Table 7 discusses the entropy change that happens as the stability phase changes from stable towards chaotic

Table 5: Lyapunov Characteristic Exponent Values for different parameters values at (0.1, 0.1) near (0,0)

	For $a_1 = 3.5$, $b_1 = -0.1$, $a_2 = 3.5$, $b_2 = -0.15$			*For $a_1 = 3.8$, $b_1 = -0.1$, $a_2 = 3.8$, $b_2 = -0.15$*		
Time	*Eigenvalue1 λ_1*	*Eigenvalue2 λ_1*	*Behaviour*	*Eigenvalue1 λ_1*	*Eigenvalue2 λ_1*	*Behaviour*
t = 10.0000	-2.14636	-2.79089	As λ_1 and λ_2 both are negative, thus the neighborhood point (0.1, 0.1) at $a_1 = 3.5$, $b_1 = -0.1$, $a_2 = 3.5$, $b_2 = -0.15$ is in the equilibrium.	3.433661	-3.53331	As $\lambda_1 > 0$ and $\lambda_2 < 0$ but their sum is negative, thus the neighborhood point (0.1, 0.1) at $a_1 = 3.8$, $b_1 = -0.1$, $a_2 = 3.8$, $b_2 = -0.15$ is in the strange chaotic state.
t = 20.0000	-2.43619	-3.15046		3.42683	-3.66666	
t = 30.0000	-2.53281	-3.2703		3.424554	-3.7111	
t = 40.0000	-2.58112	-3.33023		3.423415	-3.73333	
t = 50.0000	-2.6101	-3.36618		3.422732	-3.74666	
t = 60.0000	-2.62942	-3.39015		3.422277	-3.75555	
t = 70.0000	-2.64323	-3.40727		3.421952	-3.7619	
t = 80.0000	-2.65358	-3.42011		3.421708	-3.76666	
t = 90.0000	-2.66163	-3.4301		3.421518	-3.77037	
t = 100.000	-2.66807	-3.43809		3.421366	-3.77333	

Table 6: Lyapunov Dynamic Indicators for different parameters values at (0.1, 0.1) near (0, 0)

	For $a_1 = 3.5$, $b_1 = -0.1$, $a_2 = 3.5$, $b_2 = -0.15$		*For $a_1 = 3.8$, $b_1 = -0.1$, $a_2 = 3.8$, $b_2 = -0.15$*	
	Observation	*Behaviour*	*Observation*	*Behaviour*
DLI	For number of iterations n, $1000 < n < 3000$, the DLI values varies from 0 to 1.25 and 2.5 to 3.5 and shows a definite pattern. No value of DLI lies between 1.25 and 2.5.	DLI for $a_1 = 3.5$, $b_1 = -0.1$, $a_2 = 3.5$, $b_2 = -0.15$ follows Regular motion.	For number of iterations n, $6000 < n < 9000$, DLI values varies from 0.5 to 3.5 and does not show a definite pattern. DLI shows randomness and Brownian motion.	DLI for $a_1 = 3.8$, $b_1 = -0.1$, $a_2 = 3.8$, $b_2 = -0.15$ varies randomly thus follow a chaotic motion.
FLI	For number of iterations n, $200 < n < 300$, the FLI values increase gradually from 20 to 140. Thus, FLI shows regular motion.	FLI for $a_1 = 3.5$, $b_1 = -0.1$, $a_2 = 3.5$, $b_2 = -0.15$ follows Regular motion.	For number of iterations n, $200 < n < 300$, FLI values increase suddenly and then stabilizes around 280.	FLI for $a_1 = 3.8$, $b_1 = -0.1$, $a_2 = 3.8$, $b_2 = -0.15$ varies from 0 to 3.5×10^{39} thus follow a chaotic motion.
SALI	For number of iterations n, $200 < n < 300$, the SALI values show a great variation from 200-220 and then stabilizes to zero from 220 to 300. The values of SALI varies from 0 to 3.5×10^{-7}.	SALI for $a_1 = 3.5$, $b_1 = -0.1$, $a_2 = 3.5$, $b_2 = -0.15$ follows Regular motion.	For number of iterations n, $200 < n < 300$, the SALI values increase simultaneously and decrease in the whole interval. Chaos is observed for SALI from 0 to 10^{-15}.	SALI for $a_1 = 3.8$, $b_1 = -0.1$, $a_2 = 3.8$, $b_2 = -0.15$ varies from 0 to 10^{-15} thus follow a chaotic motion.

Table 7: Entropy value showing stability change for different a_1 and a_2 values

Values of a_1 (=a_2)	*Entropy change for variable x*	*Entropy change for variable y*	*Stability changes*
3.51	0.0460	0.0652	Stable
3.56	0. 0925	0.0782	Critical
3.65	0.1654	0.1050	Chaotic
3.75	0.2737	0.1275	Chaotic
3.80	0.3608	0.1356	Strange Chaotic

level. It provides the probabilistic value of amount of disorder that happens in every event sensitive towards change in the initial pre-requisites.

Dynamic Lyapunov indicator DLI is plotted in Figure 3(a), (b) for the parameter Set I and Set II respectively. Fast Lyapunov indicator FLI is plotted in Figure 4(a), (b) for the parameter Set I and Set II respectively. Small Aligned Lyapunov Indicator SALI is plotted in Figure 5(a), (b) for the parameter Set I and Set II respectively.

From the figures and tables, it is observed that for parameters $a_1 = 3.5$, $b_1 = -0.1$, $a_2 = 3.5$, $b_2 = -0.15$, the point $\left(\dfrac{a_1 - a_2 b_1}{1 - b_1 b_2}, \dfrac{a_2 - a_1 b_2}{1 - b_1 b_2}\right) = (3.91, 3.91)$ is not a

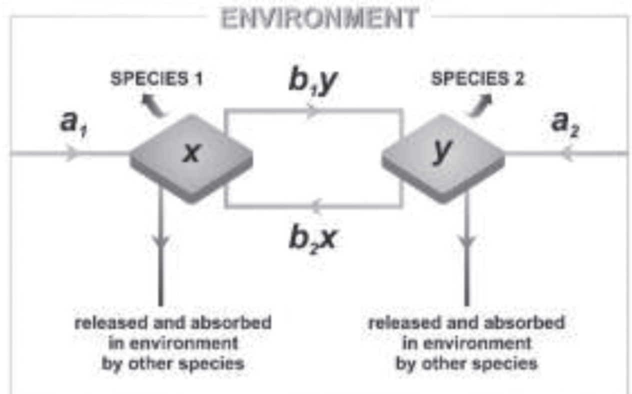

Figure 3: Compartmental diagram of the mathematical model designed.

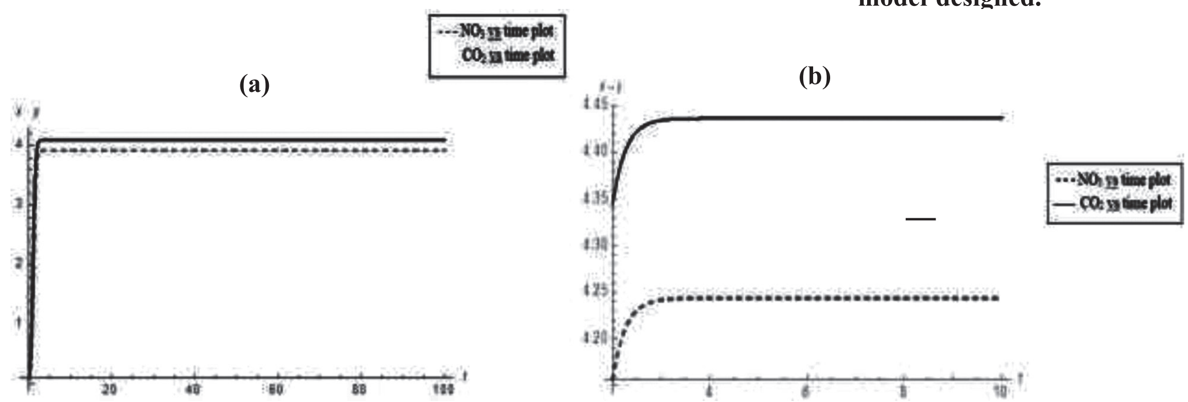

Figure 4: Time series of NO_3 and CO_2 for (a) a_1=3.5, b_1= -0.1, a_2=3.5, b_2= -0.15, Regular and (b) a_1=3.8, b_1= -0.1, a_2=3.8, b_2= -0.15, Chaotic.

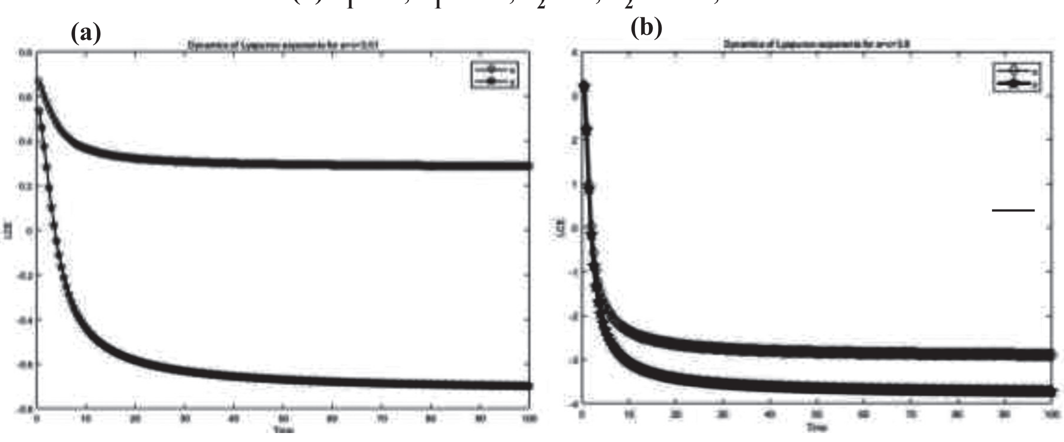

Figure 5: Lyapunov Characteristic Exponent of NO_3 and CO_2 for (a) a_1=3.5, b_1= -0.1, a_2=3.5, b_2= -0.15, Regular and (b) a_1=3.8, b_1= -0.1, a_2=3.8, b_2= -0.15, Chaotic.

stable point. The point $(a_1, 0) = (3.5, 0)$ and $(0, a_2) = (0, 3.5)$ is a stable point. In these cases, as one of the chemical compound either NO_3 or CO_2 vanishes in the atmosphere, systems does not maintain the sustenance and the life cycles in the atmosphere get affected; thus, not useful for study. The point (0, 0) is an unstable point. Therefore, the point (0.1, 0.1) in the neighbourhood of (0, 0) shows the changes from regular to chaotic motion as initial parameters are changed from $a_1 = 3.5$ ($a_2 = 3.5$) to $a_1 = 3.8$ ($a_2 = 3.8$). Thus, it is observed that as the system parameters varies, the system follows chaotic motion. Thus, for mutual sustenance, both the chemical compounds should interact in the atmosphere to avoid the catastrophe.

It is observed that in the neighbourhood of (0, 0) i.e. for (0.1, 0.1) at $a_1 = 3.5$, $b_1 = –0.1$, $a_2 = 3.5$ and $b_2 = –0.15$ the eigenvalues are negative, thus the point (0.1, 0.1) is in equilibrium. Also, DLI has two parallel regions i.e. from DLI = 0 to 1.25 and 2.5 to 3.5 and shows a definite pattern; thus regular behaviour is observed. FLI values increase gradually from 20 to 140. Thus, FLI shows regular motion. SALI values show a great variation from 200-220 and then stabilizes to zero from 220 to 300. The value of SALI varies from 0 to 3.5×10^{-7}. Thus, it has been shown from different indicators that the systems follow a regular motion.

Also, it is observed that in the neighbourhood of (0, 0) i.e. for (0.1, 0.1) at $a_1 = 3.8$, $b_1 = –0.1$, $a_2 = 3.8$, $b_2 = –0.15$ the eigenvalues are positive and negative, but the sum of eigenvalues is negative, thus the point (0.1, 0.1) is in strange chaotic state. DLI values vary from 0.5 to 3.5 and do not show a definite pattern; thus shows randomness and Brownian motion. FLI values increase suddenly and then stabilize around 280. Thus, FLI shows chaotic motion. SALI values increase simultaneously and decrease in the whole interval. Chaos is observed for SALI from 0 to 10^{-15}. The two indicators give very clear indications about orbit's nature whenever applied; computation is fast and easy. Only few hundreds of iterations are sufficient to

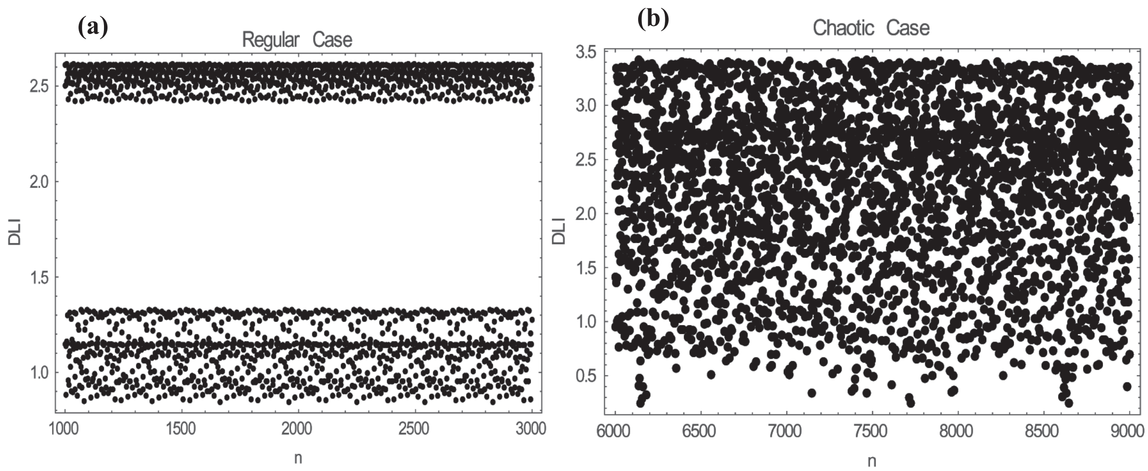

Figure 6: DLI of NO_3 and CO_2 for (a) a_1=3.5, b_1= -0.1, a_2=3.5, b_2= -0.15, Regular and (b) a_1=3.8, b_1= -0.1, a_2=3.8, b_2= -0.15, Chaotic.

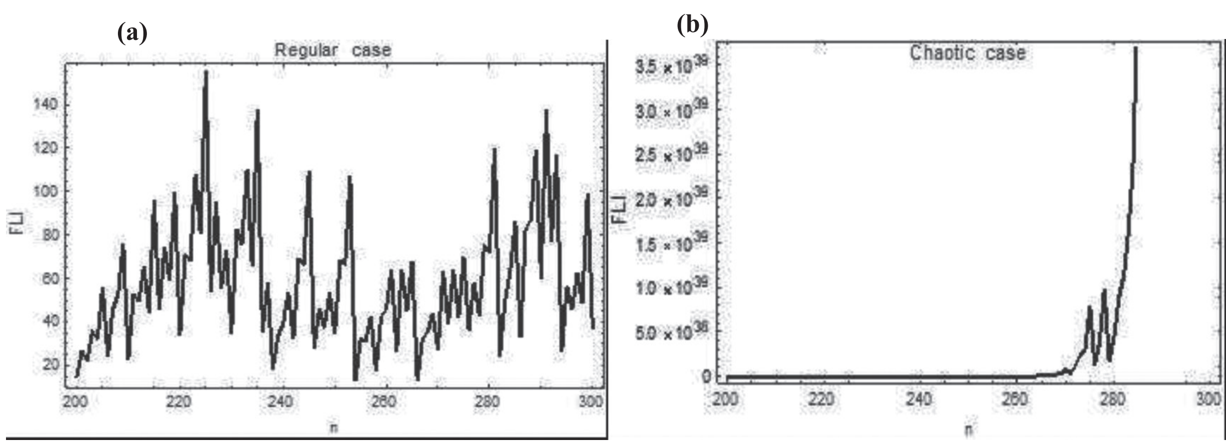

Figure 7: FLI of NO_3 and CO_2 for (a) a_1=3.5, b_1= -0.1, a_2=3.5, b_2= -0.15, Regular and (b) a_1=3.8, b_1= -0.1, a_2=3.8, b_2= -0.15, Chaotic.

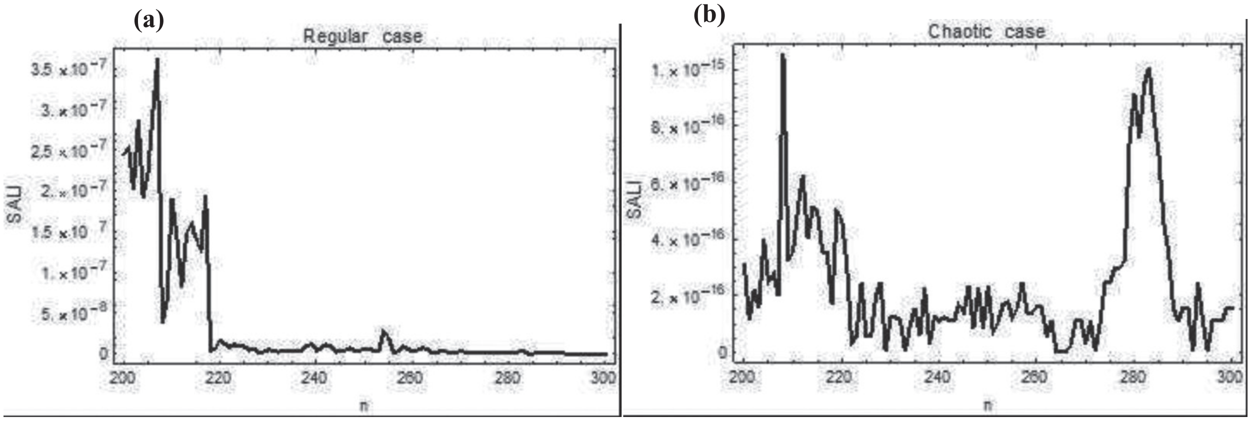

Figure 8: SALI of NO_3 and CO_2 for (a) a_1=3.5, b_1= -0.1, a_2=3.5, b_2= -0.15, Regular and (b) a_1=3.8, b_1= -0.1, a_2=3.8, b_2= -0.15, Chaotic.

get a conclusion. There is a simultaneous increase and decrease. Thus, it can be concluded that the balance should be maintained and the chemical compounds may exist in the same amount.

Conclusions

The chemical compounds NO_3 and CO_2 are present in the same environment and, therefore, the production rate of one affects the production rate of the other. Thus, in the atmosphere if one is produced it uses more oxygen; thus less availability of oxygen for the other pollutant. The mathematical model for the interaction of NO_3 and CO_2 pollutant is developed logistically. Using Routh's stability criteria, the stable points, fixed point and equilibrium points are obtained. Lyapunov Exponents depict the behaviour of the system over a period of time and the transition from regular to chaotic state. It can be observed that the values of FLI and DLI fluctuate vastly between regular and chaotic orbit. In chaotic state, values of SALI vary differently for the number of iterations with simultaneous increase and decrease. The system exhibits regular and chaotic behaviour as the system parameters vary. The parameters considered in the system govern the direction in which environmental cycle evolves.

Rate of change in entropy takes place during stability phase change which happens when the system moves from stable towards randomness. This shows that energy is released in the surroundings by the structure undergoing the evolution. This can be also referred as the disorder that the complete system undergoes when an event takes place. For variable x, the entropy increases as: 0.0460, 0.0925, 0.1654, 0.2737 and 0.3608 as the values of a_1 and a_2 changes as 3.51, 3.56, 3.65, 3.75 and 3.80 respectively. For variable y, entropy changes as 0.0652, 0.0782, 0.1050, 0.1275 and 0.1356 as the values of a_1 and a_2 changes as 3.51, 3.56, 3.65, 3.75 and 3.80 respectively.

DLI is very efficient in giving correct conclusions for regular and chaotic orbits. FLI is another powerful tool to differentiate between regular motion and chaos in the intricate systems. SALI proves to be an effective indicator which would discriminate certainty between the two types of motion. DLI has two parallel regions from 0 to 1.25 and 2.5 to 3.5 for regular case and varies randomly for chaotic orbits. The dynamical indicators give very clear suggestions about orbit's nature whenever applied; working out is fast and easy, iterations upto some hundreds are sufficient to reach towards the conclusion. FLI increases and decreases very fast over number of iterations, n. FLI shows a great variation for regular orbits and increases gradually from n = 200 to n = 270 and then there is a sudden increase around 280 for chaotic orbits.

The SALI has a great variation for n = 200 to 220 and then gradually tends to 0 for n = 220 to 300 for the regular case. In chaotic state, values of SALI vary differently for n = 200 to 300. There is a simultaneous change of highs and lows. It is observed that the dynamical indicators show the changes in regular and chaotic motion. It is observed that it is necessary to encourage mutual sustenance of NO_3 and CO_2—both in a balanced manner so that none of the environmental cycles get disrupted.

It is concluded that massive afforestation is needed for effective elimination of CO_2 sparing oxygen supply for the formation of nitrogen oxides in the requisite amount in atmosphere for prevention of ozone layer depletion by excess chlorine radicals and global warming.

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