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Article

A quasi chemical approach for the modeling of predator-prey interactions

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Abstract

We aim to develop the reaction diffusion equation for different types of mechanism of the predator-prey interactions with quasi chemical approach. The chemical reactions representing the interactions obey the mass action law. Since the cell-jump models may be considered as the proper diffusion models by themselves, the territorial animal like fox is given a simple cell as its territory. Under the proper relations between coefficients, like complex balance or detailed balance, this system demonstrated globally stable dynamics.

Keywords quasi-chemical approach; predator-prey interactions; modeling fox and rabbit interactions.

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1 Introduction

The Lotka Voltera equations are a pair of first order non linear differential equations these are also known as the predator prey equations .i.e. when the growth rate of one population is decreased and the other increased then the populations are in a predator-prey situation. The Lotka–Volterra equations are frequently used to describe the dynamics of biological in which two species interact, one as a predator and the other as prey.

In this review paper, we aim to study the interactions between the territorial animals like foxes and the rabbits. The territories for the foxes are considered to be the simple cells. The interactions between predator and its prey are represented by the chemical reactions which obey the mass action law. In this sence, we aim to study the mass action law for Lotka-Volterra predator prey models and consider the quasi chemical approach for the interactions between the predator and its prey. We also aim to develop the reaction diffusion equation for different types of mechanism of the predator prey interactions. The principle of detailed balance, however can also be introduced in some cases. Since the cell-jump models may be considered as the proper diffusion models by themselves, the territorial animal like fox is given a simple cell as its territory. The sense in which the discrete equations for cells converge to the partial differential equations of diffusion is that the cell models give the semi-discrete approximation of the partial differential equations for diffusion which result in a system of ordinary differential equations in cells. There are jumps of concentrations on the boundary of cells. The system of semi discrete models for cells with “no-flux” boundary conditions has all the nice properties of the chemical kinetic equations for closed systems. Under the proper relations between coefficients, like complex balance or detailed balance, this system demonstrated globally stable dynamics.

Here in this review paper, we will give background of the development of the different models of Lotka-Volterra types of reaction-diffusion equation along with different approaches that were acquired by the different scientist in the ecology and mathematical biology. Then we come to our goals, where we borrowed the properties of the chemical reactions for our approach to develop the reaction-diffusion equation of Lotka Volterra type.

The Lotka Volterra predator prey models were originally introduced by Alfred J. Lotka (1920) in the theory of autocatalytic chemical reactions in 1910 this was effectively the logistic equation which was originally derived by Pierre Francois Verhulst. In 1920 Lotka extended the model to "organic systems" using a plant species and an herbivorous animal species as an example and in 1925 he utilized the equations to analyze predator-prey interactions in his book on biomathematics arriving at the equations that we know today.

In 1926, Vito Volterra (Voltera, 1926), made a statistical analysis of fish catches in the Adriatic independently investigated the equations. V. Voltera applied these equations to predator prey interactions; consist of a pair of first order autonomous ordinary differential equations.

Since that time the Lotka–Voltera model has been applied to problems in chemical kinetics, population biology, epidemiology and neural networks. These equations also model the dynamic behavior of an arbitrary number of competitors. The Lotka–Volterra system of equations is an example of a Kolmogorov model, which is a more general framework that can model the dynamics of ecological systems with predator-prey interactions, competition, disease, and mutualism.

Lotka Volterra is the most famous predator prey model. According to Volterra if $x(t)$ is the prey population and $y(t)$ that of the predator at time t then Volterra’s model is (Murray, 2003),

$$\frac{dx}{dt} = x(a - by) \tag{1}$$

$$\frac{dy}{dt} = y(cx - d) \tag{2}$$

where *a*, *b*, *c* and *d* are positive constants. Often some necessary modifications are possible here e.g. for an absent predator a limited growth of prey can be introduced. The assumptions in the model are:

- In the absence of any predation the prey grows unboundedly in a Malthusian way; this is the ax term in equation (1).
- The effect of the predation is to reduce the prey’s per capita growth rate by a term proportional to the prey and predator populations; this is the $-bxy$ term.
- In the absence of any prey for sustenance the predator’s death rate results in exponential decay, that is, the $-dy$ term in equation (2).
- The prey’s contribution to the predators’ growth rate is cxy; i.e. it is proportional to the available prey as well as to the size of the predator population.
- The xy terms are representing the conversion of energy from one source to another.
- bxy is taken from the prey and cxy accrues to the predators.

The model (1) and (2) are known as the *Lotka–Volterra model* but this model has serious drawbacks. Nevertheless it has been of considerable value in posing highly relevant questions and is a jumping-off place for more realistic models; this is the main motivation of study here (Murray, 2003).

2 Interacting Population Models

The population dynamics of each species is affected whenever two or more species interact. Generally there consist whole webs of interacting species; those webs which consist structurally for complex communities are called a trophic web. The dynamics outcomes of the interactions are very sensitive to initial data and parameter values. The interactions lead to the following possible outcomes,

- Competitive exclusion;
- Total extinction, i.e., collapse of the whole system;
- Coexistence in the form of positive steady state;
- Coexistence in the form of oscillatory solutions;
- A better and friendly competitor can save a otherwise doomed prey species.

Two or more species models consist in case of concentrating particularly on two-species systems. There are three main types of interactions.

- If the growth rate of one population is decreased and the other increased the populations are in a predator–prey situation.
- If the growth rate of each population is decreased then it is competition.
- If each population’s growth rate is enhanced then it is called mutualism or symbiosis (Murray, 2003).

3 The Effect of Complexity on Stability

To explain the relationship between structural complexity and stability of ecosystems an extensive literature is available. Theoretical study reviews shows that the term stability is mostly used to mean the condition that whereby species densities, when perturbed from equilibrium, again return to that equilibrium. Analytically this condition can be made tractable by assuming that the populations are perturbed slightly so that linear approximations can be made to the nonlinear equations.

To know the effect of complexity on stability briefly let us take the generalized Lotka–Volterra predator–prey system where there are n prey species and n predators, which prey on all the prey species but with different severity. Then in place of (1) and (2) it can be written as,

$$\begin{aligned} \frac{dx_i}{dt} &= x_i\left[a_i - \sum_{j=1}^{n} b_{ij} y_j\right] \\ \frac{dy_i}{dt} &= y_i\left[\sum_{j=1}^{n} c_{ij} x_j - d_i\right] \end{aligned} \qquad i = 1, 2, 3, \ldots, n \qquad (3)$$

and all of the a_i, b_{ij}, c_{ij} *and* d_i are positive constants (Murray, 2003).

4 Realistic Predator–Prey Models

Though the Lotka–Volterra model is unrealistic because one of the unrealistic assumption is that growth of the prey population is unbounded in the absence of predation and the other is that there is no limit to the prey consumption but it suggests that simple predator–prey interactions can result in periodic behaviour of the populations. Since it is not unexpected that if a prey population increases then it encourages growth of its predator and more predators consume more prey due to which its population starts to decline. With the less food around the predator population declines and when it is low enough, this allows the prey population to increase and the whole cycle starts over again. Depending on the detailed system such oscillations can grow or decay or go into a stable *limit cycle* oscillation or even exhibit chaotic behaviour, although in the latter case there must be at least three interacting species, or the model has to have some delay terms. A limit cycle solution is a closed trajectory in the predator–prey space which is not a member of a continuous family of closed trajectories. A stable limit cycle trajectory is such that any small perturbation from the trajectory decays to zero.

One of the unrealistic assumptions in the Lotka–Volterra models, (1) and (2), and generally (3), is that the prey growth is unbounded in the absence of predation.

In the form we have written the model (1) and (2) the bracketed terms on the right are the density-dependent per capita growth rates. To be more realistic these growth rates should depend on both the prey and predator densities as,

$$\frac{dx}{dt} = xF(x,y), \ \frac{dy}{dt} = yG(x,y). \tag{4}$$

where the forms of F and G depend on the interaction, the species and so on. A more realistic prey population equation might take the form,

$$\frac{dx}{dt} = xF(x,y), \ F(x,y) = r\left(1-\frac{x}{k}\right) - yR(x). \tag{5}$$

where $R(x)$ is one of the predation term and K is the constant carrying capacity for the prey when $P=0.$

The predator population equation, the second of (5), should also be made more realistic than simply having $G=-d+cx$ as in the Lotka–Volterra model (2). Possible forms are,

$$G(x,y) = k\left(1-\frac{hy}{x}\right), \ G(x,y) = -d + eR(x) \tag{6}$$

where *k*, *h*, *d* and *e* are positive constants. The first of (6) says that the carrying capacity for the predator is directly proportional to the prey density (Murray, 2003).

5 Competitioning Models

Here, for a common food source two species compete to each other. For example, competition may be for territory which is directly related to food resources. Mathematically, carrying capacity of one species is reduced by the other species and vice versa. When two or more species compete for the same limited food source or in some way inhibit each other's growth, a very simple competition model which demonstrates a fairly general principle which is observed to hold in nature is that in the competition for the same limited resources one of the species usually becomes extinct. The basic two species Lotka–Volterra competition model with each species n_1 and n_2 have logistic growth in the absence of the other. Inclusion of logistic growth in the Lotka–Volterra systems makes them much more realistic, but to highlight the principle the simpler model which nevertheless reflects many of the properties of more complicated models, particularly as regards stability.

$$\frac{dx_1}{dt} = r_1 x_1\left[1-\frac{x_1}{k_1}-b_{12}\frac{x_2}{k_1}\right] \tag{7}$$

$$\frac{dx_2}{dt} = r_2 x_2 \left[1 - \frac{x_2}{k_2} - b_{21}\frac{x_1}{k_2}\right] \tag{8}$$

where $r_1, k_1, r_{2,} k_{2,} b_{12}$ and b_{21} are positive constants and r's are the linear birth rates and the k's are the carrying capacities. The b_{12} and b_{21} measure the competitive effect of n_2 on n_1 and n_1 on n_2 respectively and they are not equal generally (Murray, 2003).

Note that the competition models (7) and (8) are not a conservative system like its Lotka–Volterra predator–prey counterpart and if we non dimensionalise this model by writing

$$\begin{gathered} u_1 = \frac{x_1}{k_1},\ u_2 = \frac{x_2}{k_2},\ \tau = r_{1t},\ \rho = \frac{r_1}{r_1}, \\ a_{12} = b_{12}\frac{k_2}{k_1},\ a_{21} = b_{21}\frac{k_1}{k_2} \end{gathered} \tag{9}$$

(6) and (8) become

$$\begin{aligned} \frac{du_1}{d\tau} &= u_1(1 - u_1 - a_{12}u_2) = f_1(u_1, u_2), \\ \frac{du_2}{d\tau} &= pu_2(1 - u_2 - a_{21}u_1) = f_2(u_1, u_2), \end{aligned} \tag{10}$$

The steady states, and phase plane singularities are the solutions of $f_1(u_1, u_2) = f_2(u_1, u_2) = 0$ (Murray, 2003).

6 Mutualism or Symbiosis

In these cases, the two species benefit from each other. To some extent it is the opposite of the competition model here carrying capacity of each species is increased by the other species.

There are many cases where the interaction of two or more species is to the advantage of all. In promoting and even in maintaining such species mutualism or symbiosis often plays a very crucial role. Plant and seed dispersal is an example. If the survival is not at stake even in those situations the advantage of mutualism or symbiosis can have its own importance. As a topic of theoretical ecology, even for two species, this area has not been as widely studied as the others even though its importance is comparable to that of predator–prey and competition interactions (Lotka, 1920). This is in part due to the fact that simple models in the Lotka–Volterra vein give silly results. The simplest mutualism model equivalent to the classical Lotka–Volterra predator–prey one is,

$$\frac{dx_1}{dt} = r_1 x_1 + a_1 x_1 x_2.\ \frac{dn_2}{dt} = r_2 n_2 + a_2 n_2 n_1,$$

where $r_1, r_2, a_1\ and\ a_2$ are positive constants.

Since $\frac{dx_1}{dt} > 0$ and $\frac{dx_2}{dt} > 0,$ n_1 and n_2 simply grow unboundedly (Murray, 2003).

7 Threshold Phenomena

With the exception of the Lotka–Volterra predator–prey model, the two species models, which have either a stable steady states where small perturbations die out, or unstable steady states where perturbations from them grow unboundedly or result is produced in limit cycle periodic solutions. There is an interesting group of models which have a nonzero stable state such that if the perturbation is sufficiently large or it is of the right kind, then before returning to the steady state population densities undergo large variations. Such models are said to exhibit a threshold effect (Murray, 2003). One such group of models is studied here. The model predator–prey system is

$$\begin{aligned} \frac{dx}{dt} &= x\left[F(x)-y\right] = f(x,y), \\ \frac{dy}{dt} &= y\left[x-G(y)\right] = g(x,y) \end{aligned} \qquad (11)$$

where for convenience all the parameters have been incorporated in the *F* and *G* by a suitable rescaling.

8 Discrete Growth Models for Interacting Populations

Now taking the two interacting species, each have the non overlapping generations and each species affect the other's population dynamics. In the continuous growth models, there are some main types of interaction, such as, predator–prey, mutualism and competition. Nowhere near to the same extent as for continuous models for which, in the case of two species, there is a complete mathematical treatment of the equations. In view of the complexity of solution behaviour with single-species discrete models it is not surprising that even more complex behaviour is possible with coupled discrete systems (Murray, 2003).

The interaction between the prey (x) and the predator (y) to be governed by the discrete time *(t)* system of coupled equations as,

$$x_{t+1} = rx_t\ f(x_t, y_t), \qquad (12)$$

$$y_{t+1} = x_t\ \mathrm{g}(x_t, y_t), \qquad (13)$$

where $r > 0$ is the net linear rate of increase of the prey and *f* and *g* are functions which relate the predator-influenced reproductive efficiency of the prey and the searching efficiency of the predator respectively.

9 Detailed Analysis to Predator Prey Models

Predator-dependent predator-prey model is of the form

$$\begin{aligned} \frac{dx}{dt} &= xg\left(\frac{x}{k}\right) - yP(x,y),\ \ x(0) > 0, \\ \frac{dy}{dt} &= cyP(x,y) - dy,\ \ y(0) > 0, \end{aligned} \qquad (14)$$

when $P(x,y) = \left(\frac{x}{y}\right)$ then model (14) is strictly ratio dependent. The traditional or prey-dependent model takes the form

$$\begin{aligned}\frac{dx}{dt} &= xg\left(\frac{x}{k}\right) - yP(x,y),\ \ x(0)>0,\\ \frac{dy}{dt} &= cyP(x)-dy,\ \ y(0)>0,\end{aligned} \tag{15}$$

Mathematically both the traditional prey-dependent and ratio-dependent models as a limiting cases i.e. for the former $c=0$ and for the later $a=0$ of the general predator-dependent functional response

$$P(x,y)=\frac{\theta x}{a+bx+cy}$$

when $P(x)=\dfrac{\theta x}{x+m}$ and $g(\dfrac{x}{k})=r\left(1-\dfrac{x}{k}\right)$ becomes

$$\frac{dx}{dt}=rx\left(1-\frac{x}{k}\right)-\frac{\theta xy}{m+x},\ \ x(0)>0$$

where r,k,θ,m,f,d are positive constants and the population density of prey and predator at time t is represented by $x(t),y(t)$ respectively.

In the absence of predation the prey carrying capacity *K and* grows with intrinsic growth rate *r*. The predator consumes the prey with functional response of type $\dfrac{cxy}{(m+x)}$ and contributes to its growth with rate $\dfrac{fxy}{(m+x)}$. The constant d is the death rate of predator. According to model (15) in a predator-prey system enrichment will cause an increase in the equilibrium density of the predator but not in that of the prey, and will destabilize the positive equilibrium, that is according to (15) a low and stable prey equilibrium density is not possible. Another prediction that can be made from model (15) is that the mutual extinction between the prey and predator cannot extinct simultaneously.

Recently by both mathematicians and ecologists the rich dynamics provided at the boundary and close to the origin by the strict ratio-dependent models is ignored. If there is a positive steady state in ratio dependent models both prey and predator will go extinct i.e., the collapse of the system. The extinction may occur in two different ways. One of the way is that regardless of the initial densities both species become extinct and the other way is that both species will die out if the initial prey/predator ratio is too low. In the first case, extinction often occurs as a result of high predator efficiency in catching the prey and in the second way there are interesting implications. For example, it indicates that altering the ratio of prey to predators through over-harvesting of prey species may lead to the collapse of the whole system and the extinction of both species may occur. In many aspects the richest dynamics is provided by the ratio-dependent models while in the prey-dependent models the least in dynamical behavior is provided.

In ratio dependent models there are still some controversial aspects. A specific main controversial aspect is that in the ratio dependent models the high population densities of both prey and predator species are required while the most interesting dynamics of ratio-dependent models occurs near the origin. If the area of the population interaction is large certainly it is a valid concern because in such cases rather than interfering each other most efforts are spent by the predators in searching the prey hence the functional response is likely to be much more sensible to prey density than predator density. However, if the area of the population is small for the prey and even the densities are low since predators can remain interfering effectively each other then certainly in such cases ratio dependence formulation may remain valid for very small field or patch, even when the numbers of individuals of prey and predators are low while their densities may remain high. In such cases, ratio dependence models are a valid mechanism which suggests that there is a high possibility of mutual extinction.

Some interesting and new dynamics are revealed by the analysis of the ratio dependent models. For competing predators competitive exclusion principle still holds for most parameter values, it is very often that through the result of the parameter values both can go extinct. In fact, for certain choices of initial values and parameters even the prey species can go extinct it in turn cause the extinction of both predators. Coexistence is possible for some parametric values in both the forms of positive steady state and oscillatory solutions. Most surprisingly when a predator is in a position of driving the prey and itself to extinction, the introduction of a predator which is more friendly to prey and is a stronger as compared to the existing one competitor the prey species may be saved (Berezovskaya et al., 2001).

10 The Law of Mass Action. Basic Concepts (Gorban et al., 2011)

Heat energy flows from a higher temperature region to a lower temperature region. There is no net heat energy flow in the case when both the regions have a same temperature. For example a covered cup of tea will not be colder or warmer then the room temperature after it has been there for a few hours. This phenomenon is known as equilibrium. Equilibrium happens in phase transition. The chemical equilibrium and the law of mass action are the two fundamental concepts of classical chemical kinetics. In a chemical process chemical equilibrium is the state in which concentrations of the reactants and the products have no net change over time. The law of mass action is the mathematical model that explains and predicts the behaviours of the solutions in dynamic equilibrium. This law provides an expression for a constant for all reversible reactions and concerns with the composition of reactions at equilibrium and the rate equitions for elementery reactions. Gulberg and waage (1864-1879) has proved that chemical equilibrium is a dynamic process in which rate of reactions for the forward and backward reactions must be equal. For a chemical reaction the law of mass action was first stated as follows:

" when two reactants A and B react together at a given temperature in a sub situatin reaction the affinity or chemical force between them is proportional to the active masses $[A]$ and $[B]$ each raise to a particular power".

$$\text{Affinity} = \alpha[A]^a[B]^b \qquad (16)$$

Here α, a, b were regarded as emperical constants to be determined. In 1867, the rate expression were simplified as the chemical force was assumed to be directly proportional to the product of the active masseses of the reactants.

$$\text{Affinity} = \alpha[A][B] \qquad (17)$$

In 1879 this assumption was explained in trems of collision theory so that the general condition for the equilibrium could be applied to any orbitrary chemical equilibrium.

Affinity $= k[A]^{\alpha}[B]^{\beta}$ (18)

The exponents α, β, σ and τ are explicity defined as the "stoichiometric coefficients" for the reactions so that for a general reaction of the type ,

$$\alpha A + \beta B + ... \rightleftharpoons \sigma S + \tau T + ... \quad (19)$$

Forward reaction rate $= k_{+}[A]^{\alpha}[B]^{\beta}...$ (20)

Backward reaction rate $= k_{-}[S]^{\sigma}[T]^{\tau} + ...,$ (21)

where $[A],[B],[S]$ and $[T]$ are active masses and k_{+} and k_{-} are called affinity constants or rate constants. Since at equilibrium the affinities and reaction rates for the forward and backward reactions are equal, so

$$K = \frac{k_{+}}{k_{-}} = \frac{[S]^{\sigma}[T]^{\tau} + ...,}{[A]^{\alpha}[B]^{\beta}...} \quad (22)$$

The equilibrium constant K was obtained by setting the rates of forward and backward reactions to be equal. Today the expression for the equilibrium constant is derived by setting the chemical potential of forward and backward reactions to be equal. The units of K depend on the units used for concentrations. If M is used fo all concentrations then K has the units "$M^{(\sigma+\tau)-(\alpha+\beta)}$" if the system is not at equilibrium, the ratio is different from equlibrium constants. In such cases the tatio is called "reaction quotient" denoted by Q,

$$\frac{[c]^{\sigma}[D]^{\tau}}{[A]^{\alpha}[B]^{\beta}} = Q. \quad (23)$$

A system which is not at equilibrium tends to reach at equilibrium and any changes in the system will cause changes in Q so that the value of the reaction quotient approaches the value of the equilibrium constant K, i.e., $Q \to K.$

For a list of components $A_1, A_2, ..., A_n$, where each comoponent has a real variables of particles, and for concentrations $c_1, c_2, ..., c_n$, we have algebra of reactions,

$$\alpha_1 A_1 +, ..., \alpha_n A_n, \rightleftharpoons \beta_1 A_1 +, ..., \beta_n A_n, \quad (24)$$

where $\alpha, \beta \geq 0.$ we can write the stoichiometric equation for this algebra of reactions as ,

$$R_r = k_r \prod_i c_i^{\alpha i}, \quad (25)$$

With stoichiometric vector, $\gamma_{ri} = \beta_{ri} - \alpha_{ri}$,

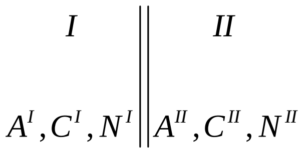

Fig. 1 Cell jump model.

11 A Simple Cell Jump Model

The standard form of reaction diffusion equation is,

$$\frac{\partial c_i}{\partial t} = f(c) + d_i \Delta c, \qquad (26)$$

where $d_i > 0,$ is diffusion coefficient and c should be literally small for very dialuted media (Gorban et al., 2011).

The thermodynamic ideality is the general requirement of a system to apply the law of mass action. Let us consider our space divided on cells, a system represented as a chain of cells each with homogeneous composition and elementary acts of transfers on the boundary (for us there are only two cells). On each cell we have some concentration for these processes. Let c^I, is the vector concentration in the first cell *I* and c^{II}, is the vector of concentration in the second cell *II* .using the general secheme of the formal kinetics which is considered to be complete if we work with list of macroscopic variables with balanced equations, a mechanism of transformation (elementary process) and the functions of the rates of these elementary processes. The mechanism of diffusion is defined as a list of elementary transitions between cells described by their stoichiometric equation. Since diffusion is a sort of jumping reaction on the border, so for these jumps the stoichiometric equation is written as,

$$\sum_i \alpha_{ri}^I A_i^I + \sum_i \alpha_{ri}^{II} A_i^{II} \rightarrow \sum_i \beta_{ri}^I A_i^I + \sum_i \beta_{ri}^{II} A_i^{II}, \qquad (27)$$

where r is the number of processes, $\alpha_{ri}^{I,II}$, and $\beta_{ri}^{I,II}$ are the stoichiometric coefficients which indicate the number of particles in cells involved in the process, where each process is is compared with the components of the stoichiometric vector defined by $\gamma_{ri}^I = \beta_{ri}^I - \alpha_{ri}^I$, also there should be sysymmetry between these cells, i.e. $A_i^I \rightleftharpoons A_i^{II}$, and diffusion coefficient d_i depends on the cell. Each elementary process is characterized by an intensive quantity, termed as velocity function $\omega_r(c^I, c^{II})$, (the number of elementary acts in a unit time per unit surface of the cell). In the absence of convection and any chemical transformation the equation of kinetics for the vector quantities, in isotropic and isothermal enviroment, is written as the equation of rate of reaction,

$$\frac{dN^I}{dt} = \frac{dN^{II}}{dt} = S \sum_r \gamma_r \omega_r, \qquad (28)$$

where S is the area of the boundary between two cells. The *i*-flux density of a substance through a unit surface of section is,

$$J_{ri}(I, II) = -\gamma_{ri}\omega_r(c^I, c^{II}). \qquad (29)$$

As a result of elementary acts of diffusion (27), the density of the total flux of the *i*-substance will be,

$$J_i = \sum J_{ri}(I, II) = -\sum_r \gamma_{ri}\omega_r, \qquad (30)$$

And the velocity function in the form of mass action law can be written as,

$$\omega(c^I, c^{II}) = k_r \prod_i (c_i^I)^{\alpha_{ri}^I} (c_i^{II})^{\alpha_{ri}^{II}}, \qquad (31)$$

where $k_r \geq 0$ is the rate constant depending upon the kinetic factors of the investigated system and its thermodynamic properties. It is necessary to fulfil the no advection condition:

$$\sum_r \gamma_r \omega_r (c,c) = 0, \tag{32}$$

which means the absence of flux at $c^I = c^{II}$, in a homogeneous composition enviroment. Introducing flux J_{ri} as the first approximation of the Taylor series expansion in ω Subject to the condition (0.2.47),

$$\overrightarrow{J_{ri}} = -\gamma_{ri} \sum_j \frac{\partial \omega_r (c^I, c^{II})}{\partial c_j^{II}} \Bigg|_{c^I = c^{II} = c(x)} . \vec{\nabla} c_j . \tag{33}$$

This expression represents the transition from flux density between the cells to the vector of the flux density. It should be noted that model will work well, especially in the selection of the suitable relationship between size of unit cell and diffusion zone (Gorban et al., 2011).

Gorban et al. (2011), Kuttler (2011), and Murray (2003) discussed a few diffusion reactions mechanisms for cell jump models and determined their reactions rates, vectors of total flux density, and their diffusion equations by using the law of mass action along with principle of detailed balance. Some of the mechanisms are presented here.

12 Models of Non Linear Diffusion

The simplest mechanism of diffusion between any two cells is the process of jumping from one cell to another. This type of mutually inverted and mutually inverse process can be written as (Gorban et al., 2011),

$$\begin{aligned} &A^I \to A^{II} \\ &A^{II} \to A^I \end{aligned} \tag{34}$$

12.1 Mechanism of sharing place

The simplest mechanism of diffusion with interaction of *n* different substances of a multi component system is given by stoichiometric equation of the form (Gorban et al., 2011):

$$\begin{aligned} &A_i^I + A_j^{II} \to A_j^I + A_i^{II} \\ &A_i^{II} + A_j^I \to A_i^I + A_j^{II} \end{aligned} \tag{35}$$

12.2 Diffusion of mechanisms of attraction and repulsion

The diffusion mechanisms leading to the inhomogeneous structures can be described by the multi solution immersed into the external conditions under which non linear mechanisms are possible with the stoichiometric equations, describing the mechanism of attraction (Gorban et al., 2011):

Repulsion:

$$\begin{aligned} &2A^I \to A^I + A^{II} \\ &2A^{II} \to A^I + A^{II} \end{aligned} \tag{36}$$

Attraction:

$$\begin{aligned} &A^I + A^{II} \to 2A^I \\ &A^I + A^{II} \to 2A^{II} \end{aligned} \tag{37}$$

12.3 Autocatalysis mechanisms

A process where a chemical is involved in its own production is called autocatalysis. Feedbacks controls exist into many biological systems. One must be familiar with how to model them because they have enormous importance. In 1978, Tyson and Othmer introduced the dynamics of metabolic feedback control systems and a theoretical models review. A process when the product of one step in a reaction sequence has an effect on other reaction steps in the sequence. The effect is generally nonlinear and may be to activate or inhibit these reactions. A very simple pedagogical example is,

$$A+Y \underset{k_2}{\overset{k_1}{\rightleftharpoons}} 2Y, \qquad (38)$$

where a molecule of Y combines with one of A to form two molecules of Y (Murray, 2003).

13 Foxes and Rabbits Interaction- A Non-Linear System

The humans are and they make open systems. Open systems interactions with the other open systems in an immeasurable set of connections of open systems. Open systems become accustomed to these connections such that their behaviour is non linear in general. It is difficult to predict the behavior of our artificial systems when they are introduced into some operational atmosphere.

It is a constant battle among the animals on a daily basis to survive. They have to find their food and avoid becoming a food. These species can be divide up on the basis that how they get their food, if they provide it they are producers (prey), if they need to find it they are consumers (predator) and if they breakdown dead material they are decomposers.

This correlation between predator and prey intertwines into a complex food chain. In the ecosystem there are various species and every one play a significant role in maintaining populations near the carrying capacity and in keeping the system in balance. In the ecosystems Predator and prey assist them through particular adaptations to compete for food resources. Predator and prey populations are directly related and they cannot survive without each other. Here this relationship is illustrated by using foxes and rabbits.

In artificial world and in the social systems non-linear behaviors are the order of the day. Rabbits and foxes share some behaviors but vary in others and their interaction is non-linear in nature.

The rabbits are proverbially very good in reproduction. In case when more rabbits are there, the more foxes will prey on them, so that the number of foxes will increase, when more foxes will predate a lot such that the number of rabbits start to decrease, swiftly it follows by falling fox numbers as there are a small amount of rabbits to sustain them therefore it is observed that the populations of rabbits and foxes are locked together in an interactive population 'dance.' This system is non-linear in its behavior. In mathematics non-linear simultaneous equations are used to represent these interactions for which there exist an infinite number of solutions.

Between the fox and rabbit populations here is a complicated and natural predator-prey relationship, since rabbits thrive in the absence of foxes and foxes thrive in the presence of rabbits. Foxes like to occupy a combination of forest and open fields. Foxes usually define their territory zones and use the transition zone or "edge" between these habitats as hunting areas. Foxes do not interfere in the defined areas of each others.

13.1 Predator prey interactions

In this idealized ecological system, two populations are considered of which one may be hunted by the second.

- Each prey gives rise to a constant number of off-spring preys each year.
- A constant proportion of the prey population is hunted by each predator each year.
- Predator reproduction is directly proportional to the constant proportion of the prey population hunted by each predator.

- A constant proportion of predator population dies each year.

If R is the number of prey population (rabbits) and F is the number of predator population (foxes), then conventionally this model has a mathematical representation as,

$$\begin{aligned} \frac{dR}{dt} &= AR - BRF, \\ \frac{dF}{dt} &= CRF - DF. \end{aligned} \tag{39}$$

The above equations are called Lotka-Volterra equations or the predator-prey equations, which are used to describe the dynamics of biological systems in which two species interact, one is a Predator-the hunter, and other is its prey-the hunted.

Here the derivatives $\frac{dR}{dt}$ and $\frac{dF}{dt}$ represent the growth of the two populations with respect to time and A, B, C and D are parameters representing the interaction of the two species in the following manner:

- A - The number of offspring per prey per year.
- B - The proportion of the prey population hunted by one predator per year.
- C - Conversion of one prey hunted and consumed by the predator into new predators.
- D - The proportion of predator population dying per year.

Physically, the Lotka-Volterra model requires a number of assumptions about the environment and evolution of the predator and prey populations such as food availability at all times to predator populations depending entirely upon the prey populations, rate of change of population which is proportional to the size of the population and an unchanged environment in favour of one species during the process.

13.2 Rabbits on the island

Taking an island inhabited by a small population of rabbits (prey) with no other animals around. The prey are assumed to have an unlimited food supply and the number of rabbits born and die in a certain period is proportional to the total number of rabbits at that time, then the change in their population can be written as:

$$\frac{dR}{dt} = rR \tag{40}$$

where R is the number of rabbits at time t and r is the growth rate of the rabbit population defined as the difference between birth and death rates. The equation has a solution as:

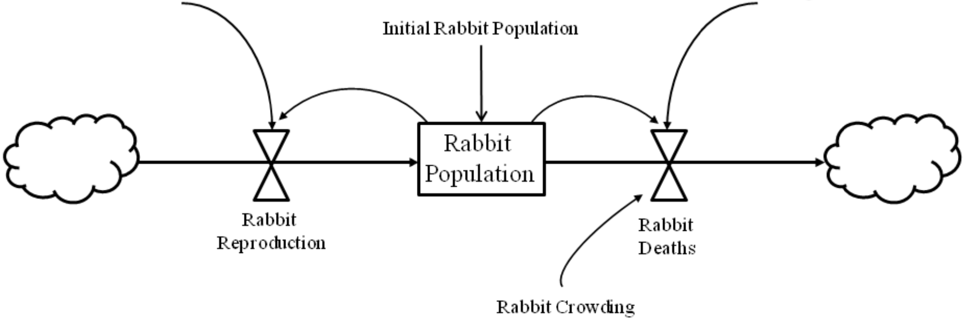

Fig. 2 Single population model-1.

$$R = R_0 e^{rt} \tag{41}$$

where R_0 is the initial population of the rabbits (prey) at time $t = 0$. This model is also called exponential growth model due exponential factor involved. The exponential growth rate will be positive if births are more than deaths and negative if deaths are dominant.

The exponential model is not very realistic because with a negative exponential growth rate, there will not be any life left on the island. On the other hand, if the growth rate is positive, the rabbits will cover the entire island with enough time. This will not happen actually because rabbits will run out of space and food due to maximum carrying capacity of island. This kind of problem was handled through the law of population growth derived by Alfred J. Lotka in 1925 by adding the concept of carrying capacity K to the exponential model. This model is called logistic model formalized by the differential equation:

$$\frac{dx}{dt} = rx\left(1 - \frac{x}{k}\right) \tag{42}$$

Clearly when $R < K,$ and $R \to k$ the equation (42) is close to the equation (40) and rabbit population stops growing. If $R > K,$ then there will be a crowding of rabbit population on the island and from equation (42) a negative sign will reduce the population growth to a manageable level. The behaviour of the model can be predicted through the growth rate r .

13.3 Fox as a predator

In the presence of hundreds of different animals on the island, the modeling of the interaction among these animals is not an easy task. However, the interaction between two species is possible taking one as a prey and the other as a predator. The same single population growth model can be used for predators (foxes), if prey (rabbits) is considered as an unlimited food supply to foxes. But Foxes are territorial animals, and in general each fox claims its own territory by marking their territories with signals that other foxes will recognize e. g., by leaving their droppings in prominent positions. They pair up only in winter. So it will be difficult for the foxes to cover the whole island without defining their own territories.

In order to describe the interaction between a predators (foxes) and its prey (rabbits), introduce a small number of fox population on the island with rabbits having unlimited food supply and following the equation (42). If R represents the rabbit's population and F is the fox's population, then population rates for each species will be affected and described by the following equations as:

$$\begin{aligned} \frac{dR}{dt} &= aR - bRF, \\ \frac{dF}{dt} &= cRF - dF. \end{aligned} \tag{43}$$

where a, b, c and d are parameters as defined for predator (fox) and its prey (rabbits). The additional terms will now be defined as:

- $-bRF$ Rabbits hunted by the foxes, reducing the rabbit population
- $+cRF$ Fox population growth by eating the rabbits

Since some of the rabbits will be hunted by the foxes (as a food), so the birth rate r is not the only factor describing the rabbit population. Without the presence of foxes, i.e., $F = 0,$ the equation (43) will reduce to a simple exponential model (40).

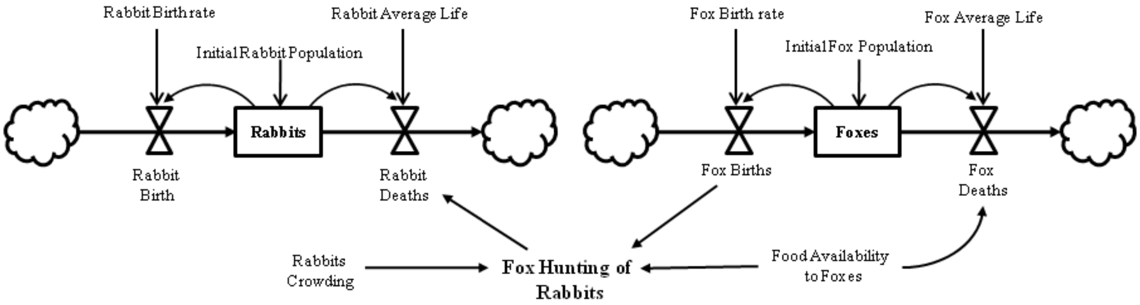

Fig. 3 Model structure.

On the other hand, without food supply $(R = 0)$ to foxes, the equation (43) will reduce to:

$$\frac{dF}{dt} = -dF \qquad (44)$$

Which means foxes will die in turn if they do not get enough food for their survival. In this case, the rabbit population will begin to increase in the absence of prey. The populations of foxes will again starts increasing with the increase in rabbit population, and this cycle will continue.

13.4 Basic reactions of foxes and rabbits

Let us suppose that our space is divided on two territories, a system represented as a chain of territories each with homogeneous composition and elementary acts of transfers on the boundary (for us there are only two territories). On each territory we have some concentrations (number of foxes and rabbits) for these processes. Let F^I (fox/ foxes in first territory) and R^I (rabbit/ rabbits in first territory) is the vector concentration in the first territory *I* and F^{II} (fox/ foxes in second territory) and R^{II} (rabbit/ rabbits in second territory) is the vector of concentration in the second territory *II.*

In any territory when foxes and rabbits both are present, the following basic mechanisms are possible in that situation;

1. When in any territory a fox (F) and total n number of rabbits (R) are present, let us suppose that r is the number of rabbits which fox (F) prey in that territory. When fox will prey rabbits (R), rabbit's population will start to decrease. The rabbits are proverbially very good in reproduction so their population will increase again; in this case the possible mechanism will be,

$$F + (n)R \rightarrow F + (n-r)R, r < n \qquad (45)$$

2. Now in the case of foxes, when two foxes, a male fox $F_{(m)}$ and a female fox $F_{(f)}$ interact, let n be the number of foxes which born as the result of that interaction, they all can be males, females or a combination of both $F_{(m+f)}$, this circle repeats itself; in this case the possible mechanism will be,

$$F_{(m)} + F_{(f)} \rightarrow (n)F_{(f+m)} \qquad (46)$$

3. Now in the case of rabbits, when two rabbits, one male $R_{(m)}$ and the other female rabbit $R_{(f)}$ interact, let n be the number of rabbits which born as the result of that interaction, they can be males, females or a combination of both sexes $R_{(m+f)}$, this circle repeats itself; in this case the possible mechanism will be,

$$R_{(m)} + R_{(f)} \rightarrow (n)R_{(m+f)} \tag{47}$$

13.5 Mechanism of circulation

The simplest mechanism of circulation between any two foxes or rabbits is the process of moving one fox or rabbit from area defined for it, to the area defined for another fox or rabbit and vise versa. This type of mutually inverted and mutually inverse processes for the case of foxes can be written as,

$$\begin{aligned} F^{I} &\rightarrow F^{II} \\ F^{II} &\rightarrow F^{I} \end{aligned} \tag{48}$$

This mechanism for the case of rabbits will be written as,

$$\begin{aligned} R^{I} &\rightarrow R^{II} \\ R^{II} &\rightarrow R^{I} \end{aligned} \tag{49}$$

As it is stated in the early lines that foxes are territorial and stay in their own territorial zones, the above mechanism may not be possible in practical in the case of foxes, but rabbits move freely in nature without any restrictions so this mechanism may or may not be possible in that case.

13.6 Mechanism of sharing place

1. The mechanism of sharing place with interaction of *n* different foxes or rabbits i.e. when a fox F_i^I is in territory one and another fox F_j^{II} is in territory two and then fox F_i^I moves from territory one to territory two and vise versa, in a multi component system is given by stoichiometric equations of the form:

$$\begin{aligned} F_i^{I} + F_j^{II} &\rightarrow F_j^{I} + F_i^{II} \\ F_i^{II} + F_j^{I} &\rightarrow F_i^{I} + F_j^{II} \end{aligned} \tag{50}$$

Practically in the case of foxes the above mechanism seems to be almost impossible because foxes usually define their territory zones and use the transition zone or "edge" between these habitats as hunting areas. Foxes do not interfere in the defined areas of each other’s and foxes fight other foxes if they find them in their territory.

2. In the case of rabbits it may or may not be possible because rabbit’s movement is free naturally without any restrictions. In that case the possible mechanisms will be,

$$R_i^{I} + R_j^{II} \rightarrow R_j^{I} + R_i^{II} \tag{51}$$

$$R_i^{II} + R_j^{I} \rightarrow R_i^{I} + R_j^{II} \tag{52}$$

3. Now in the case of mix situation i.e. by taking foxes and rabbits case together,

$$F_i^{I} + R_j^{II} \rightarrow F_i^{I} + R_j^{I} \rightarrow F_i^{I} \tag{53}$$

$$F_i^{II} + R_j^{I} \to F_i^{II} + R_j^{II} \to F_i^{II} \tag{54}$$

As the foxes are territorial while the rabbits move freely, in the above mechanism (53) it is described that when a fox is in territory one and a rabbit is in territory two, if rabbit move from territory two to territory one, the fox in that area will prey that rabbit and a similar case happens in mechanism (54) for second territory.

13.7 Mechanism of attraction and repulsion

1. Foxes are solitary and necessitate quite huge hunting areas. A fox constantly patrols its territory looking for food, using its urine to mark places it has completed searching. Foxes are territorial and fight other foxes that they find on their territory. Because they wander over such a wide area, foxes maintain several burrows and dens across their territory. The possible mechanisms of attraction and repulsion for the foxes and rabbits can be;

Repulsion:

$$\begin{aligned} 2F^{I} &\to F^{I} + F^{II} \\ 2F^{II} &\to F^{I} + F^{II} \end{aligned} \tag{55}$$

Attraction:

$$\begin{aligned} F^{I} + F^{II} &\to 2F^{I} \\ F^{I} + F^{II} &\to 2F^{II} \end{aligned} \tag{56}$$

Both the mechanisms of attraction are unnatural in the case of foxes because foxes are territorial and fight other foxes that they find on their territory so two or more foxes cannot stay in the same territory thus we will have to move towards mechanisms of repulsion consequently there will be no attraction in the case of foxes.

2. Now taking the mechanisms of attraction and repulsion for the case of rabbits the following mechanisms are possible,

Attraction:

$$\begin{aligned} R^{I} + R^{II} &\to 2R^{I} \\ R^{I} + R^{II} &\to 2R^{II} \end{aligned} \tag{57}$$

Repulsion:

$$\begin{aligned} 2R^{I} &\to R^{I} + R^{II} \\ 2R^{II} &\to R^{I} + R^{II} \end{aligned} \tag{58}$$

In this case the above stated both the mechanisms of attraction and repulsion may or may not be possible because rabbits move freely in nature without any restrictions. If two rabbits are in two different territories and they both move in the same territory then it is described by mechanisms of attraction and if two rabbits are in the same territory and one of them leaves that territory and moves to another territory in that case, it is described by mechanisms of repulsion.

3. Now for the mix situation i.e. when in any territory the mechanisms of attraction and repulsion are considered for both, the foxes and the rabbits at a time, the following mechanisms for attraction and repulsion are possible,

Attraction:

$$\begin{aligned} R^{I} + F^{I} &\to F^{I} \\ R^{II} + F^{II} &\to F^{II} \end{aligned} \tag{59}$$

In attraction mechanism when both the rabbit and the fox are in the same territory, then fox will prey the rabbit and the result will be the fox.

Repulsion:

$$\begin{aligned} R^{I} + F^{I} &\rightarrow F^{I} + R^{II} \\ R^{II} + F^{II} &\rightarrow F^{II} + R^{I} \end{aligned} \qquad (60)$$

In repulsion mechanism when both the rabbit and the fox will be in the same territory then it is possible that a rabbit may change its territory but fox does not do so because foxes are territorial. When rabbit in the first territory will change its territory then the fox of that territory will not be in a position to prey that rabbit so it will survive that fox but fox present in that territory will be in a position to prey that rabbit and vise versa.

13.8 Pair wise interaction

In pair wise interaction the following mechanisms are possible because foxes are territorial while rabbits move freely in nature and rabbits change their territories regularly while foxes does not do so. In this situation the possible mechanisms will be;

$$(R^{I} + F^{I}) + (R^{II} + F^{II}) \rightarrow (R^{II} + F^{I}) + (R^{I} + F^{II}) \qquad (61)$$

$$(R^{I} + F^{I}) + (R^{II} + F^{II}) \rightarrow (R^{I} + R^{I} + F^{I}) + F^{II} \qquad (62)$$

$$(R^{I} + F^{I}) + (R^{II} + F^{II}) \rightarrow F^{I} + (R^{II} + R^{II} + F^{II}) \qquad (63)$$

In the above mechanism (61) a rabbit and a fox are present in territory one and a similar situation is in the territory two. In mechanism one, rabbit from territory one moves to territory two and vise versa. Other possibilities are that both the rabbits move to territory one or both of them move to territory two. These possibilities are described in mechanism (62) and (63) respectively.

13.9 Autocatalysis *m*echanisms

Autocatalysis is the procedure whereby a chemical is involved in its own production. In the following mechanisms, in the case of foxes, when two foxes, a male fox $F_{(m)}$ and a female fox $F_{(f)}$ interact, let n be the number of foxes which born as the result of that interaction, they all can be males, females or a combination of both $F_{(m+f)}$, this circle repeats itself; in this case the possible mechanism will be,

$$F_{(m)} + F_{(f)} \rightarrow (n)F_{(f+m)} \qquad (64)$$

Now in the case of rabbits, when two rabbits, one male $R_{(m)}$ and the other female rabbit $R_{(f)}$ interact, let n be the number of rabbits which born as the result of that interaction, they can be males, females or a combination of both s $R_{(m+f)}$, this circle repeats itself; in this case the possible mechanism will be,

$$R_{(m)} + R_{(f)} \rightarrow (n)R_{(m+f)} \qquad (65)$$

14 The Observations

The sense in which the discrete equations for cells converge to the partial differential equations of diffusion is that the cell models give the semi-discrete approximation of the partial differential equations for diffusion.

They result in a system of ordinary differential equations in cells. Such approximation appears often in finite element methods and cells are discontinuous finite elements. There are jumps of concentrations on the boundary of cells. The Taylor expansion of the right hand sides of the discrete system of ordinary differential equations for cells produces the second order in the cell size approximation to the continuous diffusion equation (the standard result for the central differences).

Significant difference from the classical finite elements is in construction of right hand sides of the ordinary differential equations for concentrations in cells: there are flows in both directions: from cell 1 to cell II and from cell II to cell I. These flows have a simple mass action law construction and the resulting diffusion flow is the difference between them. The kinetic constants should be scaled with the cell size to keep $kl = d$ (k is the kinetic constant, l is the cell size, d is the diffusion coefficient for the particular mechanism).

This is the approximation of the right hand sides. The approximation of solutions is a more difficult problem and depends upon the properties of solutions of PDE. It seems a good hypothesis that for obtained diffusion systems with convex Lyapunov functional and “no-flux” boundary conditions in bounded areas with smooth boundaries the cell model gives the uniform approximation to the solution of the correspondent PDE.

The system of semi-discrete models for cells with “no-flux” boundary conditions has all the nice properties of the chemical kinetic equations for closed systems. Under the proper relations between coefficients, like complex balance or detailed balance, this system demonstrated globally stable dynamics. This global stability property can help with the study of the related PDE.

Finally, the cell-jump models may be considered as the proper diffusion models by themselves, for the finite physically reasonable cell size, without limit. This size may be quite large for the coarse-grained models (it depends on the medium microstructure and on the smoothness of the concentration fields).

14.1 For mechanisms of circulation

For this mechanism,

$$F^{I} \to F^{II}$$
$$F^{II} \to F^{I}$$
$$R^{I} \to R^{II}$$
$$R^{II} \to R^{I}$$

It is stated in the early lines that the above stated mechanism is not possible in the case of foxes because the foxes are territorial and does not change their territory while it may or may not be possible in the case of rabbits because their movement is free naturally and if this mechanism occurs in their case, then the equation of kinetics for the above mechanism the condition of absence of flux in a homogenous environment with the rate of constant of direct and inverted processes as $k_i^{+} = k_i^{-} = k_i$ give the following form of the diffusion equation,

$$\frac{\partial c_i}{\partial t} = k_i \Delta c_i .$$

14.2 For sharing place mechanism

Sharing place mechanism is also not possible in the case of foxes due to the fact that the foxes are territorial and does not change their territory while it may or may not be possible in the case of rabbits because their movement is free naturally and if this mechanism occurs in their case, then for the mechanisms of sharing place the diffusion equations for the above mechanism using stoichiometric vectors $\vec{\gamma}_{ri}$, fluxes of the substances F_i and F_j and the functions w_1 and w_2 for the first and second elementary process are calculated as,

For process: $$F_i^I + F_j^{II} \to F_j^I + F_i^{II}$$

$$\gamma_{1i} = -1 \qquad \gamma_{1j} = 1 \qquad w_1(c^I, c^{II}) = k_1 c_i^I c_j^{II}$$

$$\vec{J}_{1i} = k_1 c_i \overset{\rightarrow}{\nabla} c_j \qquad \vec{J}_{1i} = -k_1 c_i \overset{\rightarrow}{\nabla} c_j$$

$$w_1 = div\left(k_1 c_i \overset{\rightarrow}{\nabla} c_j \right) = k_1 \left(c_i \Delta c_j + (\overset{\rightarrow}{\nabla} c_i, \overset{\rightarrow}{\nabla} c_j) \right)$$

For process: $$F_i^{II} + F_j^I \to F_i^I + F_j^{II}$$

$$\gamma_{2i} = 1 \qquad \gamma_{2j} = -1 \qquad w_1(c^I, c^{II}) = k_k c_j^I c_i^{II}$$

$$\vec{J}_{2i} = -k_2 c_j \overset{\rightarrow}{\nabla} c_i \qquad \vec{J}_{1i} = k_2 c_j \overset{\rightarrow}{\nabla} c_i$$

$$w_2 = div\left(k_2 c_j \overset{\rightarrow}{\nabla} c_i \right) = k_2 \left(c_j \Delta c_i + (\overset{\rightarrow}{\nabla} c_i, \overset{\rightarrow}{\nabla} c_j) \right)$$

The equation for mutual diffusion for *i*th and *j*th substances was determined as,

$$\frac{\partial c_i}{\partial t} = k(c_j \Delta c_i - c_i \Delta c_j)$$
$$\frac{\partial c_j}{\partial t} = k(c_i \Delta c_j - c_j \Delta c_i)$$

The above equation describes the diffusion on the surface of the catalyst for the mechanism of jumping to a neighboring free space (Gorban et al., 2011).

15 Our Objectives

Our goals are:

(a) To build up a brief study of complex biological systems by taking a study case of foxes and rabbits.

(b) To tackle key research questions about our case study by proposing new techniques and algorithms that are inspired by those complex biological systems.

Further for our case study we want to study, and aim to extend these ideas to all other possible mechanisms complete in all aspects between foxes and rabbits. We aim a comparative study for all the possible mechanisms like, mechanism of attraction and repulsion, pair wise attraction, and for autocatalysis mechanisms between foxes and rabbits and want to determine their reactions rates, vectors of total flux density, and their diffusion equations by using the law of mass action along with the principle of detailed balance and aim to check their stability for these interactions.

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