RESEARCH ARTICLE | NOVEMBER 20 2023

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AIP Conf. Proc. 2953, 050002 (2023)
https://doi.org/10.1063/5.0177556

A Chemical Reaction Network of a Predator-prey Model with the SEIR and the SEIRS Epidemic in the Prey Population

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Abstract. A predator-prey model with an epidemic model of SEIR (Susceptible-Exposed-Infected-Recovered) and SIERS (Susceptible-Exposed-Infected-Recovered-Susceptible) in the prey population is introduced. The epidemic disease had been described by the SEIR and the SEIRS models. A logistical growth function appears in the susceptible prey population. The predation function is given in the five nonlinear ordinary differential equations. They present the dynamics' of the species' population. The main focus of this article is to propose an eco-epidemiological model that can be implemented by a chemical reaction network. The studied chemical reaction network is a mathematical-chemical apparatus through which a parallel between the change of reactant concentrations and the dynamics of the populations can be made. The authors present a chemical reaction network which describes the considered model indicating the obtained differential equations. The main law that is used is the law of mass action kinetics. Some numerical experiments are given.

INTRODUCTION: ECO-EPIDEMIOLOGICAL AND CHEMICAL REACTION NETWORK THEORY

Epidemiology is a science that studies the causes of the occurrence and spread of various types of diseases (infections) in human organisms and animal species. Based on the scientific information through the years, some scientists strive to predict the development of diseases over time in order to limit or eliminate the spreading of infections. Mathematical ecology and epidemiology are two distinct areas of applied mathematics in the field of biology. Their combination is called eco-epidemiology and it has been a subject of research since 1990. The purpose of the eco-epidemiological models is to describe the ecosystems which give the interactions between the individual populations in the presence of an infection. The discovery of the epidemiological model SIRS (Susceptible-Infected-Recovered-Susceptible) by Kermack-McKenrick [1], gave impetus to the development of mathematical epidemiology. Nowadays a lot of researchers are interested in mathematical models of infectious diseases like SI (Susceptible-Infected), SIS (Susceptible-Infected-Susceptible), SIR (Susceptible-Infected-Recovered) and SEIR (Susceptible-Exposed-Infected-Recovered) and are trying to apply them to the Lotka-Volterra model or also known as a predator-prey model [2].

These eco-epidemiological models can be classified depending on the prevalence of contagion into three distinct categories:

(i) contagion in the prey [3, 4, 5];
(ii) contagion in the predator [6];
(iii) contagion in both animal species [7, 8].

The infection in the predator occurs after the consumption of the victim (it is the so-called predation) [7, 8].

Application of Mathematics in Technical and Natural Sciences
AIP Conf. Proc. 2953, 050002-1–050002-16; https://doi.org/10.1063/5.0177556
Published by AIP Publishing. 978-0-7354-4720-2/$30.00

Chemical reaction network theory (CRNT) is an area of applied mathematics that describes the behavior of the chemical systems in the real world. The chemical kinetics similar to the formal kinetics of transfer phenomena describe the course of the reactions by using the apparatus of the kinetic equations. These equations show the change in the concentration of the participating chemical substances in time [9]. Since their appearance in the 1864 [21, 22, 23], chemical kinetics has become an object of interest in the research community due to its application in biochemistry and theoretical chemistry. The application of the chemical reactions of the living systems can be found in enzyme-catalytic reactions, destruction of biopolymers, coupled reactions and in the nonlinear chemical systems of closed and open type. Another application that is an object of scientific interest is the study of the dynamics of various mathematical, physical, chemical and biological models. For example, the description of the populations' dynamics can be given by biological growth-decay functions. In ecological or eco-epidemiological models it can be represented by kinetic equations [10,11,12,13,14]. When we speak about a chemical system we have to keep in mind the basic principle of converting the chemical reactions into a corresponding set of kinetic (rate) equations by using the law of mass action. Usually, rate equations describe the change in the concentration of the given chemical substance of the corresponding reaction in time, see [15,16]. The set of kinetic equations forms an ordinary differential system which can be linear or non-linear.

There are two approaches of forming a relationship between the chemical equations and a given mathematical model:

(i) "direct" method – when the chemical equation is given, then the mathematical model represented by ordinary differential equations is constructed;

(ii) "inverse" method – when from a given mathematical model described by ordinary differential equations we can obtain the corresponding chemical equations;

The reaction network (RN) is a mathematical-chemical apparatus by which a parallel between the change in concentrations of the chemical substances and the dynamics of the populations can be made. The RNs consists of a set of chemical species or compounds denoted by X and a set of chemical reactions denoted by R. Each of these sets convert a multiset of educts into a multiset of products [20]. Depending on the application, this simple construction may be enlarged by assigning properties such as mass, energy, sum formulas or structural formulas to the compound. On the other hand, not all RNs necessarily admit a chemical interpretation. A good advantage of the RNs is that they may contradict some fundamental principles of physics such as the conservation of energy and mass or the reversibility of chemical reactions when they are compared with epidemic models. Knowledge of the reaction networks' structure allows the given model to compute better the epidemic dynamics at the population scale from the individual-level behavior of infections [19]. The main focus of this paper is to show a relationship between a given eco-epidemiological model and its corresponding chemical reaction network using the inverse approach. As a result the structure of the resulting reaction network gives more information about the dynamics of the considered epidemic.

The present paper is constructed in four sections. The introductory part is given in Section 1. The chemical reaction networks' theory and the transformation into ODEs using the law of mass action is given in Section 2. In this section we introduce an example of a chemical reaction network for a "direct" method of achieving an eco-epidemic predator - prey model in the presence of the SIS disease. Section 3 has two subsections where the focus is on the reaction network of a predator-prey model with the SEIR and the SEIRS epidemic in the prey population. In Section 4 we give the relationship between the dynamics of a pair of individual populations and a pair of concentrations of the chemical substances corresponding to the considered animal species. This relationship is illustrated by some graphics which are obtained by using the online software SmoWeb [17]. The main emphasis of the paper is on the biological interpretation of the chemical equations through which the reaction networks of the given model are formed.

PRELIMINARIES: REACTION NETWORKS AND THEIR TARNSFORMATION INTO ORDINARY DIFFERENTIAL EQUATIONS

This section aims to acquaint the reader with the basics of the chemical reaction network theory and its application in mathematical modeling. The method of a reaction network's "translation" into a system of ordinary differential equations (ODEs) by using the principle of "kinetic mass action" is illustrated by an example. Using this method of translation, the reaction network becomes a unique mathematical apparatus through which the bio-chemical interpretation of the chemical equations can be easily understood. The ordinary differential equations system determines the change in masses (concentrations, densities) of the species. In the chemical systems' theory

the fundamental principle of transformation from a chemical reaction network to a set of ordinary differential equations which in chemistry are called kinetic equations is accomplished by the law of mass action. In chemistry these equations are called kinetic equations. The simple (elementary) reactions can be given by:

$$Reactants \xrightarrow{k} Products, \tag{1}$$

where the rate of the homogeneous chemical reaction is determined by the change in the concentration of one of the chemical species involved in it per unit time.

Let the chemical species *A*, *B*, *C* and *D* be given in such a way that *n* molecules of the species *A* and *m* molecules of the species *B* react to *p* molecules of the species *C* and *q* molecules of the species *D*. Then the chemical reaction is the following:

$$n\,A + m\,B \xrightarrow{k} p\,C + q\,D$$
$$v = -\frac{d[A]}{dt}, \tag{2}$$

The sign (-) indicates that the concentration of the species *A* decreases in time. The concentration's change of the chemical species *A* is connected with the change of the remaining species *B*, *C* and *D*, as it is shown in the stoichiometric equation (2). As the products *C* and *D* increase in time, $\mu=\frac{d[C]}{dt}$ then the rate that describes the change in their concentration will have a positive sign, *i.e.* (+). The rate of the concentration's change can be defined as:

Reaction rate = - rate of consuming one unit of reactant = + rate of creating one unit of product

In this case we obtain:

$$Rate = \frac{1}{p}\frac{d[C]}{dt} = \frac{1}{q}\frac{d[D]}{dt} = -\frac{1}{n}\frac{d[A]}{dt} = -\frac{1}{m}\frac{d[B]}{dt} = kA^{n'}B^{m'} \tag{3}$$

where the constant *k* is a rate constant and it represents the reaction's rate under the standard conditions [A] = [B] = 1 mol/l.

Let us consider some of the basic chemical reactions and their kinetic equations, applying the law of mass action:

a) **Constant supply**: The product *A* appears in the system with a constant rate *k*.

$$(source) \xrightarrow{k} A \Rightarrow \frac{d[A]}{dt} = k.$$

This is called a zero-order reaction because the rate does not depend on the concentration of either reactant (reagent).

b) **Decay substance:** The substance *A* is transformed into waste at rate *k* (*i.e.*, *A* decays and is removed from the system).

$$A \xrightarrow{k} \varnothing\ (waste) \Rightarrow \frac{d[A]}{dt} = -kA.$$

This reaction is called a first-order reaction because the rate depends linearly on the concentration of the single reactant.

c) **Transformation:** The reactant *A* is consumed with the product *B*, being produced from *A*.

$$A \xrightarrow{k} B \Rightarrow \frac{d[A]}{dt} = -kA, \quad \frac{d[B]}{dt} = kA.$$

This reaction is the simplest reaction network, having two distinct concentrations evolving due to a single reaction.

d) **Compound formation:** The interaction between chemical substances *A* and *B* gives *C*.

$$A + B \xrightarrow{k} C \Rightarrow \frac{d[A]}{dt} = -kAB, \quad \frac{d[B]}{dt} = -kAB, \quad \frac{d[C]}{dt} = kAB.$$

The production rate of *C* being proportional to the product of the reactant concentrations follows from a probabilistic description of the collision of independent molecules.

Let us denote the concentration of the chemical species *A* by $[A]_t \geqq 0$. Then the total production's rate of the chemical species *A* will be determined by its creation and/or consumption depending on each reaction where it is involved, *i.e.*,

$$\frac{d[A]}{dt} = +\sum_{i=1}^{N}(creation\ rate)_i - \sum_{i=1}^{N}(consumption\ rate)_i. \tag{4}$$

In formula (4) we denote the number of chemical reactions in which the chemical species *A* is involved by *i*. Then *N* is the total number of the chemical reactions in the reaction network. For given systems without losses or sources of chemical, as in the case of c), the physical expectations which are based on the conservation law suggest that *A+B = constant*. This can be confirmed by evaluating the expression $\frac{d([A]+[B])}{dt}$ using the kinetic equations or the rate equations. This law is called a conservation law and it gives the connection between the products and reactants [18].

The reaction order ϑ is a sum of the exponents to which the concentrations in the kinetic equation (3) are raised. In this case $\vartheta = n' + m'$. The molecularity *m* is the number of the particles involved in the chemical reaction. It characterizes the course of an elementary reaction while the reaction order ϑ is related to the course of the entire chemical reaction which consists of a series of elementary reactions. For a given elementary reaction, if the degrees *n'* and *m'* from the kinetic equation (3) match with the stoichiometric coefficients *n* and *m*, then the order and the molecularity will also match, *i.e.*, $\vartheta = m$. If the reactions proceed in a way that is not reflected correctly by their stoichiometric equation then the degrees *n'* and *m'* of the kinetic equation will not coincide with the stoichiometric coefficients *n* and *m*, see [9].

Let us consider some chemical reaction networks' examples by using the "direct" approach in obtaining the eco-epidemiological model with a presence of the SI disease.

Example:

Let the chemical species *S*, *I* and *P* be given by the following chemical reaction networks:

$$(1)\ P+S \xrightarrow{k} 2P, \quad (2)\ P \xrightarrow{\mu} S, \quad (3)\ S+I \xrightarrow{\eta} 2I, \quad (4)\ I \xrightarrow{\rho} S,$$

where k, μ, ρ, η are positive rate constants. The constructed reaction networks are in a canonical form.

TABLE 1: The chemical reactions and their equations

No	Chemical reactions	Kinetic equations
1.	$P + S \xrightarrow{k} 2P$	$\frac{d[P]}{dt} = kPS$ $\frac{d[S]}{dt} = -kPS$
2.	$P \xrightarrow{\mu} S$	$\frac{d[S]}{dt} = \mu P$ $\frac{d[P]}{dt} = -\mu P$
3.	$S + I \xrightarrow{\eta} 2I$	$\frac{d[I]}{dt} = \eta SI$ $\frac{d[S]}{dt} = -\eta SI$
4.	$I \xrightarrow{\rho} S$	$\frac{d[I]}{dt} = -\rho I$ $\frac{d[S]}{dt} = \rho I$

We denote the strictly positive concentrations of the chemical species *S*, *I* and *P* by [S], [I], [P]. Let the rate of change of the chemical substances correspond to the change of the animal species' populations – a prey and a predator. Here the function *S(t)* represents the population of the susceptible prey, *I(t)* is the infected prey and the

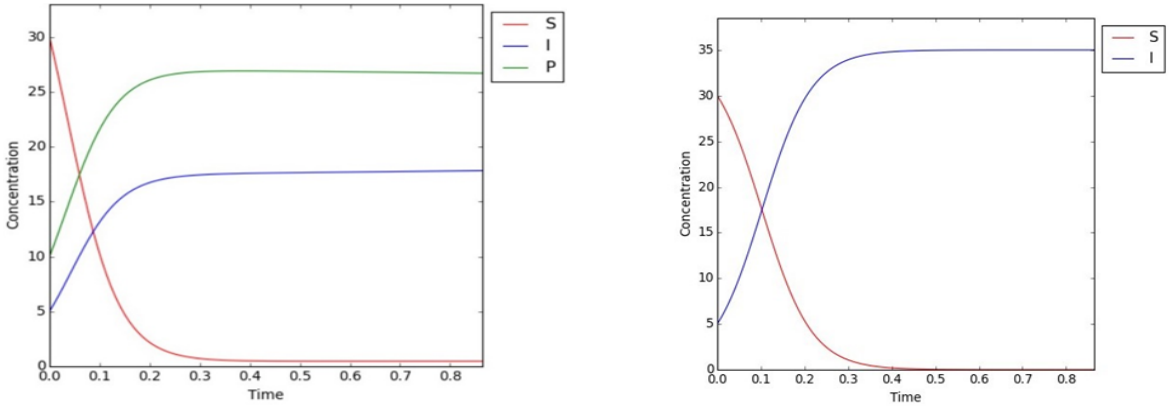
function *P(t)* represents the predator. In Table 1 we introduce four main chemical reactions and their kinetic equations. The chemical interpretations of the kinetic equations are given in Table 6 from Appendix A.

The chemical species *S*, *I* and *P* have a total rate of a production which is obtained as a sum of the right-hand members of each reaction in which they participate. We will pay attention to the following main models which are constructed by two systems of ordinary differential equations:

$$\begin{cases} \dfrac{d[S]}{dt} = -\eta SI - kPS + \mu P + \rho I \\ \dfrac{d[I]}{dt} = \eta SI - \rho I \\ \dfrac{d[P]}{dt} = kPS - \mu P \end{cases} \tag{5}$$

$$\begin{cases} \dfrac{d[S]}{dt} = -\eta SI + \rho I \\ \dfrac{d[I]}{dt} = \eta SI - \rho I \end{cases} \tag{6}$$

Model (5) is a predator-prey eco-epidemiological model with a presence of the SI disease in the prey population. If we look carefully at model (5) we will see that we have some terms colored in red. It is important to say that these terms arise from the basic SI model given in (6). Model (6) is the basic SI model. For the models (5) and (6) we construct two graphics which show the concentration's variance of the chemical species *S*, *I* and *P*.



(a) (b)

FIGURE 1: The graphics above show the variation of the concentrations of chemical species *S, I, P* corresponding to the following models: (a) the predator-prey eco-epidemiological model with the presence of SI disease; (b) the SI epidemiological model

It can be seen that there exists a correspondence in the variation of the concentrations of the chemical species *S* and *I* for the given two models which are represented by red for *S* and by blue for *I* colored lines.

A REACTION NETWORK OF A PREDATOR-PREY MODEL WITH SEIR AND SEIRS EPIDEMIC IN THE PREY POPULATION

The Mathematical Model

The presence of the epidemiological SEIR (Susceptible-Exposed-Infected-Recovered) disease or the SEIRS (Susceptible-Exposed-Infected-Recovered-Susceptible) disease is given in the prey population of the predator-prey model. The response function in the predator-prey model has a Lotka-Volterra type. The eco-epidemiological model is described by two systems of five non-linear ordinary differential equations (ODEs) which are given in formula (7). The mathematical model describes the behavior of two populations. The first population has a density denoted by $N(t)$ and the second population is called a predator population and it is denoted by $P(t)$ where *t* is a time variable.

The population of a prey is divided into four groups depending on the stage of the disease in the epidemiological model SEIR (or SEIRS). It is described by the following functions: *S(t)* – susceptible prey; *E(t)* –

exposed to disease prey; *I(t)* – infected prey and *R(t)* – recovered prey. The total prey population at time *t* is: $N(t) = S(t) + E(t) + I(t) + R(t)$. Then the ordinary differential system is:

$$\begin{cases} \dfrac{dS}{dt} = rS\left(1 - \dfrac{S+E+I+R}{K}\right) - \beta.SI - q_1SP - d_1S - m_1S + \xi R \\ \dfrac{dE}{dt} = \underset{infection}{\beta SI} - \underset{predation}{q_2EP} - \underset{\substack{exposed\ species\\ become\\ infective}}{\sigma E} - d_2E - m_2E \\ \dfrac{dI}{dt} = \sigma E - \underset{\substack{infected\\ species\\ become\\ recovered}}{\gamma I} - q_3IP - d_3I - m_3I - \underset{\substack{mortality\\ by\\ the\\ infection}}{cI} \\ \dfrac{dR}{dt} = \gamma I - q_4RP - \underbrace{d_4R}_{mortality} - \underbrace{m_4R}_{migration} - \xi R \\ \dfrac{dP}{dt} = q_1SP + q_2EP + q_3IP + q_4RP - d_5P - m_5P \end{cases} \tag{7}$$

with initial data $S(0) = S_0 \geq 0,\ E(0) = E_0 \geq 0,\ I(0) = I_0 \geq 0,\ R(0) = R_0 \geq 0,\ P(0) = P_0 \geq 0$ where ξR in the first equation is a notation for the recovered species that become susceptible, *S(t)* - susceptible prey, *E(t)* – exposed prey, *I(t)* – infected prey, *R(t)* – recovered prey and *P(t)* – predator.

In the literature the eco-epidemiological model is represented by some mathematical assumptions. This model can also be presented in its non-dimensional version (8). The theorems for positivity and the system's boundary conditions for (7) have also been proven. The existence of the equilibrium points under certain conditions has also been established [5].

$$\begin{cases} \dfrac{d\bar{s}}{d\bar{t}} = \bar{s}[1 - (\bar{s} + \bar{e} + \bar{i} + \bar{r})] - \bar{\beta}\,\bar{s}\,\bar{i} - \bar{q}_1\,\bar{s}.\bar{p} - \bar{d}_1\bar{s} - \bar{m}_1\bar{s} + \bar{\xi}\bar{r} \\ \dfrac{d\bar{e}}{d\bar{t}} = \bar{\beta}\bar{s}\bar{i} - \bar{q}_2\bar{e}.\bar{p} - \bar{\sigma}\bar{e} - \bar{d}_2\bar{e} - \bar{m}_2\bar{e} \\ \dfrac{d\bar{i}}{d\bar{t}} = \bar{\sigma}\bar{e} - \bar{\gamma}\bar{i} - \bar{q}_3\bar{i}.\bar{p} - \bar{d}_3\bar{i} - \bar{m}_3.\bar{i} - c.\bar{i} \\ \dfrac{d\bar{r}}{d\bar{t}} = \bar{\gamma}\bar{i} - \bar{q}_4\bar{r}\bar{p} - \bar{d}_4\bar{r} - \bar{m}_4\bar{r} - \bar{\xi}\bar{r} \\ \dfrac{d\bar{p}}{d\bar{t}} = \bar{q}_1\bar{s}\bar{p} + \bar{q}_2\bar{e}\bar{p} + \bar{q}_3\bar{i}.\bar{p} + \bar{q}_4\bar{r}\bar{p} - \bar{d}_5\bar{p} - \bar{m}_5\bar{p} \end{cases} \tag{8}$$

with initial data $\bar{s} \geq 0,\ \bar{e}(0) \geq 0,\ \bar{i}(0) \geq 0,\ \bar{r}(0) \geq 0,\ \bar{p}(0) \geq 0.$

Due to the fact that these mathematical models combine in themselves the epidemiological model SEIR or SIERS it is necessary to find the reproduction number R_0. The reproduction number R_0 is described in detail in [5] and its formula is given by:

$$R_0 = \frac{\bar{\sigma}\bar{\beta}\bar{s}^*}{(\bar{q}_2\bar{p}^* + \bar{\sigma} + \bar{d}_2 + \bar{m}_2)(\bar{q}_3\bar{p}^* + \bar{\gamma} + \bar{d}_3 + \bar{c} + \bar{m}_3)}.$$

From this reproduction number depends the spreading of the infection. If $R_0 > 1$, then the infection will be quickly spread in the population and if $R_0 < 1$, then the infection will die out in the long run. The reproduction number can be estimated by using the non-dimensional parameters and the values of the equilibrium coordinates in the disease-free equilibrium point *E* ($\bar{s}^*$, 0, 0, 0, $\bar{p}^*$).

The Model's Chemical Reaction Network

Using the "direct" approach given in the example of the previous section, we show how from given chemical equations we can create a mathematical model by using their kinetics' equations. In this subsection we introduce the "inverse" method. It is a method that shows how from a mathematical model described by a system of ordinary differential equations we can obtain the corresponding chemical equations.

TABLE 2: The chemical reactions, their kinetic equations and their ordinary differential equations

No	Chemical reactions	Kinetic Equations	ODEs
1.	$X_1 \xrightarrow{\bar{r}} X_1 + X_1$	$\frac{d[X_1]}{dt} = \bar{r}.[X_1]$	$\bar{s}' = \bar{r}.\bar{s}$
2.	$X_1 + X_1 \xrightarrow{\bar{p}} X_1$	$\frac{d[X_1]}{dt} = -\bar{p}.[X_1]^2$	$\bar{s}' = -\bar{p}.\bar{s}^2$
3.	$X_1 + X_2 \xrightarrow{\bar{\phi}} X_2 + X_2$	$\frac{d[X_1]}{dt} = -\bar{\phi}[X_1][X_2]$, $\frac{d[X_2]}{dt} = \bar{\phi}[X_1][X_2]$	$\bar{s}' = -\bar{\phi}\,\bar{s}.\bar{e}$, $\bar{e}' = \bar{\phi}\,\bar{s}.\bar{e}$
4.	$X_1 + X_2 \xrightarrow{\bar{\phi}} X_1$	$\frac{d[X_2]}{dt} = -\bar{\phi}[X_1][X_2]$	$\bar{e}' = -\bar{\phi}\,\bar{s}.\bar{e}$
5.	$X_1 + X_3 \xrightarrow{\bar{z}} X_1$	$\frac{d[X_3]}{dt} = -\bar{z}[X_1][X_3]$	$\bar{\imath}' = -\bar{z}\,\bar{s}.\bar{\imath}$
6.	$X_1 + X_3 \xrightarrow{\bar{z}} X_3 + X_3$	$\frac{d[X_1]}{dt} = -\bar{z}[X_1][X_3]$, $\frac{d[X_3]}{dt} = \bar{z}[X_1][X_3]$	$\bar{s}' = -\bar{z}\,\bar{s}.\bar{\imath}$, $\bar{\imath}' = \bar{z}\,\bar{s}.\bar{\imath}$
7.	$X_1 + X_3 \xrightarrow{\bar{\beta}/2} X_3 + X_3$	$\frac{d[X_1]}{dt} = -\frac{\bar{\beta}}{2}[X_1][X_3]$, $\frac{d[X_3]}{dt} = \frac{\bar{\beta}}{2}[X_1][X_3]$	$\bar{s}' = -\frac{\bar{\beta}}{2}\,\bar{s}.\bar{\imath}$, $\bar{\imath}' = \frac{\bar{\beta}}{2}\,\bar{s}.\bar{\imath}$
8.	$X_1 + X_4 \xrightarrow{\bar{\theta}} X_4 + X_4$	$\frac{d[X_1]}{dt} = -\bar{\theta}[X_1][X_4]$, $\frac{d[X_4]}{dt} = \bar{\theta}[X_1][X_4]$	$\bar{s}' = -\bar{\theta}\,\bar{s}.\bar{r}$, $\bar{r}' = \bar{\theta}\,\bar{s}.\bar{r}$
9.	$X_1 + X_4 \xrightarrow{\bar{\theta}} X_1$	$\frac{d[X_4]}{dt} = -\bar{\theta}[X_1][X_4]$	$\bar{r}' = -\bar{\theta}\,\bar{s}.\bar{r}$
10.	$X_1 + X_5 \xrightarrow{\overline{q_1}} X_5 + X_5$	$\frac{d[X_1]}{dt} = -\overline{q_1}[X_1][X_5]$, $\frac{d[X_5]}{dt} = \overline{q_1}[X_1][X_5]$	$\bar{s}' = -\overline{q_1}\,\bar{s}.\bar{p}$, $\bar{p}' = \overline{q_1}\,\bar{s}.\bar{p}$
11.	$X_1 \xrightarrow{\overline{d_1}} 0$	$\frac{d[X_1]}{dt} = -\overline{d_1}[X_1]$	$\bar{s}' = -\overline{d_1}\,\bar{s}$
12.	$X_1 \xrightarrow{\overline{m_1}} 0$	$\frac{d[X_1]}{dt} = -\overline{m_1}[X_1]$	$\bar{s}' = -\overline{m_1}\,\bar{s}$
13.	$X_1 + X_3 \xrightarrow{\bar{\beta}/2} X_2 + X_2$	$\frac{d[X_1]}{dt} = -\frac{\bar{\beta}}{2}[X_1][X_3]$, $\frac{d[X_3]}{dt} = -\frac{\bar{\beta}}{2}[X_1][X_3]$, $\frac{d[X_2]}{dt} = \bar{\beta}[X_1][X_3]$	$\bar{s}' = -\frac{\bar{\beta}}{2}\,\bar{s}.\bar{\imath}$, $\bar{\imath}' = -\frac{\bar{\beta}}{2}\,\bar{s}.\bar{\imath}$, $\bar{e}' = \bar{\beta}\,\bar{s}.\bar{\imath}$

14.	$X_2 \xrightarrow{\overline{d_2}} 0$	$\frac{d[X_2]}{dt} = -\overline{d_2}\,[X_2]$	$\overline{e}' = -\overline{d_2}\,\overline{e}$
15.	$X_2 \xrightarrow{\overline{m_2}} 0$	$\frac{d[X_2]}{dt} = -\overline{m_2}\,[X_2]$	$\overline{e}' = -\overline{m_2}\,\overline{e}$
16.	$X_2 + X_5 \xrightarrow{\overline{q_2}} X_5 + X_5$	$\frac{d[X_2]}{dt} = -\overline{q_2}\,[X_2][X_5]$, $\frac{d[X_5]}{dt} = \overline{q_2}\,[X_2][X_5]$	$\overline{e}' = -\overline{q_2}\,\overline{e}.\overline{p}$, $\overline{p}' = \overline{q_2}\,\overline{s}.\overline{p}$
17.	$X_2 \xrightarrow{\bar{\sigma}} X_3$	$\frac{d[X_2]}{dt} = -\bar{\sigma}\,[X_2]$, $\frac{d[X_3]}{dt} = \bar{\sigma}\,[X_2]$	$\overline{e}' = -\bar{\sigma}\,\overline{e}$, $\overline{\imath}' = \bar{\sigma}\,\overline{e}$
18.	$X_3 \xrightarrow{\overline{d_3}} 0$	$\frac{d[X_3]}{dt} = -\overline{d_3}\,[X_3]$	$\overline{\imath}' = -\overline{d_3}\,\overline{\imath}$
19.	$X_3 \xrightarrow{\overline{m_3}} 0$	$\frac{d[X_3]}{dt} = -\overline{m_3}\,[X_3]$	$\overline{\imath}' = -\overline{m_3}\,\overline{\imath}$
20.	$X_3 + X_5 \xrightarrow{\overline{q_3}} X_5 + X_5$	$\frac{d[X_3]}{dt} = -\overline{q_3}\,[X_3][X_5]$, $\frac{d[X_5]}{dt} = \overline{q_3}\,[X_3][X_5]$	$\overline{\imath}' = -\overline{q_3}\,\overline{\imath}.\overline{p}$, $\overline{p}' = \overline{q_3}\,\overline{\imath}.\overline{p}$
21.	$X_3 \xrightarrow{\bar{\gamma}} X_4$	$\frac{d[X_3]}{dt} = -\bar{\gamma}\,[X_3]$, $\frac{d[X_4]}{dt} = \bar{\gamma}\,[X_3]$	$\overline{\imath}' = -\bar{\gamma}\,\overline{\imath}$, $\overline{r}' = \bar{\gamma}\,\overline{\imath}$
22.	$X_4 + X_5 \xrightarrow{\overline{q_4}} X_5 + X_5$	$\frac{d[X_4]}{dt} = -\overline{q_4}\,[X_4][X_5]$, $\frac{d[X_5]}{dt} = \overline{q_4}\,[X_4][X_5]$	$\overline{r}' = -\overline{q_4}\,\overline{r}.\overline{p}$, $\overline{p}' = \overline{q_4}\,\overline{r}.\overline{p}$
23.	$X_4 \xrightarrow{\overline{d_4}} 0$	$\frac{d[X_4]}{dt} = -\overline{d_4}\,[X_4]$	$\overline{r}' = -\overline{d_4}\,\overline{r}$
24.	$X_4 \xrightarrow{\overline{m_4}} 0$	$\frac{d[X_4]}{dt} = -\overline{m_4}\,[X_4]$	$\overline{r}' = -\overline{m_4}\,\overline{r}$
25.	$X_5 \xrightarrow{\overline{d_5}} 0$	$\frac{d[X_5]}{dt} = -\overline{d_5}\,[X_5]$	$\overline{p}' = -\overline{d_5}\,\overline{p}$
26.	$X_5 \xrightarrow{\overline{m_5}} 0$	$\frac{d[X_5]}{dt} = -\overline{m_5}\,[X_5]$	$\overline{p}' = -\overline{m_5}\,\overline{p}$
27.	$X_3 \xrightarrow{\bar{c}} 0$	$\frac{d[X_3]}{dt} = -\bar{c}\,[X_3]$	$\overline{\imath}' = -\bar{c}\,\overline{\imath}$
28.	$X_4 \xrightarrow{\bar{\xi}} X_1$	$\frac{d[X_4]}{dt} = -\bar{\xi}\,[X_4]$, $\frac{d[X_1]}{dt} = \bar{\xi}\,[X_4]$	$\overline{r}' = -\bar{\xi}\,\overline{r}$, $\bar{s}' = \xi\, r$

Let X_1, X_2, X_3, X_4 and X_5 be the concentrations of the chemical species corresponding to the population of the animal species *S(t), E(t), I(t), R(t)* and *P(t)* given in models (7) and (8). The main goal in this subsection is to

determine the kinetic equation for each term on the right side of the given differential equation. After that for each kinetic equation it is important to determine the corresponding specific chemical reaction network. Using the law of mass action for each species in Table 2, we introduce the kinetic (rate) equations, the corresponding chemical reaction networks and the induced ordinary differential equations. The biological interpretation of these chemical reactions can be followed in Table 7 from Appendix B.

The predator-prey model with the presence of an epidemiological disease SEIR in the prey population is represented by the first 27 chemical equations given in Table 2. The model with a presence of a disease is described by the epidemiology SIERS model with all 28 reactions.

The total rate of the production of the chemical species X_1, X_2, X_3, X_4 and X_5 is obtained as a sum of the right-hand members of each reaction in which they participate. Thus, the differential system (9) given below is obtained. If we put the speed constants to be equal i.e. $p = \phi = z = \theta = r/K$, then the system (9) resembles system (7). If the rate constants in the chemical reactions 3, 4, 5, 6, 7, 8, 9 and 13 are different, then some new additional terms in each differential equation will appear, *i.e.*, $\frac{dX_i}{dt}$ for $i = \overline{1,5}$.

$$\begin{cases} \frac{d[X_1]}{d\bar{t}} = [X_1][\bar{r} - (\rho[X_1] + \phi[X_2] + z[X_3] + \theta[X_4])] - \bar{\beta}[X_1][X_3] - \bar{q}_1[X_1][X_5] - \bar{d}_1[X_1] - \bar{m}_1[X_1] + \bar{\xi}[X_4] \\ \frac{d[X_2]}{d\bar{t}} = \bar{\beta}[X_1][X_3] - \bar{q}_2[X_2][X_5] - \bar{\sigma}[X_2] - \bar{d}_2[X_2] - \bar{m}_2[X_2] \\ \frac{d[X_3]}{d\bar{t}} = \sigma[X_2] - \bar{\gamma}[X_3] - \bar{q}_3[X_3][X_5] - \bar{d}_3[X_3] - \bar{m}_3[X_3] - \bar{c}[X_3] \\ \frac{d[X_4]}{d\bar{t}} = \bar{\gamma}[X_3] - \bar{q}_4[X_4][X_5] - \bar{d}_4[X_4] - \bar{m}_4[X_4] - \bar{\xi}[X_4] \\ \frac{d[X_5]}{d\bar{t}} = \bar{q}_1[X_1][X_5] + \bar{q}_2[X_2][X_5] + \bar{q}_3[X_3][X_5] + \bar{q}_4[X_4][X_5] - \bar{d}_5[X_5] - \bar{m}_5[X_5] \end{cases} \quad (9)$$

with initial data $X_1(0) = X_1^0 \geq 0,\ X_2(0) = X_2^0 \geq 0,\ X_3(0) = X_3^0 \geq 0,\ X_4(0) = X_4^0 \geq 0,\ X_5(0) = X_5^0 \geq 0.$

If we want to obtain the dimensionless model (8), then the rate constants *r, p, z, θ, φ* in the differential system (9) must be equal to one. Thus, we can obtain the ordinary differential system (10) which describes the change in the concentrations of the chemical species X_1, X_2, X_3, X_4 and X_5 corresponding to the non-dimensional system (8) of the considered predator-prey model with the presence of an epidemiological disease SEIR or SEIRS in the prey population.

$$\begin{cases} \frac{d[X_1]}{d\bar{t}} = [X_1][1 - ([X_1] + [X_2] + [X_3] + [X_4])] - \bar{\beta}[X_1][X_3] - \bar{q}_1[X_1][X_3] - \bar{d}_1[X_1] - \bar{m}_1[X_1] + \bar{\xi}[X_4] \\ \frac{d[X_2]}{d\bar{t}} = \bar{\beta}[X_1][X_3] - \bar{q}_2[X_2][X_5] - \bar{\sigma}[X_2] - \bar{d}_2[X_2] - \bar{m}_2[X_2] \\ \frac{d[X_3]}{d\bar{t}} = \bar{\sigma}[X_2] - \bar{\gamma}[X_3] - \bar{q}_3[X_3][X_5] - \bar{d}_3[X_3] - \bar{m}_3[X_3] - \bar{c}[X_3] \\ \frac{d[X_4]}{d\bar{t}} = \bar{\gamma}[X_3] - \bar{q}_4[X_4][X_5] - \bar{d}_4[X_4] - \bar{m}_4[X_4] - \bar{\xi}[X_4] \\ \frac{d[X_5]}{d\bar{t}} = \bar{q}_1[X_1][X_5] + \bar{q}_2[X_2][X_5] + \bar{q}_3[X_3][X_5] + \bar{q}_4[X_4][X_5] - \bar{d}_5[X_5] - \bar{m}_5[X_5] \end{cases} \quad (10)$$

with initial data $X_1(0) = X_1^0 \geq 0,\ X_2(0) = X_2^0 \geq 0,\ X_3(0) = X_3^0 \geq 0,\ X_4(0) = X_4^0 \geq 0,\ X_5(0) = X_5^0 \geq 0.$

NUMERICAL EXPERIMENTS

In this section we give three numerical experiments which are carried out using the online platform SmoWeb when the Biochemical Reactions application is selected [17]. This application has three directories: (1) Reactions, (2) Species and (3) Settings. For each directory the user can enter the following necessary data:

(1) **Reaction** - the chemical reactions and the numerical value of the rate constants are entered by the user. The rate constant in the given chemical reaction is measured in 1 mol/l under some standard conditions.

(2) **Species** – the initial numerical values of the chemical species in the measurement unit which is chosen by the user.

(3) **Settings** – the user enters a pair of chemical substances, simulation time and printing interval so that the phase portrait can be drawn.

TABLE 3: **Case 1 (unstable case):** Numerical values of the rate constants given in chemical reactions for system (10)

$\bar{r}$	$\bar{\beta}$	$\overline{q_1}$	$\overline{q_2}$	$\overline{q_3}$	$\overline{q_4}$	$\overline{d_1}$	$\overline{d_2}$	$\overline{d_3}$	$\overline{d_4}$
1	25	1.25	3.75	12.50	1.25	0.10	0.0875	0.05	0.0375
$\overline{d_5}$	$\overline{m_1}$	$\overline{m_2}$	$\overline{m_3}$	$\overline{m_4}$	$\overline{m_5}$	$\bar{c}$	$\bar{\sigma}$	$\bar{\gamma}$	$\bar{\xi}$
0.075	0.50	0.125	0.0625	0.1875	0.3125	0.20	0.625	0.3125	0.025

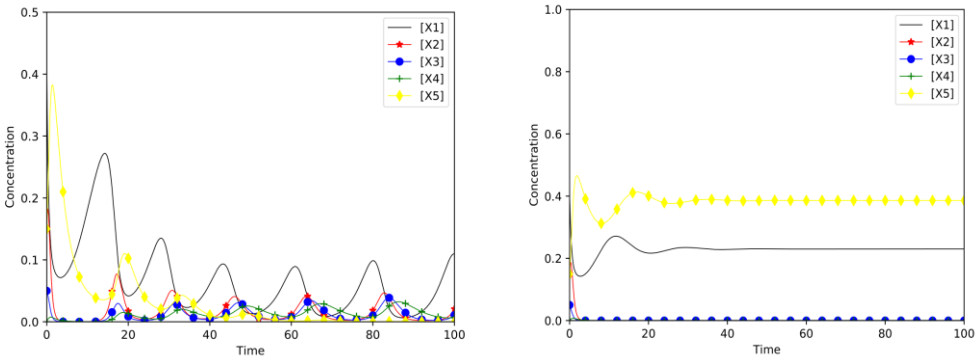
TABLE 4: **Case 2 (stable case)** Numerical values of the rate constants given in chemical reactions for system (10)

$\bar{r}$	$\bar{\beta}$	$\overline{q_1}$	$\overline{q_2}$	$\overline{q_3}$	$\overline{q_4}$	$\overline{d_1}$	$\overline{d_2}$	$\overline{d_3}$	$\overline{d_4}$
1	25	1.25	3.75	12.50	1.25	0.0375	0.05	0.0625	0.0375
$\overline{d_5}$	$\overline{m_1}$	$\overline{m_2}$	$\overline{m_3}$	$\overline{m_4}$	$\overline{m_5}$	$\bar{c}$	$\bar{\sigma}$	$\bar{\gamma}$	$\bar{\xi}$
0.075	0.25	0.125	0.0625	0.1875	0.25	0.25	0.50	0.375	0.025

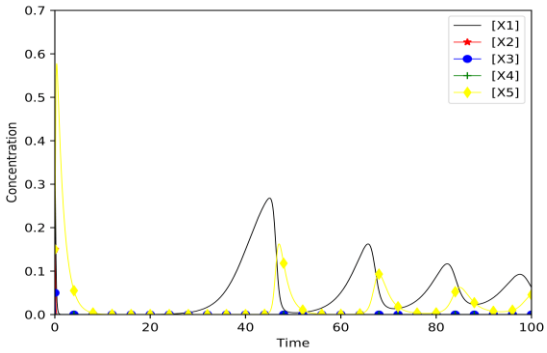
TABLE 5: **Case 3 (unstable case)** Numerical values of the rate constants given in chemical reactions for system (10)

$\bar{r}$	$\bar{\beta}$	$\overline{q_1}$	$\overline{q_2}$	$\overline{q_3}$	$\overline{q_4}$	$\overline{d_1}$	$\overline{d_2}$	$\overline{d_3}$	$\overline{d_4}$
1	25	12.50	25	75	12.50	0.0375	0.05	0.05	0.0375
$\overline{d_5}$	$\overline{m_1}$	$\overline{m_2}$	$\overline{m_3}$	$\overline{m_4}$	$\overline{m_5}$	$\bar{c}$	$\bar{\sigma}$	$\bar{\gamma}$	$\bar{\xi}$
0.05	0.625	0.375	0.125	0.50	0.625	0.1875	0.375	0.4375	0.025

In Figure 2 we introduce three graphics of the variations of the concentrations of five chemical species where the numerical values of the rate constants are given in Tables 3, 4, and 5. It is important to say that the numerical value of the constant ζ in the predator-prey model in the presence of an epidemiological disease SEIRS does not change the graphic, which is obtained for the model with a SEIR disease. The initial data that we use for the three experiments are: $X_1(0) = 0.40\text{m/l}$, $X_2(0) = 0.15\text{m/l}$, $X_3(0) = 0.05\text{m/l}$, $X_4(0) = 0\text{m/l}$ и $X_5(0) = 0.15\text{m/l}$.



(a) (b)



(c)

FIGURE 2: Graphs of the variation of the concentrations of the five chemical species with time variation for the following experiments: (a) first - Table 3, (b) second - Table 4 and (c) third - Table 5

The graphics presented in Figure 2 show that the numerical values which are used in cases (a) and (c) of the given system predict an unstable state. Of particular note is the presence of some oscillations in the graphics which resemble the oscillations of the basic predator-prey model. On this base we can see the existence of a parallel between the eco-epidemiological models and the chemical reaction networks constructed for them. In the case (b) after t_{30} the system goes to an equilibrium state.

Two other functionalities that the online platform SmoWeb provides are as follows:

(1) A collection of tables that shows the concentration of the chemical species changes in time, see Figure 3.

(2) Phase portrait of the pair of the chemical species that can be used to trace how these two chemicals interact with each other in time, see Figures 4 and 5.

	time [s]	X1 [M]	X2 [M]	X3 [M]	X4 [M]	X5 [M]
1	0.000	0.400	0.150	0.050	0.00	0.10
2	0.100	0.342	0.176	0.051	0.00	0.11
3	0.200	0.292	0.193	0.051	0.00	0.12
4	0.300	0.249	0.202	0.052	0.00	0.14
5	0.400	0.213	0.204	0.052	0.01	0.15
6	0.500	0.182	0.201	0.051	0.01	0.17
7	0.600	0.157	0.193	0.050	0.01	0.18
8	0.700	0.136	0.181	0.047	0.01	0.20
9	0.800	0.119	0.168	0.044	0.01	0.21
10	0.900	0.105	0.153	0.040	0.01	0.22
11	1.000	0.094	0.138	0.036	0.01	0.23
12	1.100	0.085	0.123	0.032	0.01	0.24
13	1.200	0.078	0.109	0.028	0.01	0.25
14	1.300	0.072	0.095	0.025	0.01	0.25

◄ ► 1 2 10 70 72

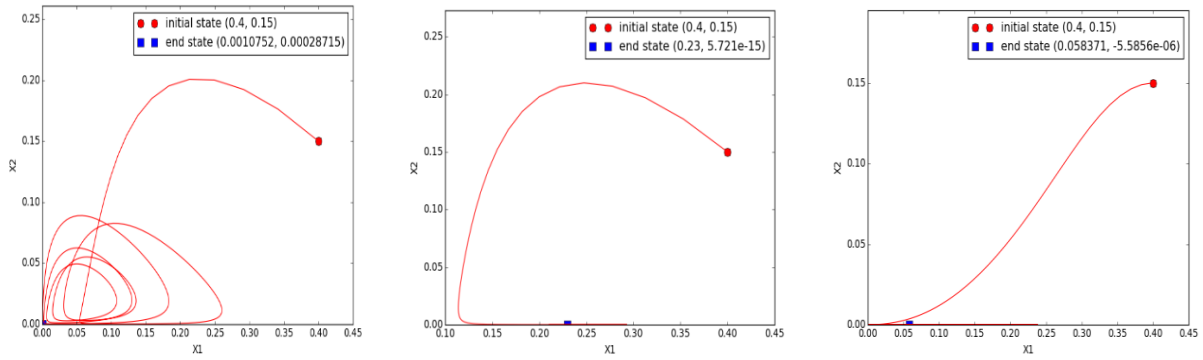
	time [s]	X1 [M]	X2 [M]	X3 [M]	X4 [M]	X5 [M]
687	68.600	0.000	0.000	0.003	0.03	0.00
688	68.700	0.000	0.000	0.003	0.03	0.00
689	68.800	0.001	0.000	0.002	0.03	0.00
690	68.900	0.001	0.000	0.002	0.03	0.00
691	69.000	0.001	0.000	0.002	0.03	0.00
692	69.100	0.001	0.000	0.002	0.03	0.00
693	69.200	0.001	0.000	0.002	0.02	0.00
694	69.300	0.001	0.000	0.002	0.02	0.00
695	69.400	0.001	0.000	0.002	0.02	0.00
696	69.500	0.001	0.000	0.002	0.02	0.00
697	69.600	0.001	0.000	0.001	0.02	0.00
698	69.700	0.001	0.000	0.001	0.02	0.00
699	69.800	0.001	0.000	0.001	0.02	0.00
700	69.900	0.001	0.000	0.001	0.02	0.00

◄ ► 1 10 40 49 50 51 60 70 72

	time [s]	X1 [M]	X2 [M]	X3 [M]	X4 [M]	X5 [M]
967	96.600	0.000	0.004	0.021	0.06	0.00
968	96.700	0.000	0.003	0.020	0.06	0.00
969	96.800	0.000	0.003	0.019	0.06	0.00
970	96.900	0.000	0.003	0.018	0.06	0.00
971	97.000	0.000	0.003	0.017	0.06	0.00
972	97.100	0.000	0.002	0.017	0.05	0.00
973	97.200	0.000	0.002	0.016	0.05	0.00
974	97.300	0.000	0.002	0.015	0.05	0.00
975	97.400	0.000	0.002	0.014	0.05	0.00
976	97.500	0.000	0.002	0.013	0.05	0.00
977	97.600	0.000	0.002	0.013	0.05	0.00
978	97.700	0.000	0.002	0.012	0.05	0.00
979	97.800	0.000	0.001	0.011	0.05	0.00
980	97.900	0.000	0.001	0.011	0.05	0.00

◄ ► 1 10 60 69 70 71 72

FIGURE 3: Some screenshots of the collection of tables



(a) (b) (c)

FIGURE 4: Phase portraits of the chemical species X_1, X_2 for the three experiments: (a) first - Table 3, (b) second - Table 4 and (c) third - Table 5

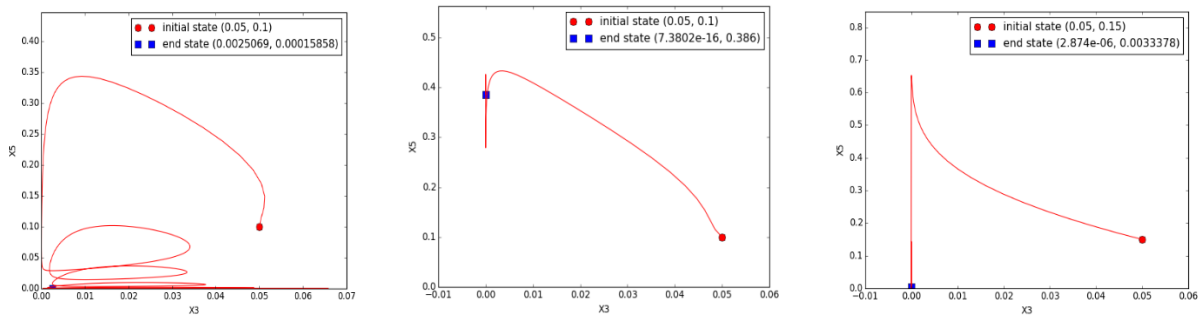


FIGURE 5: Phase portraits of the chemical species X_3, X_5 for the three experiments: (a) first - Table 3, (b) second - Table 4 and (c) third - Table 5

Since the real system, unlike the deterministic models, tends to be a subject of a random background noise so the unstable steady-state solution is unlikely to be observed in practice. Instead of this, some stable oscillations or some other types of attractors may appear. Such attractors can be seen in Figures 4 and 5. The phase portrait of the chemical species X_1, X_2 in case (a) from Figure 4 shows the decreasing of the species X_1 while the species X_2 increases in time. In case (b) from Figure 4 the same trend is initially observed - X_1 decreases and X_2 increases in time. The concentration of both species decreases until the species X_2 almost disappears. In case (c) from Figure 4 it is seen that the concentration of both species decreases in time. In Figure 5 the phase portrait of the chemical species X_3, X_5 in case (a) shows how the concentration of the species X_3 decreases while the concentration of X_5 increases in time t_M. After that the concentration of both substances decrease. In case (b) from Figure 5 a rapid increase is seen in the concentration of the species X_5 while the species X_3 decreases. We find the same trend in case (c) from Figure 5 but after time t_N a sharp decrease in the concentration of both species is observed.

CONCLUSION

Using the theory of chemical reaction networks, we can easily analyze the relationships between some different processes like growth/decay, migration, transmission of infection, loss of immunity, etc. In this work a predator-prey model with the SEIR and the SEIRS epidemic was introduced in the prey. The inverse method was applied to construct the chemical reaction network using the presented eco-epidemical models. The law of mass action was used to create links between the chemical reactions (equations) and the given system of ordinary differential equations. The numerical experiments which are carried out through the online platform SmoWeb show that if we use the same initial concentrations of the chemical species but use different rate constants, it will lead to a reaction network which can be in an unstable or a stable state. The presented phase portraits show how the two concentrations interact with each other in time. The obtained results give a relationship between the interaction of the pair of chemical concentrations and the dynamics of separate pairs of populations corresponding to the animal species described in the epidemiological models.

ACKNOWLEDGEMENTS

This work has been accomplished with the partial support by the grant No BG05M2OP001-1.001-0003, financed by the Science and Education for Smart Growth Operational Program (2014-2020) and co-financed by the European Union through the European structural and Investment funds as well as by ~~a~~ grant No 30 from CAF America. The authors would like to thank Atanas Pavlov, Milen Borisov and Ivaylo Mihaylov who created the online platform SmoWeb.

APPENDIX A

TABLE 6: The kinetic equations and their chemical interpretation

No	Kinetic equations	Chemical interpretation of the kinetic equations

1.	$\frac{d[P]}{dt} = kPS$ $\frac{d[S]}{dt} = -kPS$	In this "logistic" reaction the species *P* acts as a catalyst because it accelerates its own production. This type of catalysis is called an autocatalysis.
2.	$\frac{d[P]}{dt} = -\mu P$ $\frac{d[S]}{dt} = \mu P$	This reaction causes an exponential decay of the species *P* and an exponential growth for the species *S.*
3.	$\frac{d[I]}{dt} = \eta SI$ $\frac{d[S]}{dt} = -\eta SI$	In this "logistic" reaction, species *I* is the catalyst because it accelerates its own production. This type of catalysis is called an autocatalysis.
4.	$\frac{d[I]}{dt} = -\rho I$ $\frac{d[S]}{dt} = \rho I$	This reaction causes an exponential decay of the species *I* and an exponential growth for the species S.

APPENDIX B

TABLE 7: The chemical equations and their biological interpretation

No	Chemical equations	Biological interpretation of the chemical equations
1.	$X_1 \xrightarrow{\bar{r}} X_1 + X_1$	In the absence of infection, the number of susceptible increases depending on the birth rate.
2.	$X_1 + X_1 \xrightarrow{\bar{p}} X_1$	For a time period *t*, the number of susceptible decreases twice with rate $\bar{p}$.
3.	$X_1 + X_2 \xrightarrow{\bar{\phi}} X_2 + X_2$	In contact between susceptible and exposed to the disease, the number of exposed doubles.
4.	$X_1 + X_2 \xrightarrow{\bar{\phi}} X_1$	In contact between susceptible and exposed to the disease are likely to remain susceptible.
5.	$X_1 + X_3 \xrightarrow{\bar{z}} X_1$	In contact between susceptible and infected, remain susceptible, provided that the infected have died.
6.	$X_1 + X_3 \xrightarrow{\bar{z}} X_3 + X_3$	In contact between susceptible and infected, the number of infected doubles.
7.	$X_1 + X_3 \xrightarrow{\bar{\beta}/2} X_3 + X_3$	In contact between susceptible and infected, the number of infected doubles.
8.	$X_1 + X_4 \xrightarrow{\bar{\theta}} X_4 + X_4$	In contact between susceptible and recovered, the number of recovered doubles if it is assumed that the susceptible are not infected and they are considered to be healthy.

9.	$X_1 + X_4 \xrightarrow{\overline{\theta}} X_1$	In contact between susceptible and recovered, the number of recovered occurs susceptible species, if it is assumed that the recovered species has migrated or died.
10.	$X_1 + X_5 \xrightarrow{\overline{q_1}} X_5 + X_5$	In contact between susceptible prey and a predator, the number of predator increases.
11.	$X_1 \xrightarrow{\overline{d_1}} 0$	Natural mortality in susceptible prey.
12.	$X_1 \xrightarrow{\overline{m_1}} 0$	Migration process for susceptible prey. In this way their number is reduced.
13.	$X_1 + X_3 \xrightarrow{\frac{\overline{\beta}}{2}} X_2 + X_2$	In contact between susceptible and infected species at a rate $\frac{\overline{\beta}}{2}$, the number of exposed species to the infection gets double.
14.	$X_2 \xrightarrow{\overline{d_2}} 0$	Natural mortality in exposed prey.
15.	$X_2 \xrightarrow{\overline{m_2}} 0$	Migration process for exposed prey. In this way their number is reduced.
16.	$X_2 + X_5 \xrightarrow{\overline{q_2}} X_5 + X_5$	In contact between exposed prey and a predator, the number of predators increases.
17.	$X_2 \xrightarrow{\overline{\sigma}} X_3$	The exposed prey becomes infected at the rate of incubation $\overline{\sigma}$.
18.	$X_3 \xrightarrow{\overline{d_3}} 0$	Natural mortality in infected prey.
19.	$X_3 \xrightarrow{\overline{m_3}} 0$	Migration process for infected prey. In this way their number is reduced.
20.	$X_3 + X_5 \xrightarrow{\overline{q_3}} X_5 + X_5$	When infected prey come in contact with a predator, the number of predators increases.
21.	$X_3 \xrightarrow{\overline{\gamma}} X_4$	Infected species heal at a speed of recovery $\overline{\gamma}$.
22.	$X_4 + X_5 \xrightarrow{\overline{q_4}} X_5 + X_5$	In contact between recovered prey and predators, the number of predators increases.
23.	$X_4 \xrightarrow{\overline{d_4}} 0$	Natural mortality in recovered prey.
24.	$X_4 \xrightarrow{\overline{m_4}} 0$	Migration process for recovered prey. In this way their number is reduced.
25.	$X_5 \xrightarrow{\overline{d_5}} 0$	Natural mortality in predator.

26.	$X_5 \xrightarrow{\overline{m_5}} 0$	Migration process for predator. In this way their number is reduced.
27.	$X_3 \xrightarrow{\bar{c}} 0$	Mortality in infected prey caused by the disease.
28.	$X_4 \xrightarrow{\bar{\xi}} X_1$	Recovered prey become susceptible to infection at a rapid rate $\bar{\xi}$.

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