Qualitative Study on the Jatropha Curcas Plant Resources and Production of Biodiesel for Societal Benefits

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CERTIFICATE FROM THE SUPERVISOR(S)

This is to certify that the thesis entitled "**Qualitative Study on the Jatropha Curcas Plant Resources and Production of Biodiesel for Societal Benefits**" is submitted by Mr. Arunabha Sengupta whose name was registered vide INDEX NO. 219/16/Maths./25 dated 23.11.2016 for the award of Doctor of Philosophy (Science) degree of Jadavpur University, Kolkata 700032. This thesis is absolutely based upon his own work under my supervision and is worthy of consideration for the award of Ph.D. (Sc.) degree. Neither this thesis nor any part of this work has been submitted to any other University or Institute for the award of any degree/diploma or any other academic award.

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I dedicate my thesis to

my parents

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Abstract

Biodiesel can be produced from any material that contains fatty acids, be they linked to other molecules or present as free fatty acids. Biodiesel (BD) is manufactured by chemically reacting lipids (Triglycerides) e.g., present in Jatropha oil, with alcohol-producing fatty acid esters. It is basically an ester derived from glycerol and three fatty acids (tri + glyceride). Globally Jatropha curcas plant is one of the most promising resources for biodiesel. Present biodiesel is a liquid fuel, which is obtained by methyl esterification of fatty acid. The main constituent is fatty acid methyl ester. Production of such chemically enriched energy compounds is a subject of intense research worldwide. The reaction commonly called “transesterification” was being researched both in light of chemical diversity as well as mathematically refined parameters to enhance the reaction process. From an economical point of view, BD production is limited to the high price of oils and purification of secondary product glycerol. The production of biodiesel from terrestrial (Jatropha curcus Oil) sources is the prime focus area in developing nations and how to develop a renewable resource for future-ready energy demands is a serious thought in the global scenario. We have already initiated thematic research on the Jatropha curcus plant to yield biodiesel for future energy demands and provided sound production parametric resolutions entirely on mathematically obtained analytical findings and numerically verified process parameters like mass resistance, molar ratio of the reactants, use of catalysts, stirring effect rpm, etc. We have also produced some research on the plant ecology which serves as the raw material for the production of the oil seeds theoretically. Biodiesel is produced from Jatropha seeds by extracting the crude oil. A healthy plant will benefit us in producing a greater amount of biodiesel. Since the Jatropha plants are not disease resistant and the cost-effective production is still to be addressed in the view of societal benefits in the developing countries, the focus has now been shifted to how to get pest-free plants as well as the maximum production of biodiesel with less production cost. If we can resist or minimize the pest attack on the Jatropha plant, consequently it will lead to a steady production of alternative fuel, i.e., biodiesel. Securing clean and uninterrupted energy means growing the economy. On a large-scale production system, such ventures must be validated on cost-benefit accountability which is yet to be explored under different technological domains. Mathematical comparative product features are yet to be arrived at under different phases of the cumulative biodiesel production process without catalysts. We will focus our research on this direction as well as find the enhanced production from different technical and chemical processes without catalysts with mathematical studies. It will lead us to arrive at a balanced production where the optimized cost-benefit trade-off is achieved. This is for the overall betterment of societal aspirations, as such holistic studies will create entrepreneurial and job opportunities, decrease pollution environmentally, and boost the national economy with self-reliance in energy demands. Building mathematical models using different mathematical as well as numerical techniques, would be predicted under the studies, what is to be controlled and how to be controlled of certain reaction parameters for extraction and conversion of biodiesel from natural resources effectively and with sustainable yield.

Keywords: Jatropha curcas plant; Pest control; Pesticides; Stability; Functional response; Biodiesel; Supercritical; Optimization; Impulse, Cost-effectiveness.

Contents

Chapter 1

Introduction

“*I think the cost of energy will come down when we make this transition to renewable energy.*” – **Al Gore**

In the present global scenario, fossil fuels (oil, coal, and natural gas) are considered the main energy sources. Fossil fuels have a very important key role in the economic progress of today’s world. Eventually, these energy resources will decay in the near future as resources of conventional fuels are ultimately finite and non-renewable. As a result, the demand for fossil fuels is increasing worldwide and the cost of fossil fuels increases from time to time (Mucino et al. (2014)). Also, the emission of harmful particles and greenhouse gases into the atmosphere due to the burning of fossil fuels affects humans as well as the earth as a whole negatively. Accordingly, globally it encourages researchers to investigate new and alternative energy resources that will be sustainable, renewable, biodegradable, and environment friendly (Nas and Berktay (2007)).

There is enormous potential for renewable energy sources as they can fulfil the world's energy demand in the future. The future security of global energy resources will be enhanced by inventing new energy resources using recent conversion technologies. It will also provide a chance to reduce greenhouse gas emissions in order to control greenhouse gas levels in nature. Renewable energy resources can reduce the price of commonly used fuels in the future worldwide.

Renewable energy resources are generally the resources that we get from nature such as plants, the Sun, wind, water, etc. Renewable energy technologies turn these energy resources into heat, biofuel, chemical, electrical or mechanical power. Biomass produces heat directly through burning. Hence it is called the most effective resource amongst all the renewable energy resources. We can convert biomass directly into liquid fuels, i.e., biodiesel by various processes.

Nowadays biodiesel is being considered as one of the useful alternatives for fossil fuels which reduces our dependency on petroleum diesel. Biodiesel is biodegradable and possesses high energy density. Using biodiesel as a vehicle fuel increases energy security, improves the quality of air, and provides safety benefits. So, biodiesel is more eco-friendly than that of common fuels. It can reduce the emission of greenhouse gases, such as SO2, and hydrocarbons into the atmosphere. Therefore, the requirement for biodiesel has been increasing day by day for the last few decades (Nas and Berktay (2007)).

Biodiesel can be produced from animal fat and vegetable oil. Biodiesel can be produced from various vegetable seed oil like Cottonseed oil, Rapeseed oil, Sunflower seed oil, Soybean seed oil, Palm oil, Jatropha seed oil, etc (Anitescu and Bruno (2012)). It can be produced from algae also. But amongst all these resources of biodiesel, Jatropha curcas is the most promising, popular, and used crop for producing biodiesel as it produces the best quality of biodiesel intrinsically with the fuel grade mineral biodiesel oil. Jatropha seeds contain a higher amount of non-edible oil. Jatropha curcas has recently created a huge potential for the cultivation of this crop in global agronomy and has greatly uplifted the social and economic conditions of marginal farmers in developing countries.

Jatropha curcas plant commonly known as a purging nut or Barbados nut is a drought-resistant flowering plant, belonging to the spurge family, Euphorbiaceae species. We can find this plant in tropical and sub-tropical regions throughout the world. Jatropha plant can be used for medicinal purposes, and for producing pesticides. It also prevents soil erosion and contains or excludes farm animals when grown as living fences. The cultivation cost of Jatropha curcas is very affordable as it can grow anywhere even on barren land without any effort. For these reasons, the Jatropha curcas plant is considered the most suitable renewable resource for producing non-conventional fuel biodiesel.

Jatropha curcas plant is not resistant to some insects or pests for natural growth. There are more than 40 species of insects that affect Jatropha plant (Sharma et al. (2011)). Insect pests affecting Jatropha curcas include armyworms, aphids, mealy bugs, citrus root weevils, etc. which result in flower and fruit abortion. More than twelve types of pests damaging Jatropha curcas have been reported by Manoharan et al. (Manoharan et al. (2006)). The second year of plantation of this plant experiences high damage from the pests (Terren et al. (2012)). Devi et al. (Devi et al. (2008)) said that Morosaphycita morosalis is a major threat in Jatropha curcas cultivation. This pest feeds on the leaves and the stem of the plant. It can cause severe damage to the shrub. A single female Pempelia morosalis can lay nearly 60 whitish, flat, oval-to-round eggs. Eggs turn into larvae within 5 to 7 days. The pupal stage has been developed from Larvae which has a 7 to 8 days average longevity period. Adult male pupae were slightly smaller than female. The Pempelia morosalis species in the larval stage is a potential pest for Jatropha curcas plant (Rouamba (2011)).

Jatropha curcas plant must be protected from pest attack to get maximum seed production. Local agronomic practices advise to apply pesticides and antimicrobial agents in the plantation, which restore the normal vitality of plants by protecting disease and pest invasion. Now the farmers mainly use chemical pesticides to control pests which has resulted in pest resurgence, pollution, and uneconomic crop production. There is now immense evidence that most of these chemical pesticides are potentially risky to humans. Approximately one million people across the world die every year due to poisoning from pesticides and chronic diseases (Aktar et al. (2009)). Hence, to overcome this problem, the concept of Integrated Pest Management (IPM) has been introduced. Day by day it has been becoming more popular among farmers. The ideas given by the researchers are recently being applied in the field by marginal farmers.

Biopesticide (such as nuclear polyhedrosis virus (NPV)) is one of the such alternatives to control pests. Theoretical population ecologists led by Anderson and May studied the dynamics of insect-pathogen interactions. After this, many research articles on biological control have been reported. Investigation of the role of microbial pesticides in the IPM has been performed by Dent et al. (Dent (1997)), which has been recently reviewed for agriculture, forestry, and public health. Bhattacharya et al. (Bhattacharya and Karan (2004)) have shown that an integrated approach of bio-pesticide can control pests significantly. In North America and European countries, the real vindication of using viruses against insect pests is observed (Franz and Huber (1979)). Falcon et al (Falcon (1971)) listed the experimental and field use of pathogenic viruses.

However, there are some disadvantages of biological control as it is an elongated and costly process compared to controlling by chemical pesticides. But the key advantage of biological control is that it is eco-friendly. Chemical pesticides annihilate pests very fast but cause high environmental loss. Considering the environmental and economic issues, a combination of chemical and biological pesticides can deliver better results. Integrated control has been introduced for various agrarian crops and is being widely applied in many countries as a harmonious solution to plan operative pest management with environmental safety. Ray F. Smith (Smith (1962)) sought the effect of the simultaneous use of biological and chemical pesticides to manipulate pest insects and mites using fundamental ecological principles. Ghosh and Bhattacharya (Ghosh and Bhattacharya (2010)) formulated Integrated Pest Management (IPM) model to enhance the combined use of chemical and biological measures to control the insect pest dynamics regulating crop damage. Chitra et al. (Chitra et al. (2006)) suggested chemical insecticide as the main agent for pest management and Stegodyphus spider as the biological control agent. The integrated control programs have been established to highlight the application of both chemical and biological methods because these two techniques are our main standbys in the struggle against insect pests.

The diseases affect the growth of the plant as well as the oil production. How to control pests for this plant is a global problem in agricultural ecosystem management (J. Chowdhury et al. (2016)). Hence controlling pests for the healthy growth of the plant and for the improvement of oil productivity is urgently required. Many researchers have formulated mathematical models for controlling pests and they have studied the different perspectives of pest management tools with probable results by analyzing the system within the mathematical illustration. Chemical pesticides affect our health and plant growth and they also cause environmental pollution, and health problems and affect economic crop production (Georghiou (1990)). This leads us to find out biological control methods for plant pests. Besides that, the most effective measures in pest management are determined by the ecology of a pest. Thus, the concept of Integrated Pest Management (IPM) (Thomas (1999)) is being generated. Its application has been increased in the field by the farmers recently.

IPM reduces reliance on pesticides by emphasizing biological control methods. Bio-pesticides, components of an integrated approach, can play an effective role in pest control (Bhattacharya and Karan (2004)). Potentially, the use of viruses is one of the most significant biological methods for pest control. In American and

European countries, practical evidences of where the virus is used against insect pests are being noticed (Franz and Huber (1979)). The experimental and field use of pathogenic viruses in Europe is listed by Falcon et al.

As the importance of fuel crops is economically very high, our aim is to provide protection to the crop from exigency and increase its oil production. Pests are the main obstacles for Jatropha curcus plant to grow naturally. Jatropha plants are attacked by many pests but less than ten types of pests occur quite often, e.g., the leaf miner Stomphastis thraustica, the leaf and stem miner Pempelia morosalis, and the shield-backed bug Calidea panaethiopica etc. (Terren et al. (2012)). The natural enemy (predator) in the system survives consuming the susceptible and infected pests. Since the viral infection makes some behavioral changes and sub-lethal effects on the host, the predator consumes the infected pest in linear mass action.

In mathematical models, we have taken a real-world biological phenomenon and written it logically as mathematical problems by sets of nonlinear differential equations. The mathematical problem is then solved and its solution is construed in terms of the real-world problem. Then, we have checked the validation of the solution in the background of the real-world problem. So, formulation, solution, interpretation, and validation are the stages involved in mathematical modelling.

Though, generally the relationship between density and per capita growth for pest population is considered linear (Liang et al. (Liang et al. (2016)), Bhattacharya et al. (Bhattacharya and Karan (2004)), the relationship between the size of the biomass and its growth rate is a serious understanding in population ecology concern. The relationship between population density and per capita growth for pest population is a noteworthy biological process of existing creatures.

From ecological aspect, functional response possesses significant interpretation. In our work functional response on predator is important to study pest eradication and to keep the biological balance of the ecosystem. Generally, there are three kinds of functional response namely Holling type I or Linear functional response, Holling type II or Hyperbolic functional response and Holling type III or Sigmoid functional response. Here I have used Linear and Hyperbolic functional response of the form $f(S) = \beta S$ and $f(x) = \frac{\beta S}{a+S}$ respectively.

To get maximum production of Jatropha seeds, we formulate eco-epidemiological mathematical models for reducing the pest and thus controlling the diseases of the plant. At first fruits from the plant are harvested. Then seeds are removed from it. Next those seeds are dried under the sun for three weeks. Seeds can be dried also in an oven at 221°F. After that, oil from Jatropha seeds is extracted. Screw extruder apparatus is required for this process. $70 - 80$ % oil is extracted from first pass and up to 91 % oil is extracted from second pass. The reaction which converts the extracted oil to biodiesel is called the transesterification reaction. This reaction takes place with the help of chemical catalyst, biological catalyst or by supercritical processes which are non-catalytic processes. Transesterification reaction is dependent on some reaction conditions such as temperature, catalyst concentration, speed of stirrer, molar ratios of oil, alcohol, and water.

Transesterification of triglycerides with methanol and ethanol $i.e.$ alcohol is the catalytic process which is broadly used for biodiesel production. The effect of different catalyst for biodiesel production has been investigated by Atadashi et al. (Atadashi et al. (2013)). Potassium hydroxide, Potassium methoxide, Sodium hydroxide and Sodium methoxide are most commonly used catalysts in biodiesel production. However, industrially Sodium hydroxide and Potassium hydroxide are mainly used as their price is low (Fukuda et al. (2001)).

Worldwide many researchers have shown that biodiesel production is extremely dependent on temperature of the reaction system. It has been detected that with an increasing reaction temperature, conversion of oil increases pointedly. Bambase et al. (Bambase et al. (2007)) reported that, mass transfer rate is directly proportional to its temperature at constant stirring and catalyst amount. The major drawback of using base catalytic method is the saponification of glycerides. Berchmans et al. (Berchmans et al. (2013)) observed that catalyst used in the reaction reacts with reactants and complicates the process by forming soap. Some other type of drawbacks to produce biodiesel from Jatropha oil are catalysts are unsuitable for direct use in the transesterification reaction as Jatropha oil contain high amount of free fatty acid (Al Basir et al. (2015)). H. J. Berchmans et al. (Berchmans and Hirata (2008)) tested that the high content of FFA will lead to side formation of soap. As a consequence, biodiesel production becomes less. Thus alkaline catalyst is involved in the transesterification reaction only when Jatropha oil contains less than 1 % free fatty acid level., hence Jatropha oil undergoes an expensive pre-treatment process to reduce free fatty acid. Also, catalytic transesterification method leads side formation of soap and lessens the quantity of biodiesel.

According to Lascaray, hydrolysis is mainly a homogeneous reaction occurring in the oil phase and only a minor portion of the reaction takes place at the oil and water interface during the induction period. Hydrolysis of triglyceride (TG) from fats and oils to glycerol and free fatty acids (FFA) is an important reaction for the oleochemical industry. Hydrolysis involves three stepwise reversible reactions where triglyceride (TG) is first hydrolyzed to diglyceride (DG) and then to monoglyceride (MG) and glycerol. In each step we get free fatty acid (FFA) which later reacts with methanol to produce biodiesel. Generally, hydrolysis occurs at $100-260$°C and $100-7000\ kPa$ using $0.4\text{–}1.5$ (w/w) initial water to oil molar ratio with or without catalysts. The hydrolysis reaction rate is initially low and then gradually increases up to its normal level. This is due to an induction period that obscures the kinetics of the hydrolysis of oil (Hartman (1951)).

There are many research articles on biodiesel production through different processes, such as transesterification with chemical catalysts (Srivastava and Prasad (2000), Y. Zhang et al. (2003)), biochemical catalysts, SCMTR method (Hartman (1951), A. Demirbas (2009), G. T. Ang et al. (2015)) etc. Transesterification is a process to produce biodiesel from vegetable oils and animal fats with the aid of different alcohols. Alkaline catalysts processes form soap as side product and reduce the production of biodiesel as Jatropha oil contains free fatty acids (FFAs) and water. Therefore, there include complex and energy-consuming separation and purification steps in homogeneous chemical catalyst processes. In addition, we face difficulties to recover glycerol due to the solubility of excessive methanol and catalyst (F. Al Basir et al. (2015)). Although, because of low temperature requirement, catalyst method has an advantage in commercialization of the process with the low cost of apparatus.

Supercritical Carbon dioxide ($SC-CO_2$) has also received increasing attention as reaction media for lipids (Fujita and Himi (1995), Moquin and Temelli (2006)). Fujita and Himi (Fujita and Himi (1995)) conducted hydrolysis of triolein in $SC-CO_2$ media and reported, using thin-layer chromatography, that the hydrolysis efficiency was almost 100 percent at $8MPa$ and 250°C, and less than half of that at 200°C while no hydrolysis occurred at 100°C. One of the advantages of conducting hydrolysis in $SC-CO_2$ was that the hydrolysis vessel could also serve as an extraction vessel for FFA by simply decreasing the temperature from 250°C to 80°C and increasing the pressure from $8MPa$ to

$20MPa$. Our initial aim in conducting his study is to investigate the hydrolysis reaction in $SC - CO_2$ media to improve our understanding as $SC - CO_2$ is an excellent reaction medium and it eases the separation of the FFA from the product mixture (Moquin and Temelli (2006)). However, based on the literature review summarized above it is apparent that a better understanding of the hydrolysis reaction in $SC - CO_2$ is needed for potential industrial applications.

Here our focus has been shifted to the non-catalytic supercritical carbon dioxide ($SC - CO_2$) method to overcome the difficulties of the chemical catalytic transesterification reaction method. During the supercritical transesterification reaction, oil and methanol are heated and pressurized to their critical point at which the mixture of oil and methanol possesses unique solvating and transport properties. At the supercritical state, the oil and alcohol become a homogeneous phase after getting merged. In the SCM method, the critical temperature and pressure of alcohol can range up to $239°C$ and $8.1\ MPa$. These conditions reduce the solubility parameter of alcohol to a value near triglycerides which forms a single-phase solution. In addition, as no catalyst is needed in the process, it leads to easier separation and purification steps of biodiesel.

Even though, the Supercritical Carbon dioxide method has a vital disadvantage for commercialization. Because of the requirements of higher temperature and methanol to oil molar ratio, this process needs costly apparatus. Ang et al. (Ang et al. (2015)) established a kinetic model of supercritical reaction for biodiesel production from sea mango oil. They have shown that high temperature ($380°C$) and higher methanol to triglycerides molar ratio (45:1) are required to achieve only 78 percent biodiesel. This is due to the initial low speed of the transesterification reaction for biodiesel production to mass transfer limitations between the methanol and oil phase (Hou et al. (2007)). This problem can be evaded by applying stirring on the system. Roy et al. (Roy et al. (2014)) showed the effect of stirring on mass transfer in the transesterification of Jatropha oil. They have shown that mass transfer resistance is insignificant after a certain level of stirring.

Optimal control has got special interest in the industrial and academic fields as it provides useful information to design and control the reaction process. In general, a solution to these problems involves finding the time-dependent profiles of the control variable so as to optimize a particular performance index (Benavides and Diwekar (2012)). Pontryagin's maximum principle is widely used in optimal control, in the presence of constraints for the state variables. It is important to solve a Hamiltonian for optimal control strategy along with the optimal state trajectory. This is a maximum condition of the control Hamiltonian.

Hence, our main objectives in this thesis are dual. At first, we have formulated ecological mathematical models and analyzed the pest-controlling measures on the Jatropha curcas tree plantation in order to minimize its damage due to pest attack. Next, we have formulated mathematical models to optimize the production of biodiesel from Jatropha oil with the supercritical carbon dioxide method by determining the optimal condition with the help of simple mathematical techniques. The thesis is presented as follows.

In chapter 2, we have formulated a five-dimensional mathematical model containing the plant, pest, predator, and virus population. Here we have applied the viral pesticide to reduce the pest density and to get a healthy production of the Jatropha plant. We want to show the change in nature of the various biomass of the system due to the consumption of susceptible pests by predators with the Holling type I functional response by means of mathematical and numerical analysis. Our study indicates that virus replication may help effectively in controlling the pest population.

In chapter 3, we have extended our study to the comparison between Holling type I and Holling type II functional responses between pests and predators. Here we have studied the control of pests using bio-pesticides. A comparative analysis between two different functional responses has been analyzed to find the most effective measure to control the pest.

In chapter 4, a six-dimensional mathematical model has been formulated by us for the production of Free Fatty Acid (FFA) from Jatropha oil. Here we have studied the effect of molar ratio of water in the Supercritical Carbon dioxide medium to get maximum production of FFA. Our study reveals that water-to-oil molar ratio plays an important role in the cost-effective production of FFA. We have also studied the effect of the addition of water to the reaction system in an impulsive way.

In chapter 5, we have studied the dual effect of the molar ratios of the reactants and temperature of the reaction medium for the cost-effective production of biodiesel in the $SC - CO_2$ medium. Here it has been noticed that due to the use of water in the extraction of FFA stage, the methanol to oil molar ratio for the maximum production of biodiesel is less and thus it leads to more cost-effectiveness. From the analytical as well as numerical findings and discussion, it has been depicted that $SC - CO_2$ medium is a good reaction medium as it increases the reaction speed by diminishing the mass transfer resistance of the reactants. There is a certain effect of the temperature of the reaction medium and the molar ratio of the reactants to produce biodiesel from Jatropha curcas oil.

In chapter 6, we will conclude our findings from all the previous chapters which validates our work to get a healthy plantation of Jatropha curcas tree and to achieve a cost-effective production of biodiesel from Jatropha curcas plant resources for our societal benefits.

Chapter 2

Qualitative Study of Controlling Pest of Jatropha curcas for Linear Functional Response

Biodiesel is one of the most useful alternative fuels which is renewable, clean-burning, and cost-effective. The higher oil content and non-edible nature of the seed have made Jatropha curcus one of the most effective resources for biodiesel. Among many biodiesel-producing resources like Soybean oil, Mustard oil, Palm oil, etc. Jatropha oil is the most promising resource because it produces the purest quality of biodiesel. Jatropha plants are generally affected by pests. This affects the growth of the plant as well as the oil production. In this chapter[1], a nonlinear system has been formulated based on the relationship of various biomass and functional relation among the pest, predator, virus and plant population for the pest management of Jatropha plant by applying virus.

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[1]The major portion of this chapter is published in International Journal of Mathematics and Computer Research, Volume 11 Issue 10, pp. 3789-3793, 2023.

2.1 Formulation of The Mathematical Model

A five-dimensional mathematical model has been formulated, which consists of the biomass of Jatropha curcas plant $J(t)$, susceptible pest $S(t)$, infected pest $I(t)$, predator $P(t)$, and virus population $V(t)$. Plant growth normally follows a logistic fashion where r_J is the maximum growth rate and k_J is the carrying capacity of the said plant. Here we have described two classes of pest populations, i.e., Susceptible pests and Infected pests. The plant resource is consumed by pests at a rate α which is again converted into the susceptible pest with r_S as the maximum growth rate. k_S is considered as the carrying capacity of the susceptible pest. The virus population attacks the susceptible pests and converts them into infected pests at a rate λ. Here we have considered the linear functional response of the predator population on the susceptible pest population which helps the predators in their growth at a rate θ_1. The predators consume the infected pests at a rate *l*. Infected pests have a natural death rate ξ. d_P is the natural mortality rate of predators and ε_P denotes the intra-specific competition coefficient among predators present in the predatory guild of infected pests. The predators grow at a rate θ_2, due to predation of the infected pests. π_V is assumed as the constant recruitment rate of the virus to the system and κ is the virus replication rate. The reduction rate constant of the virus population is γ. The mortality rate of the virus population is assumed as μ_V.

With the above assumptions, the following mathematical model has been formulated.

$$\frac{dJ}{dt} = r_J J\left(1 - \frac{J}{k_J}\right) - \alpha JS$$

$$\frac{dS}{dt} = \mathrm{r_S} JS\left(1 - \frac{S+I}{k_S}\right) - \lambda SV - \beta SP$$

$$\frac{dI}{dt} = \lambda SV - \xi I - lIP$$

$$\frac{dP}{dt} = P(-d_P - \epsilon_P P) + \theta_1 \beta SP + \theta_2 IP$$

$$\frac{dV}{dt} = \pi_V + \kappa\xi I - \mu_V V - \gamma SV \qquad (2.1.1)$$

where,

$J(0) \geq 0, S(0) \geq 0, I(0) \geq 0, P(0) \geq 0, V(0) \geq 0$

and all the parameters are assumed to be non-negative.

2.2 Dynamics of the system

In this section, we will show the different equilibria of the system (2.1.1) and analyze the stability of the system around the equilibrium points.

2.2.1 Existence of Equilibria and Stability

Theorem 2.2.1: *The axial equilibrium point* $E = (0, 0, 0, 0, \pi_V)$ *exists and the system* (2.1.1) *is unstable around* E *for all the parametric values*.

Theorem 2.2.2: *The pest-free equilibrium point* $E_0 = \left(k_J, 0, 0, 0, \frac{\pi_V}{\mu_V}\right)$ *exists and the system* (2.1.1) *is stable around* E_0 *if* $k_J < \frac{\lambda \pi_V}{r_S \mu_V}$.

Pest-free equilibrium: $E_0 = \left(k_J, 0, 0, 0, \frac{\pi_V}{\mu_V}\right)$.

The Jacobian matrix for pest-free equilibrium point is given by,

$$J = \begin{bmatrix} -r_J & -\alpha k_J & 0 & 0 & 0 \\ 0 & r_S k_J - \dfrac{\lambda \pi_V}{\mu_V} & 0 & 0 & 0 \\ 0 & \dfrac{\lambda \pi_V}{\mu_V} & -\xi & 0 & 0 \\ 0 & 0 & 0 & -d_P & 0 \\ 0 & -\dfrac{\gamma \pi_V}{\mu_V} & \kappa\xi & 0 & -\mu_V \end{bmatrix}$$

At E_0 the above system is stable if $k_J < \frac{\lambda \pi_V}{r_S \mu_V}$.

Theorem 2.2.3: *The predator-free equilibrium point* $E_1(\bar{J},\ \bar{S},\ \bar{I}, 0, \bar{V})$ *exists if* $\kappa > \frac{\gamma}{\lambda}$ *and* $\frac{r_J}{\alpha} < \bar{S} < \frac{\mu_V}{k\lambda - \gamma}$ *and the system* (2.1.1) *is stable around* E_1 *for condition* (2.2.1.3).

The predator-free equilibrium point: $E_1(\bar{J},\ \bar{S},\ \bar{I}, 0, \bar{V})$.

Where $\bar{S}$ is the positive root of the cubic equation

$$A\bar{S}^3 + B\bar{S}^2 + C\bar{S} + D = 0 \qquad (2.2.1.1)$$

Where

$$A = \frac{A'}{r_J k_S \xi[\mu_V - (\kappa\lambda - \gamma)\bar{S}]}$$

$$B = \frac{B'}{r_J k_S \xi[\mu_V - (\kappa\lambda - \gamma)\bar{S}]}$$

$$C = \frac{C'}{r_J k_S \xi [\mu_V - (\kappa\lambda - \gamma)\bar{S}]}$$

$$D = \frac{D' - \lambda \pi_V r_J k_S \xi}{r_J k_S \xi [\mu_V - (\kappa\lambda - \gamma)\bar{S}]}$$

and

$$A' = r_S k_J \alpha \xi (\gamma - \kappa\lambda)$$

$$B' = r_S k_J (\alpha \xi k_S \kappa \lambda - \alpha \xi k_S \lambda + \alpha \xi \mu_V + \xi r_J \kappa \lambda - r_J \xi \gamma + \alpha \mu \lambda)$$

$$C' = r_S k_J (\xi \lambda k_S r_J - \alpha \xi \mu_V k_S - \xi k_S r_J \kappa \lambda - r_J \mu_V \xi - \lambda \mu_V r_J)$$

$$D' = \xi \mu_V r_S k_J k_S$$

$$\bar{V} = \frac{\pi_V}{\mu_V - (\kappa\lambda - \gamma)\bar{S}}$$

$$\bar{J} = k_J \left(1 - \frac{\alpha \bar{S}}{r_J}\right)$$

$$\bar{I} = \frac{\pi_V \lambda \bar{S}}{\xi [\mu_V - (\kappa\lambda - \gamma)\bar{S}]}$$

The predator-free equilibrium exists when $\kappa > \frac{\gamma}{\lambda}$ and $\frac{r_J}{\alpha} < \bar{S} < \frac{\mu_V}{k\lambda - \gamma}$.

The Jacobian matrix for predator-free equilibrium point for Holling type I functional response is given by -

$$
J = \begin{bmatrix} a^{11} & a^{12} & 0 & 0 & 0 \\ a^{21} & a^{22} & a^{23} & a^{24} & a^{25} \\ 0 & a^{32} & a^{33} & a^{34} & a^{35} \\ 0 & 0 & 0 & a^{44} & 0 \\ 0 & a^{52} & a^{53} & 0 & a^{55} \end{bmatrix}
$$

where,

$a^{11} = r_J - \alpha\bar{S} - 2\bar{J}\frac{r_J}{k_J}, a^{12} = -\alpha\bar{J}, a^{21} = r_S\bar{S}(1 - \frac{\bar{S}+\bar{I}}{k_S}),$

$a^{22} = r_S\bar{J}\left(1 - \frac{\bar{S}+\bar{I}}{k_S}\right) - \frac{r_S}{k_S}\bar{J}\bar{S} - \lambda\bar{V}, a^{23} = -\frac{r_S}{k_S}\bar{J}\bar{S},$

$a^{24} = -\beta\bar{S}, a^{25} = -\lambda\bar{S}, a^{32} = \lambda\bar{V}, a^{33} = -\xi,$

$a^{34} = -l\bar{I}, a^{35} = \lambda\bar{S}, a^{44} = -d_p + \theta_1\beta\bar{S} + \theta_2\bar{I},$

$a^{52} = -\gamma\bar{V}, a^{53} = k\xi, a^{55} = -(\mu_V + \gamma\bar{S}).$

The characteristic equation corresponding to the variational matrix at predator-free equilibrium point given before is,

$$
\lambda^5 + b_1\lambda^4 + b_2\lambda^3 + b_3\lambda^2 + b_4\lambda + b_5 = 0 \qquad (2.2.1.2)
$$

where b_is $(i = 1, 2, 3, 4, 5)$ are given as follows:

$$
b_1 = -\sum a^{ii},
$$

$$
b_2 = \sum a^{ii}a^{jj} - \sum a^{ij}a^{ji},
$$

$$
b_3 = -\sum a^{ii}a^{jj}a^{kk} + \sum a^{ij}a^{ji}a^{kk} - \sum a^{ij}a^{jk}a^{ki},
$$

$$
b_4 = \sum a^{ii}a^{jj}a^{kk}a^{ll} - \sum a^{ij}a^{ji}a^{kk}a^{ll} + \sum a^{ij}a^{jk}a^{ki}a^{ll} - \sum a^{ij}a^{ji}a^{kl}a^{lk}
$$

$$b_5 = -\sum a^{ii}a^{jj}a^{kk}a^{ll}a^{mm} + \sum a^{ij}a^{ji}a^{kk}a^{ll}a^{mm} - \sum a^{ij}a^{jk}a^{ki}a^{ll}a^{mm} + \sum a^{ij}a^{ji}a^{kl}a^{lk}a^{mm}$$

$$(i, j, k, l, m = \{1, 2, 3, 4, 5\} \; and \; i \neq j \neq k \neq l \neq m)$$

Then by Routh-Hurwitz criterion, it follows that the predator-free equilibrium point $E_1(\bar{J},\ \bar{S},\ \bar{I}, 0, \bar{V})$ is locally asymptotically stable if

- $b_i(i = 1, 2, 3, 4, 5) > 0$
- $b_1b_2b_3 > b_3^2 + b_1^2b_4$
- $(b_1b_4 - b_5)(b_1b_2b_3 - b_3^2 - b_1^2b_4) > b_5(b_1b_2 - b_3)^2 + b_1b_5^2$ (2.2.1.3)

Theorem 2.2.4: *The interior equilibrium point* $E^*(J^*, S^*, I^*, P^*, V^*)$ *exists if* $S^* < \frac{r_J}{\alpha}$ *and the system* (2.1.1) *is stable around* E^* *for condition* (2.2.1.6).

The interior equilibrium: $E^*(J^*, S^*, I^*, P^*, V^*)$.

Here $J^* = k_J(1 - \frac{\alpha S^*}{r_J})$,

I^* is the positive root of the equation $c_1{I^*}^2 + c_2I^* + c_3 = 0.$ (2.2.1.4)

where c_is $(i = 1, 2, 3)$ are given as follows:

$c_1 = l\mu_V\theta_2\epsilon_PS^* + \gamma l\theta_2,$

$c_2 = k\lambda\xi - \mu_V\xi - \frac{l\mu_V\theta_1\beta}{\epsilon_P} - \frac{l\mu_Vd_P}{\epsilon_PS^*} - \gamma\xi - \frac{\gamma l}{\epsilon_P}(\theta_1\beta S^* - d_P),$

$c_3 = \lambda\pi_V.$

$$P^* = \frac{\theta_1\beta S^* + \theta_2I^* - d_P}{\epsilon_P}$$

$$V^* = \frac{I^*[\xi\epsilon_P + l(\theta_1\beta S^* + \theta_2 I^* - d_P)]}{\epsilon_P\lambda S^*}$$

The interior equilibrium point E^* exists when $S^* < \frac{r_J}{\alpha}$.

For the single variation of sign, by Descartes' Rule of Sign there should be unique positive root. Therefore $c_2 < 0$.

$$i.e., \qquad k\lambda\xi - \mu_V\xi - \frac{l\mu_V\theta_1\beta}{\epsilon_P} - \frac{l\mu_V d_P}{\epsilon_P S^*} - \gamma\xi - \frac{\gamma l}{\epsilon_P}(\theta_1\beta S^* - d_P) < 0$$

$$\Rightarrow l\gamma\theta_1\beta S^* + (\epsilon_P\mu_V\xi + l\mu_V\theta_1\beta + \epsilon_P\gamma\xi - k\epsilon_P\xi - l\gamma d_P)S^* + l\mu_V d_P > 0.$$

This can be written as $(S^* - a)(S^* - b) > 0$. $\qquad (a < b)$

a, b are given as follows:

$$a = \frac{-(\epsilon_P\mu_V\xi + l\mu_V\theta_1\beta + \epsilon_P\gamma\xi - k\epsilon_P\xi - l\gamma d_P) - \sqrt{(\epsilon_P\mu_V\xi + l\mu_V\theta_1\beta + \epsilon_P\gamma\xi - k\epsilon_P\xi - l\gamma d_P)^2 - 4l^2\gamma\theta_1\beta\mu_V d_P}}{2l\gamma\theta_1\beta}$$

$$b = \frac{-(\epsilon_P\mu_V\xi + l\mu_V\theta_1\beta + \epsilon_P\gamma\xi - k\epsilon_P\xi - l\gamma d_P) + \sqrt{(\epsilon_P\mu_V\xi + l\mu_V\theta_1\beta + \epsilon_P\gamma\xi - k\epsilon_P\xi - l\gamma d_P)^2 - 4l^2\gamma\theta_1\beta\mu_V d_P}}{2l\gamma\theta_1\beta}$$

The Jacobian matrix for the interior equilibrium point, Holling type I functional response is given by,

$$\mathrm{J} = \begin{bmatrix} a_{11} & a_{12} & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} \\ 0 & a_{32} & a_{33} & a_{34} & a_{35} \\ 0 & a_{42} & a_{43} & a_{44} & 0 \\ 0 & a_{52} & a_{53} & 0 & a_{55} \end{bmatrix}$$

where,

$$a_{11} = r_J - \alpha S^* - \frac{2J^* r_J}{k_J},$$

$$a_{12} = -\alpha J^*,$$

$$a_{21} = r_S S^* \left(1 - \frac{S^* + I^*}{k_S}\right),$$

$$a_{22} = r_S J^* \left(1 - \frac{S^* + I^*}{k_S}\right) - \frac{r_S}{k_S} J^* S^* - \lambda V^* - \beta P^*,$$

$$a_{23} = -\frac{r_S}{k_S} J^* S^*,$$

$$a_{24} = -\beta S^*,$$

$$a_{25} = -\lambda S^*,$$

$$a_{32} = \lambda V^*,$$

$$a_{33} = -\xi - l P^*,$$

$$a_{34} = -l I^*,$$

$$a_{35} = \lambda S^*,$$

$$a_{42} = \theta_1 \beta P^*,$$

$$a_{43} = \theta_2 P^*,$$

$$a_{44} = -d_P - 2\epsilon_P P^* + \theta_1 \beta S^* + \theta_2 I^*,$$

$a_{52} = -\lambda V^*,$

$a_{53} = k\xi,$

$a_{55} = -\mu_V - \gamma S^*.$

The characteristic equation corresponding to the variational matrix at the interior equilibrium point given before is,

$$\lambda^5 + d_1\lambda^4 + d_2\lambda^3 + d_3\lambda^2 + d_4\lambda + d_5 = 0 \qquad (2.2.1.5)$$

where d_is $(i = 1, 2, 3, 4, 5)$ are given as follows:

$$d_1 = -\sum a_{ii} ,$$

$$d_2 = \sum a_{ii}a_{jj} - \sum a_{ij}a_{ji} ,$$

$$d_3 = -\sum a_{ii}a_{jj}a_{kk} + \sum a_{ij}a_{ji}a_{kk} - \sum a_{ij}a_{jk}a_{ki} ,$$

$$d_4 = \sum a_{ii}a_{jj}a_{kk}a_{ll} - \sum a_{ij}a_{ji}a_{kk}a_{ll} + \sum a_{ij}a_{jk}a_{ki}a_{ll} - \sum a_{ij}a_{ji}a_{kl}a_{lk}$$

$$d_5 = -\sum a_{ii}a_{jj}a_{kk}a_{ll}a_{mm} + \sum a_{ij}a_{ji}a_{kk}a_{ll}a_{mm} - \sum a_{ij}a_{jk}a_{ki}a_{ll}a_{mm} + \sum a_{ij}a_{ji}a_{kl}a_{lk}a_{mm}$$

$$(i, j, k, l, m = \{1, 2, 3, 4, 5\} \; and \; i \neq j \neq k \neq l \neq m)$$

Then by Routh-Hurwitz criterion, it follows that the interior equilibrium point $E^*(J^*, S^*, I^*, P^*, V^*)$ is locally asymptotically stable if

- $d_i(i = 1, 2, 3, 4, 5) > 0$
- $d_1d_2d_3 > d_3^2 + d_1^2d_4$
- $(d_1d_4 - d_5)(d_1d_2d_3 - d_3^2 - d_1^2d_4) > d_5(d_1d_2 - d_3)^2 + d_1d_5^2$

(2.2.1.6)

2.3 Numerical Simulation

In this section, we have shown the numerical simulation results using Matlab to validate our analytical findings. We have introduced virus spraying to reduce the pest population. Here our main goal is to control the pest population with the help of virus for healthy Jatropha plantation. This numerical simulation has been performed under parameters given in Table 2.1.

Table 2. 1: Parameters value used for numerical simulation (Chowdhury et al. (2016), Bhattacharya and Bhattacharya (2006), Venturino et al. (2016))

Parameters	Definition	Values (Unit)
r_J	The growth rate of plant biomass	$0.03 kg\ day^{-1}$
k_J	The carrying capacity of plant biomass	$50\ kg\ plant^{-1}$
r_S	Maximum growth rate of susceptible pest	$0.05\ day^{-1}$
k_S	The carrying capacity of susceptible pest	$300\ plant^{-1}$
α	Interaction rate between pest and plant	$0.0001\ plant^{-1}day^{-1}$
γ	Reduction rate constant of virus	$0.008\ day^{-1}$
λ	The infection rate of pest by virus	$0.003\ pest^{-1}day^{-1}$
ξ	The mortality rate of infected pest	$0.01\ day^{-1}$
d_P	Death rate of predator	$0.006\ day^{-1}$
ϵ_P	Intra specific competition coefficient	$0.002\ day^{-1}$
θ_1	Conversion factor for predator	0.05
θ_2	Conversion factor for predator	0.01
μ_V	Decay rate of virus	$0.1\ g\ day^{-1}$
β	Consumption rate of susceptible pest by predator	$0.015\ pest^{-1}day^{-1}$
l	Consumption rate of infected pest by predator	$0.7\ pest^{-1}day^{-1}$

In Figure 2.1, we have plotted the model variables as function of time. It is clear that the system moves towards its stable region as time increases. The trajectories of plant biomass, susceptible pest, infected pest, predator and virus population for Holling type I functional response have been shown. Here we can see that the system moves towards stability after a certain time. It has been also observed that susceptible pest is transformed into infected pest for and exterminated by the virus interference. The predator population is initially slightly decreased and then increased gradually, finally reaches its steady state.

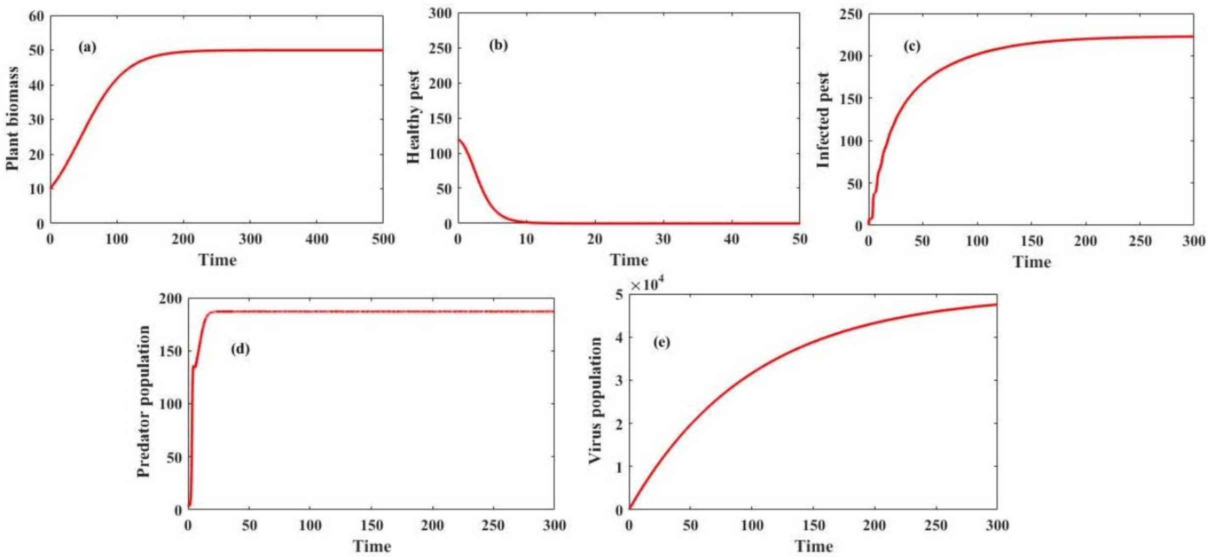

Fig. 2.1: Trajectories for different biomass: Plant biomass, Healthy pest, Infected pest, Predator population and Virus population for Holling type I Functional response at κ = 500, other parameter values are given in Table 2.1.

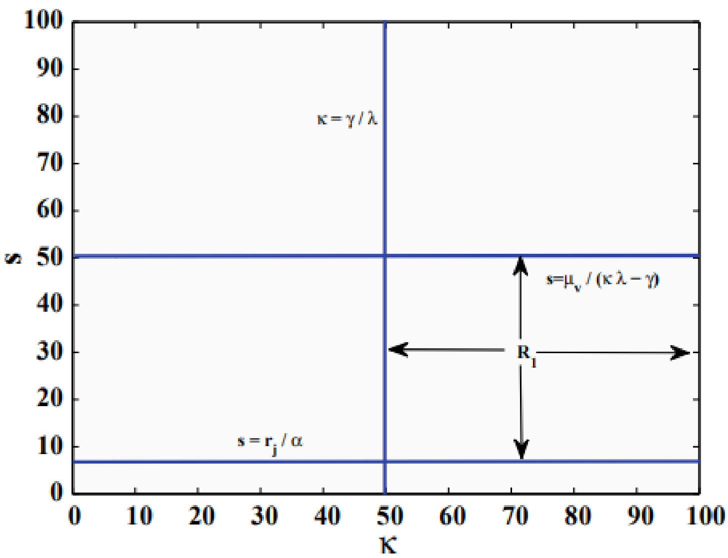

Fig. 2.2: The existence region of predator-free equilibrium point for the system with linear functional response, using the parameter values are given in Table 2.1.

Figure 2.2 depicts the region of existence for different equilibria. Here, R_1 is the existence region of predator-free equilibrium point for the system with linear functional response, whereas R_2 is the existence region of interior equilibrium points, which is represented by Figure 2.3.

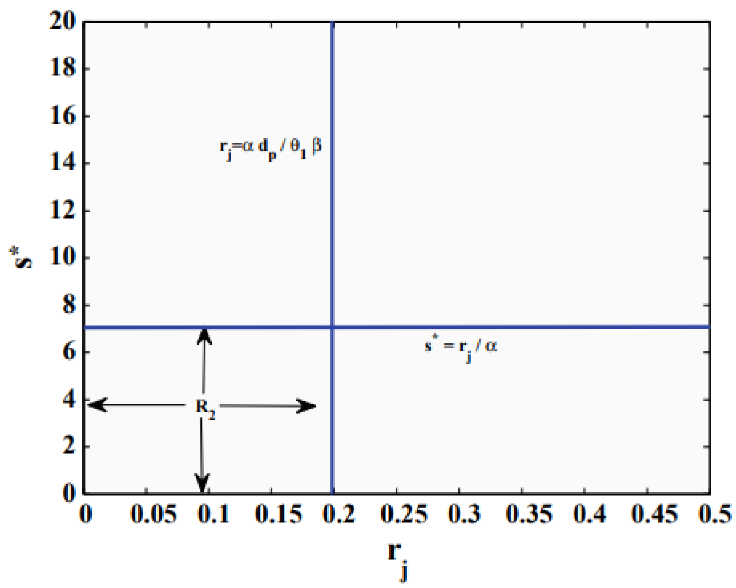

Fig. 2.3: The existence region of interior equilibrium point for the system with linear functional response, using the parameter values are given in Table 2.1.

In Figure 2.4, we have shown a mesh plotting in κ − λ-susceptible pest plane. This figure shows that for Holling type I functional response with the increasing value of κ and λ, though the pest population does not get eradicated totally from the system, it has been decreased significantly.

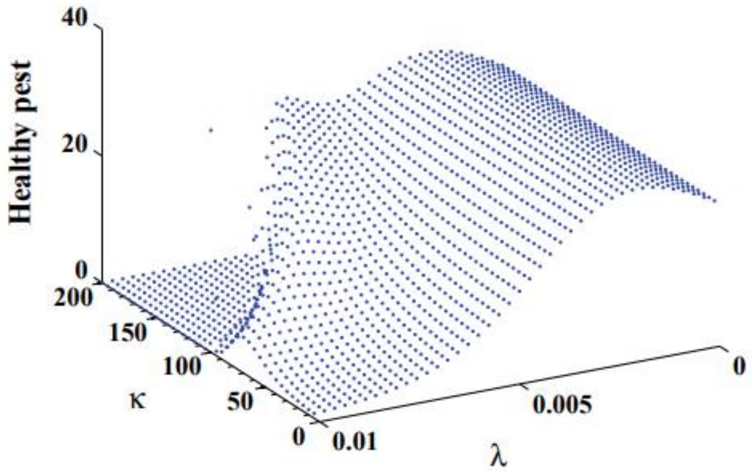

Fig. 2. 4: Mesh plotting for linear functional response in $\kappa - \lambda$-susceptible pest plane, using the parameter values are given in Table 2.1.

2.4 Discussion and Conclusion

In this chapter, we aim to control pest of Jatropha curcas plant. We have formulated a mathematical model for Jatropha curcas pest management. To do so, here we have used virus as controlling agent. The stability and existence of the system have been inspected analytically. We have checked the local stability at pest-free equilibrium, predator-free equilibrium point and interior equilibrium point for Holling type I or linear functional response on predator. Numerically, we have also examined the effect of virus replication. The dynamical behavior of all the biomass, considered in this study, have been studied and depicted with respect to different time intervals. If the pest becomes dominant in the system, then Jatropha plant will get affected severely which will lead to economic loss and consequently production of biodiesel will not be maximum. On the other hand, if the prey density becomes very less or they become extinct, the natural predator will be evanished which may also affect the biological balance of the ecosystem. Thus, it is very important to maintain the biological balance of the ecosystem in such a way so that on one hand crop yield will be maximized and predators also survive. We can easily see that linear functional response is effective in controlling and reducing the pest population within 150 days in order to get healthy plant production when spraying of virus is administered.

Chapter 3

Pest Control of Jatropha curcas Plant for Different Response Functions

It is well known fact that the natural enemy (predator) in the system survives on the susceptible and infected pest. The predator consumes the infected pest in linear mass action due to the fact that the viral infection makes some behavioral changes and sub lethal effect on host. In this chapter[1], we want to compare the change in nature of the system due to the consumption of susceptible pest by predator with Holling type I, II functional responses in the view of mathematical and numerical analysis.

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[1]The major portion of this chapter is published in Mathematical Analysis and Applications in Modeling, Springer Proceedings in Mathematics & Statistics 302, pp. 385-401, 2020.

3.1 Formulation of The Mathematical Model

Here we have formulated a five-dimensional mathematical model, containing biomass of Jatropha plant $J(t)$, susceptible pest $S(t)$, infected pest $I(t)$, predator $P(t)$ and virus population $V(t)$. Individual plant growth follows logistic fashion where r_J denotes the maximum growth rate and k_J denotes the carrying capacity of the plant. The pest population is partitioned into two classes, Susceptible and Infected pest. Pest consumes the plant resource at a rate α which is further converted into the susceptible pest with maximum growth rate r_S. The carrying capacity of the susceptible pest is assumed to be k_S. The virus population interact with the susceptible pests and turn them into infected pest class at a rate λ. Here we have considered the functional response $f\ (S)$ of the predator population on the susceptible pest population as linear and hyperbolic which helps the predators in their growth at a rate θ_1. The predators consume the infected pests at a rate l. ξ is the natural mortality rate of the infected pests. d_P is the natural death rate of predators and ε_P is the intra-specific competition coefficient among predators present in the predatory guild of infected pest. θ_2 is the growth rate of the predator due to predation of the infected pests. π_V is the constant recruitment rate of the virus. κ is the virus replication rate. The mortality rate of the virus population is μ_V.

With these suitable assumptions, the following mathematical model has been formulated.

$$\frac{dJ}{dt} = r_J J\left(1 - \frac{J}{k_J}\right) - \alpha JS$$

$$\frac{dS}{dt} = \mathrm{r_S} JS\left(1 - \frac{S+I}{k_S}\right) - \lambda SV - f(S)P$$

$$\frac{dI}{dt} = \lambda SV - \xi I - lIP$$

$$\frac{dP}{dt} = P(-d_P - \epsilon_P P) + \theta_1 f(S)P + \theta_2 IP$$

$$\frac{dV}{dt} = \pi_V + \kappa\xi I - \mu_V V - \gamma SV \qquad (3.1.1)$$

where,

$J(0) \geq 0, S(0) \geq 0, I(0) \geq 0, P(0) \geq 0, V(0) \geq 0$

and all the parameters are assumed to be non-negative.

The function $f\ (s)$ is of two different following types:

(i) ***Holling Type I or linear functional response***.

(ii) ***Holling Type II or hyperbolic functional response***.

3.1.1 Linear Functional Response

We first consider the Linear functional response or Holling type-I functional response. We consider the equilibria of the above system and discuss their local stability properties. For linear functional response, system takes the following form:

$$\frac{dJ}{dt} = r_J J\left(1 - \frac{J}{k_J}\right) - \alpha JS$$

$$\frac{dS}{dt} = \mathrm{r_S} JS\left(1 - \frac{S+I}{k_S}\right) - \lambda SV - \beta SP$$

$$\frac{dI}{dt} = \lambda SV - \xi I - lIP$$

$$\frac{dP}{dt} = P(-d_P - \epsilon_P P) + \theta_1 \beta SP + \theta_2 IP$$

$$\frac{dV}{dt} = \pi_V + \kappa \xi I - \mu_V V - \gamma SV \qquad (3.1.1.1)$$

3.1.1.1 Existence of Equilibria and Stability

Theorem 3.1.1.1: *The axial equilibrium point* $E = (0, 0, 0, 0, \pi_V)$ *exists and the system* (3.1.1.1) *is unstable around E for all the parametric values*.

Theorem 3.1.1.2: *The pest-free equilibrium point* $E_0 = \left(k_J, 0, 0, 0, \frac{\pi_V}{\mu_V}\right)$ *exists and the system* (3.1.1.1) *is stable around* E_0 *if* $k_J < \frac{\lambda \pi_V}{r_S \mu_V}$.

Theorem 3.1.1.3: *The predator-free equilibrium point* $E_1(\bar{J}, \bar{S}, \bar{I}, 0, \bar{V})$ *exists if* $\kappa > \frac{\gamma}{\lambda}$ *and* $\frac{r_J}{\alpha} < \bar{S} < \frac{\mu_V}{k\lambda - \gamma}$ *and the system* (3.1.1.1) *is stable around* E_1 *for condition* (2.2.1.3).

Theorem 3.1.1.4: *The interior equilibrium point* $E^*(J^*, S^*, I^*, P^*, V^*)$ *exists if* $S^* < \frac{r_J}{\alpha}$ *and the system* (3.1.1.1) *is stable around* E^* *for condition* (2.2.1.6).

3.1.2 Hyperbolic Functional Response

To catch a susceptible pest, predators need some time to search for its food. Hence the searching efficiency of the predators can play an important role in the system. Hence the objective of this subsection is to introduce the model with hyperbolic functional response to observe the dynamics of the system. For hyperbolic functional response, the system (3.1.1) takes the following form:

$$\frac{dJ}{dt} = r_J J\left(1 - \frac{J}{k_J}\right) - \alpha JS$$

$$\frac{dS}{dt} = \mathrm{r_S} JS\left(1 - \frac{S+I}{k_S}\right) - \lambda SV - \frac{\beta SP}{a+S}$$

$$\frac{dI}{dt} = \lambda SV - \xi I - lIP$$

$$\frac{dP}{dt} = P(-d_P - \epsilon_P P) + \theta_1 \frac{\beta SP}{a+S} + \theta_2 IP$$

$$\frac{dV}{dt} = \pi_V + \kappa\xi I - \mu_V V - \gamma SV \qquad (3.1.2.1)$$

Where a is the searching efficiency of the predator.

3.1.2.1 Existence of Equilibria and Stability

Theorem 3.1.2.1: *The axial equilibrium point* $E^{11} = (0,0,0,0,\pi_V)$ *exists and the system* (3.1.2.1) *is unstable around* E^{11} *for all the parametric values*.

Theorem 3.1.2.2: *The pest-free equilibrium point* $E_0^{11} = \left(k_J, 0, 0, 0, \frac{\pi_V}{\mu_V}\right)$ *exists and the system* (3.1.2.1) *is stable around* E_0^{11} *if* $k_J < \frac{\lambda \pi_V}{r_S \mu_V}$.

The Jacobian matrix for pest-free equilibrium point is given by,

$$J = \begin{bmatrix} -r_J & -\alpha k_J & 0 & 0 & 0 \\ 0 & r_S k_J - \dfrac{\lambda \pi_V}{\mu_V} & 0 & 0 & 0 \\ 0 & \dfrac{\lambda \pi_V}{\mu_V} & -\xi & 0 & 0 \\ 0 & 0 & 0 & -d_P & 0 \\ 0 & -\dfrac{\gamma \pi_V}{\mu_V} & \kappa\xi & 0 & -\mu_V \end{bmatrix}$$

At E_0^{11} the above system is stable if $k_J < \frac{\lambda \pi_V}{r_S \mu_V}$.

Theorem 3.1.2.3: *The predator-free equilibrium point* $E_1^{11}(\hat{J},\ \hat{S}, \hat{I}, 0, \hat{V})$ *exists if* $\kappa > \frac{\gamma}{\lambda}$ *and* $\frac{r_J}{\alpha} < \hat{S} < \frac{\mu_V}{k\lambda - \gamma}$ *and the system* (3.1.2.1) *is stable around* E_1^{11} *for condition* (3.1.2.1.3).

The predator free equilibrium: $E_1^{11}\left(\hat{J},\ \hat{S}, \hat{I}, 0, \hat{V}\right)$.

Where $\hat{S}$ is the positive root of the cubic equation

$$\grave{A}\hat{S}^3 + \grave{B}\hat{S}^2 + \grave{C}\hat{S} + \grave{D} = 0 \qquad (3.1.2.1.1)$$

Coefficients $\grave{A}, \grave{B}, \grave{C}, \grave{D}$ are as follows:

$$\grave{A} = \frac{\tilde{A}}{r_J k_S \xi \left[\mu_V - (\kappa\lambda - \gamma)\hat{S}\right]}$$

$$\grave{B} = \frac{\tilde{B}}{r_J k_S \xi \left[\mu_V - (\kappa\lambda - \gamma)\hat{S}\right]}$$

$$\grave{C} = \frac{\tilde{C}}{r_J k_S \xi \left[\mu_V - (\kappa\lambda - \gamma)\hat{S}\right]}$$

$$\grave{D} = \frac{\widetilde{D} - \lambda \pi_V r_J k_S \xi}{r_J k_S \xi \left[\mu_V - (\kappa\lambda - \gamma)\hat{S}\right]}$$

where,

$$\tilde{A} = r_S k_J \alpha \xi (\gamma - \kappa\lambda)$$

$$\tilde{B} = r_S k_J (\alpha \xi k_S \kappa \lambda - \alpha \xi k_S \lambda + \alpha \xi \mu_V + \xi r_J \kappa \lambda - r_J \xi \gamma + \alpha \mu_V \lambda)$$

$$\tilde{C} = r_S k_J (\xi k_S \lambda r_J - \alpha \xi k_S \mu_V - \kappa \xi k_S \lambda r_j - \xi r_J \mu_V - \mu_V \lambda r_J)$$

$$\widetilde{D} = \xi\mu_V r_J r_S k_J k_S$$

and

$$\hat{V} = \frac{\pi_V}{\mu_V - (\kappa\lambda - \gamma)\hat{S}}$$

$$\hat{J} = k_J(1 - \frac{\alpha\hat{S}}{r_J})$$

$$\hat{I} = \frac{\pi_V \lambda \hat{S}}{\xi[\mu_V - (\kappa\lambda - \gamma)\hat{S}]}$$

The predator-free equilibrium exists when $\kappa > \frac{\gamma}{\lambda}$ and $\frac{r_J}{\alpha} < \hat{S} < \frac{\mu_V}{k\lambda - \gamma}$.

The Jacobian matrix for predator-free equilibrium point for Holling type II functional response is given by

$$J = \begin{bmatrix} b^{11} & b^{12} & 0 & 0 & 0 \\ b^{21} & b^{22} & b^{23} & b^{24} & b^{25} \\ 0 & b^{32} & b^{33} & b^{34} & b^{35} \\ 0 & 0 & 0 & b^{44} & 0 \\ 0 & b^{52} & b^{53} & 0 & b^{55} \end{bmatrix}$$

where,

$$b^{11} = r_J - \alpha\hat{S} - 2\hat{J}\frac{r_J}{k_J},$$

$$b^{12} = \alpha\hat{J}$$

$$b^{21} = r_S\hat{S}\left(1 - \frac{\hat{S} + \hat{I}}{k_S}\right),$$

$$b^{22} = r_S\hat{J}\left(1 - \frac{\hat{S} + \hat{I}}{k_S}\right) - \frac{r_S}{k_S}\hat{J}\hat{S} - \lambda\hat{V}$$

$b^{23} = -\frac{r_S}{k_S}\hat{J}\hat{S},$

$b^{24} = -\beta\frac{\hat{S}}{\alpha + \hat{S}},$

$b^{25} = -\lambda\hat{S}$

$b^{32} = \lambda\hat{V},$

$b^{33} = -\xi,$

$b^{34} = -l\hat{I},$

$b^{35} = \lambda\hat{S}$

$b^{44} = -d_P + \theta_1\beta\frac{\hat{S}}{\alpha + \hat{S}} + \theta_2\hat{I}$

$b^{52} = -\gamma\hat{V},$

$b^{53} = \kappa\xi,$

$b^{55} = -\mu_V - \gamma\hat{S}$

The characteristic equation corresponding to the variational matrix at predator-free equilibrium point given before is,

$$\mu^5 + B_1\mu^4 + B_2\mu^3 + B_3\mu^2 + B_4\mu + B_5 = 0 \qquad (3.1.2.1.2)$$

where B_is $(i = 1, 2, 3, 4, 5)$ are given as follows:

$$B_1 = -\sum b^{ii}$$

$$B_2 = \sum b^{ii}b^{jj} - \sum b^{ij}b^{ji}$$

$$B_3 = -\sum b^{ii}b^{jj}b^{kk} + \sum b^{ij}b^{ji}b^{kk} - \sum b^{ij}b^{jk}b^{ki},$$

$$B_4 = \sum b^{ii} b^{jj} b^{kk} b^{ll} - \sum b^{ij} b^{ji} b^{kk} b^{ll} + \sum b^{ij} b^{jk} b^{ki} b^{ll} - \sum b^{ij} b^{ji} b^{kl} b^{lk}$$

$$B_5 = -\sum b^{ii} b^{jj} b^{kk} b^{ll} b^{mm} + \sum b^{ij} b^{ji} b^{kk} b^{ll} b^{mm} - \sum b^{ij} b^{jk} b^{ki} b^{ll} b^{mm} + \sum b^{ij} b^{ji} b^{kl} b^{lk} b^{mm}$$

$$(i, j, k, l, m = \{1, 2, 3, 4, 5\} \; and \; i \neq j \neq k \neq l \neq m)$$

Then by Routh-Hurwitz criterion, it follows that the predator-free equilibrium point $E_1^{11}(\hat{J},\ \hat{S}, \hat{I}, 0, \hat{V})$ is locally asymptotically stable if

- $B_i (i = 1, 2, 3, 4, 5) > 0$
- $B_1 B_2 B_3 > B_3^2 + B_1^2 B_4$
- $(B_1 B_4 - B_5)(B_1 B_2 B_3 - B_3^2 - B_1^2 B_4) > B_5 (B_1 B_2 - B_3)^2 + B_1 B_5^2$

(3.1.2.1.3)

Theorem 3.1.4.4: *The interior equilibrium point* $E_*^{11}(J_*, S_*, I_*, P_*, V_*)$ *exists if* $S_* < \frac{r_J}{\alpha}$ *and the system* (3.1.2.1) *is stable around* E_* *for condition* (3.1.2.1.6).

The interior equilibrium: $E_*^{11}(J_*, S_*, I_*, P_*, V_*)$.

Here

$$S_* = \frac{r_J}{\alpha}(1 - \frac{J^*}{k_J}),$$

$$P_* = -\frac{d_P}{\epsilon_P} + \frac{\theta_1 \beta r_J (k_J - J_*)}{\epsilon_P \left(a\alpha k_J + r_J (k_J - J_*)\right)} + \frac{\theta_2}{\epsilon_P} I_*$$

$$V_* = \frac{\alpha k_J}{\lambda r_J (k_J - J_*)} [\xi I_* + l I_* (-\frac{d_P}{\epsilon_P} + \frac{\theta_1 \beta r_J (k_J - J_*)}{\epsilon_P \left(a\alpha k_J + r_J (k_J - J_*)\right)} + \frac{\theta_2}{\epsilon_P} I_*)]$$

J_* is the positive root of the equation

$$C_1 J_*^2 + C_2 J_* + C_3 = 0. \qquad (3.1.2.1.4)$$

Coefficients $C_1, C_2,$ and C_3 are given by

$$C_1 = \pi_V \lambda \epsilon_P r_J^2 + \kappa \xi \lambda \epsilon_p r_J^2 - \gamma \xi \varepsilon p r_J^2 I_* - \gamma \theta_1 \beta r_J^2 + \gamma \theta_2 \alpha k_J a r_J - \gamma \theta_2 r_J I_*,$$

$$\begin{aligned} C_2 = & -\pi_V \lambda r_J \epsilon_P a \alpha k_J - \kappa \xi \lambda r_J \epsilon_P a \alpha k_J I_* - 2\pi_V \lambda r_J^2 \epsilon_P k_J - 2\kappa k_J \xi \lambda r_J^2 \epsilon_P \\ & + \xi \mu_V \alpha k_J r_J \epsilon_P I_* - \mu_V \alpha k_J l d_P r_J I_* + \theta_1 \beta r_J + \theta_2 I_* + \gamma \xi \epsilon_P a \alpha r_J k_J I_* \\ & + 2\gamma \xi \epsilon_P r_J^2 k_J I_* - \gamma r_J d_P a l \alpha I_* - \gamma r_J^2 d_P k_J l I_* + \gamma r_J^2 \theta_1 \beta k_J \\ & + \gamma r_J k_J \theta_1 \beta + \gamma r_J k_J^2 \theta_2 a \alpha + \gamma r_J^2 \theta_2 k_J I_* + \gamma r_J k_J \theta_2 I_*, \end{aligned}$$

$$\begin{aligned} C_2 = & \pi_V \lambda r_J \epsilon_P a \alpha k_J^2 + \kappa k_J^2 \xi \lambda r_J^2 \epsilon_P + \kappa \xi \lambda r_J k_J^2 \epsilon_P a \alpha I_* - \xi \mu_V \alpha^2 k_J^2 \epsilon_P \\ & - \xi \mu_V \alpha k_J^2 \epsilon_P I_* + \mu_V \alpha^2 k_J^2 l d_P a I_* + \mu_V \alpha k_J^2 l d_P r_J I_* - \theta_1 \beta r_J k_J \\ & - \theta_2 a \alpha k_J I_* - \theta_2 r_J k_J I_* - \lambda \xi \epsilon_P a \alpha r_J k_J^2 I_* - \gamma \xi \epsilon_P r_J^2 k_J^2 I_* \\ & + \gamma r_J k_J^2 d_P a l \alpha I_* + \gamma r_J^2 k_J^2 d_P l I_* - \gamma r_J^2 k_J^2 \theta_1 \beta - \gamma r_J^2 k_J^2 \theta_2 I_*. \end{aligned}$$

The interior equilibrium exists if $k_J > J_*$.

The Jacobian matrix for the interior equilibrium point for Holling type II functional response is given by,

$$
\mathrm{J} = \begin{bmatrix} b_{11} & b_{12} & 0 & 0 & 0 \\ b_{21} & b_{22} & b_{23} & b_{24} & b_{25} \\ 0 & b_{32} & b_{33} & b_{34} & b_{35} \\ 0 & b_{42} & b_{43} & b_{44} & 0 \\ 0 & b_{52} & b_{53} & 0 & b_{55} \end{bmatrix}
$$

where,

$$b_{11} = r_J - \alpha S_* - \frac{2J_* r_J}{k_J},$$

$$b_{12} = -\alpha J_*,$$

$$b_{21} = r_S S_* \left(1 - \frac{S_* + I_*}{k_S}\right),$$

$$b_{22} = r_S J_* \left(1 - \frac{S_* + I_*}{k_S}\right) - \frac{r_S}{k_S} J_* S_* - \lambda V_* - \frac{a\beta P_*}{(a + S_*)^2},$$

$$b_{23} = -\frac{r_S}{k_S} J_* S_*,$$

$$b_{24} = -\frac{\beta S_*}{a + S_*},$$

$$b_{25} = -\lambda S_*,$$

$$b_{32} = \lambda V_*,$$

$$b_{33} = -\xi - l P_*,$$

$$b_{34} = -l I_*,$$

$$b_{35} = \lambda S_*,$$

$$b_{42} = \frac{a\theta_1 \beta P_*}{(a + S_*)^2},$$

$b_{43} = \theta_2 P_*,$

$$b_{44} = -d_P - 2\epsilon_P P_* + \frac{\theta_1 \beta S_*}{a + S_*} + \theta_2 I_*,$$

$b_{52} = -\lambda V_*,$

$b_{53} = k\xi,$

$b_{55} = -\mu_V - \gamma S_*.$

The characteristic equation corresponding to the variational matrix at the interior equilibrium point given before is,

$$\mu^5 + D_1\mu^4 + D_2\mu^3 + D_3\mu^2 + D_4\mu + D_5 = 0 \qquad (3.1.2.1.5)$$

where D_is $(i = 1, 2, 3, 4, 5)$ are given as follows:

$$D_1 = -\sum b_{ii}$$

$$D_2 = \sum b_{ii}b_{jj} - \sum b_{ij}b_{ji}$$

$$D_3 = -\sum b_{ii}b_{jj}b_{kk} + \sum b_{ij}b_{ji}b_{kk} - \sum b_{ij}b_{jk}b_{ki},$$

$$D_4 = \sum b_{ii}b_{jj}b_{kk}b_{ll} - \sum b_{ij}b_{ji}b_{kk}b_{ll} + \sum b_{ij}b_{jk}b_{ki}b_{ll} - \sum b_{ij}b_{ji}b_{kl}b_{lk}$$

$$D_5 = -\sum b_{ii}b_{jj}b_{kk}b_{ll}b_{mm} + \sum b_{ij}b_{ji}b_{kk}b_{ll}b_{mm} - \sum b_{ij}b_{jk}b_{ki}b_{ll}b_{mm} + \sum b_{ij}b_{ji}b_{kl}b_{lk}b_{mm}$$

$$(i, j, k, l, m = \{1, 2, 3, 4, 5\}\ and\ i \neq j \neq k \neq l \neq m)$$

Then by Routh-Hurwitz criterion, it follows that the predator-free equilibrium point $E_*^{11}(J_*, S_*, I_*, P_*, V_*)$. is locally asymptotically stable if

- $D_i(i = 1, 2, 3, 4, 5) > 0$
- $D_1 D_2 D_3 > D_3^2 + D_1^2 D_4$
- $(D_1 D_4 - D_5)(D_1 D_2 D_3 - D_3^2 - D_1^2 D_4) > D_5(D_1 D_2 - D_3)^2 + D_1 D_5^2$

(3.1.2.1.6)

3.2 Numerical Simulation

In this section, we will present some numerical simulation results to validate our analytical findings. To reduce the pest, we introduce virus spraying. Here our main objective is to compare Holling type I and Holling type II functional responses between pest and predator to control the pest population by applying virus to get healthy Jatropha plant. This numerical experiment and simulation is done under parameters given as Table 3.1.

Table 3.1: Parameters value used for numerical simulation (Chowdhury et al. (2016), Bhattacharya and Bhattacharya (2006), Venturino et al. (2016))

Parameters	Definition	Values (Unit)
r_j	The growth rate of plant biomass	0.03 $kg\ day^{-1}$
k_j	The maximum density biomass of plant	50 $kg\ plant^{-1}$
r_s	Conversion factor of susceptible pest	0.05 day^{-1}
k_s	The pest carrying capacity	300 $plant^{-1}$
α	The interaction rate between pest and plant	0.0001 $plant^{-1}day^{-1}$
γ	reduction rate constant of virus	0.008 day^{-1}
λ	The infection rate of pest by virus	0.003 $pest^{-1}day^{-1}$
ξ	The mortality rate of infected pest	0.01 day^{-1}
d_p	The mortality rate of predator	0.006 day^{-1}
ε_p	lysis of predator due to competition	0.002 day^{-1}
θ_1	conversion factor for predator	0.05
θ_2	conversion factor for predator	0.01
μ_v	The decay rate of virus	0.1 $gm\ day^{-1}$
β	consumption rate of susceptible pest by predator	0.015 $pest^{-1}day^{-1}$
l	consumption rate of infected pest by predator	0.7 $pest^{-1}day^{-1}$
a	the half-saturation coefficient	0.5 (constant)

In Figure 3.1, we plotted the model variables as function of time. It is clear that the system moves towards its stable region as time increases. In figure (a) the trajectories of plant biomass for Holling type I and II functional responses have been compared. Here we can observe that for hyperbolic functional response the plant biomass reaches its stability faster than other functional responses. We can also observe from figure (b) and (c) that susceptible pest is transformed into infected pest for and exterminated by the virus interference. For hyperbolic functional response transformation of susceptible pest to infected pest is more rapid than other functional responses. The figure (d) shows that the predator population is initially decreased to a certain level and then increased gradually. By figure (e), we have shown the trajectories for virus population. Finally, predator population assumes a steady state (Figure 3.2).

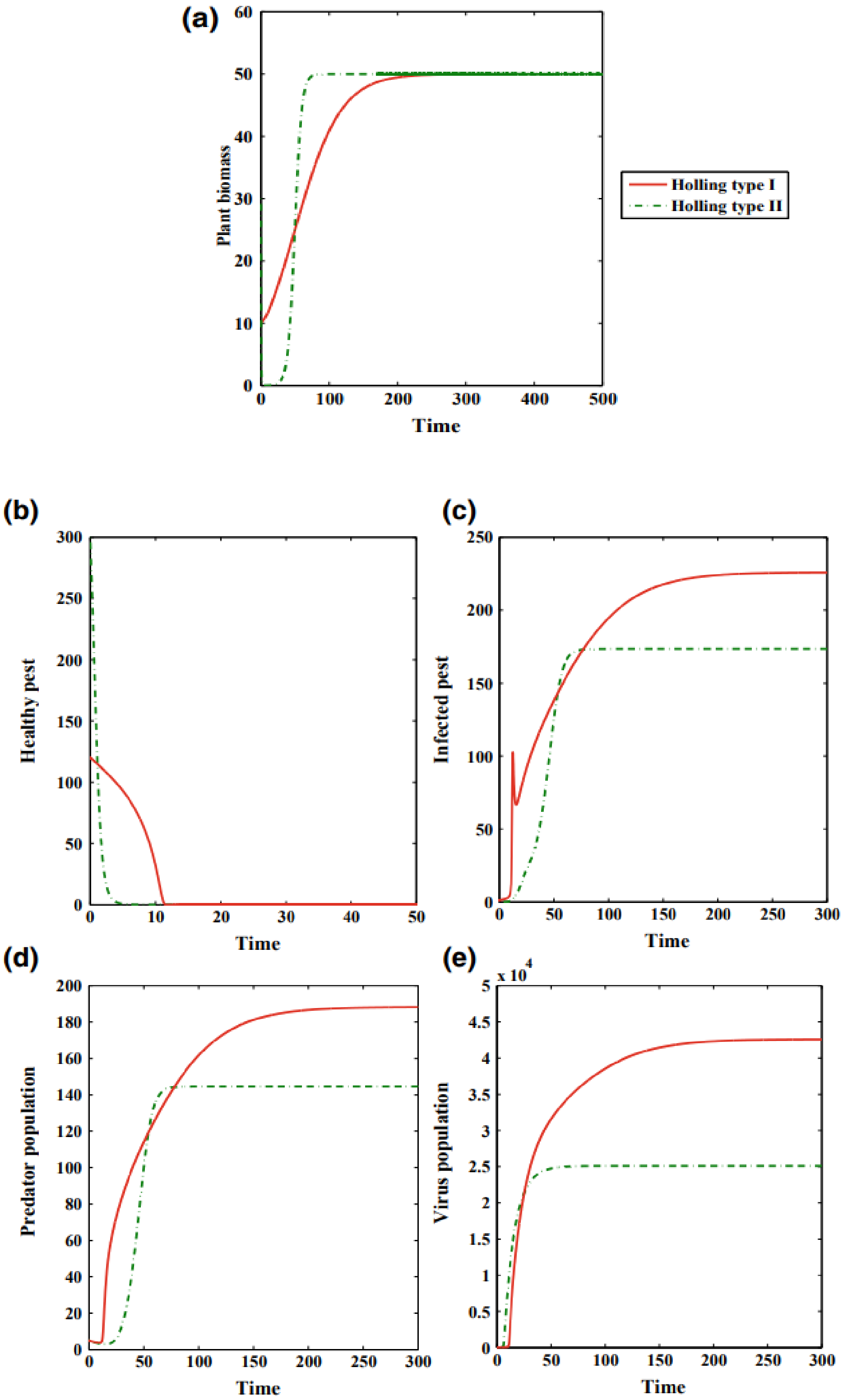


Fig. 3.1: Comparison of trajectories for different functional responses for: Plant biomass, Healthy pest, Infected pest, Predator population and Virus population at $\kappa = 500$, other parameter values are given in Table 3.1.

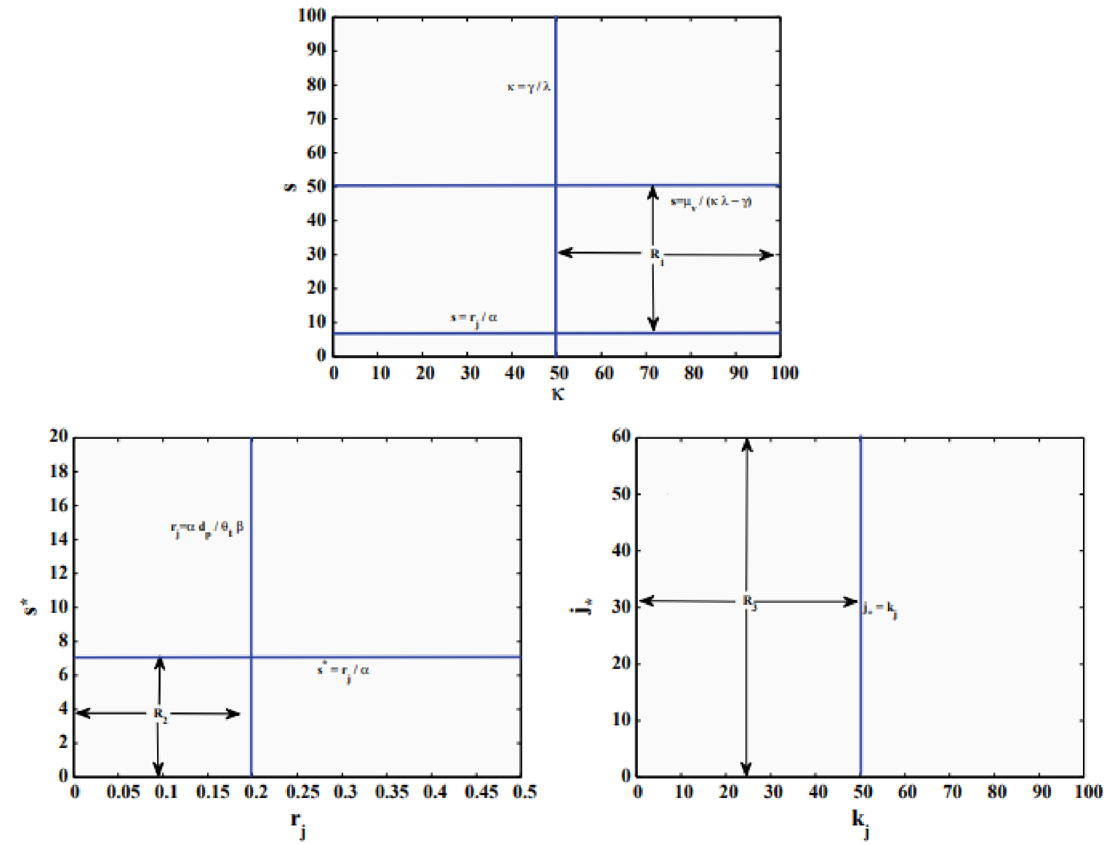


Fig. 3.2: Region of existence for different equilibria. Here R1 is the existence region of predator free equilibrium points for the system with both the functional responses, R2 and R3 are the existence regions of interior equilibrium points for the system with functional response I and II respectively.

Figure 3.3 depicts the effect of the virus replication parameter κ on different biomass. We vary the value of κ from 5 to 500. For less value of κ the system becomes unstable. Since κ is the virus replication parameter, with the increasing value of κ the virus population is increasing. Consequently, the susceptible pest population is readily converted into infected pest and susceptible pest population size is decreased. Here the model system moves towards stable pest-free equilibrium point at $\kappa = 500$. As a result, plant biomass is reaching its maximum value within 100 days.

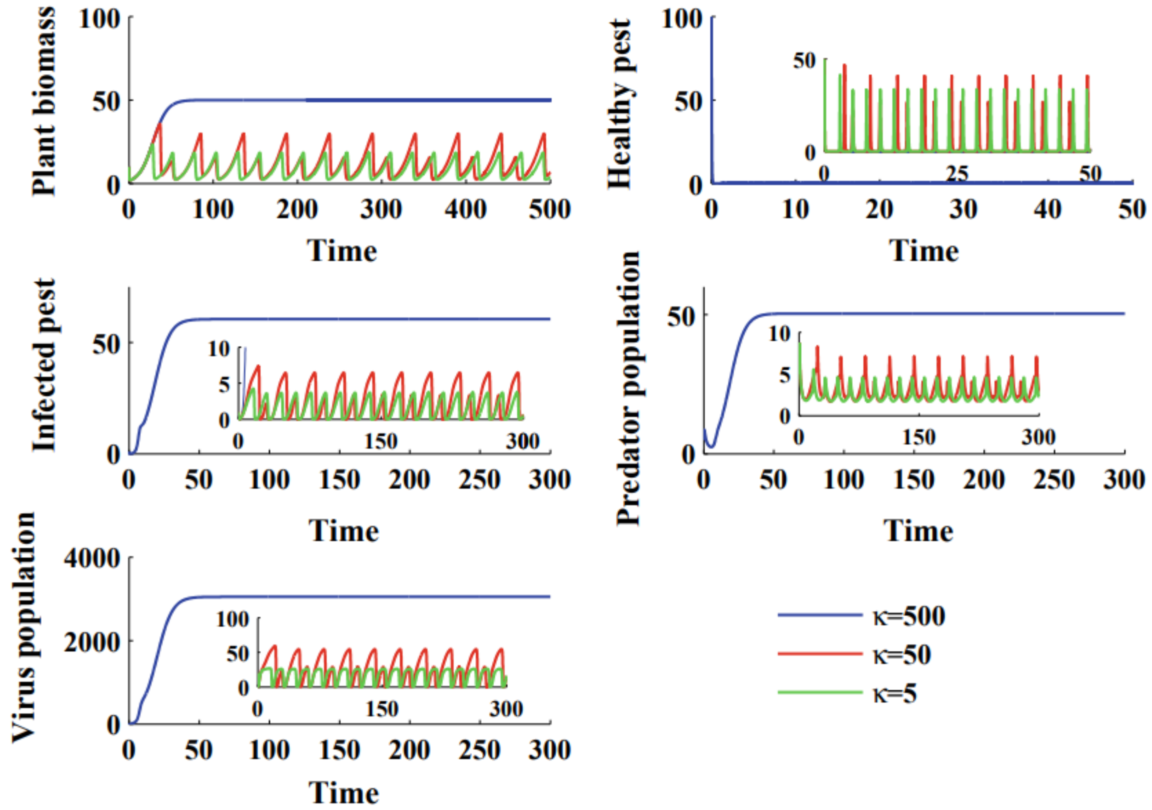


Fig. 3.3: Dynamics of the system with different values of κ for Holling type II functional responce, other parameter values are given in Table 3.1.

Figures 3.4 and 3.5 represent the time series solution of the model equation for hyperbolic functional response in virus-plant-healthy pest plane with initial values $[50, 100, 50]$, $[20, 200, 20]$, $[5, 300, 100]$ and $[30, 300, 60]$, $[20, 200, 20]$, $[10, 100, 40]$ respectively. Figure 3.4 describes that as time increases the system converges to pest-free equilibria for $\kappa = 500$. Figure 3.5 depicts that as time increases the system converges to endemic equilibria for $\kappa = 100$.

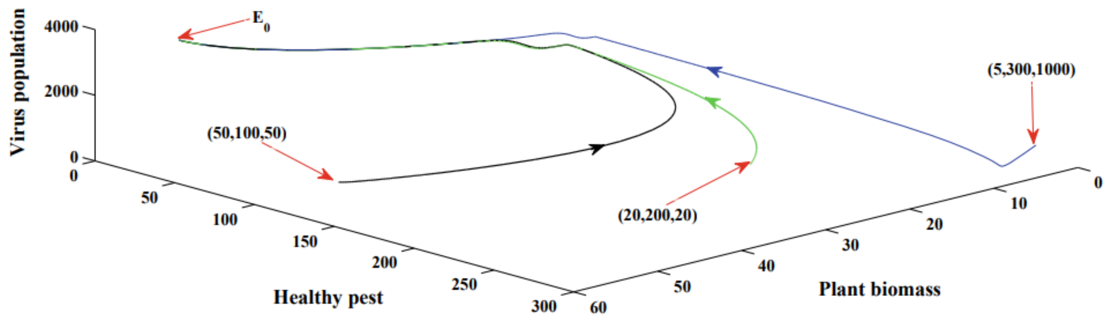


Fig. 3.4: Phase portrait in virus-plant-healthy pest plane showing that the system moves towards pest-free equilibrium point and the system becomes stable for Holling type II functional response at $\kappa = 500$, other parameter values are given in Table 3.1.

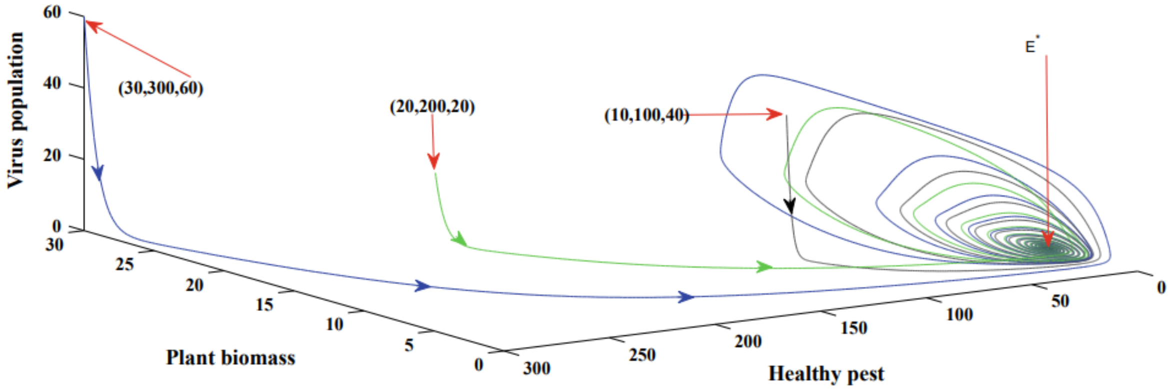
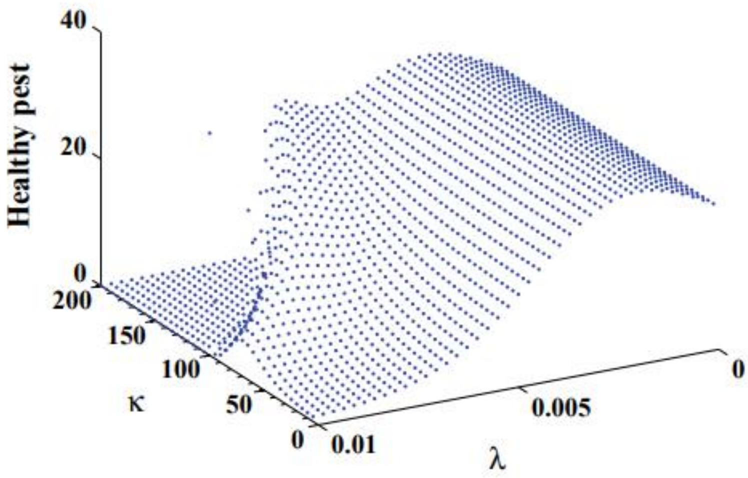
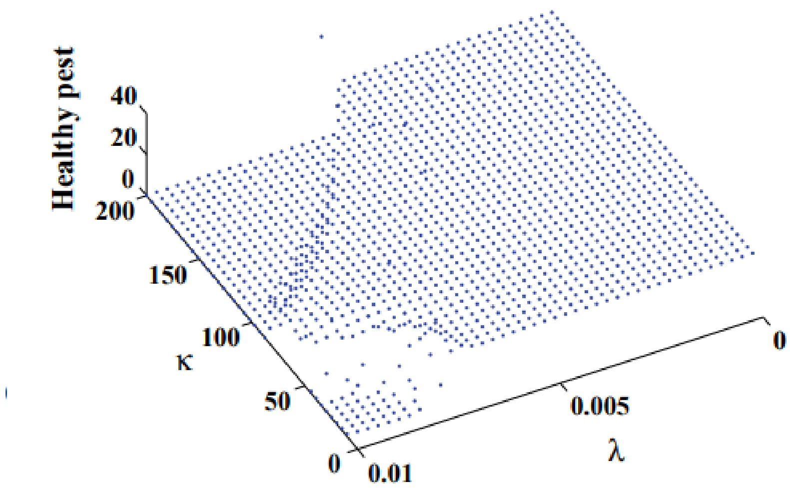


Fig. 3.5: Phase portrait in virus-plant-healthy pest plane showing that the system moves towards endemic equilibrium point and the system becomes stable for Holling type II functional response at $\kappa = 100$, other parameter values are given in Table 3.1.

In Figure 3.6, we have shown a mesh plotting in $\kappa - \lambda - susceptible\ pest$ plane. Figure (a) shows that for Holling type I functional response with the increasing value of κ and λ, the pest population decreases but not gets eradicated totally. In figure (b) we have seen that for Holling type II functional response, the healthy pests are exterminated when κ lies between 85 to 200 and λ lies between 0.005 to 0.01.



(a)



(b)

Fig. 3.6: Mesh plotting for (a) linear and (b) hyperbolic in $\kappa - \lambda - susceptible\ pest$ plane

3.3 Discussion and Conclusion

In this chapter, our main aim is to compare between linear and hyperbolic functional responses of predator on pest population to control the pest of Jatropha curcas plant using virus as controlling agent. Analytically we inspected the system from the viewpoint of stability and existence. We have checked the local stability at pest free equilibrium, predator free equilibrium points and interior equilibrium point for different functional responses. Numerically, we have examined the effect of virus replication. Here, we observe the changes of dynamical behavior with respect to different time intervals. The reason for using different types of Holling functional responses is to observe which functional response would be a suitable candidate to represent pest eradication. If the pest becomes dominant, then Jatropha will be affected heavily with economic loss. Also, if the prey becomes extinct, then the natural predator will die out, that may affect the biological balance of the ecosystem. Thus, it is very important to maintain the biological balance of the ecosystem in such a way so that in one hand crop yield will be maximized and predators also survive. We can easily see that hyperbolic functional response is more effective than that of linear functional response as within 60 days higher number of infected pests will be saturated and the system becomes stable, whereas for linear functional response it will take 150 days to stabilize the system. Also, for Holling type II functional response the virus population assumes its steady state more quickly than that of for Holling type I functional response. Hence virus population does not increase so much to show negative impact on the plant biomass. Finally, our work reveals that an introduction of predators/natural enemies with a hyperbolic functional response would be most effective to control pest and maximize healthy plant production.

Chapter 4

A Mathematical Study on the Effect of Water to Oil Molar Ratio for Free Fatty Acid Production in $SC-CO2$ Medium

In this chapter[1], a set of nonlinear differential equations has been formulated based on concentrations of Triglyceride, Diglyceride, Monoglyceride, Free Fatty Acid (FFA), Water and Glycerol. Our study is based on the effect of the molar ratio of water as well as the addition of water to the reaction medium in impulsive way and how we can get a cost-effective and stable production of FFA that ultimately leads to the production of biodiesel which we will show in the next chapter. The validity of our model is attained by experimental results. The analytical results are also verified by our numerical findings.

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[1]The major portion of this chapter is published in International Journal of Mathematics and Computer Research, Volume 11 Issue 09, pp. 3729-3733, 2023.

4.1 Formulation of The Mathematical Model

To illustrate a mathematical model for hydrolysis of vegetable Jatropha curcas oil, the following assumptions have been made:

- $\boldsymbol{A1}$: The hydrolysis of Jatropha curcas oil with water consists of three stepwise consecutive and reversible reactions.

- $\boldsymbol{A2}$: In the three reversible steps, triglycerides (TG) are initially hydrolysed to diglycerides (DG), then to monoglycerides (MG) and finally to glycerol. Each of these reaction steps produces one molecule of free fatty acids (FFA). The schematic diagram for hydrolysis of Jatropha curcas oil is as follows:

$$TG + H_2O \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} DG + FFA$$
$$DG + H_2O \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} MG + FFA$$
$$MG + H_2O \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} GL + FFA$$

- $\boldsymbol{A3}$: Here k_1, k_2, k_3 are forward reaction rates and k_{-1}, k_{-2}, k_{-3} are backward reaction rate constants respectively. These reaction rate constants follow Arrhenius equation given by:

$$k_i = a_i e^{\frac{-b_i}{T}}$$

where,

T - reaction temperature,

a_i - frequency factor,

$b_i = \frac{Ea_i}{R}$

in which

Ea_i - activation energy for each component

R - Universal Gas Constant.

Based on these assumptions the following system of differential equations characterizing the stepwise reaction has been formed.

$$\frac{dx_T}{dt} = -k_1 x_T x_H + k_{-1} x_D x_F$$

$$\frac{dx_D}{dt} = k_1 x_T x_H - k_{-1} x_D x_F - k_2 x_D x_H + k_{-2} x_M x_F$$

$$\frac{dx_M}{dt} = k_2 x_D x_H - k_{-2} x_M x_F - k_3 x_M x_H + k_{-3} x_G x_F$$

$$\frac{dx_H}{dt} = -k_1 x_T x_H + k_{-1} x_D x_F - k_2 x_D x_H + k_{-2} x_M x_F - k_3 x_M x_H + k_{-3} x_G x_F$$

$$\frac{dx_F}{dt} = k_1 x_T x_H - k_{-1} x_D x_F + k_2 x_D x_H - k_{-2} x_M x_F + k_3 x_M x_H - k_{-3} x_G x_F$$

$$\frac{dx_G}{dt} = k_3 x_M x_H - k_{-3} x_G x_F \qquad (4.1.1)$$

with the following initial conditions:

$$x_T(0) = x_{T_0}, \quad x_D(0) = 0, \quad x_M(0) = 0,$$
$$x_H(0) = x_{H_0}, \quad x_F(0) = x_{F_0}, \quad x_G(0) = 0, \tag{4.1.2}$$

4.2 System with Impulse on Water

In this section, we have considered the stepwise addition of water with time intervals t' and t'' for maximum biodiesel production. Therefore, the above system (4.1.1) becomes an impulsive system with an impulse on water. Hence the impulsive form of the above system is as follows:

$$\frac{dx_T}{dt} = -k_1 x_T x_H + k_{-1} x_D x_F \qquad t \neq t_k$$

$$\frac{dx_D}{dt} = k_1 x_T x_H - k_{-1} x_D x_F - k_2 x_D x_H + k_{-2} x_M x_F \qquad t \neq t_k$$

$$\frac{dx_M}{dt} = k_2 x_D x_H - k_{-2} x_M x_F - k_3 x_M x_H + k_{-3} x_G x_F \qquad t \neq t_k$$

$$\frac{dx_H}{dt} = -k_1 x_T x_H + k_{-1} x_D x_F - k_2 x_D x_H + k_{-2} x_M x_F - k_3 x_M x_H + k_{-3} x_G x_F \qquad t \neq t_k$$

$$\frac{dx_F}{dt} = k_1 x_T x_H - k_{-1} x_D x_F + k_2 x_D x_H - k_{-2} x_M x_F + k_3 x_M x_H - k_{-3} x_G x_F \qquad t \neq t_k$$

$$\frac{dx_G}{dt} = k_3 x_M x_H - k_{-3} x_G x_F \qquad t \neq t_k$$

and impulse is given by

$$x_H(t_k^+) - x_H(t_k^-) = r x_H \qquad t = t_k$$

(4.2.1)

With the following conditions

$$x_T(0) = x_{T_0}, \quad x_D(0) = 0, \quad x_M(0) = 0,$$
$$x_H(0) = x_{H_0}, \quad x_F(0) = x_{F_0}, \quad x_G(0) = 0 \qquad (4.2.2)$$

Here r is the rate at which water is given to the system at time t_k.

$(k = 0,1,2,\cdots)$

4.2.1 Analytical Study of The System

To get the approximate concentration profile for water by analytical method, we have considered the following subsystem here.

$$\frac{dx_H}{dt} = -k_1 x_T x_H + k_{-1} x_D x_F - k_2 x_D x_H + k_{-2} x_M x_F - k_3 x_M x_H + k_{-3} x_G x_F$$
$$+ k_4 x_F x_{ME} - k_{-4} x_B x_H \qquad t \neq t_k$$

$$x_H(t_k^+) - x_H(t_k^-) = r x_H \qquad t = t_k \qquad (4.2.1.1)$$

Since the system is bounded, $\exists\ C \in \boldsymbol{R}^+$ such that $x_j < C$, (j stands for T, D, M, H, F, G).

Also, by Arrhenius Principle k_1, k_{-1}, k_2, k_{-2} are finite quantities. Then for some positive real numbers M and N, it can be written that,

$$\frac{1}{2}M = min\,\{k_{-1}x_D x_F, k_{-2}x_M x_F, k_{-3}x_G x_F\}$$

and

$$\frac{1}{2}N = min\,\{k_1 x_T, k_2 x_D, k_3 x_M\}$$

Then the system (4.2.1.1) becomes

$$\frac{dx_H}{dt} \le M - Nx_H, \qquad t \neq t_k \qquad (4.2.1.2)$$

$$\Delta x_H = r x_H \qquad t = t_k$$

For maximum rate of change of water, the system is re-written as,

$$\frac{dx_H}{dt} = M - Nx_H, \qquad t \neq t_k \qquad (4.2.1.3)$$

$$\Delta x_H = r x_H \qquad t = t_k$$

Here m, n are some real constants.

Therefore, for a single impulsive cycle $t_k \le t \le t_{k+1}$, the solution of the system is represented by -

$$x_H(t_{k+1}^-) = \frac{M}{N}\,[1 - e^{-N(t_{k+1}-t_k)}] + x_H(t_k^+)e^{-N(t_{k+1}-t_k)} \qquad (4.2.1.4)$$

The amount of water just before impulse and immediately after impulse are given by $x_H(t_k^-)$ and $x_H(t_k^+)$ respectively.

Hence, we have

$$x_H(t_1^-) = \frac{M}{N}$$

$$x_H(t_1^+) = \frac{M}{N}(1+r)$$

$$x_H(t_2^-) = \frac{M}{N}(1+r)e^{-N(t_2-t_1)} + \frac{M}{N}(1-e^{-N(t_2-t_1)})$$

$$x_H(t_2^+) = \frac{M}{N}(1+r)^2 e^{-N(t_2-t_1)} + \frac{M}{N}(1+r)(1-e^{-N(t_2-t_1)})$$

$$x_H(t_3^-) = \frac{M}{N}[(1+r)^2\, e^{-N(t_3-t_1)} + (1+r)e^{-N(t_3-t_2)}$$

$$-(1+r)e^{-N(t_3-t_1)} + 1 - e^{-N(t_3-t_2)}\,]$$

$$x_H(t_3^+) = \frac{M}{N}\,[(1+r)^3\, e^{-N(t_3-t_1)} + (1+r)^2\, e^{(-N(t_3-t_2))}$$

$$-(1+r)^2\, e^{-N(t_3-t_1)} + (1+r) - (1+r)e^{-N(t_3-t_2)}\,] \qquad (4.2.1.5)$$

and so on.

Hence, we can write the general solution of the subsystem as

$$\begin{aligned} x_H(t_p^-) = \frac{M}{N}\,\big[&(1+r)^{p-1}\, e^{-N(t_p-t_1)} + (1+r)^{p-2}\, e^{-N(t_p-t_2)} \\ &+ (1+r)^{p-3}\, e^{-N(t_p-t_3)} + \ldots + 1 - (1+r)^{p-2}\, e^{-N(t_p-t_1)} \\ &- (1-r)^{p-3}\, e^{-N(t_p-t_2)} \\ &- (1+r)^{p-4}\, e^{-N(t_p-t_3)} - \ldots - e^{-N(t_p-t_{p-1})}\,\big] \end{aligned} \qquad (4.2.1.6)$$

4.2.2 For Fixed Time Interval

If water is given to the system in fixed time interval, then $t_n - t_{n-1} = \tau$ is constant. Hence, the general solution is:

$$x_H(t_p^-) = \frac{M}{N}\,[1 + (1+r)e^{-N\tau}$$

$$+ (1+r)^2\, e^{-2N\tau} + \ldots + (1+r)^{p-1}\, e^{-N(p-1)\tau} - e^{-N\tau}\{1$$

$$+ (1+r)e^{-N\tau} + (1+r)^2\, e^{-2N\tau} + \ldots + (1+r)^{p-2}\, e^{-(p-2)N\tau}\}]$$

$$= \frac{M}{N}\,[\frac{1-(1+r)^p\, e^{-Np\tau}}{1-(1+r)e^{-N\tau}} - \frac{e^{-N\tau}\left(1-(1+r)^{p-1}\, e^{-N(p-1)\tau}\right)}{1-(1+r)e^{-N\tau}}]\,. \qquad (4.2.2.1)$$

Taking limit,

$$\lim_{p\to\infty} x_H(t_p^-) = \frac{M}{N}\,[\frac{1-e^{-N\tau}}{1-(1+r)e^{-N\tau}}] \qquad (4.2.2.2)$$

This is the long-term maximum value of the water (since the effect of the impulse is to be immediately reduced). To keep this under the threshold $\widehat{x_H}$, we have,

$$\frac{M}{N}\,[\frac{1-e^{-N\tau}}{1-(1+r)e^{-N\tau}}] < \widehat{x_H}$$

which implies

$$\tau < \frac{1}{N}\ln\left\{\frac{M-N(1+r)\widehat{x_H}}{M-N\widehat{x_H}}\right\} = \tau_{\max} \ \text{(say)}$$

4.3 Numerical Simulation

In this section, we have numerically solved the model systems to show the effect of water to oil molar ratio and also the impulsive effect on addition of water in $SC-CO_2$ medium to maximize the production of free fatty acid. The effect of changes in the reaction parameters are shown numerically by our model.

Table 4. 1 Kinetic parameter set for the reaction system (Diwekar and Benavides (2012))

Reaction rate constants, k_i	Values (unit)
k_1	$.00995\ moles\ L^{-1}min^{-1}$
k_{-1}	$.1219\ moles\ L^{-1}min^{-1}$
k_2	$.03\ moles\ L^{-1}min^{-1}$
k_{-2}	$.0011\ moles\ L^{-1}min^{-1}$
k_3	$1.9514\ moles\ L^{-1}min^{-1}$
k_{-3}	$.1144\ moles\ L^{-1}min^{-1}$

Figure 4.1 represents the effect of water to oil molar ratio on the reaction. From $5:1, 10:1, 15:1$, $20:1$ water to oil molar ratios $15:1$ water to oil molar ratio has been considered as the optimum molar ratio for the execution of the reaction because though for both $15:1$ and $20:1$ molar ratios we have the maximum production of FFA at the same time, but for $15:1$ water to oil molar ratio the requirement of the amount of water is less and it increases the reaction rate.

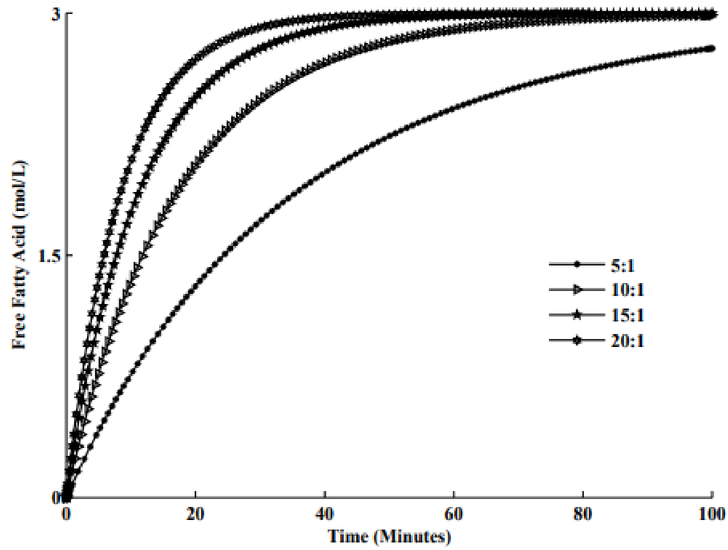

Fig. 4. 1: Effect of water to oil molar ratio in production of Free Fatty Acid through hydrolysis of Triglycerides, using parameter values given in Table 4.1.

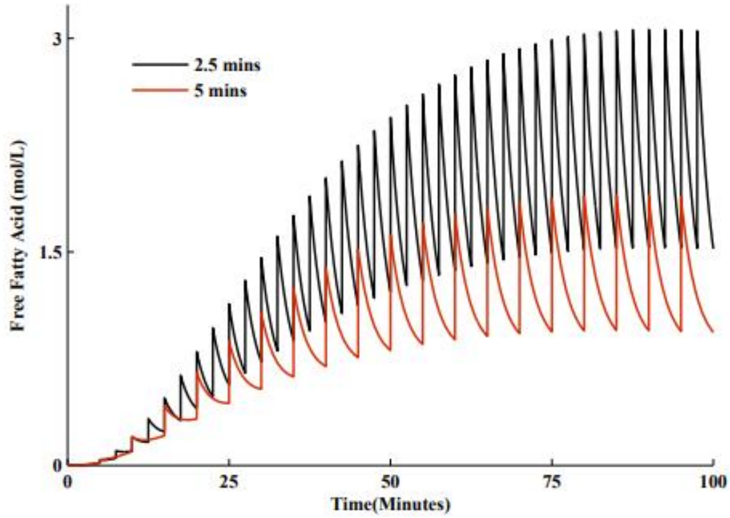

Fig. 4. 2: Concentration of Free Fatty Acid with respect to addition of water in 2.5 minutes and 5 minutes intervals, using parameter values given in Table 4.1.

Figure 4.2 compares the impulsive effect of adding the same amount of water to the reaction system for different time intervals. Here we can observe that adding water in the impulsive way with 2.5 minute interval is considerably more effective than adding water with 5 minutes interval as the reaction rate is enhanced more and ultimately results to a stable production of FFA, i.e., 3 moles/L, which is the maximum production.

4.4 Discussion and Conclusion

In this chapter, we have presented a mathematical model of hydrolysis reaction of Jatropha curcas oil with water for the maximum yield of Free Fatty Acid (FFA). By numerical simulation concentration of FFA has been calculated with respect to reaction conditions such as water to oil molar ratio and addition of water to the reaction medium in impulsive way. We have found that constant production of Free Fatty Acid is possible by the hydrolysis of triglycerides (Jatropha curcas oil) and maximum yield of free fatty acid $i.e.\ 3\,mol/L$ is attained in the $SC - CO_2$ reaction medium when water is added to the system impulsively with 2.5 minutes interval. Also, the optimized water to oil molar ratio to get maximum yield of free fatty acid has been found to be $15 : 1$. Though it can be observed that at $20 : 1$ water to oil molar ratio, we can also get the maximum production of free fatty acid, but as for both $15 : 1$ and $20 : 1$ water to oil molar ratio we have got the highest and same amount of FFA production at the same time, we have come to the point that we should choose $15 : 1$ water to oil molar ratio because of the less requirement of water. Since water is easy to get and there are plenty of sources of water in the world, this hydrolysis process is much cost-effective.

Chapter 5

Effect of Temperature and Molar Ratio on Biodiesel Production in Supercritical-Carbon Dioxide Medium

In the previous chapter we have studied and discussed the role of water to oil molar ratio in producing Free Fatty Acid (FFA) from Jatropha oil. Now we will extend our work to produce biodiesel from produced FFA when it reacts with Methanol. Methanol to oil molar ratio plays a vital role in this process. Also, the effect of the temperature of the reaction medium is highly important for producing biodiesel. In this chapter[1], our study is aimed on how we can achieve cost-effective yield of biodiesel depending on optimization of reaction temperature and the molar ratios of the reactant (methanol) using the control theoretic strategy.

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[1]The major portion of this chapter is published in Nonlinear Studies, Volume 26 No. 2, pp. 327-341, 2019.

5.1 Formulation of The Mathematical Model

To illustrate a mathematical model for hydrolysis of vegetable Jatropha curcas oil, the following assumptions have been made:

- $\boldsymbol{A1}$: The hydrolysis of Jatropha curcas oil with water consists of three stepwise consecutive and reversible reactions.

- $\boldsymbol{A2}$: In the three reversible steps, triglycerides (TG) are initially hydrolysed to diglycerides (DG), then to monoglycerides (MG) and finally to glycerol. Each of these reaction steps produces one molecule of free fatty acids (FFA). The schematic diagram for hydrolysis of Jatropha curcas oil is as follows:

$$TG + H_2O \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} DG + FFA$$
$$DG + H_2O \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} MG + FFA$$
$$MG + H_2O \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} GL + FFA$$

- $\boldsymbol{A3}$: After getting Free Fatty Acid from above reactions, methanol reacts with that FFA and produces one molecule of biodiesel (BD). This step is shown by:

$$FFA + M \underset{k_{-4}}{\overset{k_4}{\rightleftharpoons}} BD + H_2O$$

- ***A4***: Here k_1, k_2, k_3, k_4 are forward reaction rates and $k_{-1}, k_{-2}, k_{-3}, k_{-4}$ are backward reaction rate constants respectively. These reaction rate constants follow Arrhenius equation given by (Benavides and Diwekar (2012)):

$$k_i = a_i e^{\frac{-b_i}{T}}$$

where,

T - reaction temperature,

a_i - frequency factor,

$b_i = \frac{Ea_i}{R}$

in which

Ea_i - activation energy for each component

R - Universal Gas Constant.

Based on these assumptions the following system of differential equations characterizing the stepwise reaction has been formed.

$$\frac{dx_T}{dt} = -k_1 x_T x_H + k_{-1} x_D x_F$$

$$\frac{dx_D}{dt} = k_1 x_T x_H - k_{-1} x_D x_F - k_2 x_D x_H + k_{-2} x_M x_F$$

$$\frac{dx_M}{dt} = k_2 x_D x_H - k_{-2} x_M x_F - k_3 x_M x_H + k_{-3} x_G x_F$$

$$\frac{dx_H}{dt} = -k_1 x_T x_H + k_{-1} x_D x_F - k_2 x_D x_H + k_{-2} x_M x_F - k_3 x_M x_H + k_{-3} x_G x_F$$

$$+k_4 x_F x_{ME} - k_{-4} x_B x_H$$

$$\frac{dx_F}{dt} = k_1 x_T x_H - k_{-1} x_D x_F + k_2 x_D x_H - k_{-2} x_M x_F + k_3 x_M x_H - k_{-3} x_G x_F$$

$$-k_4 x_F x_{ME} + k_{-4} x_B x_H$$

$$\frac{dx_G}{dt} = k_3 x_M x_H - k_{-3} x_G x_F$$

$$\frac{dx_{ME}}{dt} = -k_4 x_F x_{ME} + k_{-4} x_B x_H$$

$$\frac{dx_B}{dt} = k_4 x_F x_{ME} - k_{-4} x_B x_H \qquad (5.1.1)$$

with the following initial conditions:

$$x_T(0) = x_{T_0}, \quad x_D(0) = 0, \quad x_M(0) = 0, \quad x_H(0) = x_{H_0}$$
$$x_F(0) = x_{F_0}, \quad x_G(0) = 0, \quad x_{ME}(0) = x_{ME_0}, \quad x_B(0) = 0 \qquad (5.1.2)$$

5.2 Optimization of Temperature

Optimal control has got special interest in the industrial and academic field as it provides useful information to design and control the reaction process. In general, a solution to these problems involves finding the time dependent profiles of the control variable so as to optimize a particular performance index (Benavides and Diwekar (2012)). Here our objective is to control temperature profile to get maximum and cost-effective production of biodiesel. To solve this problem, in this article we used the Pontryagin's maximum principle formulation. In this method, the objective function is formulated as a linear function in terms of final values of state variables (x_i) and the constant values (A_i). Thus, the objective function for this problem is shown in the following equation:

$$\text{Maximize} \quad J = \sum_{i=1}^{8} A_i x_i \tag{5.2.1}$$

Subject to the generalized form of state equations as

$$\frac{dx_i}{dt} = f(x_i, T) \tag{5.2.2}$$

For $x_i = [x_T(0), x_D(0), x_M(0), x_H(0), x_F(0), x_G(0), x_{ME}(0), x_B(0)]$.

Here x_i is the state variable that represents the concentration of each component: x_T , x_D, x_M, x_H, x_F , x_G, x_{ME}, x_B.

T (temperature) is the control variable.

A_is ($i = 0,\ldots,8$) are constants values for the linear representation of the maximum principle.

The maximum principle involves the addition of n adjoint variables (one adjoint variable per state variable), n adjoint equations, and a Hamiltonian which satisfies the following relations:

$$H = \sum_{i=1}^{8} a_i f_i \tag{5.2.3}$$

$$\frac{da_i}{dt} = -\sum_{i=1}^{8} a_j \frac{\partial f_i}{\partial x_i} \tag{5.2.4}$$

The adjoint equations can be computed as,

$$\frac{da_1}{dt} = (a_1 - a_2 + a_4 - a_5) k_1 x_H$$

$$\frac{da_2}{dt} = -a_1(k_{-1}x_F) + a_2(k_2x_H + k_{-1}x_F) + a_3(k_2x_H) - a_4(k_{-1}x_F - k_2x_H) - a_5(-k_{-1}x_F + k_2x_H)$$

$$\frac{da_3}{dt} = -a_2(k_{-2}x_F) + a_3(k_3x_H + k_{-2}x_F) - a_4(k_{-2}x_F - k_3x_H) - a_5(-k_{-2}x_F + k_3x_H) - a_7(k_3x_H)$$

$$\frac{da_4}{dt} = -a_1(k_1x_T) - a_2(k_1x_T - k_2x_D) - a_3(k_2x_D - k_3x_M) + (a_4 - a_5)(k_1x_T + k_2x_D + k_3x_M + k_{-4}x_B) - a_6(k_{-4}x_B) - a_7(k_3x_M) + a_8(k_{-4}x_B)$$

$$\frac{da_5}{dt} = -a_1(k_{-1}x_D) - a_2(k_{-2}x_M - k_{-1}x_D) - a_3(k_{-3}x_G - k_{-2}x_M) - (a_4 - a_5)(k_{-1}x_D + k_{-2}x_M + k_{-3}x_G + k_4x_{ME}) + a_6(k_4x_{ME}) + a_7(k_{-3}x_G) - a_8(k_4x_{ME})$$

$$\frac{da_6}{dt} = -(a_4 - a_5 - a_6 + a_8)k_4x_F$$

$$\frac{da_7}{dt} = -(a_3 + a_4 - a_5 - a_7)k_{-3}x_F$$

$$\frac{da_8}{dt} = (a_4 - a_5 - a_6 + a_8)k_{-4}x_H \qquad (5.2.5)$$

Now we apply the total derivative to Eq. (5.2.3) to find the derivative of the Hamiltonian. Therefore, the Hamiltonian can be calculated as:

$$\frac{dH}{dT} = \sum_{i=1}^{8} \frac{\partial H}{\partial x_i}\theta_i + \sum_{i=1}^{8} \frac{\partial H}{\partial a_i}\phi_i \qquad (5.2.6)$$

where θ_i and ϕ_i are represented by,

$$\theta_i = \frac{dx_i}{dt}$$

$$\phi_i = \frac{da_i}{dt}$$

Next to calculate the values of θ_i and ϕ_i, we consider:

$$\frac{d}{dT}\left(\frac{dx_i}{dt}\right) = \frac{d}{dt}\left(\frac{dx_i}{dT}\right) = \frac{d\theta_i}{dt}$$

$$\frac{d}{dT}\left(\frac{da_i}{dt}\right) = \frac{d}{dt}\left(\frac{da_i}{dT}\right) = \frac{d\phi_i}{dt}$$

where the differential equations for θ_i and ϕ_i are given by:

$$\frac{d\theta_i}{dt} = f(x_i, \theta_i, T)$$

$$\frac{d\theta_i}{dt} = f(x_i, \theta_i, a_i, \phi_i, T)$$

Differential equations of θ_i and ϕ_i are given as follows:

$$\frac{d\theta_T}{dt} = -\frac{dk_1}{dT}x_T x_H - k_1\theta_T x_H - k_1\theta_H x_T + \frac{dk_{-1}}{dT}x_D x_F + k_{-1}\theta_D x_F + k_{-1}\theta_F x_D \quad (5.2.7)$$

$$\frac{d\phi_T}{dt} = (\phi_T - \phi_D + \phi_H - \phi_F)k_1 x_H + (a_1 - a_2 + a_4 - a_5)(\frac{dk_1}{dT}x_H + k_1\theta_H) \quad (5.2.8)$$

$$\frac{d\theta_D}{dt} = \frac{dk_1}{dT}x_T x_H + k_1\theta_T x_H + k_1\theta_H x_T - \frac{dk_2}{dT}x_D x_H - k_2\theta_D x_H - k_2\theta_H x_D + \frac{dk_{-2}}{dT}x_M x_F + k_{-2}\theta_M x_F + k_{-2}\theta_F x_M - \frac{dk_{-1}}{dT}x_D x_F - k_{-1}\theta_D x_F - k_{-1}\theta_F x_D \quad (5.2.9)$$

$$\frac{d\phi_D}{dt} = -\phi_T k_{-1} x_F - a_1\left(\frac{dk_{-1}}{dT} x_F + k_{-1}\theta_F\right) + \phi_D(k_2 x_H + k_{-1} x_F) +$$

$$a_2\left(\frac{dk_2}{dT} x_H + k_2\theta_H + \frac{dk_{-1}}{dT} x_F + k_{-1}\theta_F\right) - \phi_M k_2 x_H -$$

$$a_3\left(\frac{dk_2}{dT} x_H - k_2\theta_H\right) - \phi_H(-k_2 x_H + k_{-1} x_F) -$$

$$a_4\left(\frac{dk_{-1}}{dT} x_F + k_{-1}\theta_F - \frac{dk_2}{dT} x_H - k_2\theta_H\right) - \phi_F(k_2 x_H - k_{-1} x_F) -$$

$$a_5\left(-\frac{dk_{-1}}{dT} x_F - k_{-1}\theta_F + \frac{dk_2}{dT} x_H + k_2\theta_H\right) \quad (5.2.10)$$

$$\frac{d\theta_M}{dt} = \frac{dk_2}{dT} x_D x_H + k_2\theta_D x_H + k_2\theta_D x_H - \frac{dk_{-2}}{dT} x_M x_F - k_{-2}\theta_M x_F -$$

$$k_{-2}\theta_F x_M + \frac{dk_3}{dT} x_M x_H - k_3\theta_M x_H - k_3\theta_H x_M + \frac{dk_{-3}}{dT} x_G x_F +$$

$$k_{-3}\theta_G x_F + k_{-3}\theta_F x_G \quad (5.2.11)$$

$$\frac{d\phi_M}{dt} = -\phi_D k_{-2} x_F - a_2\left(\frac{dk_{-2}}{dT} x_F + k_{-2}\theta_F\right) + \phi_M(k_3 x_H + k_{-2} x_F) +$$

$$a_3\left(\frac{dk_3}{dT} x_H + k_3\theta_H - \frac{dk_{-2}}{dT} x_F - k_{-2}\theta_F\right) - \phi_H(k_{-2} x_F - k_3 x_H) -$$

$$a_4\left(\frac{dk_{-2}}{dT} x_F + k_{-2}\theta_F - \frac{dk_3}{dT} x_H - k_3\theta_H\right) - \phi_F(-k_{-2} x_F + k_3 x_H) -$$

$$a_5\left(-\frac{dk_{-2}}{dT} x_F - k_{-2}\theta_F + \frac{dk_3}{dT} x_H + k_3\theta_H\right) - \phi_G k_3 x_H -$$

$$a_7\left(\frac{dk_3}{dT} x_H + k_3\theta_H\right) \quad (5.2.12)$$

$$\frac{d\theta_H}{dt} = -\frac{dk_1}{dT} x_T x_H - k_1\theta_T x_H - k_1\theta_H x_T + \frac{dk_{-1}}{dT} x_D x_F + k_{-1}\theta_D x_F +$$

$$k_{-1}\theta_F x_D + \frac{dk_2}{dT} x_D x_H - k_2\theta_D x_H - k_2\theta_H x_D + \frac{dk_{-2}}{dT} x_M x_F +$$

$$k_{-2}\theta_M x_F + k_{-2}\theta_F x_M - \frac{dk_3}{dT} x_M x_H - k_3\theta_M x_H - k_3\theta_H x_M +$$

$$\frac{dk_{-3}}{dT} x_G x_F + k_{-3}\theta_G x_F + k_{-3}\theta_F x_G + \frac{dk_4}{dT} x_F x_{ME} + k_4\theta_F x_{ME} +$$

$$k_4\theta_{ME}x_F - \frac{dk_{-4}}{dT}x_Bx_H - k_{-4}\theta_Bx_H - k_{-4}\theta_Hx_B \tag{5.1.13}$$

$$\frac{d\phi_H}{dt} = \phi_Tk_1x_T + a_1\left(\frac{dk_1}{dT}x_T + k_1\theta_T\right) - \phi_D(k_1x_T - k_2x_D) - a_2\left(\frac{dk_1}{dT}x_T + k_1\theta_T - \frac{dk_2}{dT}x_D - k_2\theta_D\right) - \phi_M(k_2x_D - k_3x_M) - a_3\left(\frac{dk_2}{dT}x_D + k_2\theta_D - \frac{dk_3}{dT}x_M - k_3\theta_M\right) + \phi_H(k_1x_T + k_2x_D + k_3x_M + k_{-4}x_B) + a_4\left(\frac{dk_1}{dT}x_T + k_1\theta_T + \frac{dk_2}{dT}x_D + k_2\theta_D + \frac{dk_3}{dT}x_M + k_3\theta_M + \frac{dk_{-4}}{dT}x_B + k_{-4}\theta_B\right) - \phi_F(k_1x_T + k_2x_D + k_3x_M + k_{-4}x_B) - a_5\left(\frac{dk_1}{dT}x_T + k_1\theta_T + \frac{dk_2}{dT}x_D + k_2\theta_D + \frac{dk_3}{dT}x_M + k_3\theta_M + \frac{dk_{-4}}{dT}x_B + k_{-4}\theta_B\right) - \phi_{ME}k_{-4}x_B - a_6\left(\frac{dk_{-4}}{dT}x_B + k_{-4}\theta_B\right) - \phi_Gk_3x_M - a_7\left(\frac{dk_3}{dT}x_M + k_3\theta_M\right) + \phi_Bk_{-4}x_B + a_8\left(\frac{dk_{-4}}{dT}x_B + k_{-4}\theta_B\right) \tag{5.1.14}$$

$$\frac{d\theta_F}{dt} = -\frac{d\theta_H}{dt} \tag{5.1.15}$$

$$\frac{d\phi_F}{dt} = -\phi_Tk_{-1}x_D - a_1\left(\frac{dk_{-1}}{dT}x_D + k_{-1}\theta_D\right) - \phi_D(k_{-2}x_M - k_{-1}x_D) - a_2\left(\frac{dk_{-2}}{dT}x_M + k_{-2}\theta_M - \frac{dk_{-1}}{dT}x_D - k_{-1}\theta_D\right) - \phi_M(k_{-3}x_G - k_{-2}x_M) - a_3\left(\frac{dk_{-3}}{dT}x_G + k_{-3}\theta_G - \frac{dk_{-2}}{dT}x_M - k_{-2}\theta_M\right) - (\phi_H - \phi_F)(k_{-1}x_D + k_{-2}x_M + k_{-3}x_G + k_4x_{ME}) - (a_4 - a_5)\left(\frac{dk_{-1}}{dT}x_D + k_{-1}\theta_D + \frac{dk_{-2}}{dT}x_M + k_{-2}\theta_M + \frac{dk_{-3}}{dT}x_G + k_{-3}\theta_G + \frac{dk_4}{dT}x_{ME} + k_4\theta_{ME}\right) \tag{5.1.16}$$

$$\frac{d\theta_G}{dt} = \frac{dk_3}{dT}x_M x_H + k_3\theta_M x_H + k_3\theta_H x_M - \frac{dk_{-3}}{dT}x_G x_F - k_{-3}\theta_G x_F - k_{-3}\theta_f x_G \quad (5.1.17)$$

$$\frac{d\phi_G}{dt} = -(\phi_M + \phi_H - \phi_F - \phi_G)k_{-3}x_F - (a_3 + a_4 - a_5 - a_7)(\frac{dk_{-3}}{dT}x_F + k_{-3}\theta_F) \quad (5.1.18)$$

$$\frac{d\theta_{ME}}{dt} = -\frac{dk_4}{dT}x_F x_{ME} - k_4\theta_F x_{ME} - k_4\theta_{ME}x_F + \frac{dk_{-4}}{dT}x_B x_H + k_{-4}\theta_B x_H + k_{-4}\theta_H x_B \quad (5.1.19)$$

$$\frac{d\phi_{ME}}{dt} = -(\phi_H - \phi_F - \phi_{ME} + \phi_B)k_4 x_F - (a_4 - a_5 - a_6 + a_8)(\frac{dk_4}{dT}x_F + k_4\theta_F) \quad (5.1.20)$$

$$\frac{d\theta_B}{dt} = -\frac{d\theta_{ME}}{dt} \quad (5.1.21)$$

$$\frac{d\phi_B}{dt} = (\phi_H - \phi_F - \phi_{ME} + \phi_B)k_{-4}x_H + (a_4 - a_5 - a_6 + a_8)(\frac{dk_{-4}}{dT}x_H + k_{-4}\theta_H) \quad (5.1.22)$$

5.3 System with Impulse on Water

In this section, we have considered the stepwise addition of water with time intervals t' and t'' for maximum biodiesel production. Therefore, the above system (5.1.1) becomes an impulsive system with an impulse on water. Hence the impulsive form of the above system is as follows:

$$\frac{dx_T}{dt} = -k_1 x_T x_H + k_{-1} x_D x_F \qquad t \neq t_k$$

$$\frac{dx_D}{dt} = k_1 x_T x_H - k_{-1} x_D x_F - k_2 x_D x_H + k_{-2} x_M x_F \qquad t \neq t_k$$

$$\frac{dx_M}{dt} = k_2 x_D x_H - k_{-2} x_M x_F - k_3 x_M x_H + k_{-3} x_G x_F \qquad t \neq t_k$$

$$\frac{dx_H}{dt} = -k_1 x_T x_H + k_{-1} x_D x_F - k_2 x_D x_H + k_{-2} x_M x_F - k_3 x_M x_H + k_{-3} x_G x_F$$

$$+k_4 x_F x_{ME} - k_{-4} x_B x_H \qquad t \neq t_k$$

$$\frac{dx_F}{dt} = k_1 x_T x_H - k_{-1} x_D x_F + k_2 x_D x_H - k_{-2} x_M x_F + k_3 x_M x_H - k_{-3} x_G x_F$$

$$-k_4 x_F x_{ME} + k_{-4} x_B x_H \qquad t \neq t_k$$

$$\frac{dx_G}{dt} = k_3 x_M x_H - k_{-3} x_G x_F \qquad t \neq t_k$$

$$\frac{dx_{ME}}{dt} = -k_4 x_F x_{ME} + k_{-4} x_B x_H \qquad t \neq t_k$$

$$\frac{dx_B}{dt} = k_4 x_F x_{ME} - k_{-4} x_B x_H \qquad t \neq t_k$$

and impulse is given by

$$x_H(t_k^+) - x_H(t_k^-) = r x_H \qquad t = t_k$$

(5.3.1)

With the following conditions

$$x_T(0) = x_{T_0}, \quad x_D(0) = 0, \quad x_M(0) = 0, \quad x_H(0) = x_{H_0},$$

$$x_F(0) = x_{F_0}, \quad x_G(0) = 0, \quad x_{ME}(0) = 0, \quad x_B(0) = 0 \qquad (5.3.2)$$

Here r is the rate at which water is given to the system at time t_k.

$(k = 0,1,2,\cdots)$

5.3.1 Analytical Study of The System

To get the approximate concentration profile for water by analytical method, we have considered the following subsystem here.

$$\frac{dx_H}{dt} = -k_1 x_T x_H + k_{-1} x_D x_F - k_2 x_D x_H + k_{-2} x_M x_F - k_3 x_M x_H + k_{-3} x_G x_F$$
$$+k_4 x_F x_{ME} - k_{-4} x_B x_H \qquad t \neq t_k$$

$$x_H(t_k^+) - x_H(t_k^-) = r x_H \qquad t = t_k \qquad (5.3.1.1)$$

Since the system is bounded, $\exists\, C \in \boldsymbol{R}^+$ such that $x_j < C$, (j stands for T, D, M, H, F, G, ME, B).

Also, by Arrhenius Principle k_1, k_{-1}, k_2, k_{-2} are finite quantities. Then for some positive real numbers M and N, it can be written that,

$$\frac{1}{2}M = min\,\{k_{-1} x_D x_F, k_{-2} x_M x_F, k_{-3} x_G x_F, k_4 x_F x_{ME}\}$$

and

$$\frac{1}{2}N = min\,\{k_1 x_T, k_2 x_D, k_3 x_M, k_{-4} x_B\}$$

Then the system (4.2.1.1) becomes

$$\frac{dx_H}{dt} \leq M - Nx_H, \qquad t \neq t_k \qquad (5.3.1.2)$$

$$\Delta x_H = rx_H \qquad t = t_k$$

For maximum rate of change of water, the system is re-written as,

$$\frac{dx_H}{dt} = M - Nx_H, \qquad t \neq t_k \qquad (5.3.1.3)$$

$$\Delta x_H = rx_H \qquad t = t_k$$

Here m, n are some real constants.

Therefore, for a single impulsive cycle $t_k \leq t \leq t_{k+1}$, the solution of the system is represented by -

$$x_H(t_{k+1}^-) = \frac{M}{N}\left[1 - e^{-N(t_{k+1}-t_k)}\right] + x_H(t_k^+)e^{-N(t_{k+1}-t_k)} \qquad (5.3.1.4)$$

The amount of water just before impulse and immediately after impulse are given by $x_H(t_k^-)$ and $x_H(t_k^+)$ respectively.

Hence, we have

$$x_H(t_1^-) = \frac{M}{N}$$

$$x_H(t_1^+) = \frac{M}{N}(1 + r)$$

$$x_H(t_2^-) = \frac{M}{N}(1 + r)e^{-N(t_2-t_1)} + \frac{M}{N}(1 - e^{-N(t_2-t_1)})$$

$$x_H(t_2^+) = \frac{M}{N}(1 + r)^2 e^{-N(t_2-t_1)} + \frac{M}{N}(1 + r)(1 - e^{-N(t_2-t_1)})$$

$$x_H(t_3^-) = \frac{M}{N}[(1+r)^2\, e^{-N(t_3-t_1)} + (1+r)e^{-N(t_3-t_2)}$$

$$-(1+r)e^{-N(t_3-t_1)} + 1 - e^{-N(t_3-t_2)}\,]$$

$$x_H(t_3^+) = \frac{M}{N}\,[(1+r)^3\, e^{-N(t_3-t_1)} + (1+r)^2\, e^{(-N(t_3-t_2))}$$

$$-(1+r)^2\, e^{-N(t_3-t_1)} + (1+r) - (1+r)e^{-N(t_3-t_2)}\,] \qquad (5.3.1.5)$$

and so on.

Hence, we can write the general solution of the subsystem as

$$\begin{aligned} x_H\left(t_p^-\right) = \frac{M}{N}\,\Big[& (1+r)^{p-1}\, e^{-N\left(t_p-t_1\right)} + (1+r)^{p-2}\, e^{-N\left(t_p-t_2\right)} \\ & + (1+r)^{p-3}\, e^{-N\left(t_p-t_3\right)} + \ldots + 1 - (1+r)^{p-2}\, e^{-N\left(t_p-t_1\right)} \\ & - (1-r)^{p-3}\, e^{-N\left(t_p-t_2\right)} \\ & - (1+r)^{p-4}\, e^{-N\left(t_p-t_3\right)} - \ldots - e^{-N\left(t_p-t_{p-1}\right)}\Big] \end{aligned} \qquad (5.3.1.6)$$

5.3.2 For Fixed Time Interval

If water is given to the system in fixed time interval, then $t_n - t_{n-1} = \tau$ is constant. Hence, the general solution is:

$$x_H\left(t_p^-\right) = \frac{M}{N}\,[1 + (1+r)e^{-N\tau}$$

$$+ (1+r)^2\, e^{-2N\tau} + \ldots + (1+r)^{p-1}\, e^{-N(p-1)\tau} - e^{-N\tau}\,\{1$$

$$+ (1+r)e^{-N\tau} + (1+r)^2\, e^{-2N\tau} + \ldots + (1+r)^{p-2}\, e^{-(p-2)N\tau}\,\}]$$

$$= \frac{M}{N} \left[\frac{1-(1+r)^p e^{-Np\tau}}{1-(1+r)e^{-N\tau}} - \frac{e^{-N\tau}\left(1-(1+r)^{p-1} e^{-N(p-1)\tau}\right)}{1-(1+r)e^{-N\tau}}\right]. \quad (5.3.2.1)$$

Taking limit,

$$\lim_{p\to\infty} x_H\left(t_p^-\right) = \frac{M}{N}\left[\frac{1-e^{-N\tau}}{1-(1+r)e^{-N\tau}}\right] \quad (5.3.2.2)$$

This is the long-term maximum value of the water (since the effect of the impulse is to be immediately reduced). To keep this under the threshold $\widehat{x_H}$, we have,

$$\frac{M}{N}\left[\frac{1-e^{-N\tau}}{1-(1+r)e^{-N\tau}}\right] < \widehat{x_H}$$

which implies

$$\tau < \frac{1}{N}\ln\left\{\frac{M-N(1+r)\widehat{x_H}}{M-N\widehat{x_H}}\right\} = \tau_{\max} \text{ (say)}$$

5.4 Numerical Simulation

In this section, we have numerically shown the effect of Methanol to oil molar ratio and also the effect of temperature of the reaction medium to maximize the production of the free fatty acid and consequently the required biodiesel. The rate of reaction depends significantly on the change of temperature of the reaction medium. The effect of changes in the reaction parameters are shown numerically by our model.

Table 5.1 Kinetic parameter set for the reaction system (Diwekar and Benavides (2012))

Reaction rate constants, k_i	Values (unit)
k_1	$.00995\ moles\ L^{-1}min^{-1}$
k_{-1}	$.1219\ moles\ L^{-1}min^{-1}$
k_2	$.03\ moles\ L^{-1}min^{-1}$
k_{-2}	$.0011\ moles\ L^{-1}min^{-1}$
k_3	$1.9514\ moles\ L^{-1}min^{-1}$
k_{-3}	$.1144\ moles\ L^{-1}min^{-1}$
k_4	$.1785\ moles\ L^{-1}min^{-1}$
k_{-4}	$.5744\ moles\ L^{-1}min^{-1}$

In Figure 5.1, we have checked the effect of temperature to the reaction system for the production of Free Fatty Acid (FFA). We have used $ode45$ to vary the temperature and to show which temperature is optimum for FFA production. Here we have assumed the water to oil molar ratio in the system to be fixed at $15 : 1$. It has been found numerically that below $240℃$ the production of FFA is ignorable. It signifies that from $240℃$ the hydrolysis of TG starts and at $343℃$ the rate of reaction of the system increases and gives a constant production of FFA, which is maximum.

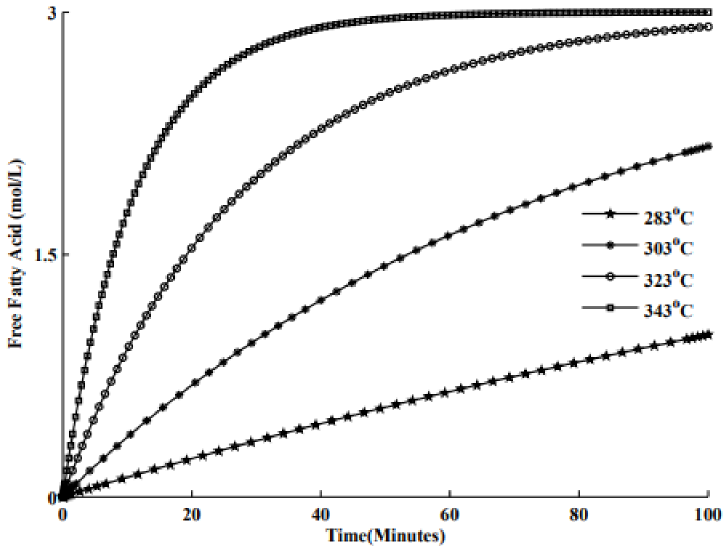

Fig. 5.1: Effect of temperature in production of Free Fatty Acid through hydrolysis of Triglycerides when the water to oil molar ratio is fixed at 15 : 1, using parameter values from Table 5.1.

Figure 5.2 represents the effect of methanol to oil molar ratio on reaction rate for conversion of biodiesel production respectively. We have seen that 3 : 1 methanol to oil molar ratio at fixed temperature 343°C is optimum for biodiesel production in Supercritical method. As for both 3 : 1 and 4 : 1 methanol to oil molar ratios, we can get the equal amount of maximum biodiesel production but for 3 : 1 methanol to oil molar ratio less amount of methanol is required.

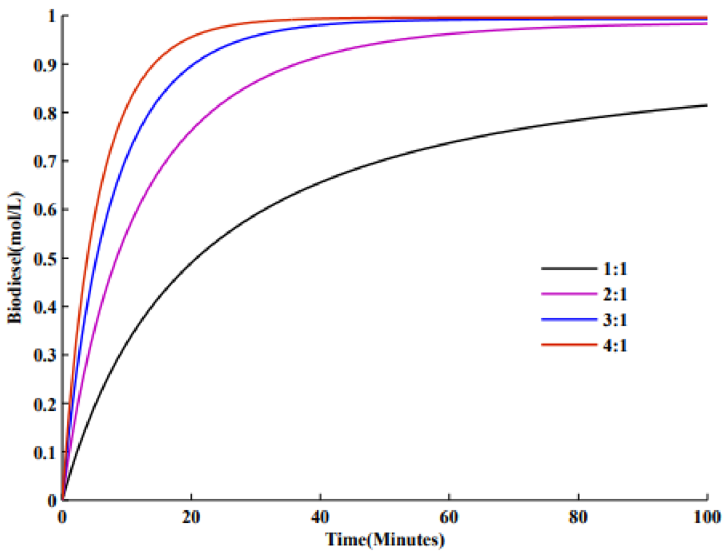

Fig. 5. 2: Concentration of biodiesel as a function of time for different methanol to oil molar ratios with constant temperature 343°C, using parameter values given in Table 5.1.

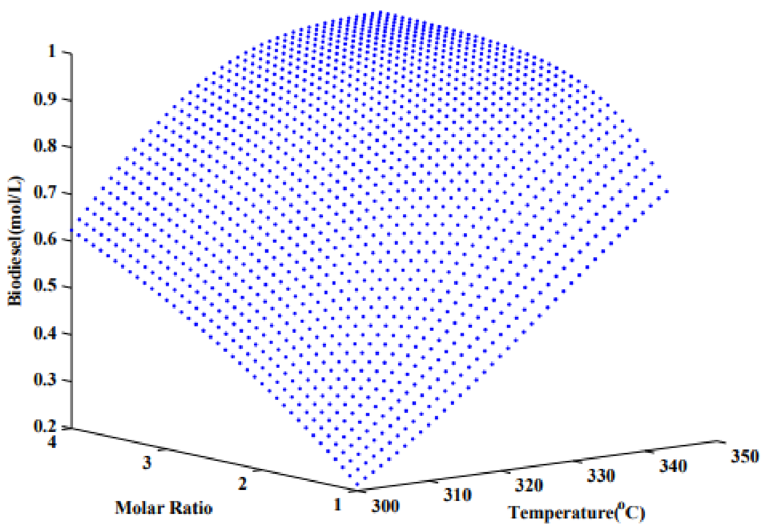

Fig. 5. 3: Concentration of biodiesel when both temperature and methanol to oil molar ratio vary, using parameter values given in Table 5.1.

In figure 5.3, we have shown a mesh plotting in temperature-molar ratio-concentration of biodiesel plane. We have varied both the temperature and methanol to oil molar ratio to get the maximum production of biodiesel. We can clearly state from this figure that with gradual increase of both temperature and methanol to oil molar ratio, the amount of produced biodiesel is also increasing and the maximum production of biodiesel is achieved when methanol to oil molar ratio is 3 ∶ 1 at the temperature of the system 343℃.

5.5 Discussion and Conclusion

In this chapter, we have presented a mathematical model of hydrolysis reaction of Jatropha curcas oil with water and alcoholysis of produced Free Fatty Acid with methanol which results into the production of desired biodiesel ultimately. By numerical simulation concentration of free fatty acid has been calculated in the previous the chapter and concentration of biodiesel has been calculated in this chapter with respect to temperature and methanol to oil molar ratio. We have numerically shown the production of biodiesel from the reaction of free fatty acid, produced by hydrolysis reaction, with methanol. In this process, at 343℃ temperature the rate of reaction of the system increases giving a constant and maximum production of FFA. Here also the effect of methanol to oil molar ratio has been illustrated. By our analytical and numerical findings, we have come to the conclusion that the minimum methanol to oil molar ratio required to achieve constant and maximum production of biodiesel is 3 ∶ 1. Also, for 4 ∶ 1 methanol to oil molar ratio, we can get the same production of biodiesel after same time. But due to the less requirement of methanol and thus to make the process more cost-effective, we have chosen 3 ∶ 1 methanol to oil molar ratio to be the optimum molar ratio. From the above analytical as well as numerical findings and discussion we can conclude that $SC - CO_2$ medium is a good reaction medium as it increases the reaction speed by diminishing the mass transfer resistance of the reactants. There is a certain effect of temperature of the reaction medium and molar ratio of the reactants to produce biodiesel from Jatropha curcas oil. Thus, with all these effects of reaction parameters we can achieve a cost-effective maximum production of the alternative fuel biodiesel.

Chapter 6

Conclusion of The Thesis

In this thesis, we aimed to control pest of Jatropha curcas plant to get healthy plantation as Jatropha is the leading most resource of alternative fuel biodiesel and also to reduce the cost of biodiesel production using non-catalytic method to get a cost-effective constant and maximum production of the fuel which will be beneficial to our society, for both environmentally and economically.

In the first part, to eradicate pests from Jatropha tree, we have used virus as controlling agent. We have studied the proposed system for Holling type I or linear functional response as well as Holling type II or hyperbolic functional response on predator. We have shown the comparison between these two response functions to display the better approach for the pest management. Numerically, we have also examined the effect of virus replication. If the pest becomes dominant in the system, then Jatropha plant will be harmed severely, which will lead to economic loss and consequently production of biodiesel will not be maximum. On the other hand, if the prey density becomes very less or they become extinct, the natural predator will be evanished which may also affect the biological balance of the ecosystem. Thus, it is very important to maintain the biological balance of the ecosystem in such a way so that on one hand crop yield will be maximized and predators also survive. This ecological phenomenon is validated by our findings where we have come to the result that hyperbolic functional response is more effective than that of linear functional response. Because in case of the hyperbolic functional response within 60 days, higher number of infected pests will be saturated and the system becomes stable, whereas for linear functional response it will take 150 days to stabilize the system. Our work reveals that an introduction of natural enemies (predators) with a hyperbolic functional response would be more effective to control pest and maximize healthy plant production. Also, for using virus as controlling agent, we can get rid of the adverse effects of using chemical pesticides which in one way or other harm our mother nature as well as the Jatropha plant. Thus, we have clearly established the measure, applying which the biological balance of the ecosystem can be maintained properly so that predators can survive, environment can be saved from harmful effects, and crop yield will be maximized.

In the second part of our thesis, we have focused on the biodiesel production from Jatropha curcas oil. At first from the hydrolysis reaction of Jatropha curcas oil with water, Free Fatty Acid (FFA) is produced. Then by the alcoholysis of previously produced FFA with methanol the required biodiesel is produced. Here we have taken the $SC - CO_2$ reaction medium to avoid mass transfer resistance of the reactants. By numerical simulation concentration of FFA has been calculated with respect to reaction conditions such as water to oil molar ratio and addition of water to the reaction medium in impulsive way. We have found that constant production of Free Fatty Acid is possible by the hydrolysis of triglycerides (Jatropha curcas oil) and maximum yield of free fatty acid $i.e.$ $3\, mol/L$ is attained when water is added to the system impulsively with 2.5 minutes interval. Also, the optimized water to oil molar ratio to get maximum yield of free fatty acid has been found to be $15 : 1$. We can get the maximum production of free fatty acid for $20 : 1$ water to oil molar ratio also at the same time. But for both $15 : 1$ water to oil molar ratio less amount of water is required. Hence, we have come to the point that we should choose $15 : 1$ water to oil molar ratio. Since there are plenty of sources of water in the world, this hydrolysis process is much cost-effective. For the production of biodiesel from the reaction of free fatty acid with methanol, the effect of methanol to oil molar ratio is significant. By our analytical and numerical findings, we have come to the conclusion that the minimum methanol to oil molar ratio required to achieve constant and maximum production of biodiesel is $3 : 1$. Though we can get the same production of biodiesel after same time also for $4 : 1$ methanol to oil molar ratio, but due to the less requirement of methanol we have chosen $3 : 1$ methanol to oil molar ratio to be the optimum molar ratio. This will make the production cost-effective. In this whole process temperature also plays a vital role. At $240℃$ the reaction starts and at $343℃$ the biodiesel yield is maximum. Therefore, we can conclude that $SC - CO_2$ medium is a good reaction medium as it increases the reaction speed by diminishing the mass transfer resistance of the reactants.

Thus, we have provided pest management measures of Jatropha curcas plant as well as the cost-effective production of biodiesel from Jatropha oil, which was our main focus throughout this work for the societal benefits.

Chapter 7

Future Direction

7.1 Basic Assumptions and Mathematical Model

In chapters 1 and 2, we have shown the effect of virus replication and Holling type I and II functional responses on predators to control the pests that affect the growth of Jatropha plant. We have used biological control as chemical pesticides have adverse effects on plants as well as on the environment. Chemical damage (called phytotoxicity) shows various symptoms including spots, blotches, leaf cupping, yellowing, stunting and also in many cases plant death. On the other hand, diminishing the pest population's size to get healthy growth of the Jatropha plant is of utmost interest. In order to do so we have to limit the pest population's size and hence Allee effects (positive density dependence) may be experienced. Allee effects that result in critical population sizes are referred to as strong Allee effects, while Allee effects causing no critical sizes are referred to as weak Allee effects.

Keeping all these in mind, we have formulated a mathematical model incorporating damage on susceptible pest population and predator population due to chemical pesticides spraying and weak Allee effects on the predator population.

In our mathematical model, the biomass for Jatropha curcas plant is denoted by $j(t)$. $s(t)$ is the susceptible pest population and $p(t)$ is the predator population. Growth of the plant and pests follow the logistic fashion. Here the growth rate of Jatropha plant is denoted by r_1 and k_1 is the carrying capacity. r_2 is the per capita growth rate of the susceptible pests and k_2 is its carrying capacity. The plant resource is consumed by pests at a rate a, which impacts negatively on the growth of the plant biomass. Predators consumes pests at a rate b and it helps prdators in their growth at a rate c. Allee effects play an important role for the growth of the predators. Here weak Allee effect has been considered where α denotes the Allee effect constant. e is the natural mortality rate of the predators. Here we have assumed θ_1 as the damaging coefficients due to the chemical pesticides spraying on the susceptible pests and θ_2 as the damaging coefficients due to the chemical pesticides spraying on the predators.

With the above assumptions, the following mathematical model has been formulated.

$$\frac{dj}{dt} = r_1 j\left(1 - \frac{j}{k_1}\right) - ajs$$

$$\frac{ds}{dt} = r_2 s\left(1 - \frac{s}{k_2}\right) + ajs - bsp - \theta_1 s$$

$$\frac{dp}{dt} = csp\frac{p}{p+\alpha} - ep - \theta_2 p \qquad (7.1.1)$$

where,

$j(0) \geq 0, s(0) \geq 0, p(0) \geq 0.$

All the parameters are assumed to be non-negative.

From the above assumptions and mathematical model, we will observe the effect of chemical pesticide spraying on the growth of Jatropha curcas plant with response to weak Allee effect on predators. This work will help us to focus on more environment friendly control measures of the Jatropha curcas plant diseases from pest attack.

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List of Publications

- **Papers Published**

1. Arunabha Sengupta, Dibyendu Biswas, Ashis Kumar Sarkar. Qualitative Study of Controlling Pest of Jatropha curcas for Linear Functional Response. International Journal of Mathematics and Computer Research, Vol. 11, Issue 10, pp. $3789-3793$, 2023.

2. Arunabha Sengupta, Jahangir Chowdhury, Xianbing Cao, Priti Kumar Roy. Pest Control of Jatropha curcas Plant for Different Response Functions. Mathematical Analysis and Applications in Modeling, Springer Proceedings in Mathematics & Statistics 302, pp. $385-401$, 2020.

3. Arunabha Sengupta, Ashis Kumar Sarkar. A Mathematical Study on the Effect of Molar Ratios of the Reactants for Biodiesel Production in $SC-CO_2$ Medium. International Journal of Mathematics and Computer Research, Vol. 11, Issue 9, pp. $3729-3733$, 2023.

4. Arunabha Sengupta, Jahangir Chowdhury, Dibyendu Biswas, Priti Kumar Roy. Effect of temperature and molar ratio on biodiesel production in supercritical-carbon dioxide medium. Nonlinear Studies, Vol. 26, No. 2, pp. $327-341$, 2019.

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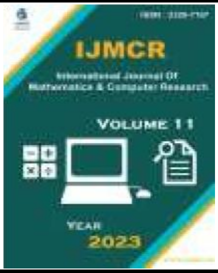

Qualitative Study of Controlling Pest of Jatropha curcas for Linear Functional Response

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ABSTRACT

In today's world, Jatropha curcas plants are a renewable energy feedstock for producing biodiesel to overcome the limitations of natural fuel. The alternative fuel biodiesel can be produced from the Jatropha plant as its seeds contain oil which is one of the important resources for biodiesel. Despite being toxic to many insects and animals, the Jatropha curcas plant is not pest and disease-free. In view of this, our research article presents the formulation and analysis of a mathematical model that describes the Jatropha plantation along with a prediction to control its natural pests by biological pesticides. We assume linear functional response of predators for susceptible pests, and infected pests as infected pests are weaker than susceptible pests and easy to catch. The dynamics of the system around each of the ecologically feasible equilibria are studied. The reduction of disease eradication and coexistence of predator and pest are observed around the predator-free and disease-free equilibrium respectively.

KEYWORDS: Jatropha curcas plant, Biodiesel, Pest control, Stability, Mathematical modeling, Functional response, Biological pesticide

I. INTRODUCTION

Conventional energy resources are very limited and due to excessive use of them, these conventional energy resources will last for maximum next few decades. To fulfill our dependency on fuel resources and maintain daily requirements, the demand for alternative energy sources is thriving. To meet these demands, the production of renewable and sustainable energy sources is greatly required. Biodiesel is one of the most useful alternative fuels which is renewable, clean-burning, and cost-effective [1]. The higher oil content and non-edible nature of the seed have made Jatropha curcus one of the most effective resources for biodiesel [2].

Among many biodiesel-producing resources like Soybean oil, Mustard oil, Palm oil, etc. Jatropha oil is the most promising resource because it produces the purest quality of biodiesel. Jatropha plants are generally affected by pests. This affects the growth of the plant as well as the oil production. How to control pests for this plant is a global problem in agricultural ecosystem management [3]. Hence controlling these pests for the healthy growth of the plant and for the improvement of oil productivity is urgently required. Many researchers have formulated mathematical models for controlling pests and they have studied the different perspectives of pest management tools with probable results by analyzing the system within the mathematical illustration. Chemical pesticides affect our health and plant growth and they also cause environmental pollution, and health problems and affect economic crop production [4]. This leads us to find out biological control methods for plant pests. Besides that, the most effective measures in pest management are determined by the ecology of a pest. Thus, the concept of Integrated Pest Management (IPM) [5] is being generated. Its application has been increased in the field by the farmers recently.

IPM reduces reliance on pesticides by emphasizing biological control methods. Bio-pesticides, components of an integrated approach, can play an effective role in pest control [6]. Potentially, the use of viruses is one of the most significant biological methods for pest control. In American and European countries, practical evidences of where the virus is used against insect pests are being noticed [7]. The

Pest Control of Jatropha curcas Plant for Different Response Functions

Arunabha Sengupta, J. Chowdhury, Xianbing Cao and Priti Kumar Roy

Abstract Nowadays Jatropha curcas plants are being considered as a renewable energy feedstock for the production of biodiesel to overcome the crisis of natural fuel. The seeds of this plant contain oil which is one of the significant resources for alternative fuel production i.e. biodiesel. Though Jatropha curcas plant is proven to be toxic to many insects and animals, it is not pest and disease resistant. On this regard our research article presents formulation and analysis of a mathematical model for Jatropha plantation with a view to control its natural pests through application of biological pesticide. We assume linear and hyperbolic functional responses of predator for susceptible pest, where for infected pest the functional response is linear, as infected pests are weaker than susceptible pest and easy to catch. We study the dynamics of the system around each of the ecological feasible equilibrium. The reduction of disease eradication and predator-pest coexistence are observed around the predator free and disease free equilibrium respectively.

Keywords *Jatropha curcas* plant · Biodiesel · Pest control · Stability · Mathematical modeling · Functional response · Biological pesticide

1 Introduction

In current global scenario the demand of alternative energy sources are highly thriving to overcome the crisis of conventional energy sources. As a result production of renewable energy sources are truly required. Biodiesel is one of the most useful

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A Mathematical Study on the Effect of Molar Ratios of the Reactants for Biodiesel Production in SC-CO_2 Medium

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ABSTRACT
The present global situation is so alarming that the conventional energy resources are decaying day by day. This adverse situation encourages us to introduce unconventional and sustainable energy resources like biodiesel. The main source of biodiesel is the non-edible vegetable oil (Jatropha curcas oil) and it is produced by chemical catalytic method. But recently supercritical method has also been proposed as an alternative cost-effective method for its production. A good quality of biodiesel can be produced in a Supercritical-Carbon dioxide medium. The productivity of biodiesel preparation through supercritical method depends on molar ratio of the reactants (water and methanol). In this research article, a set of nonlinear differential equations has been formulated based on concentrations of Triglyceride, Diglyceride, Monoglyceride, Methanol, Free fatty acid, Water, Glycerol and Biodiesel. Our study is based on the effect of the molar ratios of the reactants and how we can get a cost-effective production of biodiesel. The validity of our model is attained by experimental results. The analytical results are also verified by our numerical findings.

KEYWORDS: Jatropha curcas oil, Biodiesel, Supercritical, Molar ratio, Optimization, Cost-effectiveness.

I. INTRODUCTION

Unlimited use of fossil fuels causes the reduction of petroleum reserves. It has already been predicted that we will surely run out of fossil fuels in this century. This adverse circumstance brings significant attention to introduce and develop new alternate plant-based fuels. Also increasing environmental pollution is another threat to the world. To overcome these threats biofuel is of utmost importance because it is environmentally friendly and secures future energy supplies. As a consequence, the production and usage of biodiesel is being tremendously researched worldwide. We can derive biodiesel from vegetable oils like Jatropha curcas oil that compromises triglycerides with methanol in various processes. Biodiesel is a renewable, non-toxic, biodegradable energy source. This clean renewable fuel is superior to diesel oil in terms of sulphur and aromatic content.

Lascaray [1, 2] showed that hydrolysis is mainly a homogeneous reaction occurring in the oil phase and only a minor portion of the reaction happens at the oil and water interface during the induction period. Hydrolysis of triglyceride (TG) from fats and oils to glycerol and free fatty acids (FFA) is an important reaction for the oleochemical industry. Hydrolysis involves three stepwise reversible reactions. Triglyceride (TG) is first hydrolyzed to diglyceride (DG) and then to monoglyceride (MG) and glycerol respectively. At each step, we get one molecule of free fatty acid (FFA) which later reacts with methanol and produce biodiesel. The hydrolysis reaction rate is initially low and then gradually increases up to its normal level. This is due to an induction period that obscures the kinetics of the hydrolysis of oil [3].

Many research articles are published on biodiesel production through different processes like transesterification with chemical catalysts [4, 5], biochemical catalysts, SCMTR method [3, 4, 5, 6, 7], etc. The process of producing biodiesel from vegetable oils and animal fats with the aid of alcohols is called Transesterification. Alkaline catalysts processes form soap as a side product and reduce the production of biodiesel as Jatropha oil contains free fatty acids (FFAs) and water. Therefore, there are complex and energy-consuming separation and purification steps in the homogeneous chemical catalyst processes. It is observed that we also face difficulties in recovering glycerol due to the solubility of excessive methanol and catalyst [7].

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Effect of temperature and molar ratio on biodiesel production in supercritical-carbon dioxide medium

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Abstract. In current global scenario, the conventional energy resources are at great risk. This leads us to introduce the use of unconventional and renewable energy resources like biodiesel. Generally biodiesel is produced from non-edible vegetable oil (*Jatropha curcas* oil) by chemical catalytic method. Nowadays supercritical method is proposed as an alternative cost-effective method to produce biodiesel. In a Supercritical-Carbon dioxide medium good quality of biodiesel can be produced. The productivity of biodiesel preparation through supercritical method mainly depends on reaction temperature and molar ratio of the reactants. In this research article, a set of nonlinear differential equations has been formulated based on concentrations of Triglyceride, Diglyceride, Monoglyceride, Methanol, Free fatty acid, Water, Glycerol and Biodiesel. Our study is aimed on how we can achieve cost-effective yield of Biodiesel depending on optimization of reaction temperature and the molar ratios of the reactants (water and methanol) using the control theoretic strategy. The validity of our model is attained by experimental results. The analytical results are also verified by our numerical findings.

1 Introduction

Reduction of petroleum reserves due to the unlimited use of fossil fuels and increasing environmental pollution that causes climate change are two great threats in today's global scenario. This adverse circumstance brings significant attention to introduce and develop new alternate plant-based fuels, plant oils, and fats as promising renewable biofuel sources of energy that is environmentally friendly and secure the future energy supplies [1]. As a consequence, biodiesel has been tremendously researched

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