# Contemporary Indian Foreign Policy

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CHAKALI BRAMHAYYA

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# Contents

CHAPTER 6

# A Green and Sustainable Biocatalytic Routes to Prepare Biobased Polyols as a Precursor For Polyurethanes as Compared to Existing Biobased Polyol Technology

**Bhaskar Sharma*, Hema Tandon, Pathik Maji** and **Arti Shrivastava**

*Department of Chemistry, Guru Ghasidas Vishwavidyalaya, Bilaspur (Chhattsgarh) 495009, India*

**Abstract:** There has been great interest in the replacement of petroleum-based polyols with biobased polyols in polyurethane applications. However, current products mainly triglyceride-based polyols have many drawbacks, and also do not have the structural efficiency and physical performance characteristics that restrict them to limited applications.

To minimize all these limitations, the synthesis of low molecular weight liquid polyols can be performed *via* a robust, simple, environmentally friendly, and solvent-free 'biocatalytic route'. In contrast to chemical methods, enzyme-catalyzed reactions proceed with high enantio- and regioselectivity, under mild conditions, avoiding protection deprotection steps, providing an attractive alternative to conventional chemical methods. Bio-renewable, non-toxic and low-cost monomers, such as 2,5 dihydroxymethyl furan, 1,4 butanediol, glycerol, diglycerol, isosorbide, D-mannitol, D-sorbitol, citric acid, maleic acid, fumaric acid, succinic acid, glutaric acid, adipic acid, sebacic acid and many more can be employed in preparing biobased polyol prepolymers *via* enzymatic catalysis.

**Keywords:** Biobased polyols, Enzyme catalysis, Polyurethanes.

## INTRODUCTION

Polyurethanes have gained too much attention, and they have been referred to as "Jack of all trades" because of their tremendous use in many industries like automotive, furniture, constructions, footwear, and thermal insulations, *etc.* In general, polyurethanes are obtained by the reaction of polyisocyanates with

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CHAPTER 7

# Polymers Used as Catalyst

**Arti Srivastava***, **Bhaskar Sharma** and **Pratibha Mandal**

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**Abstract:** In general, a catalyst is used to enhance the reaction and to complete the reaction quickly or accelerate the reaction involving reactants and catalysts. In the catalysis process, only the chemical structure of reactant changes with time, but the structure of the catalyst remains unaffected throughout the course of the reaction. The varieties of chemicals that can be used as a catalyst in numerous chemical reactions are metals, acids, bases, organic compounds, inorganic complexes, enzymes and polymers. Some specific polymers have the ability to catalyse reactions with the formation of carbon-carbon and carbon-non carbon linkages. Polyvinyl pyridine and sulfonated polystyrene are very useful and simple polymers that can act as catalysts. The catalytic activity of polymers is pronounced due to modification in polymer chains. Further, polymers may also be used as a support for another catalyst. Polymer catalysis can be illustrated with soluble linear polymers, ion exchange resins, polymer-supported phase transfer catalysts, palladium catalysts on polymer supports, *etc.* The brief review of each is explained by citing important examples along with their basic principles.

## INTRODUCTION

The function of a catalyst is, to alter the rate of the reaction in order to form the product at a faster rate, and in the end, the catalyst will regenerate without any chemical changes. The catalysed reactions have a lower activation energy than uncatalysed reactions because catalyst abridged the potential energy barrier of each step of the main reaction. In this way, the catalyst provides the reduced height of the energy barrier of the split step. Eventually, the reactant can be converted into the final product with decreased Gibbs free energy without changing the overall standard Gibbs free energy of the reaction. The initial and final states of the reaction energetically remain the same. The catalytic processes are classified mainly into two types; (i) Heterogeneous and (ii) Homogeneous catalysis. In heterogeneous catalysis, the catalyst and reactants are in different phases. A typical example involves a solid catalyst with reactants as either in liquids or gases. In homogeneous catalysis, the catalyst remains in the same phase of reactants.

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*Chapter 11*

# PYRANO[2,3-C]PYRAZOLE DERIVATIVES: SYNTHESIS AND APPLICATIONS

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## ABSTRACT

Polyfunctionalized heterocyclic scaffolds have been extremely emphasized in modern organic syntheses due to their improved functional diversity which provides superior possibilities for changeable pharmacophoric groups which could react with a broad variety of receptors. In this connection, pyran-fused poly-heterocyclic scaffolds are increasingly becoming fruitful area of the study for their numerous biological activities. Among such fused hetero-polycyclic molecules, the pyrano[2,3-*c*]pyrazoles have provided a variety of scaffolds, displaying analgesic, anticonvulsant, anti-inflammatory, anti-platelet, antimicrobial, Chk1 inhibitors, anticancer, vasodilator, molluscidal and antifungal properties. Furthermore, pyranopyrazoles were found to be antioxidants and effective inhibitors to steel corrosion for lubricant oil.

Pyrano[2,3-*c*]pyrazoles are considered to be the easiest structures to obtain in association to other pyranopyrazoles from the synthetic point of view. This convenience

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CHAPTER 4

# Ball Milling: A Green Tool in Synthetic Organic Chemistry

**Subhash Banerjee*, Geetika Patel** and **Medha Kiran Patel**

*Department of Chemistry, Guru Ghasidas Vishwavidyalaya (A Central University), Bilaspur 495009 (Chhattisgarh), India*

**Abstract:** ***Background:*** Activation of covalent bonds for the initiation of chemical reactions can be achieved by all kinds of energy including light, thermal heating, microwave heating, electrical, sonochemical and mechanical energy. Among these, ball milling is an attractive alternative source of energy for the activation of bonds leading to chemical reactions due to its simplicity, ease of purification of products, mild reaction conditions and greenness of the process.

***Methods:*** Mechano-chemical reaction is defined as "a chemical reaction that is induced by the direct absorption of mechanical energy." Simply, mechanical energy can be generated by grinding using a mortar and a pestle and the process of milling is carried out in ball mills. The process of milling is more reproducible due to the regulation of parameters like time and energy entry.

***Results:*** The ball milling is mainly applicable in the industry for particle refinement processes, disagglomeration, the cracking of bacteria, *etc.* However, recently, ball milling has attracted considerable attention in organic synthesis due to its operational simplicity, economy, environment friendliness, and its potential to produce very good yields of products, and as a consequence, several research articles, review papers and book chapters have been published in recent time. The literature studies revealed that various carbon-carbon, carbon-heteroatom bond formation, condensation reactions, coupling reactions and oxidation-reduction reactions have been performed in a ball mill under mild and environmental-friendly reaction conditions.

***Conclusion:*** The aim of this review is to highlight the recent breakthrough of ball milling in organic transformation leading to the synthesis of bioactive molecules in the context of *Green Chemistry*.

**Keywords:** Ball Milling, Clean Organic Synthesis, Green Synthetic Tools, Mechanochemical Reaction, Sustainable Alternative Energy Source.

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# Catalysis: Current and Future Developments

*Volume 1*

## *Fundamentals and Prospects of Catalysis*

**Edited by**

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CHAPTER 2

# Design and Development of Bimetallic Enantioselective Salen Co Catalysts for the Hydrolytic Kinetic Resolution of Terminal Epoxides

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**Abstract:** The hydrolytic kinetic resolution of terminal epoxides catalyzed by the monometallic chiral salen Co complex follows the cooperative bimetallic mechanism and second order kinetic dependency on the catalyst. In this mechanism, one metal works as an active Lewis acid center for preferential activation of one enantiomer from a racemic substrate and the second metal center stimulates the incoming nucleophile. Mechanistically, rational design and development of bi- and multimetallic chiral complex centers within the sterically, electronically, and co-ordinatively accessible framework of chiral salen ligand provides improved activity and enantioselectivity relative to their corresponding monometallic catalysts. This chapter provides a survey of bimetallic chiral salen Co complexes used in the hydrolytic kinetic resolution of terminal epoxides to procure valuable chiral intermediates, useful for academic interest and in industrial applications.

**Keywords:** Asymmetric catalysis, Chiral salen Co complex, Kinetic resolutions, Terminal epoxides.

## BACKGROUND AND MOTIVATION

Asymmetric synthesis of chiral compounds, using enantioselective catalysts, plays a crucial role in chemical and pharmaceutical sciences [1]. The industrial need and great academic interest of enantiomerically pure (chiral) compounds in drug

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Chapter 26

# Electrochemical biosensors for monitoring of bioorganic and inorganic chemical pollutants in biological and environmental matrices

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## 26.1 Introduction

Pure water and air are the two basics, important, and valuable needs for human health and welfare, so the safety and quality of air and drinking water is vital to public health and the quality of life in any community or country. In the present era, the main causes of environmental pollution are organic and inorganic pollutants areas that are fatal for humans as well as for aquatic life. Pesticides and herbicides industries and chemical laboratories are the main sources for organic pollutants and among them, azo dyes, aromatic nitro, and phenolic compounds and their derivatives have been considered as the main organic pollutants and their continuous release may be threatening to the environment and human health (Saxena & Bharagava, 2020). For example, tetrabromobisphenol A is extensively used in brominated flame retardant but has a major impact on reproductive toxicities, immunotoxicity, and neurobehavioral disorders (Covaci et al., 2009). Azo dyes have also a very adverse effect on human health, for example, tartrazine and sunset yellow are the two main azo dyes that have been frequently used in textile products and foodstuffs, the excessive intake and long-term exposure of these dyes can cause DNA damage, allergies, and cancer disease. Apart from organic and inorganic, they have further been categorized into primary and secondary pollutants, in general, primary pollutants have detrimental impact in the form in which they are exposed into the environment and secondary pollutants, which are formed due to the chemical process occurring in the environment and they are known to be a less harmful precursor (Petrie, Barden, & Kasprzyk-Hordern, 2015; Rasheed, Bilal, Nabeel, Adeel, & Iqbal, 2019).

Most of the inorganic pollutants responsible for the contamination of water and air are mainly generated from natural phenomena such as volcanic eruption and anthropogenic activities, for example, chemical waste from industries, pesticides, fertilizer, sewage, and mining (Borah, Kumar, & Devi, 2020). The inorganic pollutants consist of different mineral acids, numerous inorganic metals (Cd, Pb, Hg, Cr, Al, As, etc.), cyanides, fluorides, nitrates, nitrites, organic and inorganic metal complexes, etc. In comparison to organic pollutants, inorganic pollutants are nonbiodegradable and cannot be detached from the environment easily. The increase of the ions of the heavy metals has an adverse effect on the aquatic organism of the earth system as they cause harmful health impacts on the kidney, liver, bones, skin, and other body systems such as nervous, gastrointestinal, circulatory, etc. (Gadd, 2010). The inorganic pollutants which are introduced into the environment come as a result of the ignition of fossil fuels are carbon monoxide, carbon dioxide, heavy metals, nitrogen, and particulates matter. Burning of fossil fuel, mining, fertilizers, industrial waste, and municipal waste is the main source of heavy metals and metalloids, which are known as the key inorganic pollutants. Heavy metals, for example, arsenic, mercury, thallium, and amalgams are highly toxic in nature as well as nonbiodegradable

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# $Zn^{2+}$ and $HPO_4$ selective arrest and bail to a trimethylbenzene -naphthalene anchored schiff base as molecular switch

**Jnana Ranjan Sahu[a], Tejaswini Sahoo [a], Rojalin Sahu[*a],Niraj Kumari[b*]**

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**Abstract-** A trimethylbenzene-naphthalene anchored Schiff base (R1) showed $Zn^{2+}$ selective conformational arrest by inhibition of its C=N isomerization leading to its fluorescent switching. The receptor is bailed by $HPO_4^{2-}$ from $Zn^{2+}$ arrest leading to its switching 'off'. This conformational arrest and bail of R1 is extremely explicit as no other ion pairs were able to show the same activity. The detection limit of the R1 for $Zn^{2+}$ is 2,47 x$10^{-7}$ M. while for $HPO_4^{2-}$ is found to be 2.27 x $10^{-6}$. The mechanistic facts for 'on-off' switching of R1 by the ion- pairs have been investigated through various spectroscopic studies .The 'on-off' switching of R1 by inputs $Zn^{2+}$ and $HPO_4^{2-}$ led it to imitate with INHIBIT logic gate.

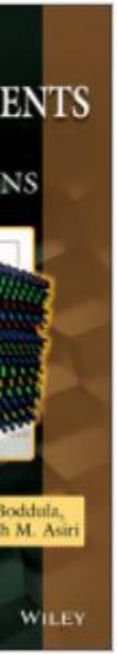
***Keywords*—Schiff base, receptor, molecular switch, logic gate.**

## Introduction

The design and synthesis of artificial new fluorescent receptors for the highly selective recognition of analyte is an eye-catching area for research in supramolecular chemistry because of their broad applications in environmental, chemical, biological, industrial and agricultural, process.[1] Zinc(II) is the second most abundant trace metal ion after iron in the human body. Biological processes, such as gene expression, apoptosis, metalloenzymes regulation and neurotransmission is significantly controlled by zinc(II) ion.[2] Severe neurological diseases, including Alzheimer's, ischemia and epilepsy are associated with the disorder of the $Zn^{2+}$ metabolism. In addition, increased levels of $Zn^{2+}$ ions in water escort to environmental problems, viz., suppressed soil microbial activity causing phytotoxic effects, creating water smelly and dirty.[3] Due to the low cost, faster response time, and low detection limit with high selectivity and sensitivity, fluorescent chemosensors has recently gained considerable interest. Therefore, the design and development of efficient fluorescent chemosensors selective to $Zn^{2+}$ are of considerable interest. Herein, we report the synthesis and sensing behavior of R1 by using various spectroscopic tools. Moreover combination of $Zn^{2+}$ and $HPO_4^{2-}$ as inputs, receptor 1 obeys the truth table of INH logic function for output. Hence receptor 1 possesses the ability to work as a molecular switch for the simplistic sensing of $Zn^{2+}$ and $HPO_4^{2-}$ through changes in its fluorescence intensity. This sensing process is also exhibited in a human cervical cancer cell lines (SiHa cells).

## Materials and methods

The reagents and solvents were obtained from commercial sources. Solvents were dried and distilled prior to their uses. Elemental analyses for C, H, and N were carried on a CE-440 Elemental




# 2D Monoelements: Properties and Applications

Inamuddin Inamuddin (Editor), Rajender Boddula (Editor), Mohd Imran Ahamed (Editor), Abdullah M. Asiri (Editor)

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## DESCRIPTION

*2D Monoelements: Properties and Applications* explores the challenges, research progress and future developments of the basic idea of two-dimensional monoelements, classifications, and application in field-effect transistors for sensing and biosensing.

The thematic topics include investigations such as:

- Recent advances in phosphorene
- The diverse properties of two-dimensional antimonene, of graphene and its derivatives
- The molecular docking simulation study used to analyze the binding mechanisms of graphene oxide as a cancer drug carrier

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# Dye Sensitized Solar Cells- Approach to Clean Energy

**Mridula Tripathi[1*] Arti Srivastava[3], Priyanka Chawla[2] and Abha Tripathi[4]**

## Introduction

Among all the available renewable energy sources like wind, tide, biomass, solar energy is considered to be most promising as it pro clean and abundant energy. To convert solar energy into electrical e solar cells devices are being used. Nowadays scientists all over the

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# Three Major dimensions of life : Environment, Agriculture and Health


**Editors :**

**Hemlata Pant , A. R. Siddiqui, Neetu Mishra , Manoj Kumar Singh, Jyoti Verma, Sandeep Kushwaha, Shishu Pal Singh, Piyush Raman Pandey**

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*Three Major dimensions of life : Environment, Agriculture and Health*
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# DETERMINATION OF ANTIOXIDANT ACTIVITY OF FLOWERS OF CASSIA GLAUCA

**Mridula Tripathi[1*], Arti Srivastava[2], Abha Tripathi[3] and Priyanka Chawla[1]**
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## Introduction

The free radicals that are produced during the normal metabolic activities in our body are responsible for some of the major diseases such as heart diseases, gout, diabetes and most recently cancer. Various studies have also shown that free radicals are also responsible for cellular necrosis[1]. Therefore reduction of these free radicals in our body is very important. Nature provides us the solution as it is an excellent store house of remedies. Natural antioxidants present in plants have the potential to scavenge free radicals present in our body[2]. An antioxidant is a molecule capable of slowing or preventing the oxidation of other molecules. Some of the common free radicals include reactive oxygen free radical species, reactive hydroxyl free radicals, the superoxide anion radical, hydrogen peroxide and peroxyl which generates metabolic products that attack lipids in the cell membranes or DNA[3].

Various synthetic antioxidants are also available like BHT (butylated hydroxy toluene), BHA (butylated hydroxy anisole) and tertiary butylated hydroquinones but these are suspected to cause various adverse side effects in body. Hence strong restrictions have been placed on their application and there is a trend to substitute them with naturally occurring antioxidants. Several studies have revealed that phenols mainly type of flavanoids, from some medicinal plants are safe and bioactive, and have antioxidant properties and exert anticarcinogenic, antimutagenic, antibacterial and anti inflammatory effects. Therefore in current years attention have been focused on such plants with antioxidant ability that may be used for human health[4].

India has rich wealth of medicinal plants and most of people still rely on traditional medicines for the treatment of common illness. *Cassia glauca* flowers are traditionally claimed for treatment of diabetes. This plant is also a good pollution tolerant and reduces chemical pollutants from the atmosphere[5].

Thus in the present research paper study was undertaken to determine the in vitro antioxidant activity of methanolic extract of flowers of *Cassia glauca* by DPPH method, reducing power method and nitrogen oxide scavenging method.

## Material and Methods

The flowers of *Cassia glauca* was collected from the local area. The flowers of *Cassia glauca* was dried crushed and was mixed into 500 ml of methanol extract was prepared using steam distillation method.

### Determination of Antioxidant Activity

The antioxidant activity was evaluated by the following methods.

### Free radical scavenging activity (DPPH* method):

The hydrogen atom or electron donating ability of the compounds and standard - BHT was determined from bleaching of purple colored methanol solution of DPPH*. This spectrophotometric assay uses the stable radical DPPH* as a reagent. The diluted working solutions of essential oils of both plants were prepared in methanol (0.062, 0.25, 0.5, 1 and 2 mg/ml).

Different concentrations of methanloic and aqueous stock solutions of beetroot were taken in each test tube and volume was made up to 2ml. Then 2ml of DPPH* solution was added in each test tube and these solutions were kept in dark for thirty minutes. DPPH* was prepared at a concentration of 0.002%. The same procedure was followed for BHT as well. All the samples were tested in triplicate. Later optical density was recorded at 517nm using UV- visible spectrophotometer. Methanol with DPPH* was used as a

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# Three Major dimensions of life : Environment, Agriculture and Health


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# SYNTHESIS AND CHARACTERIZATION OF CROSS-LINKED GRAFT COPOLYMER BASED ON CARRAGEENAN AND ACRYLAMIDE USING REDOX SYSTEM

**Arti Srivastava[1*], Rajesh Kumar[1], Mridula Tripathi[2] and Savitri Dewangan[3]**

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**Abstract**

In this research article, we have synthesizedcrosslinked graft copolymer via free radical graft copolymerization of acrylamide (AAm) onto carrageenan polymeric backbone and crosslinking occurred by using methylenebis acylamide (MBA) crosslinker. The polymerization reaction was carried out by potassium bromate and thiourea redox system in an aqueous and in nitrogen atmosphere. Infrared spectroscopy were carried out to confirm the formation of cross-linked graft copolymer between carrageenan, acrylamide and methylene bisacrylamide. Swelling ratio of the synthesized sample has also been determined.

**Introduction**

The growth of polymer science has led to the development of new materials in direct competition with natural materials, many of which have been in use since earliest times. This has caused researchers to look more critically at both natural and synthetic macromolecules in order to learn more about their underlying structures and their relation to the properties exhibited by the macromolecules. In this regard, chemical modifications have been devised to impart certain desirable properties of both natural and synthetic macromolecules, and their applications have become an integral part of such chemical modifications such as replacement transparency, good adhesion, easy handling, oxygen permeability, control of drug dosage. Various chemical modifications (e.g. change of functionality, oxidative degradation, inter- and intra-molecular gelatin, graft copolymerization), have been practiced to add improved properties to the base polymers. However, among all these methods, modification of polymers via graft copolymerization has been the subject of much interest and has made paramount contribution toward improved industrial and biomedical applications.Well-defined graft copolymers are most frequently prepared by either a "grafting through" or a "grafting from" controlled polymerization process. However the development of "click" chemistry has led to a third approach based on site specific "grafting to" chemistry [1-10]. The biomaterial is generally used to recognize materials for biomedical application. Hydrogels have been largely used in medicine, pharmacy, and life science. Their morphology and physic-chemical properties make them suitable for several applications in particular as drug controlled release system and tissue engineering. Several polysaccharides have been utilized as materials for hydrogel production. Their chemical structure can be easily modified to introduce new biological properties. We have chosen carrageenan as biomaterial and modified its degradable property with the help of vinyl monomer and make it useful in the form of hydrogel using MBA crosslinker.

➢ **Characteristics features of Carrageenan**

Carrageenan is natural polymer obtained from certain species of the red seaweed, class *Rhodophycea. The main* sources for carrageenan are the *Chondrus Crispus, Eucheuma Cottonii* and *Eucheuma Spinosum* species. Commercial carrageenan are available as stable sodium, potassium, and calcium salts or, most generally, as a mixture of these. Carrageenan can be produced via a variety of process/ techniques; alcohol extraction, potassium chloride gel press or extracted with various alkali.

Carrageenan has unique properties, which cannot be replaced by other food grade, safe and non-toxic materials. Carrageenan are far more widely used than agar as emulsifiers/stabilizers in numerous foods, especially milk based products. There are mainly three

MATERIALS SCIENCE AND TECHNOLOGIES

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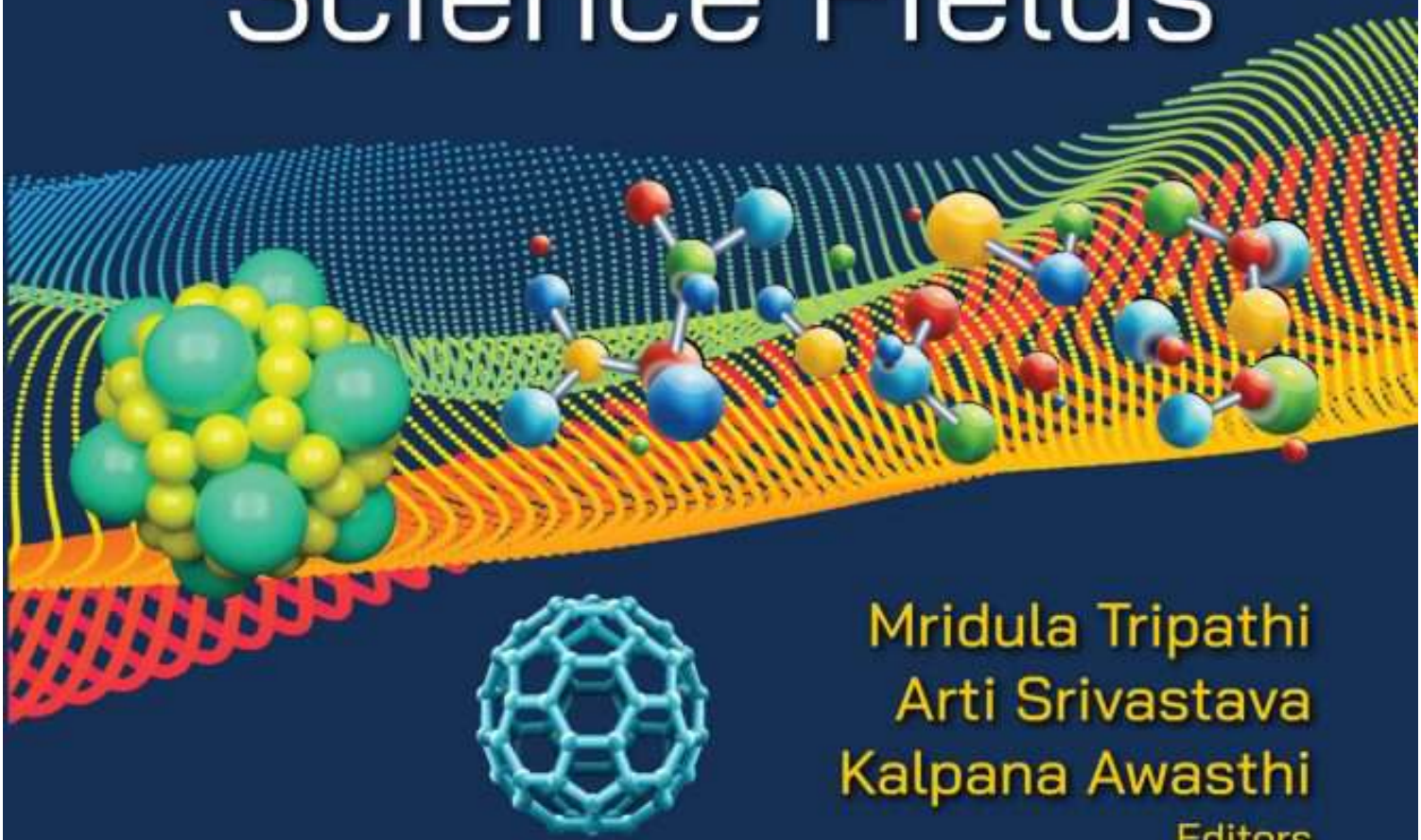

Mridula Tripathi
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# Role of phytopesticides in sustainable agriculture

15

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## 1. Introduction

According to the US Environmental Protection Agency (EPA, 2003), "Biopesticides are the certain types of pesticides derived from natural materials such as animals, plants, bacteria, and certain minerals." Biopesticides are derived from the plants' secondary metabolites, microorganisms, and insects. Substances from plants and animals have been used to manage diseases in crops, animals, and humans as well (Kumari et al., 2014). In the field of agriculture, there are various problems of pests such as insects, fungi, bacteria, and weeds from the ancient period resulting in decrease in yield and productivity of crops. Use of plant-based compounds was overtaken by the use of synthetic chemicals due to their efficacy, reliability, and quick knockdown effect with low side effect. However, synthetic pesticides have become health hazards for humans and environment due to their toxicity and various types of pollution (Halimatunsadiah et al., 2016). Biopesticides are potential alternatives to synthetic pesticides. Sources of biopesticides are readily available with the recycled material, are easily biodegradable, do not cause any kind of pollution, exhibit various modes of action, are less expensive, and have low toxicity to humans and environment. *Emblica officinalis*, *Allium sativum*, *Artemisia absinthium*, and *Citrullus colocynthis* are known sources of botanical pesticides. The microbial species of *Trichoderma*, *Bacillus*, *Pseudomonas*, and *Beauveria* have been commercialized as antimicrobic pesticides (Ndakidemi et al., 2016). Biopesticides are, however, facing with great challenges of formation, formulation, registration, commercialization in market, and most important acceptance and adoption.

Use of synthetic pesticides in agriculture may result in several adverse effects on environment including various kinds of pollution. Biopesticides have immense scope in the sustainable agriculture. In India, biopesticides cover only 2.91% of the overall pesticide market, and it is expected to exhibit an annual growth rate of about 2.4% in coming years (Gasic and Tanovic, 2013).

The use of synthetic fungicides in agriculture is a relatively very recent phenomenon, and most of the developments have taken place during the past 80 years. This has been the best way of fungal disease control in the world during the past. It is playing an

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Charu Arora

# A review on the fatal impact of pesticide toxicity on environment and human health

16

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## 1. Introduction

Many challenges confront humans to protect their crops since agriculture establishment during New Stone Age, which occurred between 7000 and 10,000 such as insects, plant diseases, weeds, and destructive animals. A wide scope of organic and nonorganic substances got from animals, plants, minerals, and microorganisms has been reported to be effective for pest control. Plant extracts (the natural pesticides) have a longer history than the other types of pesticides; the earliest agricultural natural pesticide was the nicotine which was used in the 17th century to control plum beetle. Due to the maturing chemical industry by the mid-20th century, affordable and operative synthetic pesticides were manufactured (Ujváry, 2001). In 1935, the usage of synthetic pesticides started worldwide and diffused after World War II. Pesticides were set to augment crop yields by the year of 1950, far beyond levels before World War II (Nazir et al., 2007).

According to the World Health Organization (WHO) and Food and Agricultural Organization (FAO), pesticide definition is an item or mixture of items intended to kill, repel, prevent, or lessen any pest including insects, fungi, microorganisms such as bacteria and viruses, nematodes, mice, snails and slugs, unwanted plants (weeds), birds and animals during production stages and storage, transportation, distribution, and elaboration of food and agricultural products or animal foods. Most pesticides are broad-spectrum and can kill all insects in particular area and may kill other animals and birds. Every pesticide-formulated product contains active and inert components. Active ingredients, viz., organophosphate (OP), carbamate, organochlorine, pyrethroid, and so on, are the chemical part in the pesticide that affects the target pest. While inert ingredients are inactive components of a pesticide formulation, viz., emulsifiers, solvents, carriers, aerosol propellants, fragrances, and dyes, they are

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Chapter 14

# Dye Removal From Waste Water Using Metal Organic Frameworks

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## 1 Introduction

Water is used for a number of domestic as well as industrial requirements and it plays an important and essential role in our ecosystem. Unfortunately natural resources of water are being polluted the most and the reason behind this is rapid industrialization, civilization, increased population of human beings, increased living standard and unskilled utilization of natural water resources (Bhatnagar et al., 2015; Bulgariu et al., 2019; De Gisi et al., 2016). Huge quantity of waste water containing pollutants is produced after consumption of fresh water in agricultural, industrial and domestic sectors (Anastopoulos et al., 2017). One of the major water pollutants is organic dyes used in various industries, namely, plastic, textile, paper, pulp, pigment, etc (Bulgariu et al., 2019). These industries discharge dye containing effluents to the water bodies and these effluents deteriorate the quality and quantity of water which makes it unsafe for further use (Gupta et al., 2015). Dyes are quite stable and difficult to be biodegraded due to highly complex structure (Gupta and Suhas, 2009).

Chromophores and auxochromes are main key components of a dye. Chromophores produce the color while auxochromes supplement for the chromophore and assist the molecule dissolve in water and provide enhanced affinity to attach with the fibers (Gupta and Suhas, 2009; Benkhaya et al., 2017). Natural dyes are derived from the natural sources. These can be applied on materials including fiber with the help of mordants which have an affinity for both the coloring matter and the material. Synthetic dyes are extensively used in various industries (Hunger, 2003). Dyes can be classified in several classification

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*Chapter 2*

# PHENOLIC CONTENT AND ANTIOXIDANT ACTIVITY OF *CHENOPODIUM ALBUM* LINN. AND *CURCUMA CAESIA* ROXB.

***Charu Arora[1,*], Dhruv Arora[2], Suchandra Chatterjee[3] and Vinita Tamrakar[1]***

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## ABSTRACT

Scientific finding on phenolic content and anti-oxidant properties of *Curcuma caesia* and *Chenopodium album* can be useful and interesting as this work may lead to finding new sources for natural anti-oxidants, functional food, pharmaceuticals, and nutraceuticals. A total of seven different types of extracts were investigated for phenolic content of *Curcuma caesia* and *Chenopodium album*. Antioxidant activity for both the plant species was also evaluated as these plant species are traditionally used for ethno medicine practices. Antioxidant activity was determined by DPPH and phenolic content was determined by Folin Ciocalteu method. Phenolic content was found to be higher in *Curcuma ceasia* for all types of extracts investigated. Total phenolics content was found to be a maximum of 80% in crude methanol extract for both *C. album* (2585.0 µg/g gallic acid equivalent) and *C. caesia* (6672.4 µg/g gallic acid equivalent). A good correlation has

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Charu Arora

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CHAPTER 6

# Scanning Electron Microscopy: Theory and Applications

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**Abstract:** In the present chapter, brief history, working principle, instrumentation and, recent applications of Scanning Electron Microscopy (SEM) have been enlightened. SEM is a highly sensitive and efficient magnification tool that exploits focused beams of electrons to obtain information allied to topography, morphology, and composition of materials. Utilization of SEM techniques in different fields, like various domains of materials science, forensic investigation, mechanical engineering, biological, and medical sciences has been discussed.

**Keywords:** Electron beam, Scanning electron microscopy.

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## 1. INTRODUCTION

High-energy electron beam is used to generate signals to scan the surface of solid specimen. Manfred von Ardenne [1] in 1937 developed scanning electron technique capable of magnifying the several folds of object. SEM developed by Ardenne was free from chromatic aberration. It was developed using several detection modes and theories [2] with the capability of high magnification [3]. Zworykin's group [4] worked on further modifications. Later, in 1950s and early 1960s, Charles Oatley [5 - 8] and his coworkers put their efforts to develop the first commercial SEM. The instrument was fabricated by Cambridge Scientific Instrument Company in 1965 and delivered to DuPont.

The human eye is capable of distinguishing two points that are 0.2 mm apart, by avoiding use of additional lenses. This distance is termed as resolving power of the eye. The device used to increase the resolving power is known as microscope. Advanced microscopes can achieve magnification up to 1000x. The magnification power depends on the lens quality and radiation wavelength (λ) used. The wavelength of visible light falls in the range of 400 nm to 700 nm while electrons possess relatively short wavelengths, leading to improved resolution.

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CHAPTER 5

# Transmission Electron Microscopy: Theory and Applications

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**Abstract:** Transmission Electron Microscopy (TEM) is a useful technique to explore the molecular structure, interactions and processes including structure-function relationships at cellular level using a variety of TEM techniques with resolution of one angstrom (Å) 1 to 1000 Å. Developments in modern science and technology, especially in the material science, depend significantly on microstructure characterization. In this context, novel characterization techniques are crucial to understand the properties of materials. The quality of TEM results is dependent on preparation of TEM grid. Experts are constantly working on optimization of milling parameters to reduce the potential artifacts. The resolution power of TEM makes it possible to visualize different objects with high quality images to study complex structures and tissue morphology. Thus, TEM has made a milestone towards the understating of cellular structure. This chapter includes introduction and theory of TEM including its instrumentation, sample preparation, and working applications.

**Keywords:** Backscattered electron, Instrumentation, Sample preparation, Transmission electron microscope.

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## 1. INTRODUCTION

The use of electronic microscopes is significant due to their capability to determine the details of an object by imaging. But the extent of resolution is a function of wavelength of the corresponding wavelength of light to get a highly accurate image. This concept was first proposed by Ernst Abbe in 1893. In 1932, Ernst Ruska tried to construct a new electron microscope which could produce a direct image of specimens. In the following year, by improving the resolution, normal imaging of object was attained using the electron beam [1]. Interest in electron microscopes with higher magnifications increased and the idea of developing TEM appeared. The first TEM was demonstrated by Max Knoll and Ernst Ruska with high resolution (greater than that of light) electronic microscopy

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CHAPTER 3

# Raman Spectroscopy and Its Biomedical Applications

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**Abstract:** Raman spectroscopy is a significant characterization technique using inelastic scattering of light associated with molecular vibration to gather information about chemical fingerprints of tissues, cells or biofluids. Lack of sample preparation including chemical specificity and the ability to use advanced techniques in the visible or near-infrared spectral range have led versatility in biological applications of Raman spectroscopy. By Raman spectroscopy, the changes caused by diseases in tissues and organs can be accurately investigated and it is fast, non-invasive, economic and highly specific in comparison to other diagnostic and imaging techniques. It can provide quantitative molecular information for an objective diagnosis. Raman spectroscopy can measure both chemical and morphological information in samples and provide objective diagnosis for independent tissue samples of new patients. Some specific techniques and applications presented in this chapter which will demonstrate the potential of Raman spectroscopy for medical diagnostics, as well as the versatile interest in healthcare service.

**Keywords:** Biomedical applications, Instrumentation, Raman spectroscopy, Structure determination.

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## 1. INTRODUCTION

Raman Effect was discovered by C.V. Raman (Nobel Laureate) in 1928 [1]. It is an important tool for nondestructive analysis. However, there are a number of challenges such as lack of good Raman source, lack of good detector, and interference from fluorescence.

In 1986, the first Fourier-Transform (FT) Raman spectroscopy instrument was developed. It provided a new platform of break-through to make it more convenient and sophisticated for scientists [2]. Dispersive Raman spectroscopy

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CHAPTER 7

# SEM-EDX: A Potential Tool for Studies of Medicinal Plants

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**Abstract:** Naturally obtained compounds from aromatic and therapeutic plants, herbs and shrubs have been playing a vital role in providing medicinal benefits for humans since the prehistoric period. Ancient Unani manuscripts, Egyptian papyruses, and Chinese writings have described the use of medicinal plants, herbs, and shrubs. Shreds of evidence can be found from Unani hakims, Indian Vaids, and European and Mediterranean cultures using herbs in medicine for over 4000 years. India has been known to be a rich repository of medicinal plants. The forests in India are the principal repository of various medicative and aromatic plants that are mostly collected as raw materials for the production of diverse medicine and perfumery merchandise. Treatments with these drugs are considered safe as there is minimal or no side effects. The Energy-dispersive x-ray analysis (EDX) technique is useful in the study of drugs and drug delivery. It detects nanoparticles, which are generally used to improve therapeutic performance of chemotherapeutic agents. EDX is also used for characterization of minerals accumulated in tissues. It can also be considered as a useful tool in element determination, endogenous or exogenous in the tissue, cell or any other samples. In the present chapter, potential applications of SEM-EDX in the study of valuable compounds present in medicinal plants, herbs and shrubs have been highlighted. Special reference was given to the rich biodiversity of medicinal plants found in the state of Jharkhand and the need for preserving it for the well-being of human-kind. The study provides information about the availability of some crucial minerals and phytoconstituents, which can be used to provide dietary elements and may also help in emerging new drug formulations. This chapter further highlights the role of electron microscopy coupled with analytical analysis, particularly SEM-EDX, in characterization of various primary and secondary elemental compositions. Since medicinal products based on the extracts from plants, herbs, and shrubs are eco-friendly, there is urgent need to promote extensive research in the field.

**Keywords:** Herbal drugs, Medicinal plant, Pharmacology and ailments, SEM-EDX.

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Chapter 11

# Single-source precursors for main group metal sulfides and solar cell applications

Running head: Single-source precursors

The corrections made in this section will be reviewed and approved by master copier.

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**Keywords:**

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## 11.1 Introduction

Q10 Metal sulfides are a class of substances known for their unique chemical and physical properties [1–3]. Their semiconducting nature means that they have potential in various applications. Although a variety of methods are known for the syntheses of metal sulfides, traditional methods such as solid-state reaction, chemical vapor deposition (CVD), and homogeneous precipitation methods suffer from difficulties such as temperature requirements, long reaction times, formation of impure products, mixed phases, etc. [1–6]. Compared to bulk materials, thin films of main group metal sulfides play a critical role in electronic applications such as solar cells, optical fiber communications, and full-color displays. The purity of precursors is a crucial requirement in order to limit contamination in deposited thin films [6–9]. An alternative and energy-efficient method for the synthesis of thin films is the single molecular source precursor or single-source precursor (SSP) approach where the organic/metal fragments present in the metal complexes of sulfur-containing ligands are removed and pure phase metal sulfides are reassembled under mild conditions[Instruction: reference span should be [1-10] instead of [1-9] .] [1–9].

Dual/multiple-source precursor approaches are traditionally involved in the synthesis of bulk/thin films of metal sulfides, however, single-source precursors have been suggested as a method for lowering the growth temperature. The desired synthetic reaction pathway involves adsorption of the precursor without breaking the core M-S bond but with loss of the ancillary ligands. Single-source precursors potentially display a range of advantages over conventional CVD precursors, such as limited pre-reaction owing to only one precursor, reduced toxicity, possible lower temperature growth as well as possible stability in air and moisture. However, commercialization of single-source precursors is still a challenge due to their disadvantages such as difficulties in control of stoichiometry of the final product, growth of ternary and quaternary materials, low volatility, and prevention of epitaxial growth of polynuclear decomposition fragments due to low surface mobility. Herein, we present the various methods for the synthesis of bulk materials and thin films of main group metal sulfides from single-source precursor and their use for application in solar cells.

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## 11.2 Synthetic methods

The essential requirements for a suitable precursor are synthetic ease, ability to be synthesized in good yield and purity, high volatility, stability under ambient conditions, and decomposition at elevated temperatures. Purity requires

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# Biodegradable Natural Polymeric Nanocomposite Material

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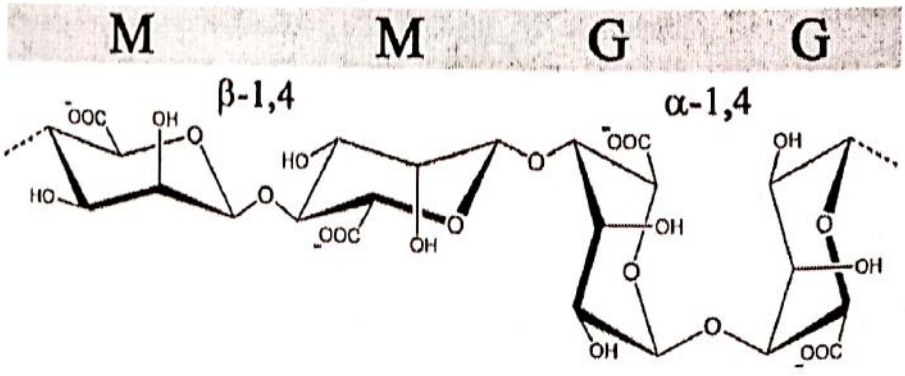
**Abstract:** Alginate is a natural polymer of carbohydrate family (polysaccharides) which is obtained from brown seaweed and having characteristics properties viz biocompability, biodegradable, non-toxic. To enhance its properties nanobased alginates are synthesized and their composites are obtained using various metals, metal oxides, nonmetallic components; which show excellent result in various field of their applications. One of the applications of biodegradable nanocomposite materials of alginate is in removing heavy metal ion pollutants from ground / surface water in order to make it potable. Another important area is Catalysis and Antimicrobial activities.

## Introduction

### what are alginates?

Alginates are natural biopolymer belonging to carbohydrate family (polysaccharides) and composed mainly of (1, 4) - linked β - D-mannuronic acid units and α – L- guluronic acid units. The main source of alginate is the cell wall of brown algae. It is a salt of alginic acid




Structure of alginate



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# 27

# COVID-19 pandemic in India: forecasting using machine learning techniques

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## 1. Introduction

The novel coronavirus disease 2019 (COVID-19) has been declared a world pandemic threat by the World Health Organization and is spreading rapidly across the world. It is an infectious disease caused by a virus called a novel coronavirus, which was also the reason for severe acute respiratory syndrome (SARS) in 2003. The SARS epidemic [1,2] was predicted by many authors using various machine learning (ML) techniques. Because of COVID-19, the number of confirmed cases and deaths are rapidly increasing in all most all countries; India has not escaped this pandemic. The first case of COVID-19 emerged in India on Jan. 30, 2020; 2 more cases were found on Feb. 3, 2020 and the number was stable until Mar. 1, 2020. The disease has since spread to most states and cities of India [3]. Few states or cities remain untouched by the COVID-19 outbreak in India. There is no vaccine to treat COVID-19 to prevent infection from one infected person to another. India has learned a lesson from other countries, and therefore the Indian government has made appropriate decisions and implemented various strategies to prevent the pandemic from spreading across the country well in advance. Many approaches were taken to stop spreading cases of COVID-19 from affected to unaffected parts of the country, including a citywide lockdown, closing all transports such as airports, railways, and local transportations, and closing markets, malls, cinemas, productions, and so on. Moreover, the isolation or quarantine of suspected patients is being done. The entire machinery of the government is fully involved to stop spreading it in the community; despite this, cases of COVID-19 positive are increasing every day. By the time of writing, there were more than 26,283 confirmed cases in India, 825 of whom died and about 5938 of whom had recovered, and the numbers keep rising [4].

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# Chapter 5
# Development of Rainfall Prediction Models Using Machine Learning Approaches for Different Agro-Climatic Zones

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## ABSTRACT

*This study focuses on modelling the changes in rainfall patterns in different agro-climatic zones due to climate change through statistical downscaling of large-scale climate variables using machine learning approaches. Potential of three machine learning algorithms, multilayer artificial neural network (MLANN), radial basis function neural network (RBFNN), and least square support vector machine (LS-SVM) have been investigated. The large-scale climate variable are obtained from National Centre for Environmental Prediction (NCEP) reanalysis product and used as predictors for model development. Proposed machine learning models are applied to generate projected time series of rainfall for the period 2021-2050 using the Hadley Centre coupled model (HadCM3) B2 emission scenario data as predictors. An increasing trend in anticipated rainfall is observed during 2021-2050 in all the ACZs of Chhattisgarh State. Among the machine learning models, RBFNN found as more feasible technique for modeling of monthly rainfall in this region.*

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## INTRODUCTION

Climate comprises a general pattern of weather conditions, seasons and weather extremes like drought, flood, heat wave and cold wave situations. Climate study is a very complicated phenomenon which contains various climatic variables, and their behaviors are also different. Climate of any region varies with space and time on account of various atmospheric forcing. Long-term systematic changes of statistical properties of the climate variables are referred to as "climate change". The statistical distribution of weather patterns with a particular long-term or extended period (decades or longer time span) indicates the climate change (Yang et al. 2010; 2015; 2017; Shi et al. 2016). In another word, climate change also refers to a shift in climate from its average weather condition eventually for the long-term period. According to United Nations Framework Convention on Climate Change (UNFCCC), climate change is directly or indirectly associated with human interventions, which alter the composition of atmospheric balance (IPCC, 2007). However, it may be caused by a hydrological cycle imbalance, phytochemical effects, biotic manners, variation in solar radiations, geological inequality, volcanic eruptions, anthropogenic activities, etc. During the recent past, the intervention of anthropogenic activities such as urbanization, population growth, industrialization, deforestation, settlements, burning of fossil fuels, etc., has increased the greenhouse gases (GHG) emission (Kumar and Sharma, 2017). Intergovernmental Panel on Climate Change (IPCC, 1996) reported that global warming is mainly due to the enhanced GHG radiation and is likely to have a significant impact on the hydrological cycle and future climate change. Alarming effects of climate change viz. severe floods, droughts and other extreme hydrological events catch the attention of the entire world to think and assess its future impact on global climate. In the recent past, various severities of adverse climatic events have been identified. Climate change seems to be more pronounced, if assessed at local and regional scale compared to global scale because globally its effects are more generalized.

In an agrarian country like India, uneven rainfall distribution may disrupt food availability and results in reduced agricultural productivity. Hence, precise knowledge about the past, present and future rainfall pattern over a region can play an important role in planning cropping pattern, finalizing the schedule of the farm operation and designing irrigation structures for effective utilization of available water resources for enhancing the agricultural production. Hence, in order to assess the climate change impacts on rainfall distribution and its future trends, the present investigation is carried out using long term monthly rainfall time series to develop an appropriate technique for the rainfall modeling in the three distinct Agro-climatic Zones (ACZs) viz., Chhattisgarh Plains, Bastar Plateau and Northern Hills ACZs of Chhattisgarh state in east central India.

In a recent decade study about possible changes in rainfall pattern over a region due to climate change is being assessed using statistical downscaling of general circulation models (GCM) products from global to local scale. Statistical downscaling methodologies are based on transfer functions, which highlight relationships between global scale predictors and local scale response variable using linear/non-linear regression equations (Wilby et al. 2002, 2004; Murphy and Timbal, 2008). GCM products provide the required the long period global scale data of various large scale climate variables, which is used as predictors for rainfall prediction. Multi-linear regression (MLR), principal component analysis (PCA) and canonical correlation analysis (CCA) are outdated statistical downscaling regression methods (Dibike and Coulibaly, 2005). Conversely, machine learning techniques such as artificial neural network (ANN), least square support vector machine (LS-SVM) and least square support vector regression (LS-SVR) are gaining popularity during the past two decades and considered under nonlinear regression models. Among

them most of the researchers have demonstrated the potential of MLR, LS-SVM (Benestad et al. 2007; Cannon and Whitfield 2002; Chen et al. 2010; Najafi et al. 2011; Ojha 2013; Cheng et al. 2008; Maheras et al. 2004; Kostopoulou et al. 2007; Schoof et al. 2007; Huth 1999, 2002, 2004), PCA (Wetterhall et al. 2005; Tolika et al. 2006), CCA (Huth 1999, 2002, 2004; Kostopoulou et al. 2007; Tomezeiu et al. 2006; Landman et al. 2001; Tolika et al. 2006), ANN (Goyal and Ohja 2012; Kostopoulou et al. 2007; Samadi et al. 2013; Tisseuil et al. 2010; Trigo and Palutikof, 2001; Tripathi et al. 2006), and SVM (Anandhi et al. 2009; Chen et al. 2010; Ghosh and Mujumdar 2008; Tripathi et al. 2006; Najafi et al. 2011; Chen et al. 2012) for modelling climate variables. Out of all discussed downscaling techniques, ANN has gained broad credit (Cannon and Whitfield, 2002; Tisseuil et al. 2010). In climate impact studies, SVM has theoretically proved better than other techniques in transfer functions (Tripathi et al. 2006). Sachindra et al. (2013) stated that LS-SVM is found to be the proper technique for statistical downscaling of General Circulation Model (GCM) outputs to stream flow than multiple linear regressions. Besides this, recently, Xu et al. (2020) developed a multiple machine learning (MML) downscaling models, based on a Bayesian model average (BMA), to downscale the precipitation simulation of 8 Coupled Model Inter comparison Project Phase 5 (CMIP5) models using model output statistics (MOS) in the upper Han River basin. Ahmed et al. (2020) developed Multi-Model Ensembles (MMEs) using machine learning algorithms; ANN, K-Nearest Neighbor (KNN), SVM and Relevance Vector Machine (RVM) for rainfall prediction over Pakistan. Vandal et al. (2018) compared Perfect Prognosis (PP) approaches, Ordinary Least Squares, Elastic-Net, and SVM, along with two machine learning methods Multitask Sparse Structure Learning (MSSL) and Autoencoder Neural Networks for downscaling of daily and extreme precipitation. Sachindra et al. (2018) also investigated four machine learning techniques, Genetic Programming (GP), ANNs, SVM, and RVM for statistical downscaling of precipitation.

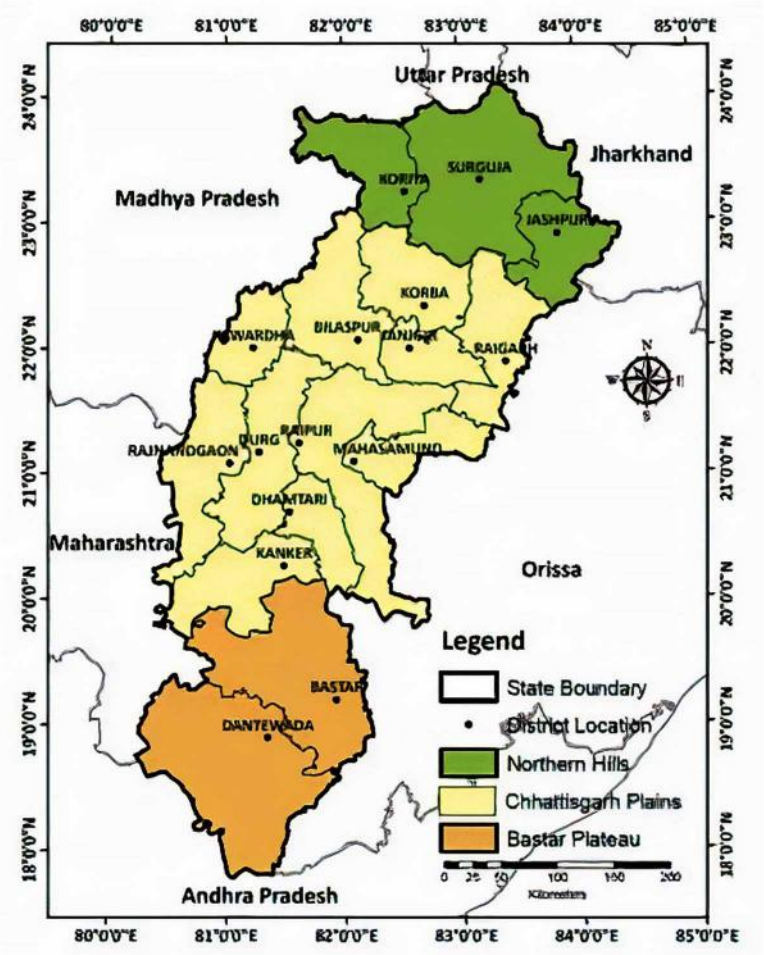
Literature review motivated the authors to conduct the present investigations and therefore an attempt has been made to develop appropriate machine learning models for monthly rainfall predictions in different ACZs of Chhattisgarh state of east-central India. Potential of most popular and conventional machine learning models, such as multi-layer artificial neural network (MLANN), radial basis function neural network (RBFNN) and least Square support vector machine (LS-SVM) are investigated to model the monthly rainfall pattern in different ACZs. These, machine learning techniques are based on transfer functions and model the relationships between predictors and the target variable. These regression techniques are mainly based on a set of supervised learning methodologies that can analyze historical long term observed rainfall time series and recognize patterns. The developed machine learning models are then applied for future rainfall trend using appropriate GCM projections. However, successful implementation of such models are highly dependent on the appropriateness of future climatic projection(s) at a regional level. Future rainfall time series obtained through these machine learning models, will be beneficial for future prospectives like sustainable planning and mitigation. The present investigation demonstrated some alternate machine learning approach for statistical downscaling of long term monthly rainfall time series and its application for future rainfall projections using appropriate climate change scenarios over Chhattisgarh state of India.

## MATERIAL AND METHODS

### Study Area

The Chhattisgarh state of east central India is acknowledged as "Bowl of Rice" with the geographical area of about 135,190 km$^2$ (Kansal et al. 2015). It contributes about 12% forest to the Indian sub-continent. However, 44% contribution itself in Chhattisgarh. The aerial extent of Chhattisgarh state lies between 17.78$^o$N to 24.11$^o$N and 80.24$^o$E to 84.39$^o$E. A total of 27 districts come under the administrative boundary of Chhattisgarh state which is located in a tropical zone due to its location near to the tropic of cancer. The Chhattisgarh state is divided into three distinct ACZs viz. Chhattisgarh Plains, Bastar Plateau and Northern Hills as depicted in Figure 1. Chhattisgarh state is a mono-cropped state with rice (*Oryza sativa*) being the main crop cultivated in 3/5$^{th}$ of the total area during the *Kharif* season. More than 80% of the population are dependent upon agriculture for its livelihood.

*Figure 1. Location map of the study area*



## Rainfall Data Collection

Long-term daily rainfall data are obtained from the fine resolution (0.25° x 0.25°) time series released by India Meteorological Department (IMD). Further, daily time series from 1948 to 2017 has been converted into monthly/annual time series using area weighted-average technique with the help of geographic information system (GIS) platform for all the 27 districts of Chhattisgarh region. Descriptive statistics of annual rainfall has been computed for finding the behavior or variability of rainfall in different ACZs. Location of meteorological stations and its spatial distribution of average annual rainfall along with descriptive statistics are shown in Table 1. No missing evidence is found in the time series. The outliers have been removed using the standard ratio method (ratio between the highest peak and the mean value of the correlation plane) as indicated by Raffel (2007). District wise monthly rainfall time series is averaged to obtain monthly rainfall time series for respective ACZs and used as target variable for calibration and validation of the proposed machine learning models.

## Selection of Predictors for Rainfall Modeling

The selection of appropriate predictors is one of the most essential and complex steps in a downscaling procedure. The selection of predictors varies with space and time, which is based on the target variable characteristics under large-scale atmospheric circulation. A different scenario provides a wide range of predictors and each and every predictor is important in downscaling techniques. It is very necessary to develop strong relationships between the target variable and predictors (Wetterhall et al., 2005). According to guidelines for use of climate scenarios developed from statistical downscaling methods the predictors should be selected as per the following criterion: (1) The large-scale predictors should be physically relevant to the local-scale features and realistically simulated by GCMs, (2) the predictors are readily available from the archives of reanalysis datasets and GCMs output and, (3) predictors have strongly correlated with target variables (Wilby et al., 2004). Hence, the monthly observed predictor data of climatic variables are derived from the National Center for Environmental Prediction (NCEP) reanalysis data on 2.5° x 2.5° grid-scale for 41 years (1948-2017) (Mishra et al. 2014). The extracted data range between 17.50°N - 24.33°N latitude and 80.11°E - 84.73°E longitude, which covers the entire Chhattisgarh state. The large-scale monthly predictors are derived from Hadley Center Coupled GCM Model, version-3 (HadCM3) for B2 future scenario which is obtained from the Climate Change Severity Index (CCSI) from 2021 to 2050 on grid resolution is 2.5° x 3.75° for future rainfall prediction. The HadCM3 B2 GCM scenario defines the world with intermediate population and its growth of economic condition under consideration of sustainability through social, economic and environmental factors, therefore, B2 scenarios is considered for Indian condition. In India, HadCM3 GCM B2 has been chosen while studying the climate change impact because of its widespread acceptance. The 26 NCEP predictors of different atmospheric pressure levels used for rainfall modelling in this study are shown in Table 2.

*Table 1. Location of meteorological stations and average annual rainfall distribution in different ACZs of Chhattisgarh state and its descriptive statistics (data base 1948-2017)*

| Districts | Long. | Lat. | Alt. | Average RF | SD | CV |
|---|---|---|---|---|---|---|
| Balod | 81.21 | 20.73 | 324 | 1210.0 | 251.5 | 20.8 |
| Balodabazar | 82.16 | 21.66 | 254 | 1127.7 | 263.8 | 23.4 |
| Bemetra | 81.54 | 21.71 | 278 | 1119.2 | 234.3 | 20.9 |
| Bilaspur | 82.13 | 22.07 | 264 | 1271.1 | 233.5 | 18.4 |
| Dhamtari | 81.54 | 20.70 | 305 | 1267.5 | 277.6 | 21.9 |
| Durg | 81.28 | 21.18 | 289 | 1179.8 | 254.9 | 21.6 |
| Gariabandh | 82.30 | 20.26 | 292 | 1226.9 | 245.8 | 20.0 |
| Janjgir-Champa | 82.57 | 22.00 | 256 | 1296.8 | 264.7 | 20.4 |
| Kanker | 81.49 | 20.27 | 388 | 1379.2 | 276.9 | 20.1 |
| Kawardha | 81.23 | 22.01 | 353 | 1126.5 | 231.2 | 20.5 |
| Korba | 82.70 | 22.34 | 316 | 1376.8 | 284.3 | 20.7 |
| Mahasamund | 82.09 | 21.10 | 318 | 1213.5 | 266.5 | 22.0 |
| Mungeli | 81.69 | 22.07 | 288 | 1203.3 | 225.2 | 18.7 |
| Raigarh | 83.39 | 21.89 | 215 | 1363.8 | 288.6 | 21.2 |
| Raipur | 81.62 | 21.25 | 298 | 1153.7 | 281.6 | 24.4 |
| Rajnandgaon | 81.03 | 21.09 | 307 | 1210.4 | 243.2 | 20.1 |
| **Chhattisgarh Plains** | | | | **1232.9** | **257.7** | **20.9** |
| Bastar | 81.93 | 19.20 | 552 | 1502.0 | 228.3 | 15.2 |
| Bijapur | 80.82 | 18.79 | 592 | 1516.0 | 302.8 | 20.0 |
| Dantewada | 81.35 | 18.90 | 362 | 1498.9 | 281.8 | 18.8 |
| Kondagaon | 81.66 | 19.59 | 593 | 1356.2 | 231.5 | 17.1 |
| Narayanpur | 81.25 | 19.72 | 408 | 1408.6 | 256.0 | 18.2 |
| Sukma | 81.66 | 18.39 | 210 | 1468.9 | 277.0 | 18.9 |
| **Bastar Plateau** | | | | **1458.5** | **262.9** | **18.0** |
| Balrampur | 83.61 | 23.61 | 441 | 1199.8 | 257.0 | 21.4 |
| Jashpur | 83.85 | 22.90 | 753 | 1422.0 | 272.9 | 19.2 |
| Koriya | 82.54 | 23.25 | 700 | 1214.3 | 253.4 | 20.9 |
| Surajpur | 82.87 | 23.21 | 528 | 1258.4 | 283.8 | 22.6 |
| Surguja | 83.19 | 22.95 | 623 | 1374.1 | 290.5 | 21.1 |
| **Northern Hills** | | | | **1293.7** | **271.5** | **21.0** |
| **Chhattisgarh** | | | | **1318.9** | **185.2** | **14.0** |

Long., Lat., Alt., RF, SD and CV denotes longitude(°N), latitude(°E), altitude(m), rainfall (mm), standard deviation (mm) and coefficient of variation(%) respectively

*Table 2. Description of all NCEP predictors used for rainfall modelling.*

| S. No. | Atmospheric Pressure Level | NCEP Variables Descriptions | Code | Units |
|---|---|---|---|---|
| A | 1013.25 hPa | Mean sea level pressure | ncepmslpas | Pa |
| B | 1000 hPa | Surface airflow strength | ncepp__fas | m/s |
| | | Surface zonal velocity | ncepp__uas | m/s |
| | | Surface meridional velocity | ncepp__vas | m/s |
| | | Surface vorticity | ncepp__zas | $s^{-1}$ |
| | | Surface wind direction | ncepp_thas | degree |
| | | Surface divergence | ncepp_zhas | $s^{-1}$ |
| C | 850 hPa | 850 hPa airflow strength | ncepp8_fas | m/s |
| | | 850 hPa zonal velocity | ncepp8_uas | m/s |
| | | 850 hPa meridional velocity | ncepp8_vas | m/s |
| | | 850 hPa vorticity | ncepp8_zas | $s^{-1}$ |
| | | 850 hPa wind direction | ncepp8thas | degree |
| | | 850 hPa divergence | ncepp8zhas | $s^{-1}$ |
| | | 850 hPa geopotential height | ncepp850as | m |
| | | Relative humidity at 850 hPa | ncepr850as | % |
| D | 500 hPa | 500 hPa airflow strength | ncepp5_fas | m/s |
| | | 500 hPa zonal velocity | ncepp5_uas | m/s |
| | | 500 hPa meridional velocity | ncepp5_vas | m/s |
| | | 500 hPa vorticity | ncepp5_zas | $s^{-1}$ |
| | | 500 hPa wind direction | ncepp5thas | |
| | | 500 hPa divergence | ncepp5zhas | $s^{-1}$ |
| | | 500 hPa geopotential height | ncepp500as | m |
| | | Relative humidity at 500 hPa | ncepr500as | % |
| E | Near surface | Surface specific humidity | ncepshumas | g/kg |
| | | Mean temperature at 2m | nceptempas | $^0$C |
| | | Near surface relative humidity | ncepr hu mas | % |

## Machine Learning Models

### Radial Basis Function Neural Network (RBFNN)

RBFNN is a category of feed forward network with a single hidden layer and an output layer formulated by Broomhead and Lowe (1988). Pictorial representation of the RBFNN is given in Figure 2. Each processing unit termed as a neuron in the hidden layer is associated with centers $c = c_1, c_2, c_3, \ldots, c_h$, and its width $\sigma = \sigma 1, \sigma 2, \sigma_3, \ldots, \sigma h$, where h is the number of neurons in the hidden layer. Each neuron in hidden layer receives the same set of input data ($x = x1, x2, x3, \ldots, x_n$). Centers of every hidden neuron have the same dimension as that of the input data, i.e. $c_i \in R^n, x \in R^n$. The output of each hidden layer neurons

($\varnothing_1, \varnothing_2, \varnothing_3 \ldots\ldots \varnothing_h$) is associated with synaptic weight (w1,$w_2$,$w_3$,... wh). Output $\varnothing_i$ of it$h^h$idden layer neuron is basically a Gaussian function and is represented by:

$$\varnothing_i\left(z\right) = e^{\frac{-z^2}{2\sigma_i^2}} \tag{1}$$

where, $z = \left\|x - c_i\right\|$, represents the Euclidian distance between input data and corresponding centers and $\varnothing_i = \varnothing(\left\|x - c_i\right\|$. The Gaussian function used in the each hidden layer neuron is actually a category of radial basis function. Finally the response of the RBFNN for a given set of input data at the output layer neuron is linear in terms of weights and computed using the following expression.

$$y = \sum_{i=1}^{h} w_i \varnothing_i \tag{2}$$

Calibration of the RBFNN network for each instant of input data and its corresponding output {*x,y*} is done in a recursive manner, by updating the network parameters {$w_i$,$c_i$,$\sigma$i$_j$ to minimize the following instantaneous error cost function.

$$e = \frac{1}{2}\left(y^d - y\right)^2 \tag{3}$$

The weight update rules to optimize the network parameters {$w_i$,$c_i$,$\sigma$i$_j$ at time t is given by following equations which are derived using a gradient descent algorithm.

$$w_i\left(t+1\right) = w_i\left(t\right) + \eta_1\left(y^d - y\right)\varnothing_i \tag{4}$$

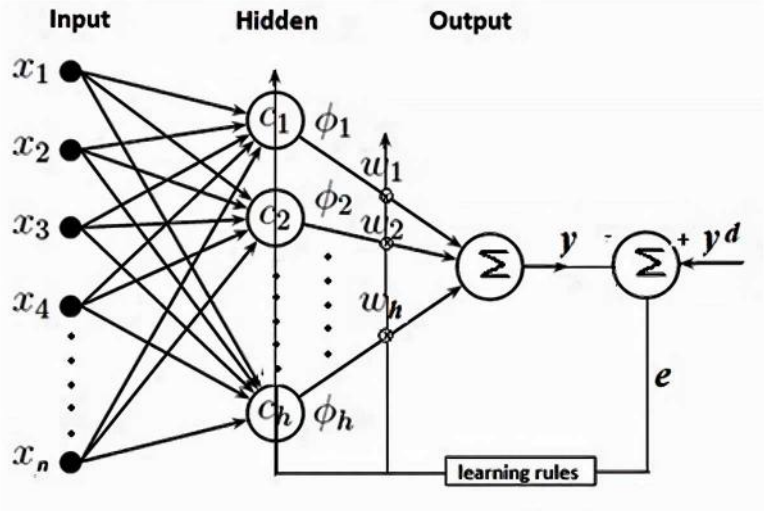
$$c_{ij}\left(t+1\right) = c_{ij}\left(t\right) + \frac{\eta_2}{\sigma_i^2}\left(y^d - y\right) w_i \varnothing_i \left(x_j - c_{ij}\right) \tag{5}$$

$$\sigma_i\left(t+1\right) = \sigma_i\left(t\right) + \frac{\eta_3}{\sigma_i^3}\left(y^d - y\right) w_i \varnothing_i z_i^{\,2} \tag{6}$$

where,

$y^d$= desired outputor target value
$c_{ij} = j^{th}$ element of $i^{th}$ center
$\eta_1, \eta_2, \eta_3$ = learning rate for network parameters {$w_i$,$c_i$,$\sigma$i$_j$ respectively.

*Figure 2. Block diagram of RBFNN based estimator*




## Least Square Support Vector Machine (LS-SVM)

Least squares support vector machines (LS-SVM) is another statistical downscaling machine learning technique. Least square version of support vector machine has been also utilized for this study. LS-SVM is based on a set of supervised learning methodology that can analyze data and it recognizes patterns which are used for categorization as well as regression analysis. In this method, the solution can be found by solving a set of linear equations instead of a convex quadratic programming (QP) problem for classical SVMs. LS-SVM classifiers (Suykens and Vandewalle, 1999; Suykens et al., 2001). LS-SVMs are a class of kernel-based learning methods. Consider a finite training sample of N patterns $\{(x_i, y_i), i = 1, . . ., N\}$, where $x_i$ denote the $i^{th}$ pattern in N-dimensional space (i.e. $x_i = [x_{1i}, . . ., x_{Ni}] \in \Re N$) constitutes input to LS-SVM and $Y_{i\in}\Re N$ is the corresponding value of the desired model output. Further, let the learning machine be defined by a set of possible mappings x→ f (x, w), where f (·) is a deterministic function which for a given input pattern x and adjustable parameters w (w ∈ℜN), always gives the same output. Calibration phase of the learning machine involves adjusting the parameters w. The parameters are estimated by minimizing the cost function ΨL ($_w$, e). The LS-SVM optimization problem for function estimation is formulated by minimizing the cost function.

$$\Psi_L\left(w,e\right) = \frac{1}{2} w^T w + \frac{1}{2} C \sum_{i=1}^{N} e_i^2 \tag{7}$$

Subject to the equality constraint

$$y_i = \hat{y}_i = e_i, i = 1,....., N \tag{8}$$

Where *C* is a positive real constant and $\hat{y}$ is the actual model output. The first term of the cost function represents weight decay or model complexity-penalty, function. It is used to regularize weight sizes and to penalize large weights. This helps in improving generalization performance. The second term of the cost function represents a penalty function. The solution of the optimization problem is obtained by considering the Lagrangian as

$$L\left(w,b,e,\alpha\right)=\frac{1}{2}w^{T}w+\frac{1}{2}C\sum_{i=1}^{N}e_{i}^{2}-\sum_{i=1}^{N}\alpha_{i}\left\{\hat{y}_{i}+e_{i}-y_{i}\right\}+b \tag{9}$$

Where $\alpha_i$ are Lagrange multipliers and *b* is the bias term. The conditions for optimality are given by

$$\begin{cases} \dfrac{\partial L}{\partial w}=w-\sum_{i=1}^{N}\alpha_{i}\varphi\left(x_{i}\right)=0 \\ \dfrac{\partial L}{\partial b}=\sum_{i=1}^{N}\alpha_{i}=0 \\ \dfrac{\partial L}{\partial e_{i}}=\alpha_{i}-Ce_{i}=0,i,.....N \\ \dfrac{\partial L}{\partial \alpha_{i}}=\hat{y}_{i}+e_{i}-y_{i}=0,i=1,.....N \end{cases} \tag{10}$$

The elimination of *w* and *e* will yield a linear system instead of a quadratic programming problem. The above conditions of optimality can be expressed as the solution to the following set of linear equations after elimination of *e* and $e_i$.

$$\begin{bmatrix} 0 & \vec{1}^{T} \\ \vec{1} & \Omega+C^{-1}I \end{bmatrix}\begin{bmatrix} b \\ \alpha \end{bmatrix}=\begin{bmatrix} 0 \\ y \end{bmatrix} \tag{11}$$

$$where, y=\begin{bmatrix} y_{1} \\ y_{2} \\ \vdots \\ y_{N} \end{bmatrix};\vec{1}=\begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}_{N\times N} \tag{12}$$

$$\alpha=\begin{bmatrix} \alpha_{1} \\ \alpha_{2} \\ \vdots \\ \alpha_{N} \end{bmatrix};I=\begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}_{N\times N} \tag{13}$$

Here, $I_N$ is an N×N identity matrix, and $\Omega \in R^{N\times N}$ is the kernel matrix defined by Ω is obtained from the application of Mercer's theorem.

$$\Omega_{i,j} = K\left(x_{i,}x_j\right) = \varphi\left(x_i\right)^T \varphi\left(x_j\right)\cdots\forall i,j \tag{14}$$

Where $\varphi(\cdot)$ represents the nonlinear transformation function defined to convert a nonlinear problem to a linear problem in a higher dimensional feature space. The resulting LS-SVM model for function estimation is:

$$f\left(x\right) = \sum \alpha_i^* K\left(x_i, x\right) + b^* \tag{15}$$

$K(\mathbf{x}_i,\mathbf{x})$ is the inner product kernel function defined in accordance with Mercer's theorem (Courant and Hilbert, 2008) and $b^*$ is the bias. There are several possibilities for the choice of the kernel function, including linear, polynomial and radial basis function (RBF). The linear kernel is a special case of RBF (Keerthi and Lin, 2003). Further, the signed kernel behaves like RBF for certain parameters (Lin and Lin, 2003). They are defined as follow.

Linear kernel:

$$K\left(x_i, x_j\right) = x_i^T x_j \tag{16}$$

Polynomial kernel:

$$K\left(x_i, x_j\right) = \left(x_i^T x_j + t\right)^d, t \geq 0 \tag{17}$$

Radial Basis Function kernel:

$$K\left(x_{i,}x_j\right) = e^{-\frac{\left\|x_i - x_j\right\|^2}{2\sigma^2}} \tag{18}$$

Where, t is the intercept and d is the degree of the polynomial, $\sigma$ is the width of RBF kernel, which can be adjusted to control the expressivity of RBF.

## Multi-Layer Artificial Neural Network (MLANN)

MLANN is a feed forward neural network suggested by Haykin (1998) with an input layer, one or more hidden layer and an output layer. A N-5-1 structure of MLANN (N=26 represents the number of input data, 5 neurons in hidden layer and one neuron at the output layers) is used in this study with different input combinations. The training of the network is done by back-propagation algorithm which is based

on the error-correcting learning rule to update the weights and biases of each neuron in different layers. Hyperbolic tangent (tanh) is used as the activation function.

## Performance Evaluation Measures

The performance of the predictive models is evaluated by computing root mean square error (RMSE), coefficient of determination ($R^2$) and Nash and Sutcliffe efficiency factor (NSE) (Kim and Kim 2008; Zhang and Govindaraju 2000; Nash and Sutcliffe 1970) between desired (FAO-PM) and estimated $ET_0$. The mathematical formula for the different evaluation measures are as follows.

$$RMSE = \sqrt{\frac{1}{T}\sum_{i=1}^{T}(Out_{est} - Out_{obs})^2} \tag{19}$$

$$R^2 = \frac{\left[\sum_{i=1}^{T}\left(Out_{obs} - \overline{Out_{obs}}\right)\left(Out_{est} - \overline{Out_{est}}\right)\right]^2}{\sum_{i=1}^{T}\left(Out_{obs} - \overline{Out_{obs}}\right)^2 \sum_{i=1}^{T}\left(Out_{est} - \overline{Out_{est}}\right)^2} \tag{20}$$

$$NSE = 1 - \frac{\sum_{i=1}^{T}\left(Out_{est} - Out_{obs}\right)^2}{\sum_{i=1}^{T}(Out_{obs} - \overline{Out_{obs}})^2} \quad (-\infty \leq EF \leq 1) \tag{21}$$

where, $Out_{obs}$ and $Out_{est}$ represent the observed and estimated values, respectively. $T$ is the total number of validation patterns and i denotes the number of particular instances. Low RMSE values represent the close association between desired and estimated output. Similarly, $R^2$ and EF values close to 1 are also an indicator of superior predictive ability of the model. (Duhan and Pandey 2015).

## Stepwise Algorithm for Model Development and Its Application

Monthly Rainfall data are considered as the target variable and climatic variables (n=26) as predictors. First of all, screening of variables has been chosen based on partial correlation coefficients. Highly positive and negative correlated variables have been selected for the same. MLANN, RBFNN, LS-SVM machine learning technique have been adopted for downscaling of monthly rainfall. There techniques are non-parametric downscaling techniques which are based on convex quadratic programming (QP) and Kernel-based learning functions. The entire downscaling process is completed by the regression/ transform function. The overall methodology is based on a set of supervised approaches which provide better results compared to traditional statistical based approach (Suykens and Vandewalle, 1999). Proposed methodology for rainfall downscaling is shown in Figure 3. The stepwise algorithm used to carry out the future projection of rainfall is as follows:

1. Obtain the monthly rainfall time series from a reliable source.
2. Check missing values and consistency for all the meteorological stations.
3. For calibration and validation purpose, NCEP data for the period 1948-2017 are utilized. However, the calibration and validation periods are taken as 1948-2010 and 2011-2017 respectively.
4. For possible future projection of the target variable (rainfall), HadCM3 B2 future scenarios is used.
5. Select the potential predictors using the screen of variables by partial correlation (Duhan and Pandey 2014).
6. Run the MLANN, RBFNN, LS-SVM machine learning models with potential NCEP predictors (Keerthi and Kin 2003; Courant and Hilbert 2008).
7. Calibrate the model by fine tuning the parameters of transfer function. (Keerthi and Kin 2003) to by minimizing the error cost function.
8. After calibrating of the machine learning models to a satisfactory level, validate the model with remaining data, which is kept reserved for validation of the models.
9. The performance of model efficiency is checked by the root mean square error (RMSE), coefficient of determination ($R^2$), Nash-Sutcliffe efficiency coefficient (NSE) (Kim and Kim 2008; Zhang and Govindaraju 2000; Nash and Sutcliffe 1970).
10. Further developed machine learning models have been applied using the predictor variables of HadCM3 B2 scenario (Chandniha and Kansal 2016) and projection of future rainfall scenarios for study locations for the period of 2021 to 2050.

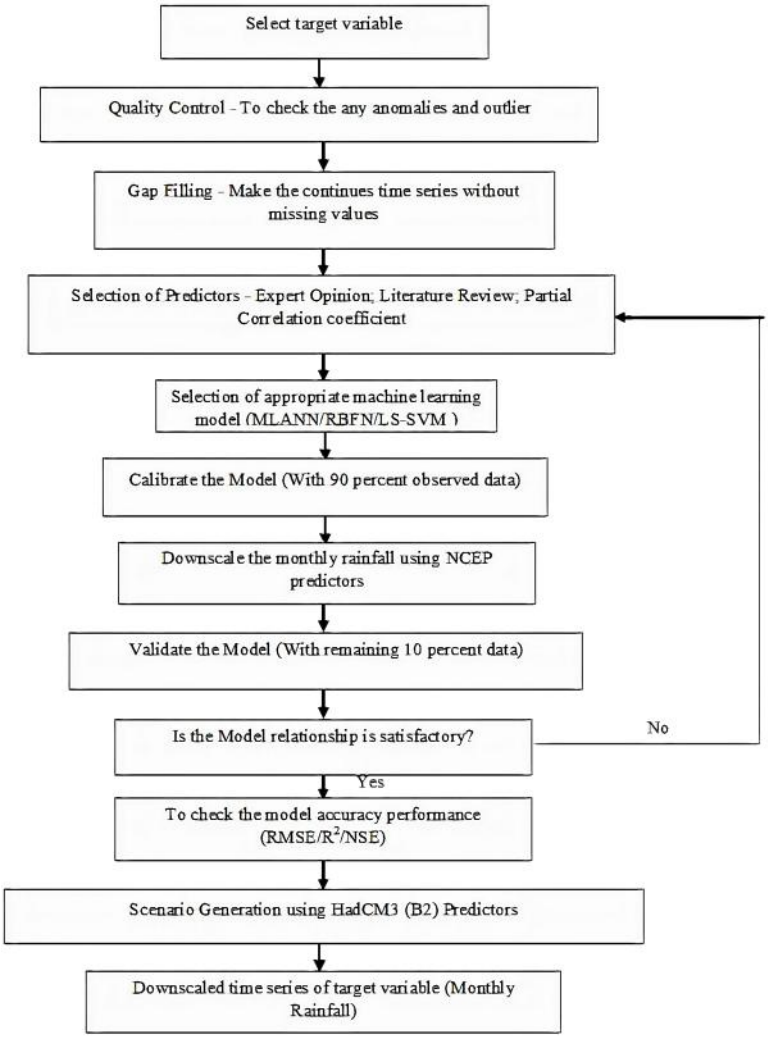
## RESULTS AND DISCUSSION

### Calibration and Validation of Machine Learning Models

In this study potential of three machine learning models, namely MLANN, RBFNN and LS-SVM are investigated for rainfall modeling. Simulation studies are carried out for modeling monthly rainfall time series for different ACZs of Chhattisgarh using NCEP predictor variables. Long term monthly NCEP predictors from 1948-2010 is considered for calibration of different machine learning models as per the methodology described in the previous section. Recent 7 years of NCEP predictors and monthly rainfall data from 2011-2017 is used for model validation in different ACZs.

To calibrate the model, NCEP predictors and desired target data is normalized between -1 to 1. Model parameters of the MLANN, RBFNN and LS-SVM i.e., learning rate, weights are initialized to random numbers between -1 to 1. Input patterns are given to the input layer of the model in a sequential manner and corresponding estimated output is obtained at the output layer after completion of the forward pass for each set of input patterns. Estimated output is compared with the target output to compute the instantaneous error which is the cost function for the proposed model. Real time update of the model parameters is done in each instance to minimize the squared error. The process continues till all the available input patterns for model calibration gets exhausted. This completes one cycle called epoch. At the end of each epoch, mean square error is computed. The iterative process is repeated several times until RMSE is minimized to a desired low value. This completes the supervised calibration process and model parameters are then fixed to constitute proposed model.

*Figure 3. Proposed methodology for rainfall downscaling*




After completion of the model calibration process, validation data sets are used and corresponding monthly rainfall estimates are obtained using the developed models. For model comparison and selection, performance evaluation measures i.e., RMSE (mm/week), NSE and $R^2$ are computed for each model under consideration and the results are presented in Table 3. It is can be easily seen that, the calibration and validation performance in terms of $R^2$, RMSE and NSE values are comparatively better in case of Chhattisgarh Plains as compared to Northern Hills and Bastar Plateau ACZs. This may be associated with a different topographic situation of respective ACZs. Also, the difference between $R^2$, RMSE and NSE values during calibration and validation phase is less in Chhattisgarh Plains with different machine learning approaches, whereas the validation performance of these machine learning models are comparatively inferior to calibration performance and the difference is more in Bastar Plateau and Northern Hills ACZs.

*Table 3. Calibration and validation performance of MLANN, RBFNN and LS-SVM machine learning techniques for monthly rainfall estimation using NCEP predictors*

| Zone | Model | Calibration Performance (1948-2010) | | | Validation Performance (2011-2017) | | |
|---|---|---|---|---|---|---|---|
| | | $R^2$ | RMSE | NSE | $R^2$ | RMSE | NSE |
| Chhattisgarh Plains zone | MLANN | 0.936 | 39.20 | 0.925 | 0.930 | 39.82 | 0.913 |
| | RBF | **0.938** | **36.14** | **0.936** | **0.931** | **39.75** | **0.913** |
| | LS-SVM | 0.907 | 43.72 | 0.907 | 0.923 | 43.30 | 0.897 |
| Bastar Plateau zone | MLANN | 0.921 | 46.10 | 0.914 | 0.888 | 60.26 | 0.853 |
| | RBF | **0.924** | **43.35** | **0.924** | **0.894** | **51.39** | **0.893** |
| | LS-SVM | 0.891 | 52.63 | 0.889 | 0.876 | 58.00 | 0.864 |
| Northern hills zone | MLANN | 0.934 | 38.29 | 0.934 | 0.890 | 49.00 | 0.879 |
| | RBF | **0.939** | **38.17** | **0.934** | **0.911** | **42.80** | **0.908** |
| | LS-SVM | 0.896 | 48.64 | 0.893 | 0.870 | 54.30 | 0.852 |
| Chhattisgarh state | MLANN | 0.930 | 41.20 | 0.925 | 0.902 | 49.70 | 0.882 |
| | RBF | **0.934** | **39.20** | **0.932** | **0.912** | **44.70** | **0.905** |
| | LS-SVM | 0.898 | 48.30 | 0.896 | 0.889 | 51.90 | 0.871 |

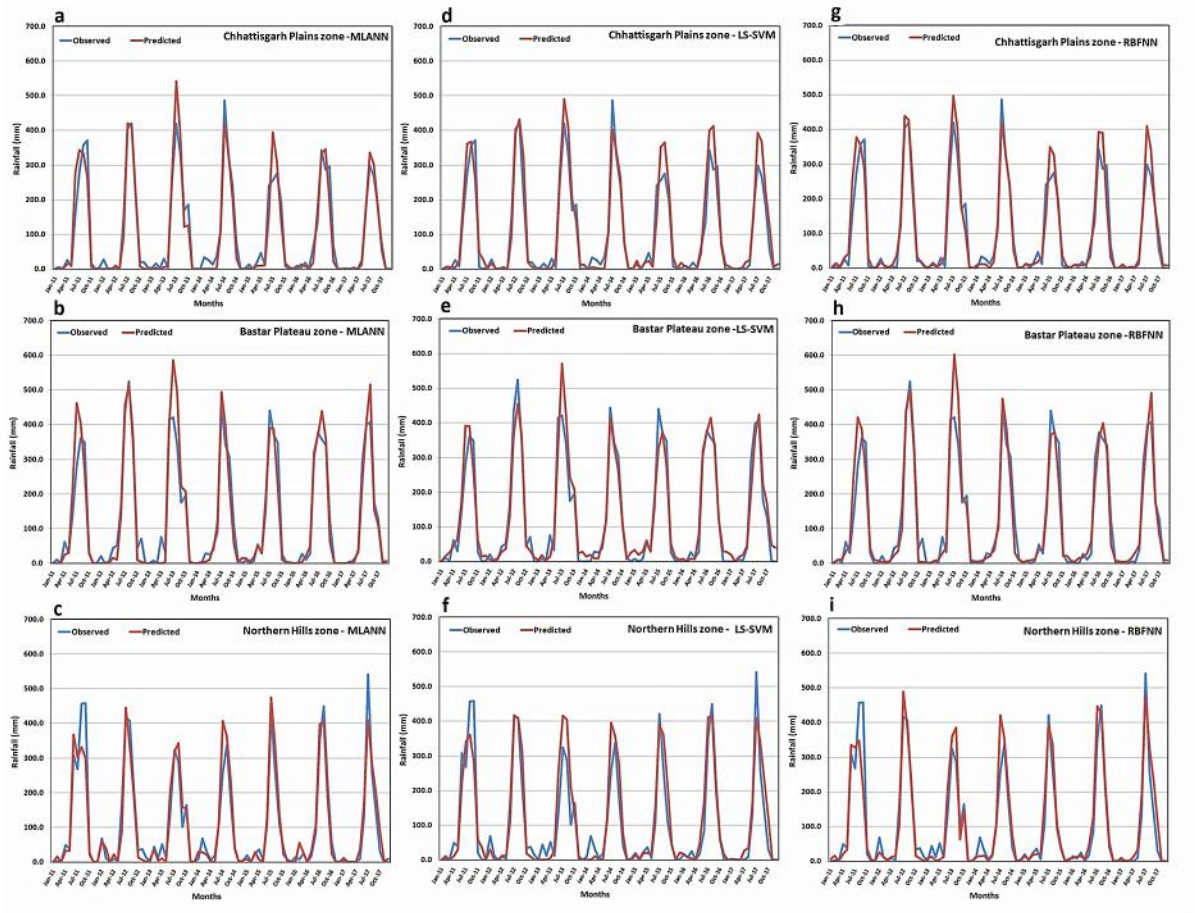
It is observed that, RBFNN models performed better in terms of $R^2$, RMSE and NSE in all the three ACZs as well as in the Chhattisgarh state and ranked first. Lower RMSE and higher $R^2$ and NSE values are highlighted by bold numbers in the Table 3. In Chhattisgarh plains, low RMSE values of 39.75 and 39.82 are obtained with RBFNN and MLANN models during the validation phase, whereas the same for LS-SVM are obtained 43.30, which is comparatively higher. At Bastar Plateau zone, RMSE ranges from a low of 51.39 for RBFNN to a high of 58.00 and 60.26 for LS-SVM and MLANN respectively. Similarly, in the Northern hills zone too, the validation performance of RBFNN models is superior (RMSE = 42.88) as compared to MLANN (RMSE =49.00) and LS-SVM (54.37).

Two more performance evaluation measures, $R^2$ and NSE are also computed for each model as model selection based on $R^2$ alone may mislead sometimes. In general, $R^2$ and NSE value close to one indicates higher prediction accuracy of any regression model. It can be seen from the Table 3 that in most of the cases, higher $R^2$ values close to 0.9 or above is obtained and hence, it becomes difficult to choose a particular model based on $R^2$ alone.

It can be seen that both $R^2$ and NSE in different ACZs during calibration and validation phase computed close to 0.9 or more with different machine approaches. This indicates that all the selected machine learning models have the potential of modeling monthly rainfall in different ACZs. However, among the machine learning approaches $R^2$ and NSE values obtained with RBFNN model is found superior as compared to MLANN and LS-SVM in all the three ACZs.

A comparison between estimated and observed monthly rainfall for different machine learning models under investigation in Chhattisgarh Plains, Bastar Plateau and Northern Hills ACZs are illustrated in Figure 4 (a to i). It can be seen that, estimated monthly rainfall during the validation period (2011-2017) in respectively ACZs matches closely with the observed monthly rainfall in all locations. However, as compare to MLANN and LS-SVM rainfall estimates, RBFNN rainfall estimates overlapped more precisely with observed rainfall in all the ACZs.

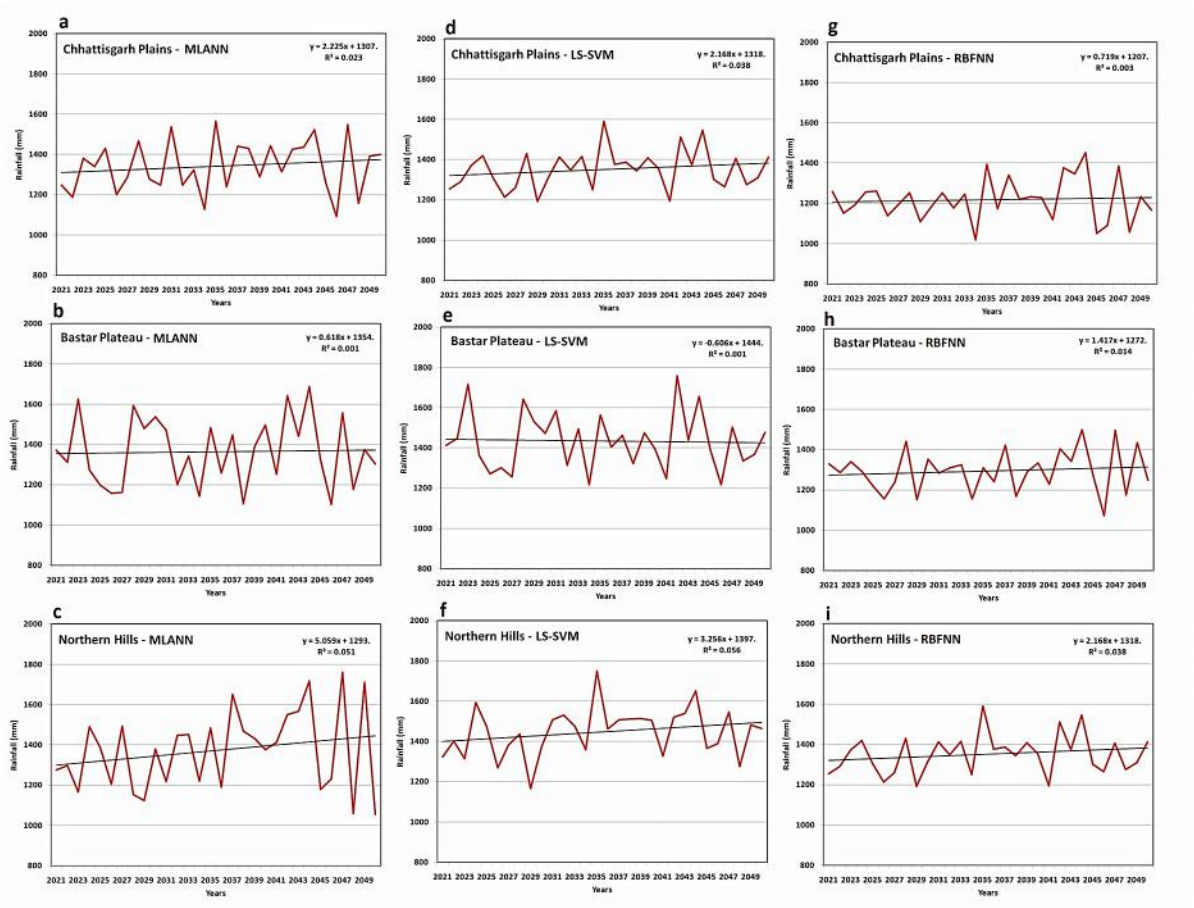
*Figure 4. Comparison of observed and predicted monthly rainfall using machine learning models (MLANN, LS-SVM and RBFNN) during validation phase (2011-2017) in different ACZs of Chhattisgarh state*




## Future Projections of Rainfall Using Hadcm3 B2 Emission Scenario

After the calibration and validation of the RBFNN, MLANN and LS-SVM models, model experiments are carried using large scale climate variables obtained through GCM outputs. For this purpose the feature vectors of predictor variable are prepared from HadCM3 GCM for B2 emission scenarios and simulations are carried out to obtain a downscaled result of future projected monthly/annual rainfall using the developed RBFNN, MLANN and LS-SVM machine learning models. The anticipated trend of future annual rainfall of Chhattisgarh Plains, Bastar Plateau and Northern hills ACZs for the period from 2021 to 2050 are obtained through RBFNN, MLANN and LS-SVM machine learning models and are shown in Figure 5 (a to i). The projected values of annual rainfall are represented as box plot arrangements to describe the decadal changes in future rainfall time series. The box plots of decadal rainfall pattern for the period 2021-2033, 2031-2040 and 2041-2050 are shown in Figure 6 (a to i). The middle line of the box plot signifies the median value while the upper and lower edges signify the 75% and the 25% of the data set respectively. The highest and lowest limits of the upper and lower vertical

*Figure 5. Linear trend of possible annual rainfall estimated by different machine learning models (MLANN, LS-SVM and RBFNN) for the period 2021-2050 using HadCM2-B2 predictors in different ACZs of Chhattisgarh state*

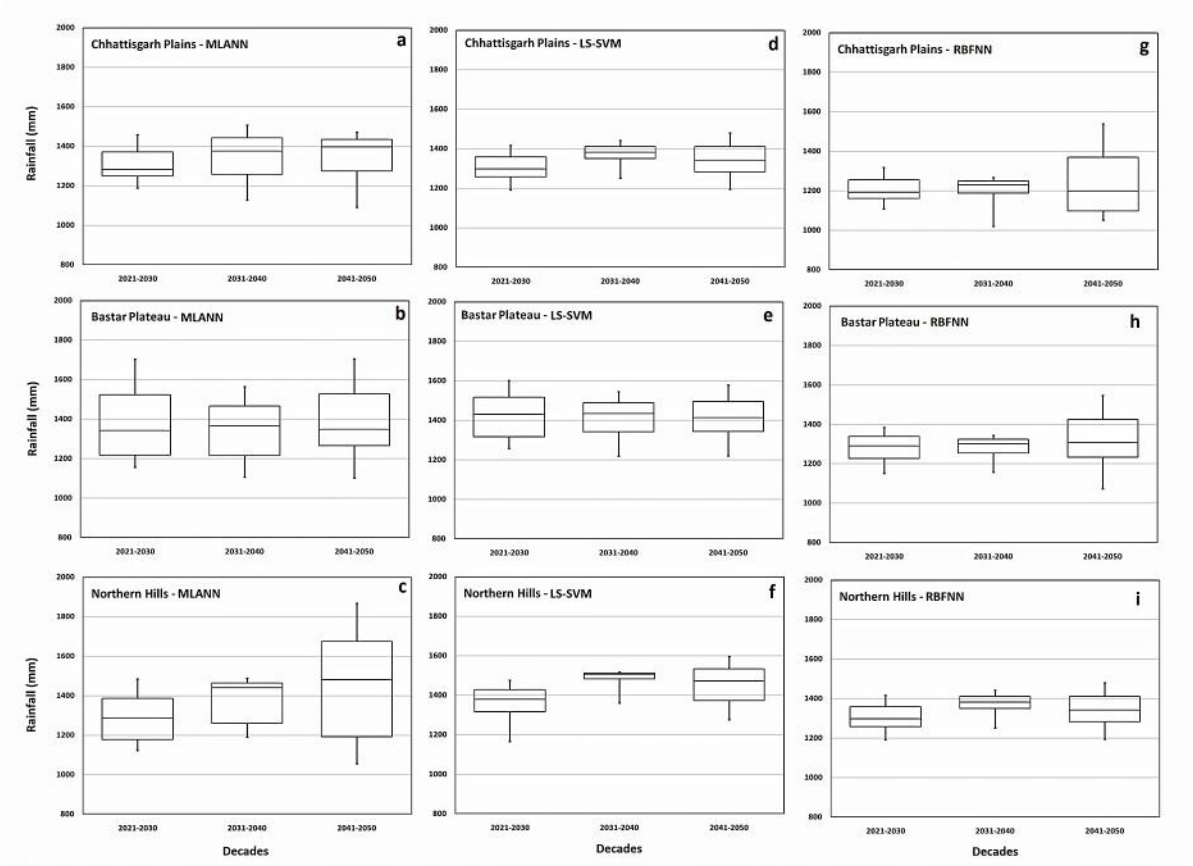



lines indicate highest and lowest values respectively. The black square depicts the simulated mean, and the straight-line shows the observed mean. The Figures, 5 & 6 and ultimate result show an increasing pattern in the future rainfall with some variations of increase and decrease within decades with most of the machine learning approaches in different ACZs. Considering the superiority of RBFNN model over MLANN and LS-SVM, future rainfall trends obtained with RBFNN model can be used for planning of regional level agricultural policies as well as for efficient water resource management under the changing climate of the region.

## CONCLUSION

In the present investigation the impact of climate change on rainfall pattern is assessed in three distinct ACZs in Chhattisgarh region of India. For this purpose the MLANN, RBFNN and LS-SVM machine learning techniques are used for statistical downscaling of the large scale climate variable from global

*Figure 6. Box plot of decadal changes in expected annual rainfall estimated by different machine learning models (MLANN, LS-SVM and RBFNN) for the period 2021-2050 using HadCM2-B2 predictors in different ACZs of Chhattisgarh state*




to local scale. For model development, calibration and validation of different machine learning approach are done using the long term NCEP variables as predictor variable and local scale rainfall time series as the target variable in different ACZs. The efficiency of the MLANN, RBFNN and LS-SVM models are evaluated by model performance criteria, i.e., $R^2$, RMSE and NSE, which shows the an excellent agreement between observed and estimated monthly rainfall during calibration and validation periods with all the machine learning approaches in different ACZs. Among the machine learning approaches considered for investigation, results obtained with RBFNN model is found superior over MLANN and LS-SVM models. The projected rainfall time series are obtained using HadCM3 GCM predictors for B2 emission scenarios with the help of proposed machine learning models. The changes in the rainfall pattern in different ACZs are discussed for the future periods i.e. 2030s, 2040s and 2050s. The projected rainfall time series shows an overall increasing trend of rainfall during the period 2021-2050 for all the ACZs. Despite uncertainties and bias always associated with the projected time series, but these machine learning models proved to be more feasible for downscaling rainfall as compared to other statistical downscaling techniques used in the past. Therefore, the present investigation will provide useful insight for planning better strategies for the management of water resources.

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# Chapter 15
# Performance Evaluation of Machine Learning Techniques for Customer Churn Prediction in Telecommunication Sector

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## ABSTRACT

*The principle objective of this chapter is to build up a churn prediction model which helps telecom administrators to foresee clients who are no doubt liable to agitate. Many studies affirmed that AI innovation is profoundly effective to anticipate this circumstance as it is applied through training from past information. The prediction procedure is involved three primary stages: normalization of the data, then feature selection based on information gain, and finally, classification utilizing different AI methods, for example, back propagation neural network (BPNNM), naïve Bayesian, k-nearest neighborhood (KNN), support vector machine (SVM), discriminant analysis (DA), decision tree (DT), and extreme learning machine (ELM). It is shown from simulation study that out of these seven methods SVM with polynomial based kernel is coming about 91.33% of precision where ELM is at the primary situation with 92.10% of exactness and MLANN-based CCP model is at third rank with 90.4% of accuracy. Similar observation is noted for 10-fold cross validation also.*

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## INTRODUCTION

Modeling of customer churn prediction(CCP) has been used in various sectors like different products, commodities, finance, social network, telecommunication, airlines, online gaming and banking(Athanassopoulos, 2000). The CCP models are developed to find out those customers whose probability or chances of churning or leaving the organization is high. It helps the organizations to focus seriously on those customers with some retention strategy. Hence it helps the enterprise to use efficiently its limited marketing budgets. Retention of consumers is highly profitable to companies because of three reasons: (1) finding out new customers is more costly than retaining existing customers(Athanassopoulos, 2000). (2) old customers are more loyal, do not attracted by other marketing competitors, require less budget to serve, and in the other hand they generate revenue for the organization through viral marketing (Farquad et. al., 2014), and (3) churn of customers means loss to organization due to reduction in sales(Ganesh et.al., 2000) . Therefore, most of the companies are now interested in retention of old customers than attracting new customers (Amin et. al., 2016). However, identification of active churners out of a large samples of customer base is a hectic job. For this reason, enterprises are now a days using predictive churn models to make their position in the competitive market.

Recently, (Höppner et. al, 2018) has proposed a expected maximum profit measure for customer churn (EMPC) using decision tree technique. Authors are employing social network analytics to predict customer churn in the telecommunication industry(Óskarsdóttira, et. al. 2017; Mitrovi et. al., 2019). The concept of classifier's certainty estimation using distance factor is presented for CCP in (Amin et. al., 2018). A predictive churn model by using big data has reported in (Shirazi et.al., 2018). ProfLogit, a classifier uses genetic algorithm during training step to maximize the EMPC has suggested in (Stripling et. al, 2018). Three new profit-driven strategies for CCP using support vector machine (SVM) is given in (Maldonado et. al. 2019).

Presently, organizations in the telecommunication sectors (TCS) have adequate data about their consumers where data mining can be applied. This enables the machine learning group to develop various predictive models to handle the CCP in TCS (Amin et.al., 2016). Prediction of churn is a binary classification problem. Using the historical data of the customers the ML models can be trained so that it can able to tell whether a new customer will churn or not. This motivates the authors to develop models using various ML techniques. The main objective of this paper is to study the performance of different machine learning techniques for the churn prediction of telecommunication data. The chapter has used Support Vector Machine (SVM), Multilayer Artificial Neural Network (MLANN), Decision tree (DT), Discriminant Analysis (DA), Naïve Bayesian classifier and Extreme Learning Machine(ELM) for developing CCP models and done the comparison between these models to find out the best model.

Rest of the chapter is organized as follows: Section 2 deals with brief description about each of the machine learning techniques used in this study. Development of a churn prediction model using multilayer artificial neural network is described in Section 3. Data collection and simulation study is given in Section 4. Discussion on results is outlined in the Section 5. Finally conclusion of the chapter is presented in Section 6.

## Methodology Used

The churn prediction model is a binary classification model. Means there is only two classes whether the customer will churn (represented as 1) or not churn(represented as 0). For this binary classification

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purpose, the entire dataset is divided into training set and testing set. The training set is used to train or develop the classifier using the error correction method and then the classifier is validated using the testing samples. In this chapter classifiers like Support Vector Machine (SVM), Multilayer Artificial Neural Network (MLANN), Decision tree (DT), Discriminant Analysis (DA), Naïve Bayesian classifier and Extreme Learning Machine(ELM) are used. A brief description of the individual classifiers is as follows:

## Multilayer Artificial Neural Network (MLANN)

Multilayer artificial neural network (ANN) is a nonlinear structure that mimics the conduct of biological brain. It includes a couple of interconnected layers and wide variety of processing elements known as neurons in every layer. Generally ANN consists of three layers: input layer, hidden layer and output layer. In churn prediction model development of a hard and fast of input neurons are defined which can be activated by way of the inputs of the training set. After elevated with weight values the inputs are transformed by way of a activation function. The outputs of these neurons are then exceeded to other neurons and the procedure is repeated until the desired result is obtained. Learning of the MLANN takes place by means of updating the weights between the neurons the usage of BP (Haykin, 2016) algorithm.

## Support Vector Machine (SVM)

SVM is a supervised technique (Han and Kamber, 2012) used more often than not for classification and regression analysis. When few records points are given belong to two groups and we want to realize to which group a new record will belong. Then it's miles a linear classification problem. SVM considers each information factors as N dimensional vector and try and separate it by way of drawing N-1 quantity of traces or hyperplanes. The hyperplane having most margin from nearest statistics point of both classes is chosen and called maximum marginal hyperplane (MMH). For nonlinear type the SVM makes clustering or agencies of the information factors and tries to restoration a new statistics factor to one in all these businesses and for this reason does the category. Kernel capabilities are used for nonlinear class of information factors. The SVMs are employing Gaussian Radial Basis, Sigmoid and Polynomial characteristic as kernels. Its primary set of rules is based totally on structural Risk minimization principle (SRM). Here the error rate of a learning device is considered to be bounded by the sum of the training error rate and a term relying on the Vapnik Chervonenkis dimension(Mitra and Acharya, 2004).

## Decision Tree (DT) Classifier

The decision tree(DT) (Höppner et.al.,2018) is a supervised and parametric method typically used for classification and regression. Based at the training records features it creates simple selection rules. The tree hence received is employed to predict the goal magnificence of checking out set. Every tuple of the training set contains quite a number of features and a category label. Each attribute within the training pattern corresponds to one node in the decision tree and every leaf node represents a class label. The mastering system divides the samples set into subsets iteratively at the attributes or till there is no further records gain. The information gain (IG) of a discrete random variable Y with probability mass function P(Y) is

$$I(Y) = -\log_2 P(Y) \tag{1}$$

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Entropy is a measure of uncertainty in case of a random variable. It helps to pick out the attribute with maximum IG for further division decreasing the uncertainty at that instant. The entropy of the random variable is given as

$$H(Y) = E[I(Y)] = E[-\log_2 P(Y)] = -\sum_i \log_2 P(y_i) \tag{2}$$

## Discriminant Analysis(DA)

Discriminant analysis (DA) (Dornaika et. al., 2020) is a statistical approach which is used for classification when the dependent variable is categorical and independent variables are interval in nature. Categorical variable means the variable divided into different categories or classes or groups. DA develops discriminate functions which can be are linear combos of independent variables that may discriminate properly among the dependent variables or target classes as given in (4).

$$DF = w_1 Y_1 + w_2 Y_2 + w_3 Y_3 + ... + w_n Y_n + c \tag{3}$$

where

DF = discriminate function
w = the discriminant coefficient or weight for that independent variable
Y = respondent's score for that independent variable
c = a constant

The weight values of the variable are selected in such as manner that it may maximize the class differences. It is a parametric technique to decide which weightings of quantitative variable nice discriminate between or more than two group of cases. The maximum quantity of functions is either the variety of predictors or the wide variety of groups minus one.

(E) K-Nearest neighbor: K-nearest neighbors(K-NN) (Han and Kamber, 2012) is a simple non-parametric algorithm that holds all training tuples and wait till it gets a checking out tuple, hence referred to as a lazy learner. On getting a new tuple for classification it classifies the new tuple primarily based on a distance measure. Here Euclidean distance is used as the space measure. A tuple is classified via majority vote of its neighbors. The tuple is assigned to the class that is most common among its K nearest neighbors measured by way of a distance function. When K = 1, then the new tuple is definitely assigned to the class of its nearest neighbor.

## Extreme Learning Machine (ELM)

Extreme learning machine (Huang, 2006) is a feed forward network with single hidden layer whose hidden layer neurons and the enter weights are randomly selected. The output weights are determined by the use of Moore-Penrose pseudoinverse method so that the output of the network is equal to the goal or desired value. The network is strong and faster because of its low computation. It completely overcomes the hassle of how to do tuning of learning rate, a way to pick wide variety of epochs and