Optimization of Hydrogen Production from Sewage Sludge using Machine Learning Methods Integrated with Genetic Algorithm

By

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Dedication

To my very Supportive, Loving,
and
Caring Family

Acknowledgement

All praise and eminence are due to "ALLAH," the undisputed architect of this world, who gave us the capacity for comprehension and sparked our curiosity about the planet as a whole. Warmest welcomes to the supreme ruler of this world and the hereafter, "Prophet Mohammed (PBUH)," a source of knowledge and benefits for all of humanity as well as for Umah.

I would like to convey my profound gratitude to **Dr. Muhammad Nouman Aslam Khan** for his leadership, motivation, helpful suggestions, dedication, and thorough oversight during the project. For his aid during my programme, I am appreciative to him. It was a fantastic privilege and an honour to work under his direction. I shall cherish this memory for my entire life.

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(Zeeshan Ul Haq)

Abstract

Hydrogen production from the supercritical water gasification (SCWG) of sewage sludge (SS) is a sustainable and efficient process. However, the challenging and intricate task for the experimental technique is to find out the correlation between proximate, ultimate analysis and gasification conditions with Hydrogen production. This process is complicated, expensive and requires many experimental techniques. To accurately predict and analyze the effect of input parameters on SCWG of SS process economically, an efficient model must be developed. Considering economic viability and ensuring optimization of hydrogen yield, this study considers four different machine learning (ML) models (Support Vector Machine, Ensembled Tree, Gaussian Process Regression (GPR), Artificial Neural Network) to predict, analyze the optimal model, and evaluate SCWG performance. The results suggests that GPR is favored for predicting Hydrogen yield ($R2 > 0.997$, RMSE 0.093), and is highly recommended for dealing with complex variable-target correlation. The partial dependence plot shows that temperature, moisture content and pressure are among the effective parameters of SCWG. Furthermore, optimization techniques such as genetic algorithms are incorporated to optimize hydrogen production by tuning the ML hyperparameters. Additionally, a Graphical User Interface was developed by utilizing the optimized GPR model for ease in computing Hydrogen yield.

KEYWORDS:

Sewage Sludge, Artificial Intelligence, Genetic algorithm, Optimization, Supercritical water gasification, Machine learning.

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Nomenclature

Sewage Sludge (SS)

Supercritical water gasification (SCWG)

Artificial Intelligence (AI)

Machine Learning (ML)

Gaussian Process Regression (GPR)

Support Vector Machine (SVM)

Artificial Neural Network (ANN)

Genetic Algorithm (GA)

Graphical User Interface (GUI)

Chapter 1:

Introduction

1.1.Sewage Sludge

Wastewater treatment produces sewage sludge, which can be utilized to generate power and heat [1]. Concerns about socio-economic and environmental issues are driving interest in alternative sewage sludge treatment and disposal [2]. Also, sewage sludge contains several organic and inorganic toxic chemicals that require long-term treatment [3]. Handling and disposal are expected to account for around half of the costs of operating secondary sewage sludge treatment processes in Europe [4]. The volume and tonnages of sewage sludge produced annually in the USA, China, and Europe were calculated at 240 MT (2010) [5]. In 2013, China produced 6.25 MT of dry solids sewage sludge, of which only 25% was correctly processed. Globally sewage sludge production was 45 dry MT in 2017 [1, 6-8]. In 2015, five EU nations (Spain, Italy, Germany, France, and UK) produced 75% of all sewage sludge [4]. In the same year, China and Taiwan produced up to 40 MT and 77,000 T sewage sludge, respectively [8, 9]. Its high moisture content (almost 98 wt%) prevents its use in many applications. However, thermal processing requires moisture content below 15% [10]. Before using thermochemical techniques, different drying processes are dependent on the moisture content and operational cost. Thermal drying, natural drying, bio drying, and mechanical drying [11] are all available options. In contrast to thermal drying, natural drying can use solar energy to minimize moisture content. A bio-drying process is analogous to composting, which takes days to dehydrate. Sludge's significant heavy metal content is a second important trait. Sludge is rich in nitrogen and phosphorus, which can be used as fertilizer in agriculture and land applications. A study shown in Figure 1 by the EU, Japan, Chine and U.S countries found that sewage sludge might be used in building materials, incineration, anaerobic digestion, and land applications depending on moisture content, contaminants, and socio-economic considerations. Incorrect dumping might also result in considerable sewage sludge disposal. Globally, the economic development of countries is linked to the disposal and treatment of sewage sludge [12, 13] .

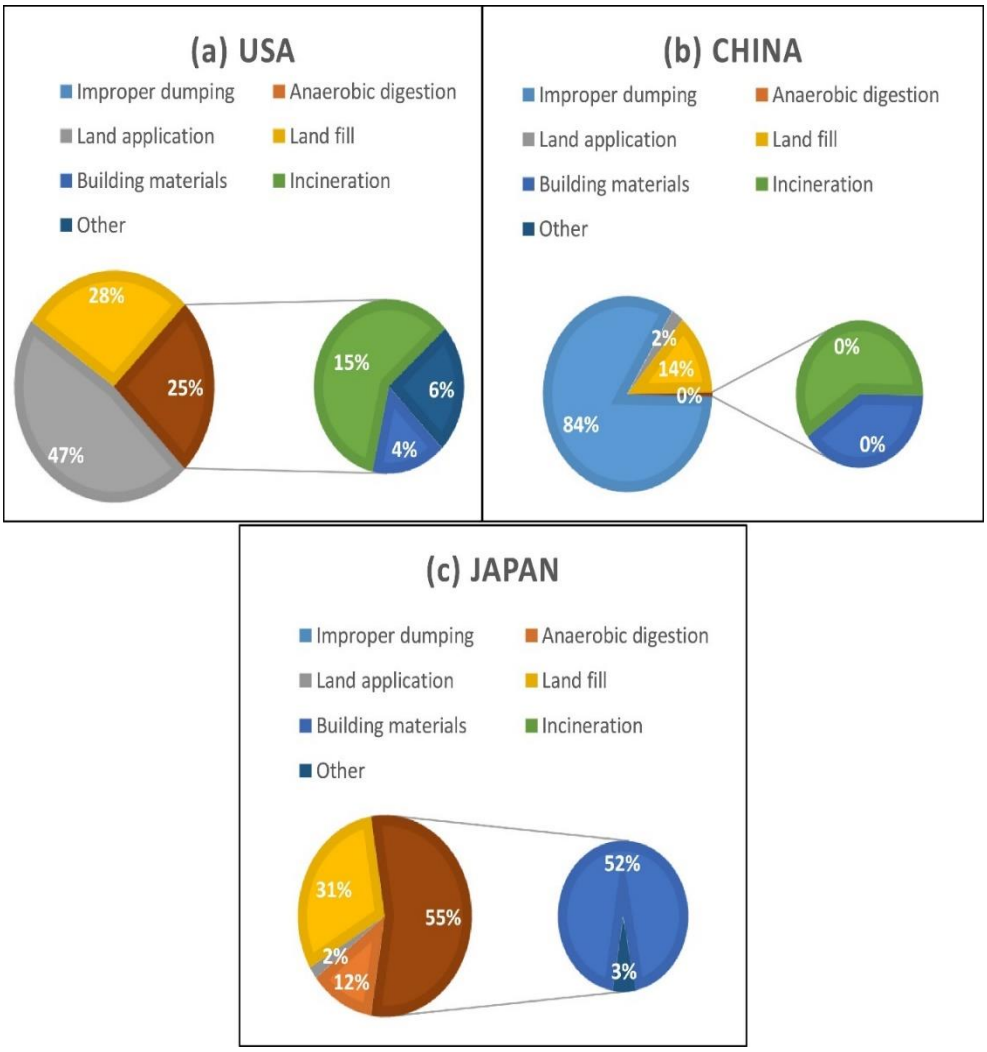

Figure 1: Sewage sludge usage in different countries [13]

Thermochemical conversion processes like pyrolysis and gasification have been recommended as alternatives to the present most effective approaches [14]. While thermo-chemical conversion requires complex equipment and processes, it may be more efficient and reduce volume than other methods of treatment. Recent research compared the benefits and drawbacks of microbiological and thermochemical approaches. Compared to thermochemical methods, anaerobic digestion demands a longer solids retention time, more room for the digesters, a smaller product diversity, and more capital investment [15]. Process intensification, sludge pollutants, resource recovery, new treatment procedures, and costs are now influencing sewage sludge management [16]. Different processes for sewage sludge gasification treatment is

shown in Figure 2 [17].

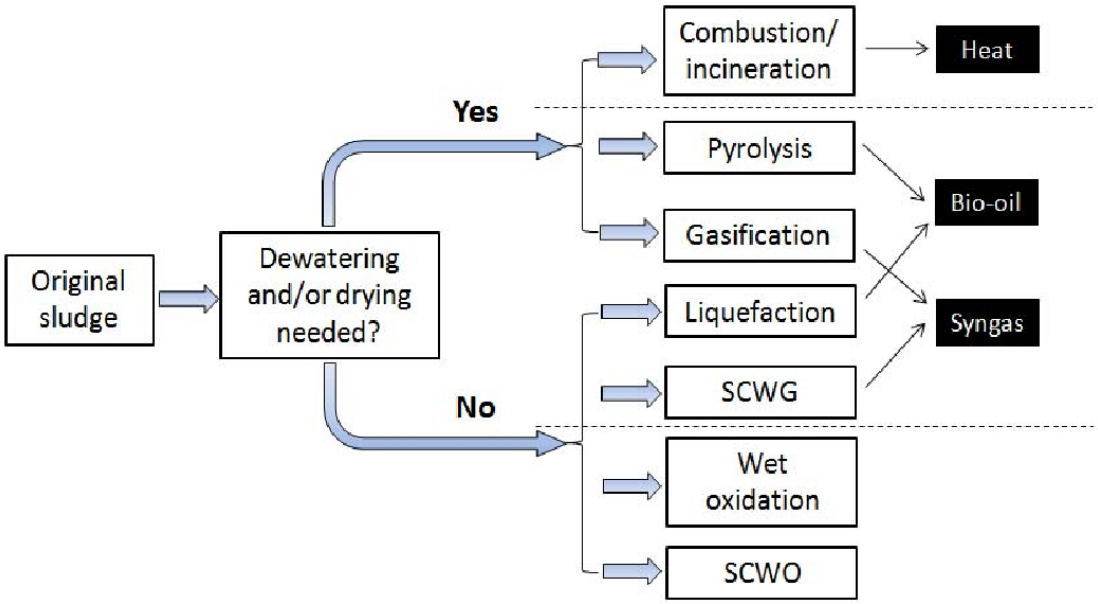

Figure 2: Sewage Sludge formation during wastewater treatment [17]

1.2. Characteristic of Sewage Sludge

1.2.1. Moisture Content

Three types of sewage sludge that can be used to generate energy: primary, waste activated, and digested [18]. In water treatment facilities, the cleaned water is extracted from the sewage sludge, which is slurry with high water content. The moisture content of sewage sludge must be reduced to a minimum before it can be used for disposal or energy recovery. Different drying processes are used sewage sludge including bio-drying, mechanical drying, and thermal drying. Tertiary thermal dryers include rotary and tunnel dryers. For mechanical dryer filter presses with belt or vacuum dryer are used [11, 19] . Wood, pre-dried feed stocks, cotton, and straws are widely used as bulking agents in co-processing sludge. Bio drying is also utilized for sewage sludge, where fungi and bacteria help remove water. The air flow rate, initial moisture content, temperature, time, and process are critical. However, it takes longer than thermal drying and removes less moisture than thermal drying [20, 21]. Under ideal processing conditions, electro-osmotic dewatering with bio drying could decrease water content from 83 to 60% in minutes [22]. Wet-drying methods can minimize pathogens in sewage sludge [23]. Solar radiation can be used to dry sewage sludge, however it requires exposure of several days and is dependent on weather.

Also, closed solar drying outperforms open solar drying [24]. Thermal drying is the best method for producing energy and fuels from sewage sludge [11]. Thermal drying is clearly advantageous for decreasing harmful pathogens and other toxic pollutants as well as increasing drying rate. Nitrogen may be recovered through continuous thermal drying at temperatures between 160 and 200 °C [25]. Water removal efficiency can be determined using energy and mass balances, which can suggest the drying process's feasibility. Conditioners or additions like CaO are widely used to dry and condition sewage sludge before employing it in thermochemical processes.

1.2.2. Heavy Metals and Organic Pollutants

Heavy metals as well as other harmful organic pollutants in sewage sludge present significant potential barriers to consumption. Industrial and municipal wastewater is treated to remove toxins, but sewage sludge continues polluted by a wide spectrum of organic micro contaminants [26]. SS is a mixture of bacteria, inorganic components, and water. Many countries have legislation to manage pathogens in sewage sludge. Undigested organic elements include protein, peptide, lipid, polysaccharide, plant polysaccharides with aliphatic structures or phenolic, and organic pollutants [27, 28]. Toxic alkyl-phenol ethoxylates are widely employed as detergents in industrial and commercial products in the United States [29]. Most research on sewage sludge's environmental impact focuses on a few chemicals or families of compounds. Some researchers have examined major extraction, cleaning, and instrumental approaches used to identify new poisons [30, 31]. So, before dumping sewage sludge or using it in agriculture, it must be thoroughly tested for developing pollutants. However, only a few countries have stringent limits for these contaminants. The heating values of activated and raw sludge were reported to be 16-23 MJ/kg and 23-29 MJ/kg, respectively [32]. The data of primary and secondary SS illustrate that energy-rich products can be produced.

Chapter 2:

Literature review

2.1.Literature Review

In recent decades, public awareness of the benefits of renewable energy sources has grown fast to fulfill the world's growing energy demand as a foundation for the development of modern world and the rapid growth of the world's population [33, 34]. Inadequate conventional production fuel supply to satisfy increasing energy demands, as well as a variety of other concerns affecting the global population have sparked considerable international interest in developing new solutions for energy conservation and environmental preservation in power generating. According to Olabi et al. [35] using renewable energy resources to reduce reliance on conventional fuel resources and provide a variety of energy demands for larger and smaller scale energy conversion systems is the most important solution.

Evidently, in the future, fossil fuel availability will be a global issue since the terminal decline in its resources and current higher investment risks caused by competition from clean renewable energy resources, tough government, and security targets as shown in Figure 3 [36] . To avoid the use of fossil fuel, an increasing trend has been observed, in which resources like waste biomass from different sectors including, food, agriculture and industrial have been used [37]. Renewable energy has recently remained the most preferred alternative for reducing reliance on non - renewable fuels. In the context of renewable energy, biomass belongs to any organic matter that is recyclable and sustainable, such as animal manure, plants, agriculture fruits and vegetables, food processing by-products, and municipal waste. Because of the focus on biomass in the power mix, it is now the world's fourth largest contributor to energy supply, behind oil, coal, and natural gas [38]. According to Khan [39], biomass is currently an significant renewable energy resource. Because biomass may be turned into gas, liquid, and solid fuels, it offers several distinct advantages. Apart from electricity generation, biomass may be used to make a wide range of chemicals, and biomass has a lot of promise because of its abundance and reasonably high heating value. Furthermore, substituting biomass for fossil fuels as a renewable resource may be an option for reducing net CO2 pollution in the environment.

Biomass is carbon-neutral, which means that the net CO2 released during combustion is used by plants through photosynthesis [40].

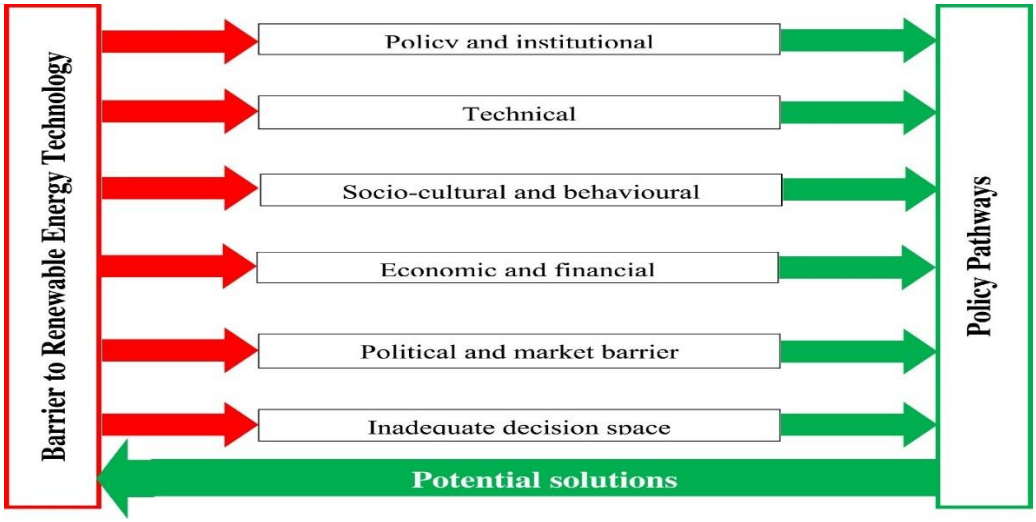

Figure 3: challenges to the use of renewable energy sources [36] .

Sewage Sludge, which is generally appeared as by-product from wastewater treatment plant, contain high calorific value organics [41], if not, timely managed can readily cause secondary pollution, such as unwanted emissions (leachate and odor) into the atmosphere, and heavy metal accumulation in soil due to high moisture contents and complex organic composition [42, 43]. The deposits of SS will continue to rise in coming decades due to factors like urbanization, industrialization, and population growth [44]. However, if biologically treated sewer sludge can have a high calorific value depending on the processed wastewater [45]. Common SS treatment procedures in past were incineration, composting and most common landfills [41]. Although most of these traditional techniques allow for a partial recovery of nutrients and energy, they fall short of fully using the sludge's potential as shown in Figure 4 [46] . However, recently different technological approaches have being established in which green hydrogen have been produced from renewable sources including Electrolysis, Photocatalysis, Thermochemical cycles, Plasmolysis and Bio H2. However, their current productivity and cost competitiveness for downstream applications are still lacking due to its high energy requirement, also these method accounts for a very small portion of global hydrogen generation [47].

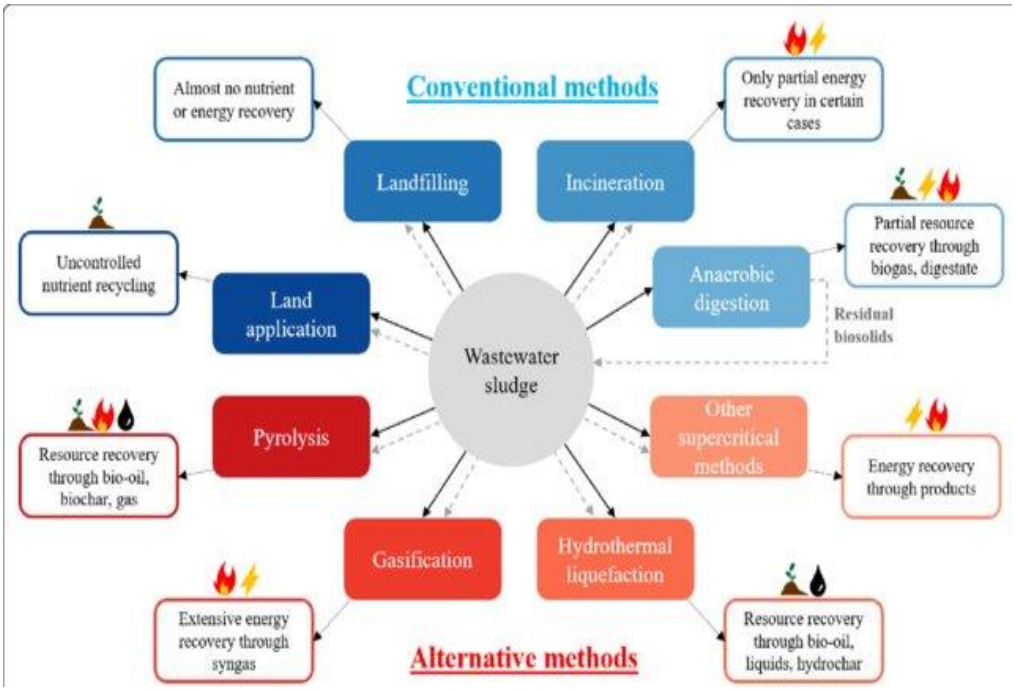

Figure 4: Conventional vs alternative processes for conversion of sludge [46]

An organic solid or liquid component is transformed into a solid phase, gas or vapor phase during gasification process of biomass. Gas phase, normally described as "syngas," has a higher heating value that can be used to produce electricity or biofuels. The organic unconverted portion and inert material left in the processed biomass make up the solid phase known as "char." This process, which involves an oxidation process of the carbon in the feeding material, is often carried out by means of a gasifying carrier such as oxygen, steam, air, N2 flow or carbon dioxide. A strategy to increase the conversion of biomass to produce energy and enable biomass utilization is gasification of biomass. As people become more aware of the potential consequences of fossil energy on the climate and as oil costs continue to rise, biomass gasification methods are being developed at a faster rate. [48]. Sewage sludge thermochemical conversion is given in Figure 5 [13].

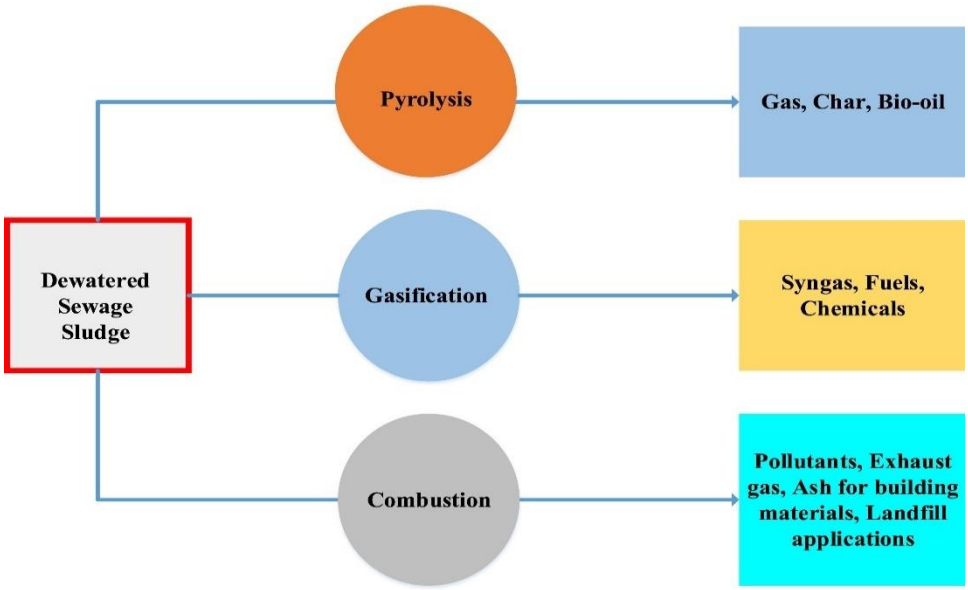

Figure 5: Thermochemical Conversion of sewage sludge into valuable products [13]

Raising the operating temperature during biomass thermal conversion processes (typically above 900 °C) allows tars to be broken down into lighter species. Between 700 and 1000 °C, CH4 and Co concentrations rise linearly whereas H2 concentrations rise exponentially [49]. It is possible to gasify organic feed in a hydrothermal medium at various temperatures, pressures, or even in the presence of catalysts. If the temperature and pressure are subcritical (225-265 °C and 2.9-5.6 MPa), it can be a catalyzed gasification process [50]. When the feedstocks' moisture content surpasses 30% weight percent, it has distinct advantages against the other conversion pathways in terms of heat consumption. On the basis of heat consumption efficiency, Figure 6 adapted from [51] compare other biomass conversion processes with SCWG methods.

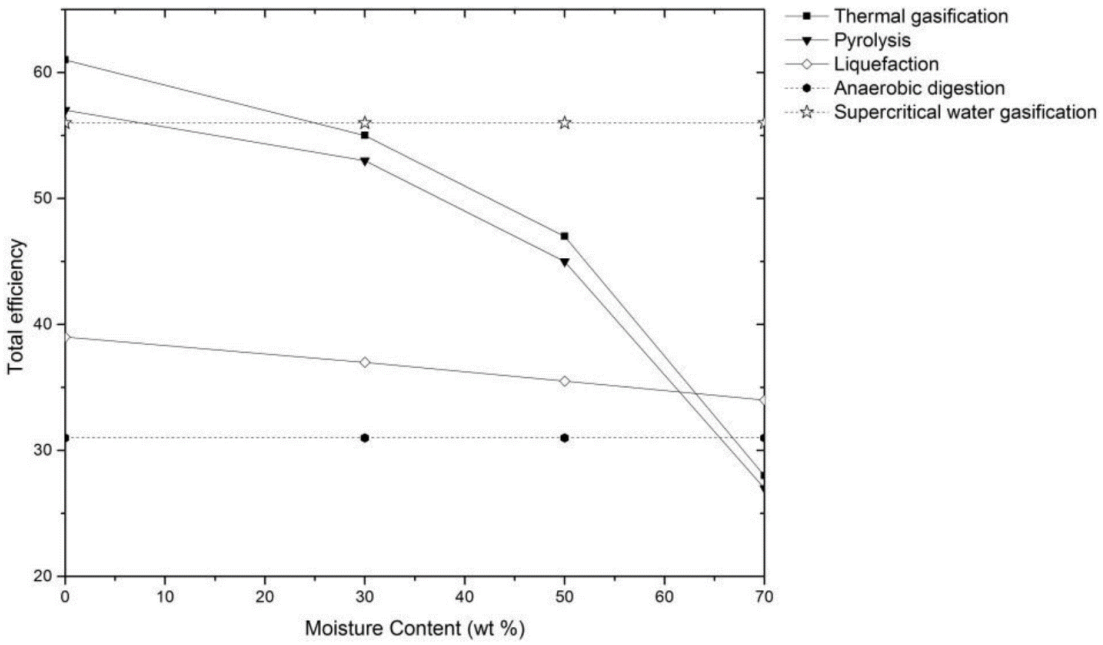

Figure 6: Moisture contents effects on total efficiency for different process [51]

Compared to other gasification techniques, SCWG of SS is an efficient process which not only reduces the need of drying but also regulates heavy metals using compressed and hot water at critical or near-critical temperatures (374.3 °C and 22.1 MPa) [52]. Biomass can be super critically gasified using various feedstocks and under various processing conditions. From minimal biomass feedstocks to complicated biomass feedstocks with or without a catalyst can be used as the feedstock under batch or continuous procedures [51].

In SCWG of SS, water acts as a reaction medium and shift the equilibrium towards H2 production in water-gas shift reactions [53, 54]. The advantageous physical characteristics of water and how they adjust in the supercritical area, which triggers water to serve as a catalyst and as a solvent, are the primary drivers of research interest on supercritical water. Additionally, water serves as a reactant in hydrolysis processes [55]. The dielectric constant, density, and viscosity of the water have a significant impact on biomass gasification. Water's physical characteristics substantially change above critical point, where it behaves like a homogenous fluid phase. the viscosity of water become like gas viscosity and density become like liquid at its supercritical condition, these are the two characteristics that improve mass transport and solvation qualities, respectively as shown in Figure 8 and 9 adapted from [51, 56]. Because of its dielectric constant, liquid water performs well as a polar solvent at normal test conditions (25 °C and 0.1 MPa). It is highly soluble in a wide

range of substances, including electrolytes, but poorly miscible with gases and hydrocarbons. The dielectric constant dramatically drops as water hits its supercritical phase. As a result, water begins to act like that of an organic, non-polar solvent, which has the effect of making inorganics poorly soluble and completely miscible with vapors and many hydrocarbons. Phase boundaries are no longer present due to its miscibility. Because of this lack, water and organic chemicals react quickly and completely in homogeneous phase [57].

Sludge gasification is modelled using three basic types of modelling approaches: kinetic models, equilibrium models, and computational fluid dynamic models [58]. CFD models may replicate a variety of physical processes, but they demand a lot of processing power and very specific data (geometry, materials, and boundary conditions). Kinetic models are suitable for simulating the effects of reactors process development parameters, but their conceptual modelling is significantly more difficult [59]. In a fluidized gasifier, petersen et al. [60] established a kinetic model for gasification of sludge that took into account both the fluid mechanics of the circulating bed and a wide range of gasification processes. kinetic rate equations for this model required axial gas concentration and temperature measurements.

Different studies were carried out to show the impact of parameters on SCWG of SS, including an experimental study discusses the effect of different catalysts, temperature and feed concentration on SCWG of SS [61] . Thermodynamic study illustrates the effect of feed concentration and temperature on the process [62]. The thermodynamical study is easy and economical, but it is difficult to achieve the condition in practical gasifiers, ultimately resulting in low prediction accuracy. Also, the Kinetic study needs a significant amount of time in formulation. However, ML models as compared to kinetic and thermodynamical studies uses the actual conditions of an experiment to show the effect of input parameters on the SCWG, but also predict the hydrogen yield accurately without taking assumptions and too much time [63]. Elmaz et al. [64] in his study collected data from the fixed bed gasifier and utilized four regression model (Multilayer perceptron, polynomial regression, Support vector regression, and decision tree) on the gasification process of biomass to predict five output ($HHV, CO_2, CO, CH_4, and\ H_2$) and compared the results of non-stoichiometric and stoichiometric studies. Decision tree and multilayer perceptron were among the best model with R2 ~ 0.9. Tang et al. [65] successfully predicted the composition and gas yield by utilizing support vector machine and random forest and

was recorded that biomass composition can contribute more than pyrolysis condition in case of CO and CH4 prediction. Additionally, pearson coefficients map shows the non-linear correlation between different feature as shown in Figure 7 adapted from [65]. Balsora et al. [66] have developed artificial neural network model from 704 data point for the prediction of pyrolysis kinetic utilizing the biomass composition as inputs and Garson equation was used to study the relative significance of input features on pyrolysis kinetics.

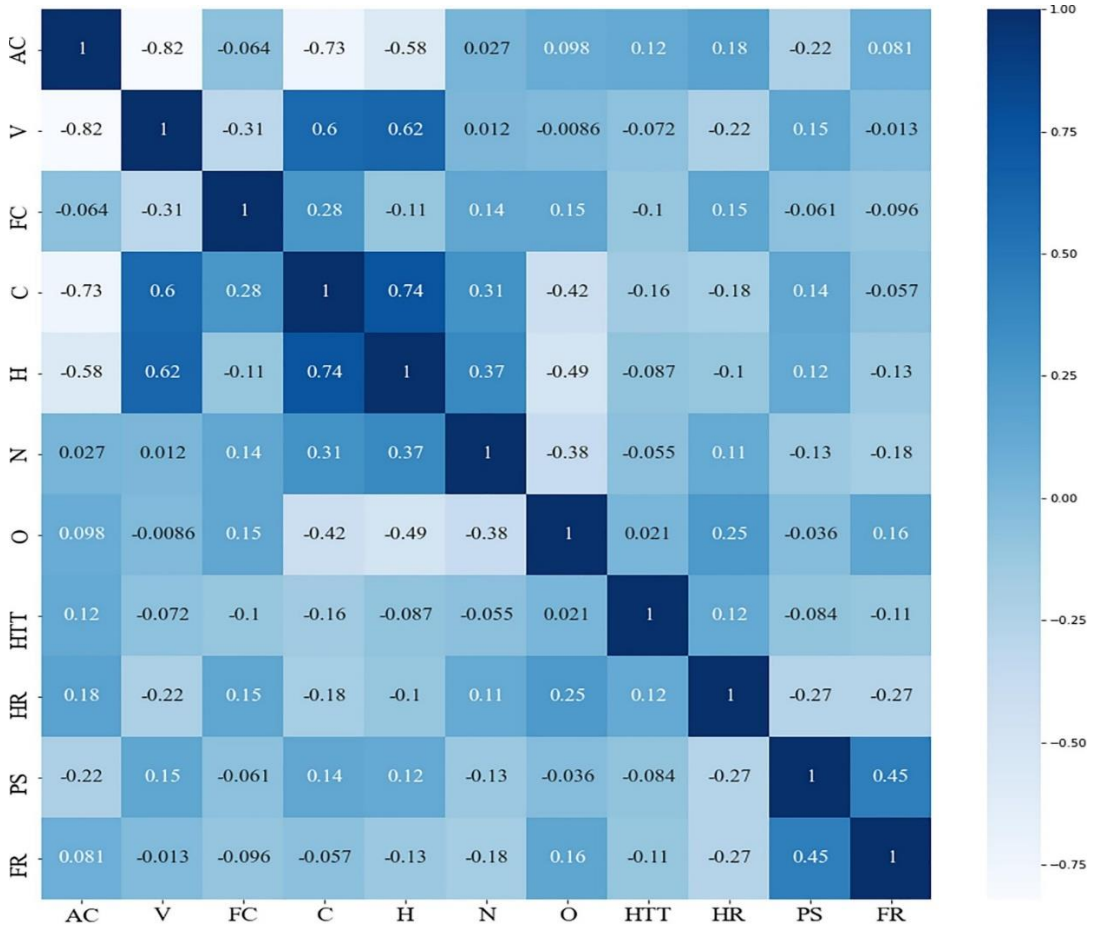

Figure 7: Pearson coefficients between variables [65]

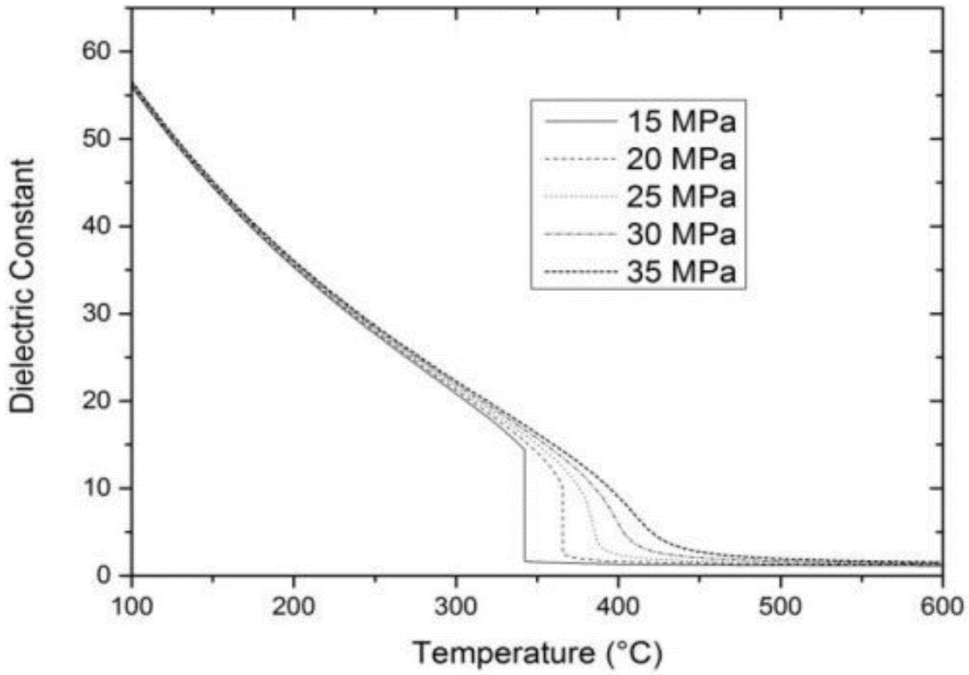

Figure 8: Dielectric constant of water at different temperature and pressure [51]

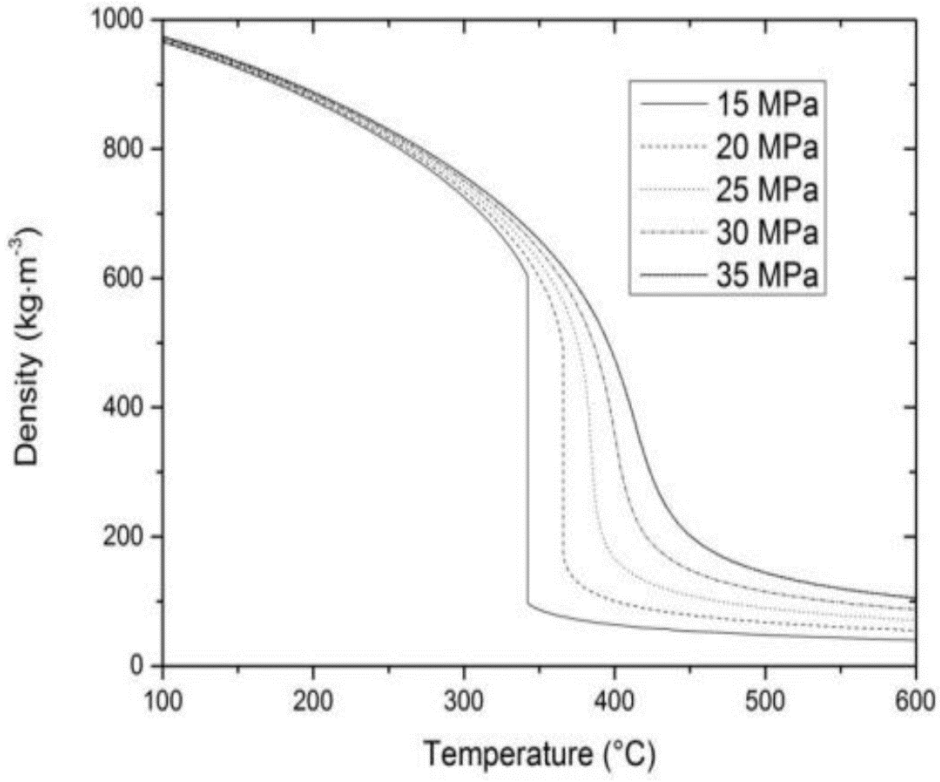

Figure 9: Density of water at different pressure and temperature [51]

To determine H_2 yield output and its relationship to input parameters (proximate, ultimate composition and gasification conditions) through the conventional methods requires extensive trailing, which is time consuming, labor-intensive, and expensive. To effectively study their combine effects on the H2, it is essential to study the

behavior of supercritical water gasification parameters with integrated consideration of SS composition utilizing artificial intelligence techniques that is machine learning (ML), deep learning (DL), and data mining. Machine learning-based models offer a practical solution in which process data is utilized to develop a model that is used for optimizing, automation, and surveillance [67]. Also, in comparison to relying on complex rule-based programs, machine learning model is based on experimental data and is a highly developed approach established on scientific computation and uses a data driven technique for learning and detecting patterns [63].

2.2. Problem Statement

Despite the fact that there are numerous study papers on gasification of sewage sludge to produce hydrogen gas. But the majority of the literature is concerned with designing and perfecting the gasification process through various experimental and mathematical techniques. The modelling of hydrogen production from sewage sludge integrated with machine learning models has not yet been covered in any literature. In a similar vein, no one has concentrated on the hybrid approach of the machine learning models integrated with optimization technique to predict the hydrogen yield. Intelligent systems have therefore been very interested in predicting the yield and increasing the effectiveness of energy management systems.

2.3. Objectives

The following will be primary contribution of this work:

- Genetic algorithm-based features selection
- Prediction of Hydrogen yield using machine learning methods.
- Optimization of model
- Influence of various parameters on hydrogen yield

Chapter 3:

Overview of developed models

This section provides a broad review of all the modelling techniques developed for this thesis. These modelling techniques include machine learning (ML) models, genetic algorithms (GA), and artificial neural network (ANN).

3.1. Genetic Algorithm

An evolutionary algorithm called a genetic algorithm (GA) imitates the course of biological evolution. In 1975, Holland proposed a theory for genetic algorithms. Darwin's theory of evolution, which simulated the preservation of better species and their genes, had an impact on GA. Numerous researchers have utilized generalized estimating equations [20] to assess the resolution of challenging issues whose performance parameters lack the qualities of continuity and differentiability [68, 69].

A genetic algorithm is a population-based feature selection algorithm that works with a group of solutions rather than selecting a single solution. Initially, the population is chosen, and each solution is encoded as a chromosome of Genes or bits. Every single chromosome has its fitness value and when combined they are called a population- the population is a set of solutions. A generation is a population at a certain time. The fitness function is a key parameter in the Genetic Algorithm as it specifies the problem to be optimized. The fitness of a chromosomal pair is employed to reproduce offspring [70].

It is an inhabitant's algorithm that is built on the ideas of genetic inheritance and natural selection. Each solution stands in for a chromosome, and each parameter denotes a gene. GA measures each population member's fitness using an objective function called fitness. A selection technique is used to arbitrarily select the best options in order to enhance poor solutions. Because probability and fitness are related, this operator is a little more likely to choose the optimal options (objective value). Additionally, there is a higher likelihood to avoid local optima while choosing incorrect answers. It suggests that excellent alternatives can be removed with the aid of other solutions if they get trapped in a local solution. Until an optimal solution is established, an extreme integer of repetitions or population is comprehended, or a

variation between solutions is smaller than a predetermined limit, this process is repeated [71, 72]. Given that the GA approach is stochastic, one can question its validity. This method is reliable and capable of calculating global optimum solution for a specific problem since it keeps the best solutions in each iteration and uses them to improve subsequent options. As a result, with each succeeding generation, the entire population gets better. This strategy benefits from mutation as well. This operator modifies the chromosomes' genes at random, maintaining population diversity and enhancing GA's enquiring nature [73]. Genetic Algorithm process flow diagram is shown in Figure 10.

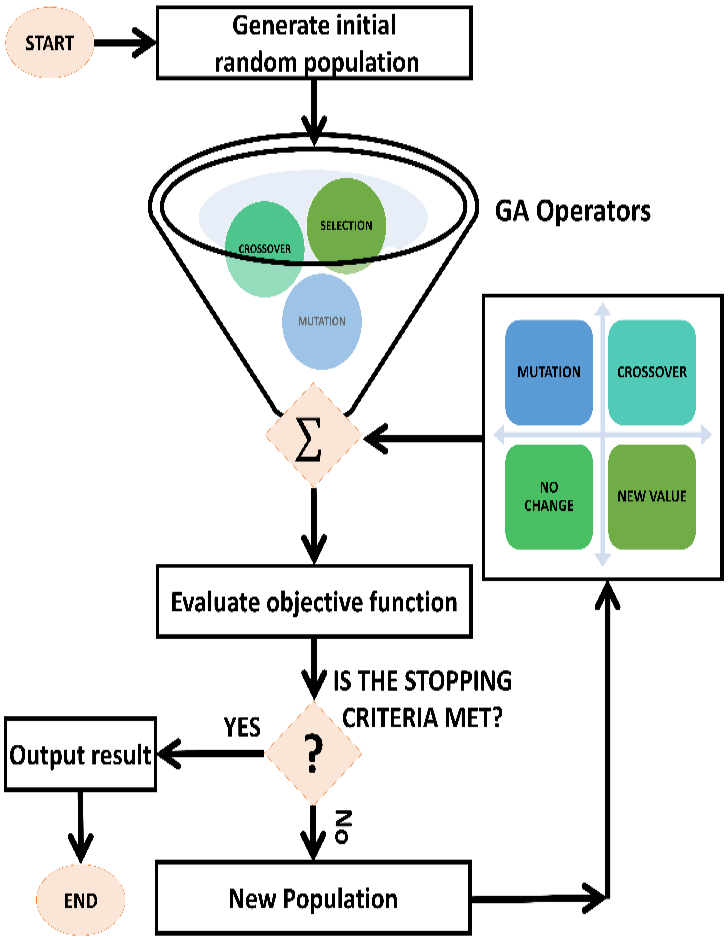

Figure 10: Genetic Algorithm workflow

3.1.1. Genetic Algorithm Methodology

3.1.1.1: Gene Representation:

Every chromosome relates to a potential answer to the specific optimization problem, as was previously stated. A chromosome is made up of many genes, which illustrates

how the parameters of the optimization problem change over time. The problem must first be stated before the vectors can be established when using the GA approach. There are two GA variants: a binary variation and a continuous form. A binary version could take two values as parameters (e.g., 0 or 1). Continuous values are used when there are upper and lower constraints on the value. Binary GA is the term used when many values need to be chosen. The variables here require the allocation of additional bits. For instance, in a problem with two parameters, each parameter can have eight different values, and each parameter will need three genes [74, 75]. In order to calculate the set of genes for choosing n discrete values, log2n is used. It has been demonstrated that real value number encoding of chromosomes leads to more effective GAs and superior solutions. It's important to remember that genes can also be objects or components of a story. As long as genes are included in a fitness equation and produce a fitness value, the GA algorithm can use them. The term "genetic programming" describes separate computer programs for each gene [76].

Initialization: A large number of distinct solutions are initially generated at random to create an initial population. The population varies in size based on the circumstance, but it typically consists from several hundred to thousands of solutions. In most cases, the population is generated at random and includes all possible outcomes. Sometimes, the best answers are "planted" where they are most probable to occur [77].

Selection: Natural range is the key driving force behind this GA algorithm element. The most physically fit people have a greater chance to find food and mates in the environment. As a possible consequence, their genes promote more to the development of the next generation of animals that are comparable [78].

The Roulette Wheel Selection is the most basic GA. This operator divides a circle into N equal parts. The ith member of the population is represented by the ith section in the circle. This sector's breadth is equivalent to the likelihood that the same person will be chosen. In this instance, the total width of the circle's intervals is one. At the selection stage, the circle is rotated N times. Each time the roulette wheel turns, a new population is created using the individual that is indicated [79] .

Crossover: Individuals who have been chosen using a selection operator must then be utilized develop new generation. Naturally, a new chromosome is generated by joining the chromosomes of the parents' genes [80]. The GA algorithm emulates it by integrating the two new solutions produced by the two answers selected by the

roulette. wheel. There are other crossover operator strategies published in the literature as well. In a single-point crossover, the genetic mutations of two parent solutions are transferred both before and after the single point. In contrast, just the chromosomes between two crossing points in a double point crossover are swapped [81].

The following additional crossover strategies are listed in the literature:

1. Standard Crossovers
a. Uniform crossover
b. Reduced surrogate crossover
c. 1-Point crossover
d. Discrete crossover
e. Flat crossover
f. K-point crossover
g. Shuffle crossover
h. Average crossover
i. Intermediate crossover
2. Binary crossovers
a. Random respectful crossover
b. Elistist crossover
c. Count preserving crossover
d. 1-Bit adaptation crossover
e. Homologous crossover
f. Masked crossover
g. Multivariate crossover

The main goal of crossover is to ensure that genes are passed, and that the progeny inherit the DNA of their parents. Crossover is the primary exploitation method in the GA. The program will attempt to validate and look for alternate combinations of genes from the parents if the crossover is carried out using a randomized pivot point for two specified parents. Therefore, without adding a single new gene, those workable methods are utilized. Notably, the GA Possibility of a Crossover (Pc) parameter depicts the likelihood of accepting a new child. A similar range of random variables is generated for each child. If this number is less than Pc, the child is passed onto next generation. In the absence of this, the parents will be transferred. When

some of the offspring do not survive, this also happens in nature [74, 82].

Mutation: Genes are altered in the ultimate evolutionary process once offspring's solutions are produced. Because substantial genetic mutations reduce GA to a crude random search, GA has a lower mutation rate. The mutation operator keeps the inhabitants diversified by establishing a further degree of uncertainty [83]. In practice, this operator increases the likelihood of eliminating local solutions and avoids alternatives from becoming similar in the GA algorithm [78].

The following list includes some of the most popular mutation strategies:

• Variable mutation probability

• Individuality mutation

selection rates, crossovers, and mutation operators are used by the majority of EAs. These operators have been used to every single generation in order to improve the supremacy of genes in the next cohort. When good solutions are preserved and handed on to the next batch intact, elitism is the norm. The main objective when utilizing the crossovers or mutation operators is to prevent deteriorating such solutions (elites). Starting with an arbitrary population of entities, the GA algorithm runs. This strategy improves the population all the way to the finish by utilizing the three operators mentioned above. The best estimate of the global optimal for a given task is taken to be the best solution in the preceding population. The selection, mutation, and crossover can all be shifted or ready to fix values throughout the optimization process. The sections that follow examine the influence of changing on GA presentation [84, 85].

The genetic operators change the population throughout generations, searching for a desirable or optimal result as shown in Fig. 8. It is vital that the population is diversified and retains adaptive traits from past generations. The selection operator seeks to select parents who are more likely to have offspring of the population with good fitting values. Selection is a key GA step used for the selection of those individual having good fitness value. Chromosomes which have higher fitting values are more likely to be picked for reproduction while Individuals with low fitting values are ignored because of the disturbance to local optima. Selection of chromosomes for reproduction is directly proportional to the fitness value [70]. Along with selection, Crossover is an important genetic algorithm operator involved in the pairing of parental features during reproduction, and as a result offspring is born, each of which contains features inherited from both of its parents. One-point, two-point, or

homologous crossover operators exchange genes between two chromosomes. Mutation operators are used for the introduction of new individuals to the populations and to prevent the loss of important information from the string. It is required to ensure population genetic variety by randomly altering one or more individual of a given population. Moreover, by altering gene code from 0 to 1 will yield binary coded gene [70].

Genetic Algorithm (GA) is population-based stochastic algorithm, which is optimize the searching tool for difficult problems on the basis of genetic selection principle [86]. It is also use for the purpose of research and development as well as for machine learning. The objective is to produce solutions to potential generations. GA stimulates the biological evolution process and is founded on genetic inheritance and natural selection.[87]. It is used to calculate the fitness of each member of the population by employing fitness function. Then, selection, mutations and crossover are used to create future populations. [88].

A genetic algorithm can vigorously change the search process in order to find the best possible solution by utilizing the probability of genetic crossing and mutation. GA has the power to modify the encoded genes. GA can analyze numerous individuals and produce multiple optimum solution. Consequently, GA offers superior worldwide search capabilities. The babies resulting from chromosomal exchange between parents are likely to destroy the admirable genetic structures and the formula of crossover is as follow $K = \frac{G+2\sqrt{g}}{3G}$ (1)

K

$= dynamically\ changing, and\ depends\ on\ the\ number\ of\ evolutionary\ generations$

$g\ =\ number\ of\ generations\ of\ the\ algorithm$

$G\ =\ total\ number\ of\ evolutionary\ generations$.[89].

- Initially a random population set was generated.

$P = \{p_1, p_2, \dots, p_{pop\_size}\} \dots\dots\dots (2)$

$p_i = \left[p_{i_1}\, p_{i_2}\, \cdots\, p_{i_j}\, \cdots\, p_{i_{no-vars}}\right]\ i = 1,2, \dots,\ pop\_size$

$j = 1,2, \dots,\ no\_vars\ \dots\dots\dots (3)\ para^{\,j}_{min} \le p_{i_j} \le\ para^{\,j}_{max} \dots\dots\dots (4)$

$pop\ size = population\ size$

$no\ of\ vars = number\ of\ variables\ to\ be\ tuned$

$p_{i_j}, i = 1,2, \dots$

- A fitness function was used to evaluate the features.

$fitness = f(p_i)$ ……. (5)

- Where objective function criterion was not met, a new set of population was generated by resetting the algorithm. Genetic operators (selection, mutation and crossover) were used to generate the population.

3.2.Machine Learning Models

In this study Gaussian Process Regression, Artificial Neural Network, Ensembled Tree, and Support Vector machine were utilized to create models for precisely estimating H2 yield via SCWG of SS based on proximate, ultimate analysis and gasification conditions. The ML models in this study were built, trained, and tested using MATLAB software. The best possible GPR and Ensembled hyper-parameters were chosen using the Bayesian optimization method. **Figure 11** shows the schematics of the machine learning methods.

3.2.1. Support Vector Machine

The SVM is a computer-based ML algorithm that is treated for both classification and regression tasks [90]. The kernel function is utilized by the support vector machine to develop a mathematical correlation amongst input and output in both regression and classification problems. The kernel function is very useful when the task is difficult as it entails nonlinearities. The kernel function transfers model parameters into high-dimensional vector to linearly split variable quantity that are not linear in nature in the lower-dimensional vector [91]. For SVM decision processes, kernel functions can be defined, and MATLAB enables users to set custom kernels. This feature allows SVM algorithm to be used to solve linear classification and regression problems without the need for hyperparameter tuning. SVMs have a unique ability to provide balanced predicted results, even in studies with small sample numbers [92]. The yield of H2 is the optimization goal in this study. The optimization of SVM parameters is important for a target–optimization problem. The SVM parameter optimization performance evaluation index is first defined, and the optimal parameter is then solved by using the MATLAB application [93].

Supervised learning technique recognized as a support vector machine (SVM) was originally developed for solving classification problems and was then developed for

regression problems as well. To distinguish between different sets of data, this algorithm is dependent on the formation of a hyperplane in a space with a large (or an infinite) dimensionality [94]. To achieve the best separation, the hyperplane should be placed as far away from the nearest training data points as possible [95]. In the feature space, SVR generates the following linear regression function shown in an equation by given feature vectors dataset $x = x_i \in R^P;\ i = 1,,,n$, and a target value $Y \in R^n$.

$$f(x) = w^T \varphi(x) + b \quad (6)$$

w ~ weight vector and b ~ bias

To determine these terms following equations are solved

$$min\ \frac{1}{2} w^T w + C \sum_{i=1}^{n} (\xi_i + \xi_i^*) \quad (7)$$

Subject to constraints:

$$yi - w^T\ \Phi(xi) - b \quad \leq \xi + \xi_i \quad (8)$$

$$w^T\ \Phi(xi) + b \quad \leq \xi_i + \xi_i^*$$

$$\xi_i, \xi_i^* \geq 0$$

ξ = error of models away from the hyperplane in which ξ_i^*, ξ depend on whether sample below or above the $\boldsymbol{\varepsilon}$ tube, C is the plenty term. The important hyperparameters are C and $\boldsymbol{\varepsilon}$,in which small value of C use fodatasetset having a lot of noise.The rediction of SVR by the lagrangian dual technique can be analyzed by following equation.

$$f(x) = \sum_{i=1}^{n} (\alpha_i + \alpha_i^*)\, K(x_i + x_j) + b \quad (9)$$

α = Lagrang multiplier of dual form,

K = Kernel function [95]

$$K(x_i + x_j) = \Phi(x_i)^T \Phi(x_j) \quad (10)$$

3.2.2. Ensembled Learning Tree

Decision tree is the most widely used machine learning technique, and it is built on tree-based models that predict output using logical principles. It creates a regression model based on the conditional statement's tree structure and does not rely on a preexisting correlation between the input and output features. DT makes decisions based on attributes in the dataset to split down data into smaller groupings. Decision nodes and leaf nodes are types of nodes present in a network. With the given 'yes' or 'no' answers, it develops a set of queries including, 'is equal' or 'is greater,' and

then meets up with another question to answer. This process continues until all questions have been answered, and then result is obtained. The data is repeatedly divided into binary segments to grow DT [96, 97]. This process was performed unless perfect homogeneity was achieved, or a predefined maximum number of nodes was attained. Overfitting is an issue with the DT, as it is with other regression techniques. The DT algorithm uses a method called "pruning" to prevent overfitting. Because of outliers, pruning is a crucial method to apply in tree building. It also addresses the issue of overfitting. Small subsets of instances may exist in datasets that are not clearly characterized. Pruning can be used to appropriately categorize them. Pruning can be divided into two categories i) online pruning ii) post pruning [96].

Multi-decision tree (DT) was used to develop the advanced algorithm known as RF. Each DT expands independently after receiving a random set of the input data (also known as a bootstrap sample). Even if each decision tree in the random forest is regarded as a poor learner, the RF as a whole is able to gain higher levels of expertise and precision when they make a prediction collectively. As samples with goal values are grouped together, a decision tree iteratively partitions the feature space, (x), using a random set of data d(x,y). The data is represented by d_m with n_m samples at node (m). The equation is as follow

$$d_m^{left} = \{(x, y) | x_p \leq t_m\} \quad (11)$$

$$d_m^{right} = d_m / d_m^{left} \quad (12)$$

The data dm is split in to two subsets (d_m left, d_m right). The candidate split into p and t_m,in which p is feature and t_m is thurshold.

These subsets are rescued until the maximum depth is allowed to be reach. RF prediction progression is as follow

$$f(x) = \frac{1}{K} \sum_{K=1}^{K} D\, T_t(x) \quad (13)$$

The ensemble learning method is a type of method that integrate many learners with specified combination strategies. In comparison to previous black-box algorithms, the tree-based ML models are simpler to perceive and understand and can tackle both linear and non - linear problems. [98]. The tree ensemble method utilized multi-objective optimization to produce effective diagnostic rules. Two models are used in the proposed method: the base learners, which are used to forecast the posterior class probabilities of a sample, and a meta-learner, which is used to predict the label of the final class by integrating the basic learners. Model combination and model selection

are examined through a different angle during development of model. For an accurate and intelligible ensemble, we use a multi-objective approach to model selection in order to maximize both accuracy and ensemble complexity at the same time. The tree ensemble method uses the hill-climbing method in order to find a stable set of rules and is based on rule selection and rule accuracy [99].

3.2.3. Gaussian Process Regression

GPR is a Bayesian tool and an effective learning model used for nonlinear regression problems. Apart from predicting, this method can also provide the coefficient of determination for each prediction point, which measures the forecast's uncertainty. Probability distributions may be considered as Gaussian processes. The mean and variance of a Gaussian distribution are used to calculate the probability of an input vector. The GPR model produces a mean and correlation vector instead of a scalar mean and variance [100]. Williams et al. apply GPR to higher-dimensional regression problems that have typically been addressed using other approaches that include, neural networks and decision trees, with promising results [101]. GPR gives a way to adjust the interpolation's locality directly and quantitatively, which is encoded in the assumption of smoothness.

GPR is a non - parametric, Stochastic attitude towards regression that is used in machine learning to determine the probability distribution across all acceptable functions.[102]. Gaussian process prior is assumed in GPR, which can be specified by using a mean function m(x) and covariance function k (x, x'). GPR assumes a Gaussian process prior, which can be described by mean of covariance function k (x, x') and function m(x).

$$f(x) \sim GP(m(x), k(x, x')) \quad (14)$$

During model selection of Gaussian process prior, form of covariance kernel and mean function is chosen. There are various options for kernel functions such as square, linear, and constant with multiple kernels composition. The kernel composition is a constant kernel with the radial basis kernel function which encodes the smooth function. Equation used for the Constant times radial basis kernel function (RBF) is as

$$k(x, x') = {\sigma_f}^2 \, exp(-\frac{1}{2l^2}\|x - x'\|^2) \quad (15)$$

There are two hyperparameters of kernel length scale *l*. and signal variance σ^2, As we conclude that

GPR has many advantages, including the ability to work with limited datasets and the ability to analyze prediction uncertainty.

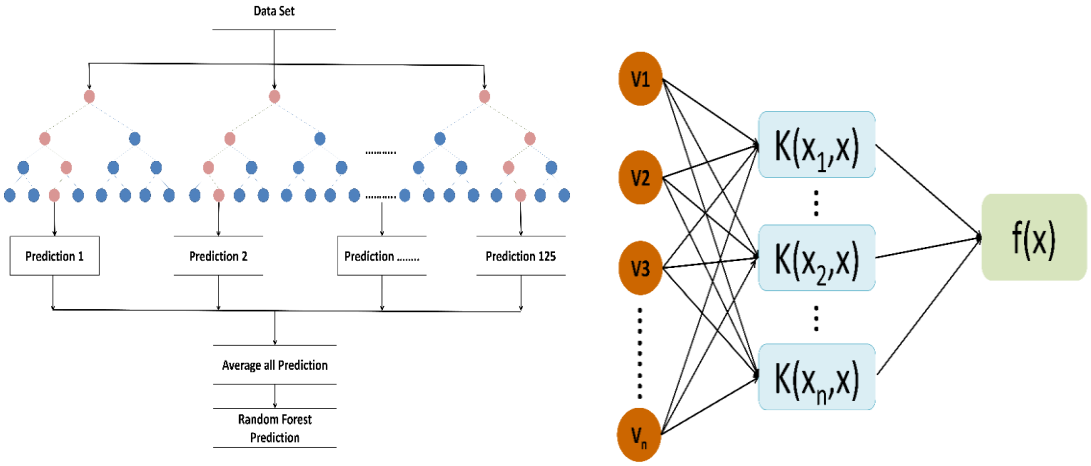

Figure 11: Schematics of Machine learning models

Artificial Neural Network

The concept of artificial neural network was originally introduced in the field of biology, where neural networks play a key part in the human body. In 1949, Hebb's rule—which was founded on theories and observations of the neurophysiologic environment—was presented as the first method for training ANNs. Computer models called ANN are modeled upon nervous system of living things. They could pick up and retain knowledge (information-based). They can be viewed as a group of units represented by neurons, linked together by numerous interconnections, and operated by synaptic weight matrices and vectors [103, 104].

3.2.4. Artificial Neural Network

ANN are advanced computing technologies that mimic functions to interpret data quantitatively through learning and training. The ANN learns and adapts itself until it meets the answer by processing data through a complicated network with feedback [105]. In Artificial neural network, neurons are the basic building blocks

which act as a simple controller taking input data from one or more features to produce output. There are three main layers in a typical network: input, hidden, and output layer. The network's inputs are frequently mapped to its outputs via a directed graph with weighted nodes [106]. The input layer receives information, signals, features, or assessments from the outer environment. These inputs are typically normalized within a training algorithm. This normalization improves the network's numerical consistency. The hidden layer neurons pull information about the system. Each neuron input has a weight that defines the input's "intensity." A neuron multiplies each input by its weight, adds the results for all inputs, and determines the output based on the computation and an activation function [107, 108].

The human brain itself and already-existing biological neural system concepts were used to construct the ANN designs. Artificial neurons are tampered-with copies of actual neurons used as processing or calculation units. These ideas were inspired by research into how the cell membrane of a neuron generates and enhances electrical signals. Activation functions in ANN model are nonlinear, have continuous outputs, and perform basic tasks including gathering data from their inputs, merging it in accordance with their operational functions, and producing an output based on their Inherent activation functions as shown in Figure 12 [109, 110].

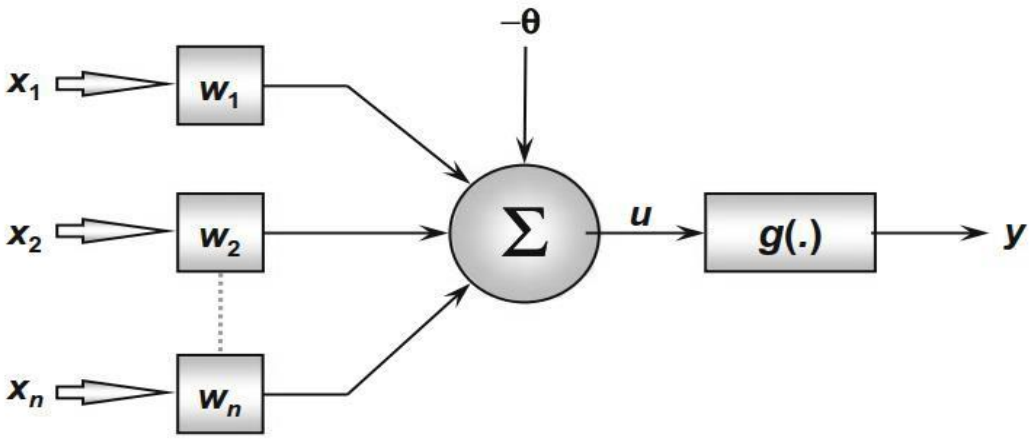

Figure 12: Artificial Neuron

3.2.4.1: ANN architecture:

Input layer, hidden layer, and output layers are typically included in ANN models, and they are described as follows:

Input layer**:** The input layer manages of collecting information from the outside environment, such as data, signals, features, or evaluations. Within the parameters of

the activation functions, these inputs are frequently normalized. The network's mathematical computations are numerically more consistent as a result of this standardization.

Hidden layer: Neurons of the hidden layers are responsible for extracting data about the system under inquiry. As much of the network's internal tasks are managed by these layers.

Output layer: This layer, like the levels before it, is called neurons and is accountable for generating and presenting the network outputs that are the result of the processing carried out by the neuron in the layer before. Given that neurons are interconnected, and their layers are undisturbed, the major designs of ANNs can be divided under the following categories: Recurrent networks, mesh networks, and feedforward networks are the four different types. Networks with a single layer and multiple layers of feedforward [111-113]

In this ANN architecture, there is only one output layer and one input layer. Figure 19 depicts a simple layer feed forward network with m inputs and n outputs. Information always moves from the source to the destination layer in a single direction (hence, unidirectional). As seen in Figure 19, networks using this architecture would always have the same set of network outputs as neurons. Solutions for these networks typically include linear filtering problems and pattern categorization [114].

Chapter 4:

Methodology

4.1. Overview of Methodology

In this work data for supercritical water gasification of sewage sludge were taken, and a machine learning models integrated with Genetic Algorithm was developed. Operational parameters include the Proximate, ultimate analysis and supercritical water gasification conditions.

MATLAB was used to import the data from the excel sheet. A single objective GA is utilized to define the importance feature and predict the hydrogen yield. The data set was also utilized to train an AI system to predict the hydrogen yield from sewage sludge under hypothetical parameters.

In this work, an GPR-GA model was established to predict the hydrogen yield while using the proximate, ultimate and gasification conditions of sewage sludge supercritical water gasification.

The present research's workflow is shown in Figure 13.

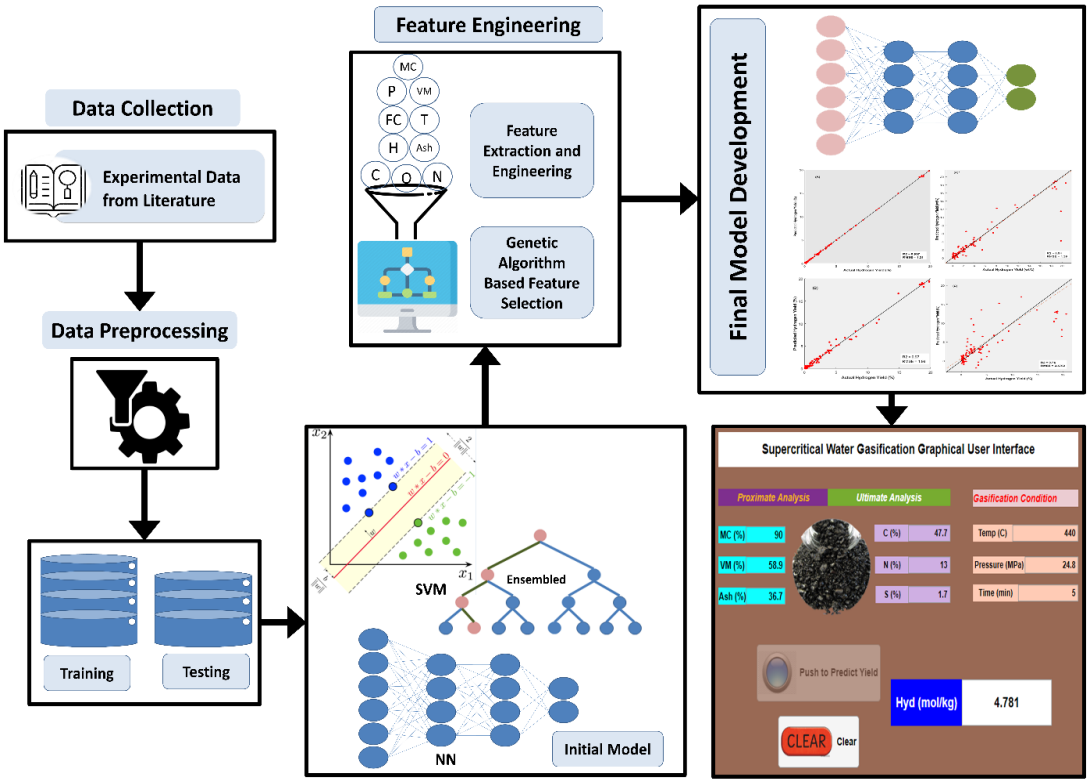

Figure 13: Research workflow

The objective of using comparative analysis was to determine the best model for selecting input parameters and architecture of ML models, ultimately improving performance of the prediction model as shown in the Figure 14.

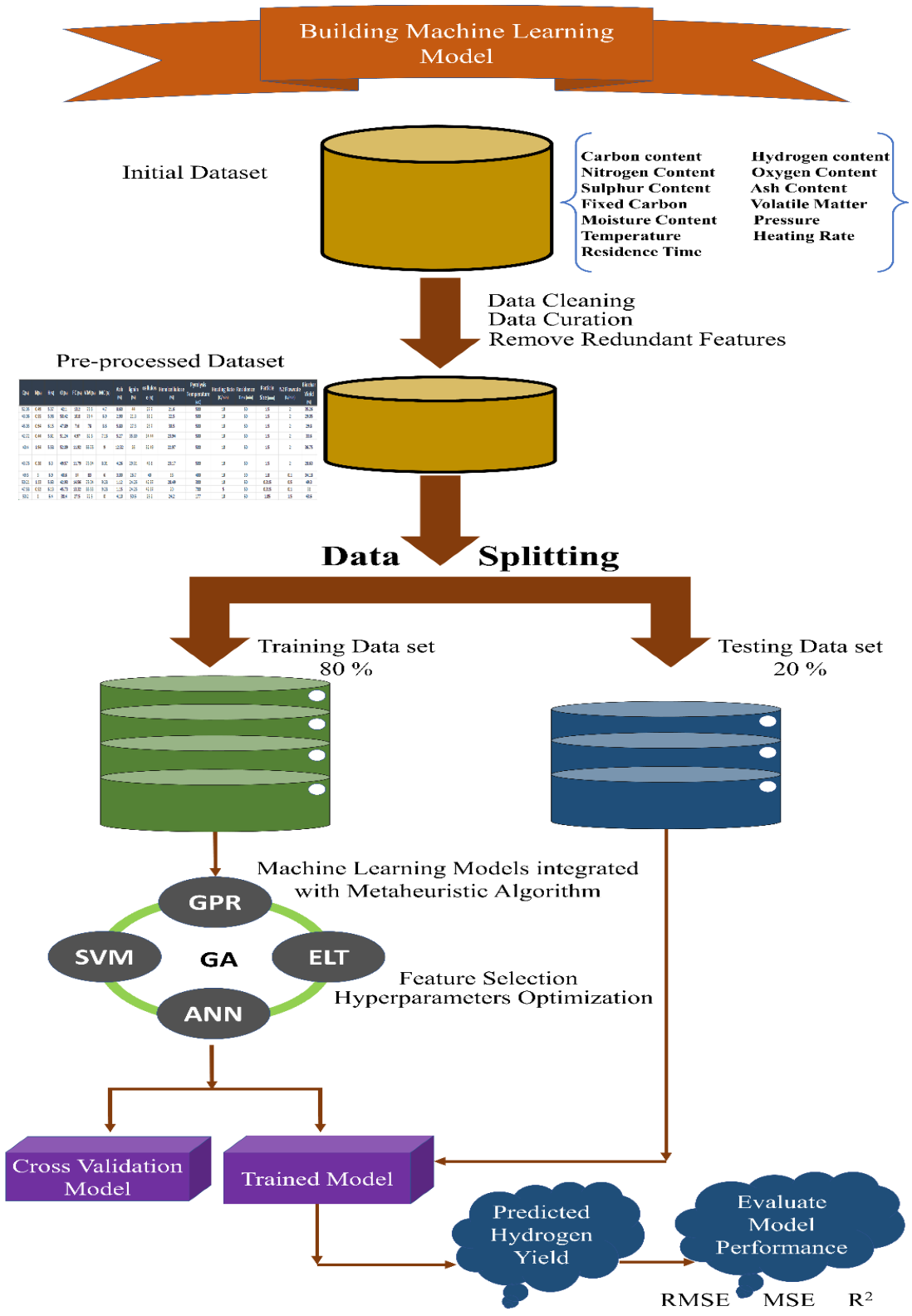

Figure 14: Machine Learning workflow for Optimum coefficient of determination

4.2. Data collection

In the present study, data is collected from comprehensive literature assessment of experimental studies reported for Supercritical water gasification (SCWG) from SS. The major criteria for the selection of the data included SS, Supercritical water gasification, and Hydrogen production. Various keywords such as hydrogen yield, supercritical water gasification, machine learning, sewage sludge, and biomass were used to search relevant articles in Web of Science, Google Scholar, and Science Direct. Following the reclamation of data from related papers, features data extraction and categorization were completed to build and test machine learning models. The data collection process used is outlined below.

- A total of 125 hydrogen yield data points were collected from 21 published papers [61-63, 115-130].
- Data of the samples were taken from gasifier based on sewage sludge proximate and ultimate composition and super critical water gasification conditions.
- Information was taken from related figures, tables, and Supplemental data in the literature.
- Data was collected on biomass proximate and ultimate analysis which included carbon, Sulphur, nitrogen, and hydrogen, and oxygen while proximate analysis consisted of fixed carbon, moisture content, volatile matter, and ash.
- Supercritical water gasification temperature, pressure, and residence time along with the proximate and ultimate analysis were used as input parameters in the super critical water gasification process.
- Hydrogen yield considered as output parameter of the gasification process.
- Table 1, 2, 3 show the data distribution of the data all.

Table 1: Proximate data distribution

Parameters	Min	Q1	Median	Mean	Q3	Max
Carbon	7.36	19.50	38.18	31.32	47.7	47.7
Nitrogen	0.37	2.79	4.67	4.57	5.78	13
Hydrogen	0.75	2.12	3.40	4.41	4.82	15.50
Oxygen	4.24	14.27	23.74	24.61	28.3	55.66
Sulphur	0	0.91	1.05	1.07	1.7	3.34

Table 2: Ultimate data distribution

Parameters	Min	Q1	Median	Mean	Q3	Max
FC	0.78	4.40	9.41	16.77	45.10	73.02
VM	23.97	52	61.63	55.81	78.80	78.8
MC	0.66	79	84	77.38	87.37	97.20
Ash	2.5	21.5	28.96	36.57	48.7	71.57

Table 3: Supercritical water gasification data distribution

Parameters	Min	Q1	Median	Mean	Q3	Max
Temp (C)	350	400	420	465.4	450	873
Time (min)	2.5	6	20	29.18	60	450
P (MPa)	22.1	24	27	28.4	35	35

Chapter 5:

Results and discussion

Taking into account the afore mentioned information discussed in the final paragraph of section Literature review while formulating this study, different ML models including, Support Vector Machine (SVM), Gaussian Process Regression (GPR), Ensembled tree, and Artificial Neural Network (ANN) were used to predict H_2 yield utilizing SS composition (proximate and ultimate analysis) and gasification conditions (temperature, pressure, and residence time). Figure 15 shows that ML models take the feed composition and gasification conditions as an input parameter that is carbon (C), Sulphur (S), Hydrogen (H), Oxygen (O), Nitrogen (N), Fixed Carbon (FC), Volatile Matter (VM), Moisture Content (MC), Ash Content (Ash), Gasification temperature (Temp), Residence time (time) and Pressure (P). These input parameters were used for data driven modeling and an optimized model is developed which is used for process validation and process prediction.

The objective of this work is to develop a genetic algorithm (GA) based optimum ML model for the prediction and evaluation of H_2 yield through SCWG using sewage sludge as a feed and to develop an intelligent GA based features selection model with improved accuracy in prediction of controlling reaction parameters. Consequently, the optimum ML method integrated with GA will be beneficial for researcher to predict the H_2 yield for the experimental work. For the first objective, ML models including support vector machine, ensembled tree, gaussian process regression and artificial neural network are used for the prediction of H_2 yield. Through genetic algorithm, parameters of ML models are tuned and optimized for the better prediction function. This integrated approach is applied on the ML models and the optimum ML model GPR is selected for the prediction of H_2 yield. For the second objective, rather than resorting to conventional methods such as filter, and wrapper methods, a GA based feature selection model is utilized. The filter method is based entirely on correlation between input and output variables rather than cross validation performance which can falsely interpret various feature selection. While, in the wrapper technique Machine Learning model is educated on each set of the properties utilizing predefined classification algorithm to predict a feature with good results. However, this method is time consuming, and a model developed on various features

might lead to over fitting. On the contrary, GA based feature selection is an advanced optimization tool which results in multiple solutions, allowing the selection of the best possible solution in a relatively less time. Finally, Graphical User Interface was developed, to predict H_2 yield, using both optimum features and machine learning algorithm with the help of MATLAB.

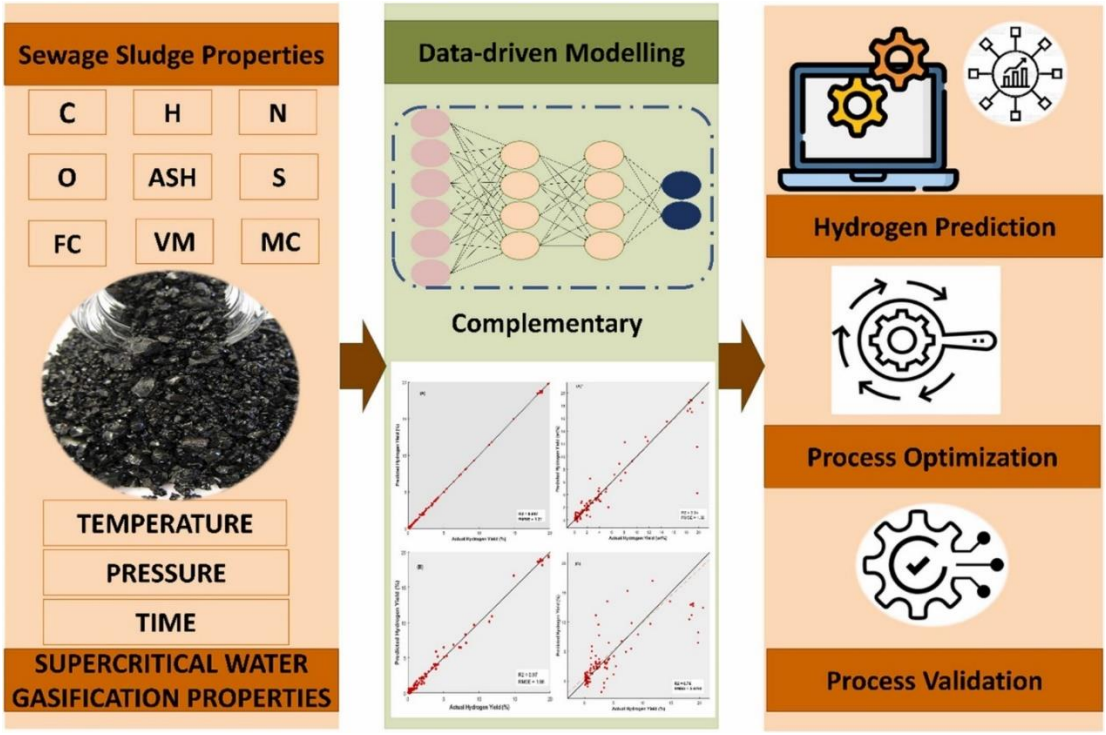

Figure 15: Process Flow Diagram for Hydrogen Prediction using Machine Learning.

5.1. Box Plot Presentation

Box Plot is a technique used to present dataset's distribution. It shows the maximum and minimum range, median, mode, tolerance, and lower and upper quartiles. Understanding the box plot's structure and origins facilitates the evaluation of data and its uses [131]. In box plot presentation, the proximate, ultimate and gasification condition were plotted against their distribution as shown in Figure 2. Ultimate analysis including Carbon (C), Sulphur (S), Hydrogen (H), Oxygen (O), and Nitrogen (N), were in the ranges of 7.36%-47.7%,0.75%-15.5%, 0.37%-13%, 4.24%-55.66%, 0%-3.34%, while in proximate analysis which included Fixed Carbon (FC), Ash, Moisture Content (MC), and Volatile Matter (VM) ranges from 0.78%-73.02%, 23.9%-78.8%,0.66%-97.2%, and 2.5%-71.57% respectively. Also, Gasification reaction conditions (Temperature (T), Residence Time (Time), and Pressure (P)) were ranges from 350-873 ^{0}C, 2.5-120 min, 22.1-35 MPa, respectively.

Box plot presentation is given in Figure 16.

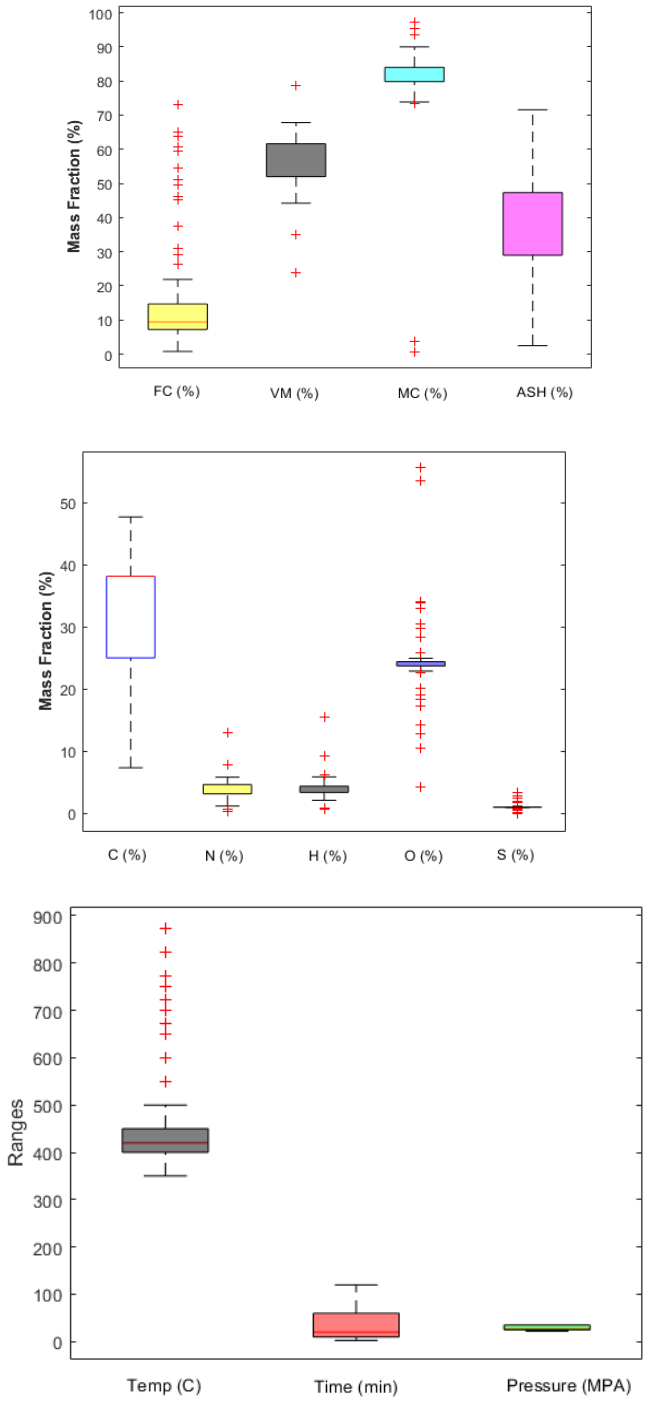

Figure 16: Box Plot representation

5.2. Performance evaluation criteria

GPR, SVM, Ensembled tree, and ANN from MATLAB library were pre-processed using default hyperparameters. Preprocessing techniques were evaluated using MSE and R^2. To pre-process and deeply model, the datasets were randomly divided into training (80%) and testing (20%) datasets. To minimize data wasting and overfitting, 5-fold cross-validation was employed to validate the created models. Ranges for the hyperparameters tuning were specified from the Regression model toolbox of each model and then optimize with the help of GA. These hyperparameters were then utilized to build and test models. The average values of the statistical indices were utilized to evaluate the validation phase's performance over the modelling procedure.

The following two criteria were used for the prediction performance of each final ML model: 1) Root-mean-squared error (RMSE) and 2) Coefficient of determination (R^2). Following are the R^2 and RMSE equations:

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (Y_i^{exp} - Y_i)^2}{\sum_{i}^{n} (Y_i^{exp} - Y_i^{exp})^2} \quad (16)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (Y_i^{exp} - Y_i)^2} \quad (17)$$

Y_i^{exp} *is experimental value,* Y_i *is predicted data and n represent number of test sample*

5.2.1. Hyperparameters Tuning

Parameters selected for tuning from different ML models were specified from the regression model toolbox with a 5-fold cross validation and standardized data True. Table 4 shows the hyperparameters selected, their ranges and optimized values. These hyper parameters were tuned and optimized with the help of Genetic algorithm for SVM, GPR and Ensembled Tree. Optimized value for SVM were box constraint value of 214.055, Kernel Scale value 432.2483, Epsilon 0.7987, and Kernel function of linear. After applying the GA to the ensembled hyperparameters, optimum values for Ensembled model hyperparameter are reported as: Number of learning cycle 10, Learning rate 1 and Selected method was LSBoost. In GPR, optimized hyperparameter after applying genetic algorithm were Sigma 30.2724, kernel function

squared exponential, basic function none, and kernel parameters [1.017314230722229 3.89396463096418]. Finally, Artificial neural network model was trained from the regression model toolbox with optimized hyperparameter values of layer sizes [10 10 10], lambda 0, standardized true, and activations Sigmoid.

Table 4: Ranges and Optimized Values for parameters selected

ML Methods	**Parameters**	**Ranges**	**Optimized Values**
SVM	Box Constraint	0.001-1000	**214.055**
	Kernel Scale	0.001-1000	**432.2483**
	Epsilon	0.0025686 – 256.8569	**0.7987**
	Kernel Function	Gaussian, Linear, Quadratic, Cubic	**Linear**
Ensembled Tree	Number of learning cycle	10-500	**10**
	Learning rate	0.001-1	**1**
	Methods	LSBoost, Bag	**LSBoost**
GPR	Sigma	0.0001-55.069	**30.2724**
	Kernel Function	Non/iso-tropic Exponential, Non/iso-tropic Matern 3/2, Non/iso-tropic Matern 5/2 Non/iso-tropic Rational Quadratic, Non/iso-tropic Squared Exponential,	**Squared Exponential**
	Basic Function	Constant, Zero, Linear	**Zero**
	Kernel Parameters	0.523-523	**1.017314 3.89396**

5.2.2. Prediction Performance

The Hydrogen yield was predicted using different ML models, such as GPR, Ensembled Tree, RF, SVM and ANN models. Based on GA-based features selection, all five machine learning models accurately predicted the Hydrogen yield. Figure 17 shows the GPR R^2 and RMSE value before feature selection which is 0.94 and 1.39 respectively. After applying GA based feature selection, R^2 value increased up to 0.997 while RMSE value decreased to 0.093. Means that the irrelevant features were present in the models and were removed after applying GA. Comparison of all four ML models is listed in Table 5, which shows that the GPR, Ensemble Tree, ANN performance was satisfactory as compared to that SVM for hydrogen yield prediction. Training and testing coefficient of determination (R^2) value for the GPR, Ensembled model, ANN were 0.997 and 0.994, 0.943, respectively. while RMSE values were 0.093, 0.560, and 1.521 as shown in Figure 18. The non-linearity of hydrogen yield with respect to input features was the root cause of SVM low performance in comparison to other ML models. The SVM model performed poorly in both training and testing (Training R^2 = 0.761 RMSE =2.479, Testing R^2 = 0.692 Testing RMSE = 2.966) compared to performance of other ML models, such as GPR, Ensembled Tree and ANN models. GPR model performed better than all other models in both training and testing. ML models have been evaluated based on coefficient of performance (R^2) and RMSE values, the performance trends for training and testing as (GPR>Ensembled>ANN>SVM). Table 6 shows the experimental yield and GPR predicted yield.

Table 5: Comparison of ML Methods

Model	**Training R^2**	**Testing R^2**	**Training RMSE**	**Testing RMSE**
GPR	0.997	0.963	0.093	0.203
Ensembled Tree	0.994	0.921	0.560	1.232
SVM	0.761	0.692	2.479	2.966
ANN	0.943	0.861	1.521	1.987

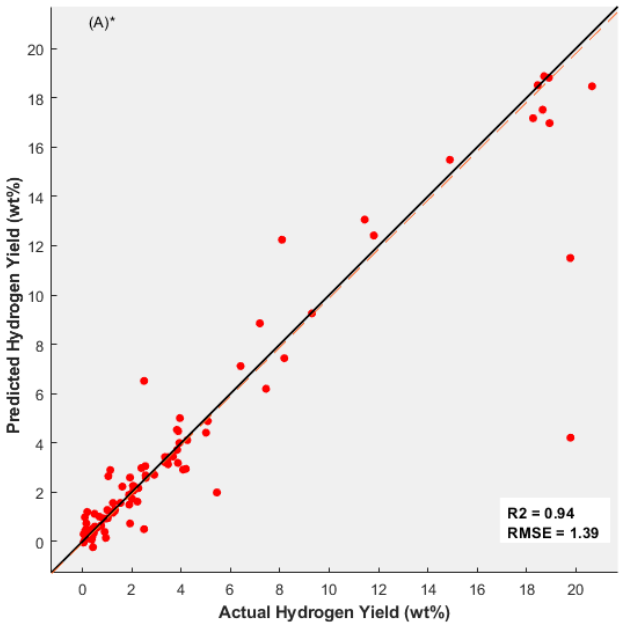

Figure 17: GPR Model before Feature Selection

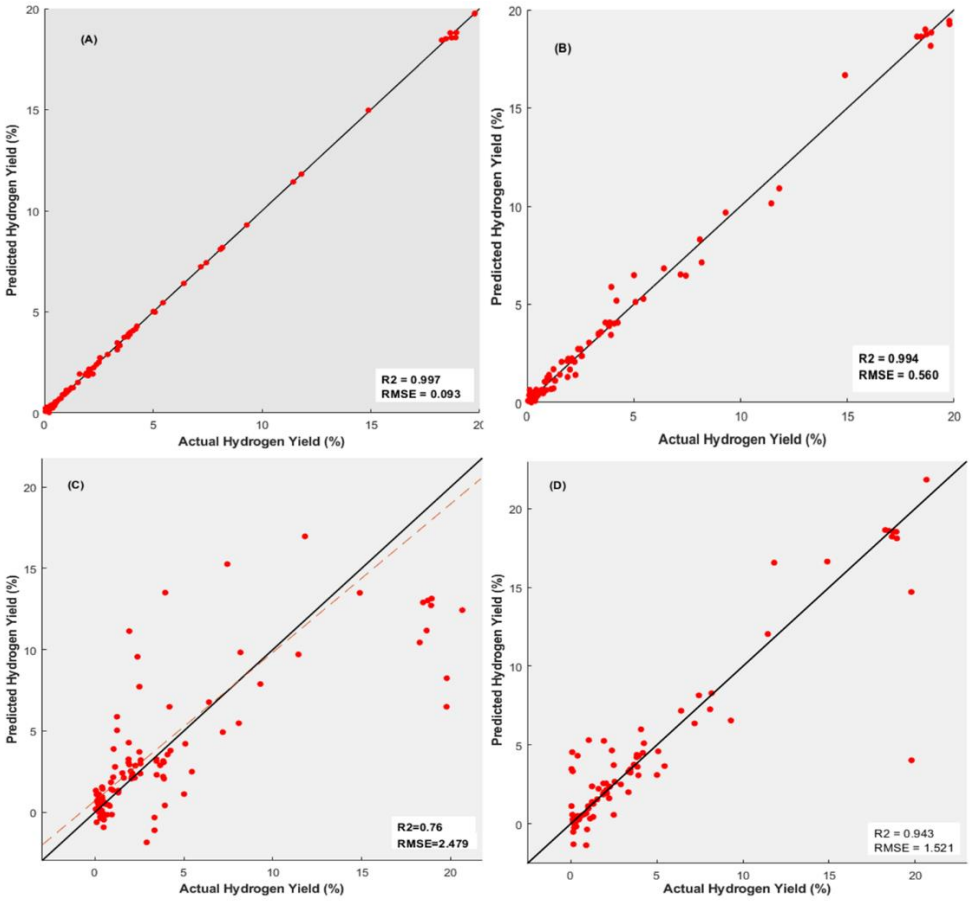

Figure 18: Comparison of the different ML models with the H2 yield (A) GPR, (B) Ensembled, (C) SVM and (D) ANN models.

Table 6: Validation of GPR Model

S.NO	Experimental Yield	GPR Predicted Yield	Difference	References
1	0.47	0.54	0.07	[116]
2	9.3	8.68	0.62	[115]
3	0.22	0.2054	0.014	[132]
4	0.4872	0.49	0.028	[61]
5	4.25	4.781	0.53	[122]

5.2.3. Features Importance

GPR model with Shapley method can accurately characterize the relationship between input parameters and H_2 production. Shapley method works based on the magnitude of feature attribution. This was used to evaluate the relative significance of different inputs parameters on H_2 yield in supercritical water gasification. Figure 19 illustrates the impact of sewage sludge composition and gasification conditions on H_2 production. The MC, H and Ash contents had a significant effect on H_2 yield, whereas the effect of C and VM concentrations on H_2 yield was minor. MC shows high effect on the hydrogen yield because of its high composition as compared to other components in sewage sludge.

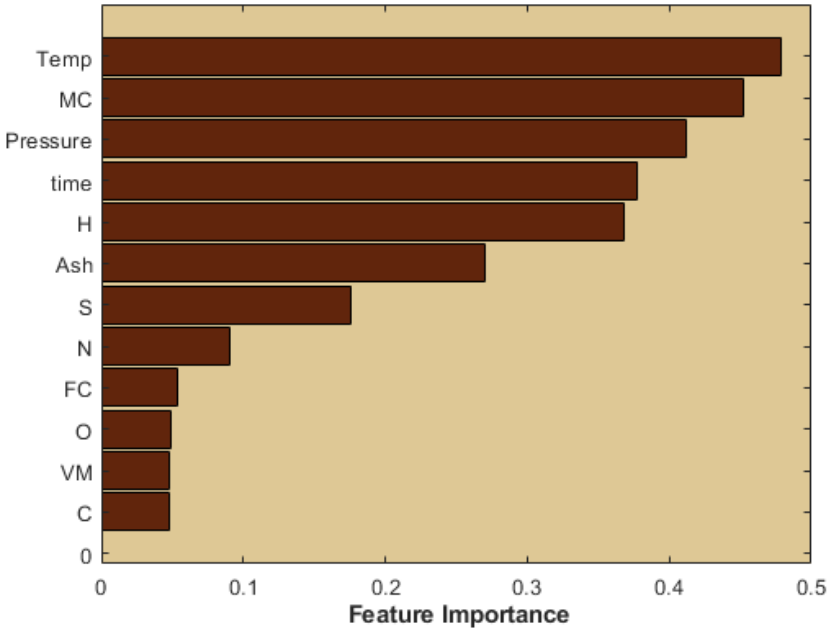

Figure 19: Feature importance of sewage sludge composition and gasification parameters on the H2 yield

Gasification conditions Temp, and pressure had a noticeable effect on H_2 yield but time showed a negligible effect as compared to other gasification conditions. Features impacts trends are T>MC>P>time. [133] et al used data of different biomasses, while in this work sewage sludge was used as a feedstock, and proximate, ultimate, and gasification conditions were used to build a machine learning model with feature importance. This study compared the impact on different parameters (H, N, O, C, MC, VM, Ash, Temp, Pressure, time) which effect the hydrogen yield prediction.

5.3. Effect of Parameters

5.3.1. Effect of parameters on Hydrogen Yield

Partial dependence (PDPs) analysis helps to determine the impact of input data variables on output. In the PDPs, only those variables were selected which have influence on the output. Selected input parameters influence on hydrogen yield are shown in Figure 20. Temperature is one of the key essential determining factors for the reaction to occur in supercritical or near supercritical water. Figure 7 demonstrates the influence of fixed carbon and temperature on sewage sludge

supercritical water gasification, Percentage yield of hydrogen shows an increasing trend as temperature was raised from 350 C to 760 C as reported by [134]. ML models suggest that gasification can be improved by raising the temperature as shown in figure 7 (A, B, and C). As a result, the gasification process was made more efficient using high temperatures. Hydrogen yield was primarily as a result of water-gas shift kinetics and steam-reforming, which were enhanced by high temperatures. Due to high temperature, hydrogen synthesis was facilitated. Heating the mixture to high temperatures improved gasification. The impact of pressure on Supercritical water gasification is difficult to predict. SCWG's key qualities must be explored in order to comprehend the impacts of pressure including dielectric constant, and density all rise with pressure. Water's ionic reaction mechanisms predominate at the critical point (22.1 MPa) due to larger densities than those found at supercritical temperatures. As a result, water's ionic product yield increases, speeding up the hydrolysis process for breaking down sewage sludge components. According to this, ionic reactions are preferred over free radical reactions at high pressures. The trend in figure (D), (E), and (F) reveals that at high pressure (30-32 MPa) hydrogen yield is optimum. Above the pressure range discussed earlier, little effect of pressure was detected on Hydrogen yield reported by [135]. As shown in Fig.7, some of the features have a minimal effect on GPR model predictions. According to the data, an increase in H_2 was recorded with an increase in MC. Increasing time increased H_2 production only for a few minutes, owing to the water-gas reaction. However, with time, the production decreases due to the methanation reaction.

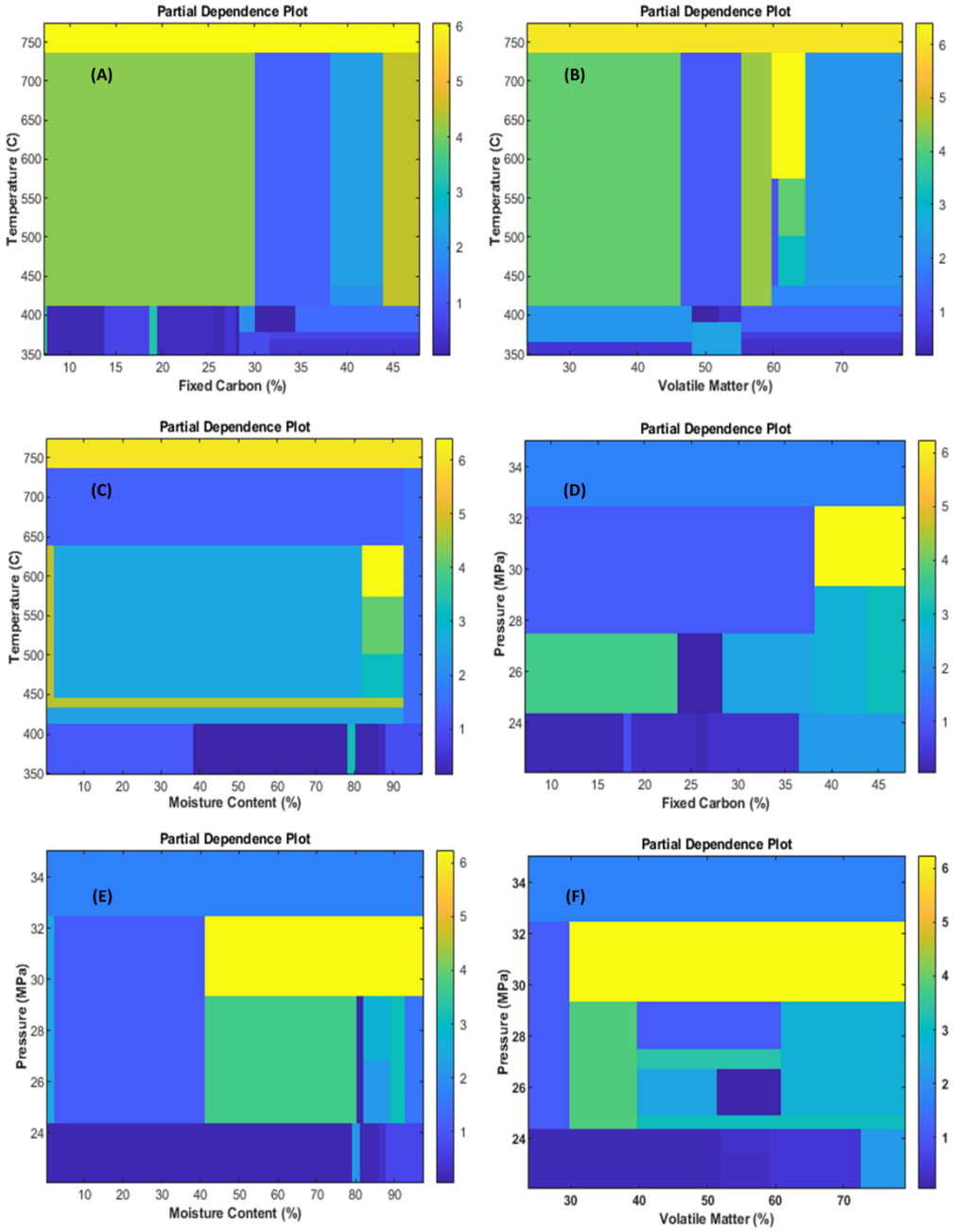

Figure 20: Three-way Partial dependence plot for Hydrogen Yield using Proximate analysis and Gasification conditions

5.4. Graphical User Interface

Graphical User Interface (GUI) accepts users to interact with electronic equipment utilizing graphical icons, symbols, and user-friendly software with a command-driven interface. The GUI presented in this paper allowed users to input data of proximate, ultimate composition and gasification conditions. GUI uses the

GPR model prediction function to predict hydrogen yield. GUI was developed in MATLAB 2021b. Figure 21 illustrates GUI for two different sewage sludge composition and gasification conditions in which the proximate analysis (MC 86.21%, VM 51.51% and Ash 47.29%), ultimate analysis (C 25.93%, N 4.58%, and S 0.75%), and gasification condition (temp 400 C, P 24 MPa, time 30 min) were inserted as an input and model was operated with the help of push button. GUI predicted the hydrogen yield as 0.2054

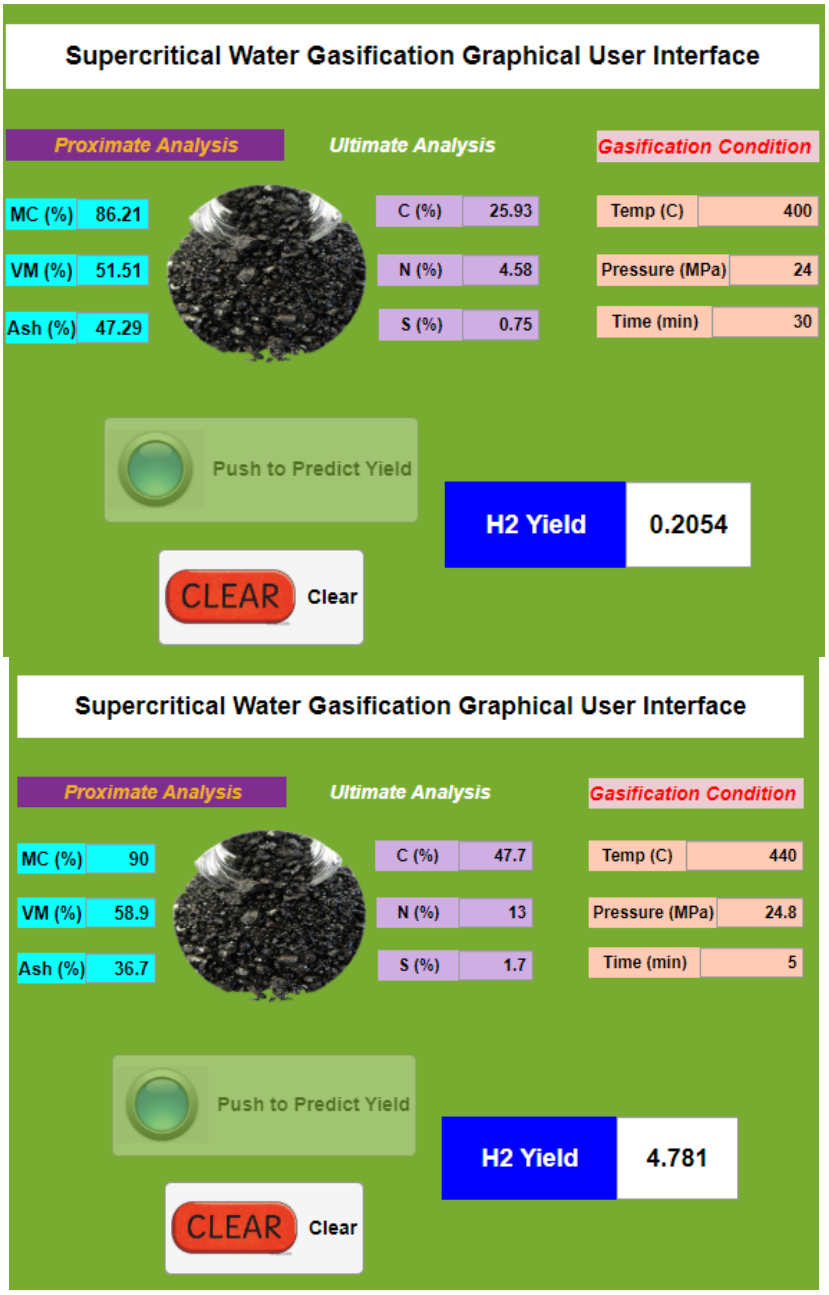

Figure 21: GUI for Hydrogen Yield Prediction

Conclusions

Machine Learning models have being used in this research to predict hydrogen production from the proximate, ultimate and gasification conditions of sewage sludge. In comparison to Ensembled Tree (R^2 0.994), ANN (R^2 0.943), and SVM (R^2 0.761), the Gaussian process regression model performed better in terms of prediction (R^2 0.997). This study provided a more precise and understandable method for predicting hydrogen yield from sewage sludge using super critical water gasification. The important features for the hydrogen prediction while utilizing the GPR model were T > MC>P. At different proximate, ultimate and gasification condition the GPR model predicted values and experimental value were 0.54–0.47, 8.68–9.3, 0.2054–0.22, 0.49–0.487, and 4.781–4.25 mol/kg respectively. GPR model suggests that gasification can be improved with high temperature (350–750 °C), pressure in the range of 30–32 MPa, and high moisture content.

Recommendations

1. The proposed method might be extended to include other chemical experimental and industrial processes.
2. To generate more accurate findings, a deep learning-based technique can potentially be implemented into the suggested framework by constructing a big database.
3. The proposed methodology might be extended to some other biomass gasification processes.

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