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The Application of Computational Modeling for the optimization of Bio Fuel Production Processes

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ABSTRACT

As the current advanced society, there is a precipitous increase in the application of computational modeling in almost every industry. Given the depletion of fossil fuels and the negative effects its burning has on the environment, one area of research gaining significant traction is bio-fuels. Computational modeling has the potential to be a cost-effective tool that enhances both productivity and economics for biofuel processes. Advances in artificial intelligence and its subclasses are making it possible to predict several items including process yields, substrate medium components and optimal process conditions among others. It has been employed in many bioprocesses such as pretreatment of lignocellulosic biomass and various biofuel production processes. Further implementation of this computer-based tool may potentially mitigate the need for preliminary experiments and in some cases, lab-scale experiments. This review highlights the application of computational modeling in biofuel production and also discusses future trends.

Key words: Computational modeling, biofuel, machine learning, artificial intelligence.

1. INTRODUCTION

With the global population expected to increase exponentially over the coming years, global energy demand is escalating simultaneously. Conventional fossil fuel sources such as coal, oil and gas, are rapidly depleting with some studies estimating their complete depletion within the next century (Moodley and Gueguim Kana, 2017). Coupled to this, is the harsh negative impacts of fossil fuel burning such as greenhouse gas emissions contributing towards climate change. All of these factors have prompted the search for alternative fuels that encourage a bio-economy within global economies (Sewsynker-Sukai et al., 2018). With this in mind, several bio-fuels have been proposed and investigated including bio-ethanol, bio-hydrogen, bio-methane and biodiesel (Kumar et al., 2020). In addition to this, several process factors have been taken into account, some of which include feedstock type and inoculum type. Each of the factors and processes have their own developmental challenges which requires further research.

In order to fully realize the potential of biofuel production, these processes must undergo a thorough modeling and optimization in order to enhance process economics and scalability. For instance, when examining the pretreatment of lignocellulosic biomass feed stocks, several parameters are considered. The pretreatment type will dictate the parameters to be considered. For example, chemical pretreatment using conventional heating will potentially include parameters such as chemical concentration, temperature, heating time and solid loading (Moodley et al., 2020). Microwave heating will include microwave power and heating time (Moodley and Gueguim Kana, 2017). Subsequent stages in the process such as enzymatic hydrolysis can include factors such as enzyme loading, solid loading, hydrolysis temperature and rotations per minute. When moving to biofuel production, there are more parameters to be considered, including temperature, pH, agitation, substrate concentration, inoculums concentration, oxygen levels etc. (Moodley and Gueguim Kana, 2015). All of the parameters play a crucial role in the manner in which the process proceeds and are also determinants in final output yield. For this reason, it is imperative that all these parameters are modeled and optimized in their respective stages to ensure maximum productivity.

Various computational modeling tools have been employed to assist in this regard, ranging from machine learning to genetic algorithms. Each of the methods has different fundamental operating principles and therefore offers different approaches. With this in mind, this review aims to detail the different modeling and optimization tools that are available for this purpose with the latter part of the review looking at how these tools have been applied in research.

2. COMPUTATIONAL MODELS AND DESIGNS

2.1 Response Surface Methodology (RSM)

RSM, a mathematical methodology allows one to extrapolate relationships between sets of data, containing independent variables correlating to one or more outputs, referred to as responses. This process allows the operational variables or parameters to be evaluated based on whether they have a significant or non-significant effect on the desired output (Myers, 1976).

2.1.1 Central Composite Design (CCD)

CCD is employed in scenarios to generate a second order polynomial model based on a set of data. In its core, CCD, a cluster of points at the center and axial points are distanced equally to the midpoint. Use either SI (MKS) or CGS as primary units. (SI units are strongly encouraged.) English units may be used as secondary

This factorial based design element is category 2k factorial. In this element, the k represents the number of parameters. Every parameter is observed at two different levels. This essentially means that every parameter has a minimum and maximum value. This model works by employing coded values, where a coded value of -1 and +1 is attached to signify the parameter at their minimum and maximum values respectively. A factorial is geometrically represented by a cube where each angle further represents factor or parameter interactions. From this point of view, a total of 8 interactions can be examined when 3 input parameters are chosen to compute the effects on the desired output.

The axial element of central composite design makes reference the values that are distanced equally from the center point of the cube that is generated during the factorial design. Consequently, there is a confident and an adverse axial value, referred to as +α and -α respectively. These axial points add two more values to the data set, emanating from more differing values in each parameter. The value of α is computed using the following equation, α = (ni)1/4. In this equation, nide notes the number of interactions achieved from the design. With this in mind, for a total of 8 interactions, α = 1.682 (Myers, 1976). The midpoint element in the CC design is the median of maximum and minimum values computed in the factorial design. To this end, the center point can be described as the optimal conditions where they potentially meet. The inclusion of the midpoint in the design enhances the level's design. Similarly, if the design has three variables, by default the design would be based on three levels. This type of model would lead to the estimation of 10 coefficients, inferring some degrees of freedom are left further indicating the generation of a reliable model particular when some experiments are prone to experimental error (Rakic et al., 2014).

2.1.2 Doehlert Design

The Doehlert design defines a sphere-like testing area and emphasizes the consistency of space. Even though this design is not orthogonal, it does not differ drastically from the value necessary for effective use (Massart et al., 2003). In the case of two parameters, the Doehlert configuration comprises one mid-point and six regular points, establishing a hexagon, and thus forms a sphere.It can be represented in three dimensions in various manners, reliant on the chosen structure with geometric characteristics. In a Doehlert design, the amount of rates differs among all the inputs (Garcıa-Campaña et al., 1997). For instance, in a two parameter design, one parameter is examined at five values, whereas the remaining variable is examined with three values. This characteristic allows select from factors which is to be allocated to a big or small number of rates freely. To determine the variables, different parameters may be used. As a rule of thumb, it is better to select a parameter with a significant effect as a factor with five rates with a view to extract a large amount of knowledge from the system. Every design is defined by taking into account the number of parameters or input factors and their respective coded values (Ci) of the experimental matrix. This association is described by the equation (1) below:

$$C_i = \left\{ \frac{X_i - X_i^0}{\Delta X_i} \right\} \alpha \qquad (1)$$

In the equation above, Ci represents the coded value for the factor level I, Xi is its actual value from the experiment, X0i is the real value at the midpoint of the navigation space, ΔXi is the real value variance phase and α is the coded value threshold for every parameter in the design.

Replicates are performed at the midpoints of the variables to authenticate the model through an experimental variance estimate. The evaluation between the aforementioned second-order models has shown that Doehlert designs and Box – Behnken designs are effective compared to composite central designs, given that the effectiveness of one experimental design is described as the amount of coefficients of the estimated model distributed by the amount of experiments conducted. An example of a Doehlert design for a three factor design is illustrated below in Table 1.

Table 1: Doehlert Matrix for a three level design

Runs	Experimental factors		
	A	*B*	*C*
1	0	0	0
2	1	0	0
3	0.5	0.866	0
4	0.5	0.289	0.817
5	-1	0	0
6	-0.5	-0.866	0
7	-0.5	-0.289	-0.817

8	0.5	-0.866	0
9	0.5	-0.289	-0.817
10	-0.5	0.866	0
11	0	0.577	-0.817
12	-0.5	0.289	0.817
13	0	-0.577	0.817

2.1.3 Box-Behnken Design

The Box Behnken design is another modeling and optimization method that has been extensively employed in various studies. The amount of experiments (N) needed for BBD processes is defined as $N=2k(k-1)+C0$ (where the count of parameters and C0 is the count of midpoints). By contrast, the amount of experiments for the former design is $N=2k+2k+C0$. A comparison among the Box-Behnken Design and additional response surface methods has shown that the Box-Behnken Design and Doehlert design are marginally more effective than the central composite design. Table 2 illustrates that three-level complete factorial designs are expensive when the number of factors is greater than two. In this table, A and -A correspond to 1 and -1 respectively. The number of experimental runs increases with increasing factors and thus has a ripple effect with the consumables and equipment needed thereby further requiring more time to conduct experiments. This can significantly reduce productivity of the process. A further benefit of the Box-Behnken Design is it does not include runs where all variables are at their maximum or minimum levels simultaneously. Consequently, these methods are valuable when avoiding experiments conducted with extreme conditions where in adequate results can be obtained. In comparison, these are not suggested for cases where the objective is to learn the extreme answers, that is, at the cube's vertices.

Table 2: Coded factors for a three-level Box-Behnken design

Run	Variable 1	Variable 2	Variable 3
1	-A	-A	0
2	A	-A	0
3	-A	A	0
4	A	A	0
5	-A	0	-A
6	A	0	-A
7	-A	0	A
8	A	0	A
9	0	-A	-A
10	0	A	-A
11	0	-A	A
12	0	A	A
C	0	0	0
C	0	0	0
C	0	0	0
C	0	0	0

2.1.4 Comparison of Response Surface Methods

By comparison, the Doehlert design is the most effective of the three for all values of k. Doehlert designs possess additional effectiveness in surveying space: adjacent hexagons may completely and efficiently load a space, since the hexagons occupy space without overlapping (Massart et al., 2003; Bosque-Sendra et al., 1995). Another advantage is its sequential ability, where experiments can be recycled where at first, the limits were chosen without motivation (Massart et al., 2003).

2.2 Genetic Algorithm

Traditional optimization approaches use a weighed approach with numerous targets and turn the problem into a single objective optimization. Weighed objective variables are decided earlier on, in terms of priorities and factors. Each collection of weighed parameters would give a singular solution to the problem of optimization, and a new solution will result in variation of the factors. The batch of solutions obtained provides a Pareto solution for the problem of multi-objective optimization. Deb (2001) reported that typical actions can be classified as multi-objective optimization constructed on choice, that involves supplementary data to turn the problem into one objective optimization. So the desired resolution can be obtained by answering the optimization of the singular goal. By contrast, a second group, termed ideal multi-objective optimization, disregards higher-level data to generate ideal solutions; nevertheless, high-level data may be applied at some point in the future to choose the best desirable resolution from the Pareto optimal solutions set. Furthermore, preferential solutions are time consuming since specific weighing factors need to be implemented for each ride. Preference strategies often need additional details and limitations for the user to solve the multi-objective optimization problem by increasing the number of goals. A method for delivering power effectively by using GA is explained (Abdul et al., 2018)

Evolutionary optimization algorithms for multi-objective optimization have now been applied because of their methodology to employing a population-based technique to create new population of solutions from one solution in a duplication in each iteration. In recent years, the key rationales for employing evolutionary methods are their suitability for broad array of functions, ease of use in various functions, and versatility for specific case studies (Deb, 2001;Abraham et al., 2005). In recent times, genetic optimization algorithms are becoming commonly employed for multi-objective problems as a collection of optimal Pareto solutions are needed for such problems and can be given in one run by these approaches (Deb 2001, Ebrahim et al., 2005, Konak et al., 2006, Siinivas and Deb, 1995; Bandyopadhyay, 2012).

A. The Non-Dominated Sorting Genetic Algorithm II (NSGA II) has received the most consideration among various evolutionary genetic optimization algorithms (Deb, 2011). The key benefits of NSGA II compared to other genetic algorithms are the addition of the crowded comparison operator across the primary space for globally optimal solutions, a decrease in computational difficulty and a growth in population variety (Yijie and Gongzhang, 2008). Overall, the key features of the NSGA II are: (i) introducing elitism that can accumulate all non-dominated solutions and further boost convergence traits; (ii)variety ensuring and range of solutions; and (iii) considering a non-dominated method to class individuals with respect to the degree of non-dominance (Konak et al., 2006; Yijie and Gongzhang, 2008; Deb et al., 2002). A survey is done on the software testing by applying genetic Algorithm (Chandraprakash et al., 2017)

When running the algorithm, in essence, every structural network signified by the gene population is evaluated and assessed based on their results. The genes are then replicated with a greater chance if their output is better. That is, the genes which generate a poorly performing network are unlikely to be copied; whereas those with desired results are likely to be replicated. Therefore, the replicating procedure creates a population with a lot of higher performing genes. If the replication procedure is complete, the genes are then "bred" by 'mating' at random points with some of the data in the network. To add a certain variety, a slight random shift is made, called a "mutation." Then repeat the whole cycle. In a given problem space, each gene codes a potential solution-called the search domain. This domain encompasses all potential solutions to the present problem. Alphabets are mostly employed but in recent years this has been expanded to comprise character-based encoding and real-evaluated encoding.

Defining a baseline GA involves the following steps:

1. Build a population of arbitrary individuals such that each individual represents a potential solution to the problem being faced.

2. Calculate increasing human fitness, that is, its capacity to solve a specific problem. This requires searching for the so-called fitness function.

3. Select individual members of the community to become parents. The fitness-proportionate selection is the basic selection method, where persons are chosen with a potential proportional to their relative fitness. This ensures that the estimated amount of times a person is selected in correspondence to their relative population results. Therefore, individuals with high fitness have a greater chance of "reproducing," whereas those with poor fitness are likely to vanish.

4. Produce offspring and introduce them to the population by recombining novel material through crossover and mutation.

5. Evaluate fitness for the kids.

6. Repeat steps (3) to (5), until a fitness criterion solution is obtained.

Selection by itself cannot bring new people into the population. The quest space uses genetically based operators such as crossover and mutation to locate novel factors. The Crossover Operator is the most significant genetic operator. The crossover process, in biological environments, results in the recombination of alleles through the swapping of sections between sets of genotypes. GA are iterative stochastic systems, which are not expected to congregate. The end instruction may be stated as a set, a maximum number of generations, or a predefined appropriate standard of fitness. It emerges from the fact that in a population of mediocre others, there might be some exceptional genotypes at the top. These genotypes take over a large part of the population in the first couple of generations, before the crossover operator can create a more diverse collection of healthy genotypes.

2.3 Fuzzy Logic

An academic at UC Berkeley first proposed Fuzzy theory in 1965, suggesting a set theory that functions over the range [0, 1]. The seminal work called "Fuzzy Sets" presented the essence of this theory. Whilst the results of Boolean logic are limited to 0 and 1, fuzzy logic findings vary from 0 to 1. In essence, Fuzzy logic determines certain transitional values including absolute truth and absolute false between sharp evaluations. This is an indication that Fuzzy sets can manage ideas that is usually encountered daily, such as very small, small, big and very big. Fuzzy logic is akin to human reasoning, since it is based on notches of real information and uses factors of language. Fuzzy logic works with fuzzy sets which have membership degrees/notches in their components. Essentially, a member element from a multiple set associated with different membership values may be an object. For example, weekdays are usually assigned from Monday to Friday; whereas weekends include Saturday and Sunday. Alternatively, it could be assumed that on Friday, individuals begin to feel the optimistic impact of the approaching weekend. Therefore, it may be thought that while Friday is classed as the "weekdays" set with a membership value of 0.95, it belongs to the "weekend" set with a value of 0.05 (Kayacan and Khanesar. 2016).A method to decrease the cloud environment latency by applying fuzzy logic is proposed (Jena et al., 2017).

Even though the definition of fuzzy logic and probability sound similar, they are very different. Even though probability allows assumptions about a specific fact, fuzzy logic stays away from claims about likelihood but characterizes membership in loosely described sets. For example, if 0.5 is known as a likelihood value for an old person, it can be assumed that the possibility is they may be old. It is unclear whether they are young or old. In fuzzy logic, though, if 0.5 is described as the degree of membership in the

set of young and old people, some information about the person is given and therefore is put in the midst of young and old (Kayacan and Khanesar. 2016). A method is discussed to improve clustering rate accuracy using Fuzzy C Means (Ramesh et al., 2018). Fuzzy Inference Vector ACO is used for detection of island and analysed the stability of power system integration (Reddy et al., 2018). Fuzzy C-Means is applied for image segmentation and extraction of island using the intensity of pixel (Rehman et al., 2018).

In nature, fuzzy logic is seen as being closer to human reasoning and innate language. With MFs, human thinking methods are achieved which determines how each factor in the input domain is surveyed to a space of membership values. Values for membership in fuzzy sets are inside [0;1]. If an adage is absolute valid, the Fuzzy sets membership value is set to be 1. Similarly, if it is totally incorrect, the Fuzzy Sets membership value is 0. An MF production is known as an antecedent (μ). While an MF's input values are smooth, these MFs transform them into fuzzy variables (Kayacan and Khanesar. 2016).

2.4 Artificial Neural Network

There has been a lot of study over the past few decades aimed at forecasting the future and aiding in good choices. These studies have contributed to many evolutions in the methodology of predictions. Many of those developments in methods were focused on mathematical techniques. These methodologies-artificial neural networks (ANNs)-actually face a new challenger. ANN has been widely praised as addressing many problems in forecasting and modeling decisions. For instance, it has been proposed that they can easily model any kind of operation, and change the input data automatically and optimally. These kinds of statements have created a lot of interest in ANN. Chatfield (1993), have had competing thoughts and has questioned if ANN has been over-sold or is just a phase.

ANN are mathematical models which are based on the biological association and functioning of neurons. There are several artificial variants of the neural network that are related to the design of the role. In addition, there are several differences in the way neurons are represented. Some concepts have these models meticulously correlate to biological neurons and concepts have the models differing greatly from biological operation. The literature indicates a variety of possible benefits that ANN has over the statistical methods. Non-linear trends may also be modeled with ANN, since it can be general operation estimators. Also, they can estimate approximations of functions piece-wise. ANN can mathematically be shown to be approximations of general operation. This means they can mechanically estimate what functional type the information is best described by. Although this characteristic is not important if the useful structure is basic (e.g. linear), it helps ANN to derive more information from the operational structures underlying it. ANN has also been shown to automatically partly change input information. Even ANN are fundamentally nonlinear. That means they can not only approximate non-linear functions efficiently, but they can also remove any undesirable elements from the data after removing linear terms. Since ANN uses many hidden layers, the networks will automatically divide the sample domain and construct various operations into various segments of the domain. This infers that ANN has a diffident ability to construct nonlinear models on a piece-wise basis. One clear example of such a model is the artificial neural network model for the exclusive OR role. A method is proposed for the improvement of torque, increase the speed and also the flux response with the application of ANN and Adaptive Neuro-Fuzzy Inference (ANFIS) (Venkateswara Rao et al., 2018). With the artificial intelligence techniques has automated IoT hub (Yasaswini et al., 2018). The classification of images of flower by using segmentation and ANN is discussed (Inthiyaz et al., 2028). An analysis on eye vessel damage, micro aneurysms and exudates using ANN is done (Reddy et al., 2018)

ANN, too, has some issues. First, the methods and modeling techniques of artificial neural networks are rapidly evolving while certain techniques of statistical modeling are established. Secondly, although programs for statistical techniques are easily accessible, viable artificial neural network tools of high quality, though. Often it lags behind in-field innovations. Third, artificial neural network models are more difficult to understand than many predictive models, and to give physical significance. Fourth, ANN includes more estimate parameters than other statistical forecasting models do; this can lead to over-fitting problems. Lastly, ANN requires more computing resources than the mathematical models.

3. CURRENT APPLICATIONS IN BIOPROCESSES

Various computational designs and models have been applied to the bioprocess sector, as outlined in Table 4. More commonly, these techniques have been employed in the modeling and optimization of lignocellulosic pretreatment methods. For instance, Mariano et al. (2020) employed the central composite design to model and optimize the release of sugar from coconut pulp through acid hydrolysis. Similarly, Iram et al. (2019) also used the central composite design to model and optimize the acid pretreatment of dried distiller's grains to produce a soluble feedstock. The Box-Behnken design was employed by Liu et al. (2018) to optimize the pretreatment of corn straw using ionic liquids. Artificial Neural Network has been employed to generate a model with the ability to predict sugar yield, based on the training using data from multiple studies involving inorganic salt pretreatment (Moodley et al., 2019). This model can provide substantial preliminary information prior to conducting lab studies thereby saving time and potentially enhancing productivity. Looking at biofuel production processes, the genetic algorithm method was employed by Abadila et al. (2020) to optimize a photovoltaic-hydrogen system. In another study by Ghaderi et al. (2018), the production of bio-ethanol from switch grass was optimized and

programmed using the fuzzy logic method. This is an illustration of the widespread use of computational models in the bioprocess and biofuel sector, owing to the many advantages these systems possess.

Table 4. Different computational models and designs employed in bioprocess design studies.

Process	Model employed	Reference
Lignocellulosic pretreatment	Central composite	Li et al., 2019
Microalgae pretreatment	Central composite	Ellison et al., 2019
Bioethanol production	Central composite	Manmai et al., 2020
Lignocellulosic pretreatment	Central composite	Mariano et al., 2020
Lignocellulosic pretreatment	Central composite	Tsegaye et al., 2020
Lignocellulosic pretreatment	Central composite	Iram et al., 2019
Lignocellulosic pretreatment	Box-Behnken	Rai et al., 2019
Biofuel production	Box-Behnken	Senol et al., 2020
Lignocellulosic pretreatment	Box-Behnken	Shahabazuddin et al., 2018
Biohydrogen production	Box-Behnken	Jung et al., 2011
Lignocellulosic pretreatment	Box-Behnken	Martin et al., 2019
Lignocellulosic pretreatment	Box-Behnken	Liu et al., 2018
Enzyme production	Genetic algorithm	Sirohi et al., 2018
Biofuel production	Genetic algorithm	Abadlia et al., 2020
Biofuel production	Genetic algorithm	Oloko-Oba et al., 2018
Bioethanol production	Fuzzy logic	Garofalo et al., 2020
Bioethanol production	Fuzzy logic	Konti and Damigos, 2018
Bioethanol production	Fuzzy logic	Ghaderi et al., 2018
Lignocellulosic pretreatment	Artificial neural network	Rego et al., 2018
Lignocellulosic pretreatment	Artificial neural network	Lee et al., 2020
Lignocellulosic pretreatment	Artificial neural network	Moodley et al., 2019
Biodiesel production	Artificial neural network	Rajendra et al., 2009
Bioethanol production	Artificial neural network	Chouaibi et al., 2020
Bioethanol production	Artificial neural network	Sorrosal et al., 2017

3.1 Lignocellulosic pretreatment

Optimizing pretreatment processes is important for the positive economic outlook of bioprocess and biofuel technologies (Tu and Hallett, 2019) and many different pre-treatments have to be evaluated on a vast range of procedural conditions. Efficient bioconversion techniques must specifically break down the building blocks and produces fractional or complete disconnection of cellulose, hemicellulose and lignin, thus reducing by-product formation as well. Integrated processes incorporating multiple pretreatment methods are effective in reducing the amount of required stages and eliminating possible inhibitors as opposed to the traditional single process (Kumar and Sharma, 2017). Biological pretreatments that use microbes (bacteria and fungi) can possess possible benefits but involve the choice of microbial inoculum to effectively pretreat unique biomass sources (Kanta et al., 2017). Lignocellulosic waste serves as a substrate for the production of bio-fuels and the pretreatment techniques rely on the constituents of agricultural sources to establish their utilization for the production of hydrogen, methane, ethanol, methanol, but anol and diesel (Zhu et al., 2020). Bio-fuels in liquid form are especially important sustainable commodities owing to existing infrastructure that are in place for their use in transport. Additionally, they have encouraged the development of new pretreatment techniques for new fuel components acquired from lignocellulosic-based carbohydrates. Bio-refinery principles dictate the range of techniques of pretreatment used for the bio-conversion of lignocelluloseto bio-fuels, owing to the residues that must be considered (Faustino et al., 2019). The valorization of lignin is an integral feature of the effective biorefinery of lignocellulose. Bioprocesses that result in the removal of lignin from the carbohydrate component can be differentiated from those resulting in the subsequent isolation of lignin into fuels and chemical (Rinaldi et al., 2016), but the pretreatment mechanisms of chemicals routes have not been adequately explored to develop techniques or to optimize the pretreatment until recently (Baruah et al., 2018). These applications should be improved by recent advances integrating de-polymerization and conversion (Wendisch et al., 2018). Depolymerized lignin is often a multifaceted combination of different molecules, so refining the native component may minimize its density through both chemical and biological techniques (Schutyser et al., 2018). The use of cascades, where lignocellulose is initially pretreated based to

its structure and features may be a choice. However, it should be taken into account that "owing to the complex structure of biomass, the single pretreatment approach has restricted enhancement of the fractionation efficiency" (Liu et al., 2019). Deep eutectic solvents, made from biomass effluent, are used for enzymatic saccharification and lignin removal pretreatments (Shen et al., 2019). This chemical is generatedfrom available materials and demonstrates lignin selectivity compared to cellulose, but these are still in their infancy.

Computational methods have become important for the identification of methodologies to evaluate chemical processes easily, accurately and automatically. Luckily, their uses for modeling bioprocesses have seen remarkable progress in recent times (Goulart et al., 2019) and their future applications for processes of pretreatment has shown immense promise (Butler et al., 2018). For example, from over 100 million molecules a groundbreaking approach to machine learning discovered highly effective novel antibiotics. The properties of molecules are learned by a neural network, a method that varies from those currently in use. Instead of searching for particular compounds, the network is equipped to search for compounds with a particular activity (Marchant, 2020). Interactions concerning fragile intermolecular forces can be explored using a machine learning model that can predict the total density of electrons. It has been trained using a dataset of minute molecular fragments and forecasts polypeptide density, and describes electrostatic connections between fragments which play a role in protein stability.

3.2 Bioprocess Modeling

Computational Intelligence (CI) is the research field that focuses on researching and utilizing strategies that are considered intelligent. These strategies can be implemented through software programs. Usually these program scan be applied to general optimization algorithms. This can further include genetic algorithm, swarming, artificial neural networks and fuzzy logic to name a few. Even though they are called computational intelligence methods, many statistical-based approaches are meticulously linked to computational intelligence methods. Commonly, hybrid systems which incorporate a strategically balanced mixture of various computational intelligence methods to counteract one another's disadvantages, and the design and implementation can also be seen as one of computational intelligence objectives. Modeling, optimization, monitoring and regulation of bioprocesses can be categorized as a division of Chemical Engineering, and recently terms bio-processing. These processes, of course, comprise upstream processes such as feedstock preparation, and downstream processes such as bio-product separation and purification, along with the center of the method: singular and multiple bio-reactors. This could be enzyme-based fermenters or micro-organism or cell culture reactors. In industry, bioreactors are typically called fermenters, even though the culturing sometimes proceeds aerobically where fermentation can be considered an unintended stream. This scientific classification was possibly inherited from the manufacture of alcoholic drinks, one of the first bioprocesses in history. The broad variety of bio-processing operations makes it impossible to explore all possibilities for CI techniques to be applied.

B. Many studies have examined either one or multiple computational intelligence methods in controlling bioprocess' in general or other specific areas (Alford, 2006; Harms et al., 2002; Komives and Parker, 2003; Glassey et al., 1997; Lee et al., 1999). Others, however, only mention them very briefly, such as (Clementschitsch and Bayer, 2006; Schugerl, 2001). An elaborate study involving a two-year investigation into the employment of neural networks for the control of processes was reported by Lennox et al. (2001). These authors provide a detailed description of the conclusions drawn from the study, while also concentrating on data problems together with neural network issues. Pertinent problems that should be addressed when employing neural networks in bioprocesses, as suggested by Karim et al. (1997), are the appropriate scaling of data, the choice of a suitable network structure – taking into account the appropriate choice of process parameters, and the role of the algorithm. Previous issues and different neural networks have been studied in their review in relation to different microbiological systems. The computation of the optimum rate of the substrate feed is of vital importance in fed-batch fermentation; the approximation process can be described as a unique control problem (Chaudhuri and Modak, 1998) and owing to this, a complicated job of optimization is to be unraveled. Additional feed regulation is a very complex process since it is quite difficult to tune and has a profound effect on the desired stream; under-feeding may cause microorganism starvation and over-feeding may result in the formation of undesired products and may interfere with the formation of the product. As a result, the development of an appropriate food strategy is crucial to the successful fermentation of fed-batch products.

The influential paper based on the algorithms for search optimization of biotech processes by Simutis & Lübbert (1997), highlights the significance of search algorithms (compared to the conventional approach linked to the Pontryagin Maximum Principle). This shows that the employment of arbitrary searches methods, which are much more rudimentary, easier to comprehend and enforce, can essentially lead to the use of random search procedures. Three randomized search procedures were employed in the analysis, viz. chemotaxis algorithm, simulated annealing and evolutionary programming. Highlights found in this study are recommendations to new investigators that "the evolutionary ANN algorithm with sigmoid-based functions should be used to evaluate the optimized control profile of complicated processes." Explaining methods to enhance the efficiency of process optimization and control models, it was concluded by Simutis et al. (1997) that "the efficiency of models can be improved." This proved to be better than using either of these

methods on a stand-alone basis. The employment of hybrid process designs was also reinforced by the thoughts and deliberations by Galvanaukas et al. (2004).

4. FUTURE PROSPECTS OF COMPUTATIONAL MODELING IN BIOFUEL PRODUCTION

The use of biomass as a substrate in biofuel production has sky-rocketed in recent times owing to the contribution towards sustainable growth in a circular economy. Process optimization of biomass-based processes to boost the yield and productivity of the bio-fuels required is crucial to the lucrative economic outlook of bioprocesses. Bioprocess design and optimization from a modeling stand point has shown to be a capable method for this purpose, in conjunction with additional tools such as genetic engineering and bioprocess monitoring, to promote methodical design and optimization studies with the objective of swiftly enhancing the productivity of the feedstock process for the development of bio-fuels. Consolidative cell and biochemical kinetic modeling may aid in the creation of fermentation techniques or in the identification of genetic modification contenders for improved bioprocess efficiency from lignocellulose to adhere to the technological and economic demands. Nevertheless, models that have been developed recently do not provide a monitoring and signaling system or cell stress reaction mechanism when cultivated in biomass supernatant, which also plays a pivotal role in computing fermentation performance. Addition of high-throughput omics data to explain cell control and genome kinetics is a likely imminent trend to continually enhance the precision of the consolidative modeling system for biomass-based design, optimization and scale up.

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