

Parametric Optimization for the Maximization of Hydrogen Production by Enterobacter Cloacae

by

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CERTIFICATION OF APPROVAL

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A project dissertation submitted to the
Chemical Engineering Programme
Universiti Teknologi PETRONAS
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Approved by,

(DR. TIMOTHY GANESAN ANDREW)

UNIVERSTI TEKNOLOGI PETRONAS

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JANUARY 2015

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

(MOHAMAD SHAKIR AMRI BIN SAIDIN)

ABSTRACT

The decrease of fossil fuel energy induces the development of sustaining renewable energy. One of the potential energy to be further developed is hydrogen energy. Most of the hydrogen resources currently come from fossil fuel energy. Besides, some biological processes also can produce hydrogen such as dark fermentation which is being focused on in this project. *Enterobacter cloacae* are used as the bacteria to be fermented in the nutrient broth. Since this process has yet to achieve economic sustainability, this project focuses on the maximization of the production of hydrogen gas by optimizing the parameters influencing the hydrogen production. The decision variables (process parameters) are the initial glucose concentration, Inoculum age and also the initial pH of the nutrient broth. By using data from the previous research, the parameters are optimized by using three numerical methods, simulated annealing, pattern search and Genetic algorithm. A comparison between these three algorithms used is done to compare the optimization results and discuss their advantages and disadvantages.

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CHAPTER 1

INTRODUCTION

1.1 Background

In current times, with fossil fuels reserves rapidly declining, the urge of renewable energy are playing and will play a vital role in meeting current and future energy needs. The key component of the sustainable development of renewable energy is to generate more environmentally friendly energy compared to the conventional fossil energy sources, which will not be depleted within the foreseeable future. Hydrogen energy is one of the renewable energy that can provide high energy density, low capital cost and easy integration with the existing energy network which is most promising contributors towards more sustainable future, in both energy demand and environmental sustainability (Enteshami and Chan, 2014).

Hydrogen gas is considered as a good energy carrier for the future due to its high energy content and clean usage of electricity production in fuel cells or for combustion with air. At present, hydrogen is produced from fossil fuels by reforming pyrolysis, biomass gasification, or electrolysis. Hydrogen also can be produced biologically through photolysis, photo-fermentation, dark fermentation, or with microbial electrolysis cells (MEC). Most of these methods are not environmentally-friendly, however, dark fermentation is the opposite of them. It has many advantages such as the process itself do not require light energy, has wide substrate versatility and high hydrogen production rate which is can be maintained at non-aseptic conditions and simple reactors (Nissila *et al.*, 2014).

Fermentative hydrogen production has got certain distinct advantages over the photo-fermentation like it does not require any light source but producing hydrogen at a faster rate. Moreover, hydrogen-producing fermentative anaerobic bacteria have potential to metabolize organic wastes as the produce cleaner and renewable energy in the process which also environmental friendly process that resulting in production of oxygen gas as their byproduct (Ghosh, Joy and Das, 2011). Thus, in order to realize this clean and environmental friendly energy production, optimization of the process is need to estimate the maximum potential yield of hydrogen that can be

produces to ensure sustainable development of the fermentative hydrogen production in the upcoming future.

Three numerical methods is test to maximize the optimization problem, which are Simulated Annealing, Pattern Search and also Genetic Algorithm. The Simulated Annealing (SA) is an iterative improvement algorithm for a global optimization. The SA algorithm imitates the process of annealing in metals as they cool from liquid to solid states. It is inspired from thermodynamic to simulate the physical process of annealing of molten metals. Thus, it exploits an analogy between the way in which a metal cools and freezes into a minimum energy crystalline structure. The algorithm employ the generation of random numbers when they search for the optimum solution. (Saruhan, 2014)

Pattern Search (PS) optimization routine is a derivative free evolutionary technique that is suitable to solve a variety of optimization problems that lie outside the scope of the standard optimization methods. Generally, PS has the advantage of being very simple in concept, and easy to implement and computationally efficient algorithm. In addition, PS possesses a flexible and well-balanced operator to enhance and adapt the global and fine tune local search. (Al-Othman *et al.*, 2013).

On the other hand, Genetic Algorithm (GA) is the stochastic global search optimization algorithm which is inspired by Darwin's theory of natural selection. GA is essentially mimicking the process of natural evolution underlying the idea of survival of the fittest, in which the fitness of individual is improved by successive iteration through processes of selection, crossover and mutation. Basically, GA is capable for solving a wide range if optimization problems, even in highly nonlinear, multidimensional search spaces. (Patel and Kheraj, 2014).

1.2 Problem Statement

Parallel to pursuing hydrogen production for renewable energy applications, cost issues have been among the major obstacles in many of the projects and ideas. Despite numerous developments in hydrogen production, the profits from the yield do not justify sustainable use of these technologies. However, with the right parametric optimization approach, these issues could be resolved in the near future.

1.3 Objectives

The main aim of this research project is to find the optimal parameters for hydrogen production by *Enterobacter Cloacae* to maximize the hydrogen production using the dark fermentation process. Based on previous research data using numerical approach, the optimal parameters was determined and reliable data can be obtained.

The objectives of the research are as follows:

- a. To optimize the fermentation process in order to get maximum yield of hydrogen production.
- b. To test three optimization algorithms (SA, PS and GA) to get higher maximum yield of hydrogen production.
- c. To compare and analyze the optimization results produced by the computational techniques.

1.4 Scope of Study

This project focuses on performing parametric optimization in order to maximize the hydrogen production by the *Enterobacter Cloacae*. By using the previous research experimental data, numerical approach methods are done in MATLAB and the optimal parameters is analyzed. This project scope basically limited to the three algorithms, simulated annealing, pattern search and Genetic algorithm that is used to optimize the parameters. The algorithms were not tuned to the optimal. Model limited to the previous data and regression analysis developed by Sen and Das (2005). Algorithms only were executed on the computer. Experimental modeling and testing was done by Sen and Das (2005).

CHAPTER 2

LITERATURE REVIEW

2.1 Enterobacter Cloacae

Enterobacter Cloacae is a rod-shaped, gram-negative bacterium from the Enterobacteriaceae family. The size of this bacteria ranges from 0.3-0.6 x 0.8-2.0 μm . Enterobacter cloacae live in the mesophilic environment with its optimal temperature at 37 °C and use its peritrichous flagella for its movement. This type of bacteria can facultative anaerobic which can make Adenosine triphosphate (ATP) by aerobic respiration when oxygen present but capable of switching to fermentation in the absence of the oxygen (Oh *et al.*, 2013)

Based on the web article by Oh *et al.*(2013), these species of bacteria can be found on human skin and tissues as well as fruits, vegetables, and devices such as a hot water treatment tank. Although this organism is mainly a pathogen for human and cause disease, Enterobacter cloacae have been used as a biological control for plant disease such as the seed-rooting oomycete in *Pythium ultimum*, control insect pests on mulberry leaves, suppress disease, and also in clean energy production which is hydrogen gas obtain through the dark fermentation process.

2.2 Dark Fermentation

Based on the article by Guo *et al.* (2010) and Nissila, Lay and Puhakka (2014), there are several methods to produce hydrogen at the present, most of the hydrogen supply in the world produce from fossil fuels by reforming, pyrolysis, biomass gasification or electrolysis. Besides that, hydrogen also can be produced biologically through photolysis, photofermentation, dark fermentation and also with microbial electrolysis (MEC). In this research paper, dark fermentation process will be in focus for the hydrogen production as the method has many advantages that have promising potential in the future development.

The advantages are:

- a. It does not require light energy
- b. Wide substrate versatility
- c. High hydrogen production rates
- d. Production can be maintained at non-aseptic conditions and in simple reactor.

According to the research by Guo *et al.* (2010), dark fermentation is a key technology for producing hydrogen from crop residues, livestock waste and food waste. Based on their findings on biohydrogen production from the agricultural by the dark fermentation, there are three categories of agricultural residue have been considered. There are the waste directly generated from agricultural production, animal manure and food waste. It is shown that all these three possess great potential as a substrate for hydrogen production by dark fermentation, with food waste shows highest potential, followed by crop residues and livestock waste.

Based on the Nissila, Lay and Puhakka (2014), dark fermentative hydrogen production from lignocellulosic hydrolyzates is also an appealing method for renewable energy alternative. For the lignocellulosic biomass to become amenable to hydrogen gas fermentation pretreatment and/or hydrolysis is required. However, these processes and utilization of their side streams have to be carefully designed to become economically feasible.

Furthermore, based on the research by Lee, Show and Su (2011), biohydrogen has been regarded as an attractive future clean energy carrier due to its high energy content and environmental-friendly conversion. The extensive research in the past two decades have reviewed promising prospect of biohydrogen production via dark fermentation. As stated in the study that there have been substantial improvement and development in both the yield and volumetric production rates of hydrogen fermentations by different bacterial species.

2.3 Simulated Annealing

Based on the article by Altomare *et al.* (2014), Kaur, Rattan and Patterh (2012) and Mirzaali *et al.* (2011), Simulated annealing algorithm is a general-purpose optimization technique and has been applied to many combinatorial optimization problem. The main idea behind Simulated Annealing is an analogy, which is categorized as a metaheuristic method, with the way in which liquids freeze and crystallize.

According to Kaur, Rattan and Patterh (2012), SA is a stochastic global optimization technique which exploits an analogy between the way that a metal cools and freezes into a minimum energy crystalline structure. The fundamental idea of Simulated Annealing is therefore that the moves made by an iterative improvement algorithm, which the re-arrangement of molecules of the liquid occur as it is cooled at the same time the energy of the molecules corresponds to the cost function which is being optimized by the iterative improvement algorithm.

The SA algorithm aims to achieve the global optimum by slowly through convergence to a final solution, which hopefully ending up in a global optimizes solution.

2.4 Pattern Search

According to Altomare *et al.* (2014), AlHajri *et al.* (2012) and Căleanu *et al.* (2011), Pattern Search is direct search method for nonlinearly constrained optimization as adaption of a bound constrained augmented Lagrangian method. Unlike many conventional optimization techniques, it does not require the gradient information to guide its search process nor does it impose certain characteristics on the objective function such as convexity or continuity. Key attractive features of this optimization algorithm are concept simplicity, ease of implementation, and computational efficiency.

Pattern Search also is an attractive alternative because it is often computationally less expensive than other optimization methods. The methods operate by searching a set of points called a pattern, which expands or shrinks depending on whether any point within the pattern has a lower objective function value than the current point. The search stops after a minimum pattern size is reached.

In the study by Al-Othman *et al.* (2012) mention that Pattern Search possesses a flexible and well-balanced operator to enhance and adapt the global and fine tune local search. The algorithm proceeds by computing a sequence of point that may or may not approaches to the optimal point and starts by establishing a set of points called mesh, around the given point. This current point could be the initial starting point. This current point could be computed from the previous step of the algorithm. The mesh is formed by adding the current point to a scalar multiple of set of vectors called pattern. If a point in the mesh is found to improve the objective function at the current point, the new point becomes the current point at the next iteration.

2.5 Genetic Algorithm

Patel and Kharej (2014), state that GA is inspired by the Darwin's theory of natural selection which is essentially mimicking the process of natural evolution underlying the idea of survival of the fittest. Basically, the fitness of individual is improved by successive iteration through the processes of selection, crossover and mutation.

Based on the article by Antoine and Batra (2015), Genetic Algorithm (GA) is a direct search method that uses ideas based on natural selection to explore the search space for finding a global optimum. Population initialization, parent selection, crossover, mutation and selection of the fittest are the common elements in most GAs which is same as stated by Patel and Kharej.

According to the article by Bagheri *et al.*(2015), GA utilize random search evolutionary algorithms for optimization of a fitness function by means of the parameters space coding. The algorithm is started with a set of random solutions called population. Solutions from one population are used to forms a new population. This is motivated by a hope that the new population will be better than the old population. In order to form a new population, GAs use genetic operators and selection process. Genetic operators are used to generate the new solutions from the current solutions. The best solution is then returned to represent the optimum solution.

2.6 Research Efforts in Optimizing Biohydrogen Production

There are many effort in optimizing biohydrogen production can be seen in the past years. Based on research by Pan *et al.* (2007), statistically based experimental designs were applied to optimizing process parameters for hydrogen production from glucose by *Clostridium* sp. Fanp2 which was isolated from effluent sludge of anaerobic hydrogen-producing bioreactor.

The important factors influencing hydrogen production, which identified by initial screening method of Plackett–Burman, were glucose, phosphate buffer and vitamin solution. Box–Behnken design were adopted to screen the key process parameters and identify optimal values that bring maximum hydrogen production. The result shows that the statistical experimental design is an effective tool for optimization of process parameters on biohydrogen production and advance of hydrogen yield.

According to Chong *et al.* (2009), bacteria named *Clostridium butyricum* EB6 successfully produced hydrogen gas from palm oil mill effluent (POME). Thus, central composite design and response surface methodology were applied to determine the optimum conditions for hydrogen production and maximum hydrogen production rate from POME. The optimized conditions were determined for hydrogen production and hydrogen production rate using variables of pH, temperature and chemical oxygen demand (COD).

Moreover, based on the study by Nath and Das (2011), stated that biohydrogen is a sustainable energy resource due to its potentially higher efficiency of conversion to usable power, non-polluting nature and high energy density.

The study basically highlights the recent studies on modeling of microbial growth, substrate utilization and product formation along with various optimization strategies. It is note that any biohydrogen process depends largely on optimization of several controlling factors in order to get feasible production yield.

Furthermore, there is also optimization research by Ghosh, Sobro and Hallenbeck (2012), which focus on hydrogen production from glucose via single-stage photofermentation by the photosynthetic bacterium *Rhodobacter capsulatus* JP91. Response surface methodology with Box-Behnken design was used to optimize the independent experimental variables of glucose concentration, glutamate concentration and light intensity, as well as examining their interactive effects for maximization of molar hydrogen yield.

Based on the result, the three independent variables studied, glucose glutamate, and light intensity all had significant interactive effects on hydrogen yield. The optimized yield obtained is higher than the previously achieved and similar to what was previously shown for two-stage systems. Thus, single stage photofermentation of glucose is found to be a promising technology to achieve economic feasibility in upcoming future.

CHAPTER 3

PROBLEM FORMULATION

Based on study Sen and Das (2005), below are experimental setup that have been use to obtain maximum hydrogen yield of *Enterobacter Cloacae*.

There are several materials were used in the experiment:

- a. The nutrient broth powder and nutrient agar were obtained from HiMedia Laboratories Ltd, Mumbai
- b. Yeast extract powder and extra pure AR D-glucose were obtain from Sisco Research Laboratories Pvt Ltd, Mumbai
- c. Malt extract and KOH were purchased from Qualigens Fine Chemicals, Mumbai
- d. AR $K_2Cr_2O_7$ was obtained from S.D Fine-Chem Ltd.

For this experiment, *Enterobacter cloacae* DM11, the double mutant strain developed at IIT Kharagpur, was maintained at 4°C on nutrient agar slants and grown in nutrient broth at 37°C. In this bacteria species, the alcohol formation pathways were blocked by using allyl alcohol, while the organic acid formation pathways were blocked by proton suicide technique using NaBr and NaBrO₃.

The growth medium made from, using the nutrient broth by suspending 13g of nutrient broth powder in 1000 ml Milli-Q water. Hydrogen production medium was MYG, in which the malt extract (1.0% w/v) and yeast extract (0.4% w/v) concentrations were kept constant. The concentration of D-glucose was varied (0.8-1.2% w/v) in steps of 0.2% (w/v). While, the initial pH was varied (4-8) in steps of 2 units with all the media were autoclaved at 103.5kPA (15 psi) pressure and 121°C for 15 min.

The bacteria cells were aseptically transferred to 100ml nutrient broth taken in a 200ml conical flask by scraping it from the surface of slants. Then, the incubation was carried out in a temperature-controlled shaker at 37°C and 200 rpm. The incubation time was varied between (5-15 h) in step of 5h.

3.1 Initiation of Hydrogen Production

400ml of MYG medium was sterilized in a 100ml flask and aseptically transferred to a sterilized 500 ml flask. 20 ml of inoculum was added to the latter with a magnetic flyer. Then, the flask is sealed with a cork containing an inlet as well as an outlet tube. The outlet was connected by silicon tubing to a CO₂ absorber unit which contains 30% of KOH solution. The CO₂ absorber was connected to water displacement unit for collecting produced gas in the space above the water. Acidified K₂Cr₂O₇ is stained into the water for visual clarity. All joint and the connections were made airtight by sealing wax and Argon was passed through the set up to make the conditions anaerobic and the flask was placed on Spinit™ magnetic stirrer. The speed setting is kept constant at 5 of 10 based on the scale. The amount of hydrogen gas produced after 10 h was noted.

3.2 Previous Experimental Result Data Input

The regression analysis was used to generate an equation, which gave an empirical relationship between the response Y (cumulative hydrogen production in millimoles after 10 h) and the variables in non-coded form:

$$Y = -119.63814 + 116.83954X_1 + 2.3818X_2 + 19.8697X_3 - 48.45834X_1^2 \\ - 0.02971X_2^2 - 1.3261X_3^2 - 0.46875X_1X_2 - 1.33243X_1X_3 \\ - 0.18393X_2X_3$$

The results of the preliminary experiments found that the cumulative hydrogen production initially increased with increasing pH and then decreased respectively as 7.1429, 13.2143 and 10 millimoles at pH 4.6, 5.6, and 6.6. Similar situation can be seen in the case of initial glucose concentration respectively as 12.857, 13.75 and 10.1786 millimoles at initial glucose concentrations at 0.8, 1.0 and 1.2% respectively. While, the inoculum age is at 7.8571, 13.3928 and 10.1429 millimoles at inoculum ages 4, 12 and 20 h respectively.

The results indicate that hydrogen yields initially increase with an increase in the initial glucose concentration, inoculum age and initial pH but fall with further increase in the values of the variables. The optimum value of the initial pH tallied with the reported value of 6.0 for *Enterobacter Cloacae* IIT-BT 08.

The optimum values of the independent variables for the maximum production of hydrogen as determined from the above equation from the Three-Box-Benken Factorial Design use :

- a. Initial glucose concentration : 1.06% (w/v)
- b. Age of inoculum : 12.96 h
- c. Initial pH : 6.06

The theoretical maximum cumulative yield of hydrogen after 10 h using these values of the process parameters was found to be 17.9093 millimoles, which tallies with 17.8571 millimoles obtained experimentally results.

CHAPTER 4

METHODOLOGY

4.1 Project Flowchart

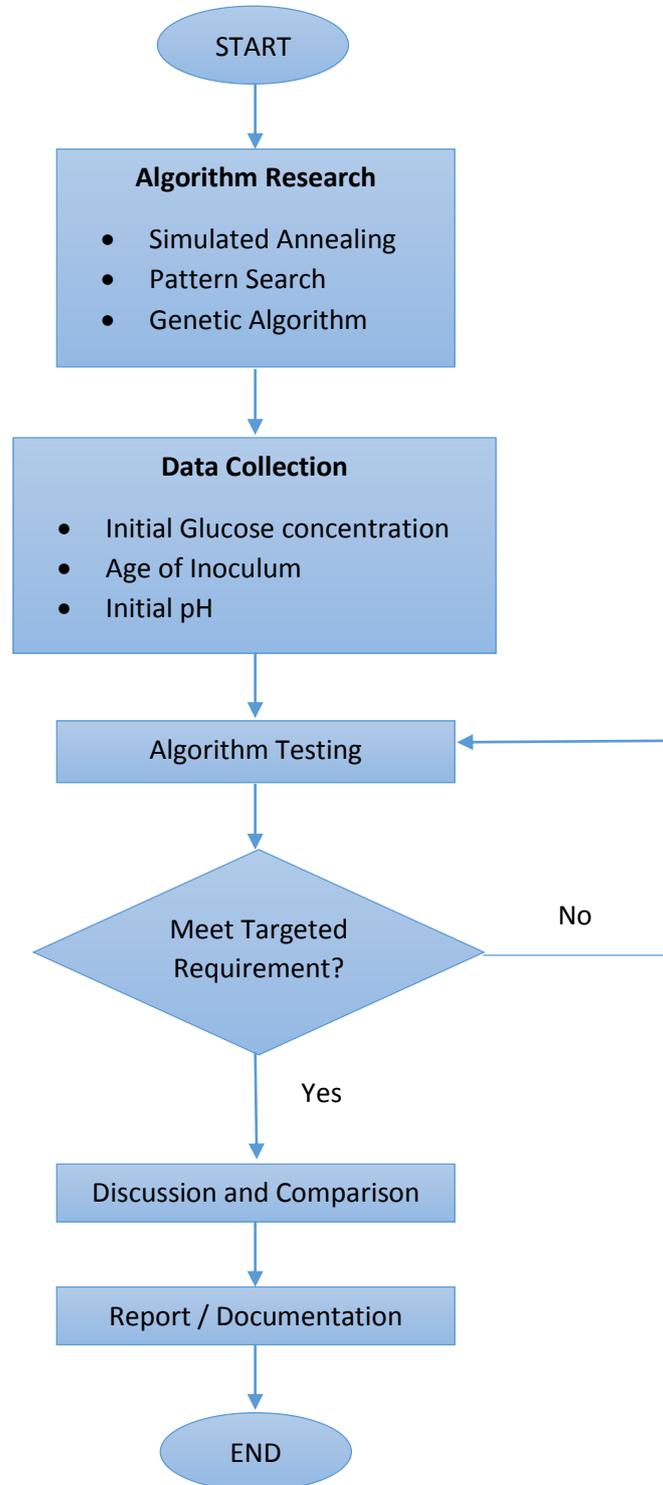


Figure 1 : Methodology Flowchart

4.2 Data Collection

The data input for the algorithm will be taken from the previous experimental data from Sen and Das (2005) using the same condition as the result they found. The data that will be used include the equation derived from the regression, the initial glucose concentration, age of inoculum and also the initial pH of the solution. These data will then be fed into the algorithm for optimization of the parameters.

4.3 Algorithm testing for optimization

The entire proposed algorithm will be tested with the prior data to optimize the parameters to increase the amount of hydrogen gas produced. The testing of the algorithm will be repeated for many times until the parameters have been optimized so that the potential of maximum hydrogen production is achieved.

4.3.1 Simulated Annealing

Based on the article by Al-Aomar (2010), Simulated Annealing (SA) is an optimization method that is based on the structural properties of materials, mainly metals, undergoing the annealing process, where materials are melted down and then cooled slowly in a controlled manner.

Such process resembles the SA search in seeking global optima while avoiding being trapped at local optima. As a global search engine, SA has become a popular tool for solving problems where mathematical programming formulations become intractable. This includes solving various combinatorial optimization problems in circuit design, scheduling, path generation, and many others.

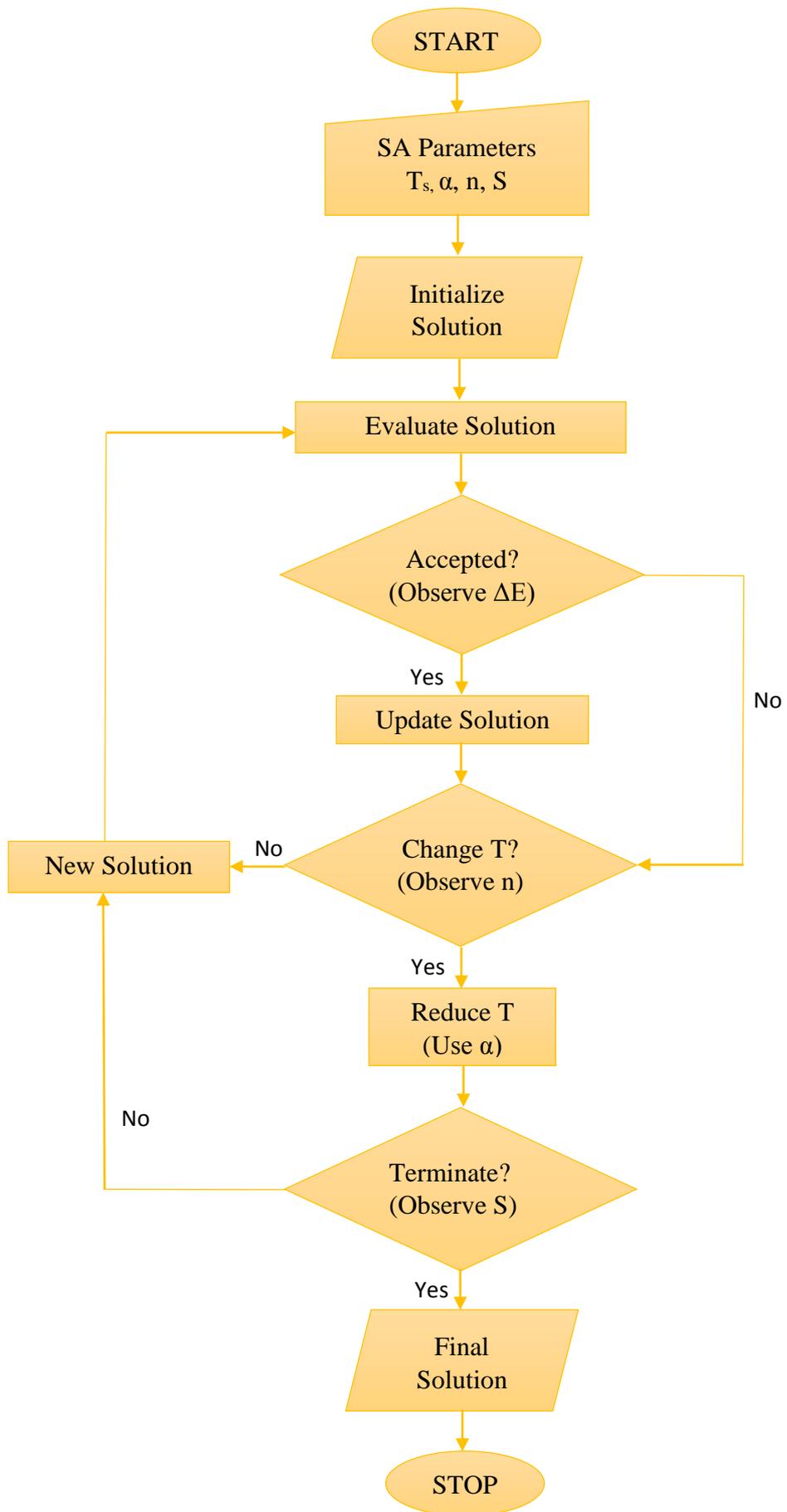


Figure 2: Flowchart SA Search Algorithm

As shown in Figure 2, SA control parameters include initial temperature (T_s), cooling parameter (α), number of T decrement steps (S), and the maximum number of iterations (n) a teach T step. The temperature T , which is modulated by a predetermined cooling schedule, controls the degree of randomness present within the search. Determining the starting initial temperature (T_s) is problem-specific that depends on the scaling of the objective function. The search will seek convergence to the local optima toward the end of the computation, when the temperature T is nearly zero.

The cooling parameter $\alpha \in [0, 1]$ controls the rate at which the temperature is reduced, where large values (typically between 0.70 and 0.99) will produce better results through slow cooling schedules. Longer temperature steps (large number of iterations n) will also produce slower cooling rate at a fixed α by allowing the system to stabilize at that temperature step.

After setting SA parameters, an initial solution is generated randomly and used as the first current solution. The initial solution, as well as future solutions, is evaluated using some objective function. The value function (VM) is analogous to the energy (E) value in thermodynamics, where higher VM (lower E) implies a closer state to thermal equilibrium.

Thus, change in energy (ΔE) is measured at each evaluated solution and the solution is accepted if $\Delta E < 0$ (newsolutionresultsin lower E). Else, Boltzmann acceptance criterion is employed where a random value $R \in [0, 1]$ is generated and compared to Boltzmann probability of acceptance $p(\Delta E)$. If $R \leq p(\Delta E)$, the new solution is accepted and current solution is updated. Otherwise another new solution is generated. Given the current temperature T and using Boltzmann constant (K), $p(\Delta E)$ is defined as follows:

$$p(\Delta E) = \exp \frac{-\Delta E}{KT}$$

The search continues in this inner loop until reaching maximum step iterations (n) where T is decremented according to the cooling parameter (α). Reducing T results in reducing Boltzmann probability for acceptance of worse solutions (those with higher energy E). Different methods can be used for reducing T in the cooling process. A commonly used simple approach is the linear method, where:

$$T_{i+1} = \alpha T_i$$

As the temperature drops, the process of finding neighboring solutions and accepting them as current solutions, if acceptance criterion is met, is repeated until termination. The algorithm is either set for terminating at a subzero final T, to run certain number of T steps (S), or when no improvement occurs in one T step.

4.3.2 Pattern Search

Based on AlHajri *et al.* (2012), Pattern Search (PS) is a derivative-free algorithm that starts from any arbitrary initial point, called Base Point (BP) $\mathbf{x}_{BP}^{(k-1)}$ where k serves as the iteration index. It searches for optimality in a sequential technique in which each step is comprised of two types of moves, exploratory and pattern moves.

In the exploratory move, the search direction starts by spanning 2n coordinate directions and generate a mesh of 2n points, i.e. $\mathbf{S} = [\mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_{2n}]$ and such mesh is centered at the current BP. The mesh itself is constructed along 2n independent positive and negative unit length coordinate vectors that belong to a finite set of \mathbf{D} vectors and \mathbf{D} is defined in a compact form as $\mathbf{D} = \{\pm u_i | i = 1, 2, \dots, n\} = \{d_i\}_{i=1}^{2n}$ or in a vector form as:

$$\mathbf{D} = [u_1, u_2, \dots, u_n, -u_1, -u_2, \dots, -u_n] = [d_1, d_2, \dots, d_{2n}]$$

where, u_i is the i th unit coordinate vector. In a subsequent step during the exploratory move, the unit coordinate vectors are multiplied by a step size control parameter, Δ , where $\Delta \in R^+$ and added to the best previously seen BP to generate the mesh points as shown in the equation below:

$$\mathbf{s}_i^{(k)} = \mathbf{x}_{BP}^{(k-1)} + \Delta d_i$$

Accordingly, those newly obtained mesh points serve as the next trial points at the current iteration. Next, the objective function is evaluated at all the mesh points, and the point \mathbf{s}^* yields the greatest decrease in the objective function, i.e. $F(\mathbf{s}^*)^{(k)}$, is chosen to be compared with that of the initial BP, $\mathbf{x}_{BP}^{(k-1)}$, as illustrated in Equations below:

$$F(\mathbf{s}^*)^{(k)} = \min\{F(\mathbf{s}_1)^{(k)}, F(\mathbf{s}_2)^{(k)}, \dots, F(\mathbf{s}_{2n})^{(k)}\}$$

$$\mathbf{x}_{BP}^{(k)} = \begin{cases} \mathbf{s}^* & \text{if } F(\mathbf{s}^*)^{(k)} < F(\mathbf{x}_{BP}^{(k-1)}) \\ \mathbf{x}_{BP}^{(k-1)} & \text{if } F(\mathbf{s}^*)^{(k)} \geq F(\mathbf{x}_{BP}^{(k-1)}) \end{cases}$$

For an unsuccessful exploratory move, PS decreases the current step size, Δ , through multiplying it by a reduction factor, i.e. $1/\tau$, where $\tau \in \mathbf{N}^+\{1\}$. A τ value of one is exempted from the positive integer numbers set, simply because it would lead to the step size of the previous failed exploratory move. Such step size adjustment is performed until it reaches a predefined tolerance of δ .

The pattern move shift the new BP, $\mathbf{x}_{BP}^{(k)}$, linearly according to equation:

$$\mathbf{x}_{BP}^{(k)+} = \mathbf{x}_{BP}^{(k)} + [\mathbf{x}_{BP}^{(k)} - \mathbf{x}_{BP}^{(k-1)}]$$

Which the resultant BP, $\mathbf{x}_{BP}^{(k)+}$, becomes the newest temporary BP at which the objective function is to be evaluated as well.

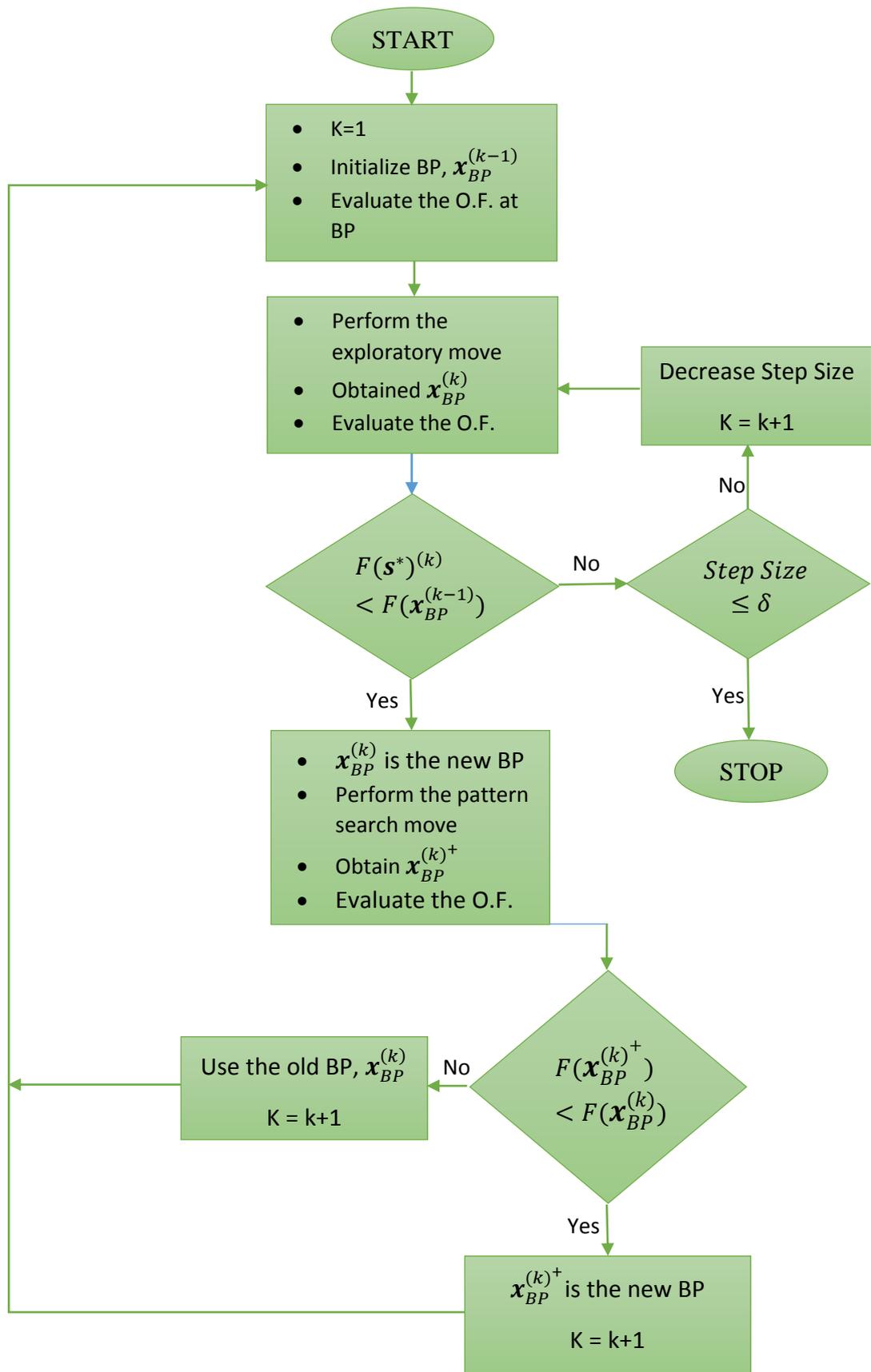


Figure 3: Flowchart of PS algorithm

4.3.3 Genetic Algorithm

Based on Silva, Cantao, and Tamakami (2012), Genetic algorithm (GA) belong to the class of evolutionary computation that simulates the process of natural evolution using stochastic optimization methods. They use the evolution principle as a search method in the solution of optimization problems.

For the structure representation, this approach represent a solution is the floating point implementation, where each chromosome has the same length as the solution vector. The vector used, $V^i = (x_1^i, x_2^i, \dots, x_n^i)$, with $i = 1, 2, \dots, \mathit{popsize}$ as a chromosome to represent a possible solution to the optimization problem, where n is the dimension.

In the Initialization process, define an integer $\mathit{popsize} = 10 * n$ as the number of chromosomes and initialize $\mathit{popsize}$ randomly for each chromosome. An interior point is choose to initialize the population, denoted by V^0 , and select $\mathit{popsize}$ individuals randomly in a given neighborhood of this point. Define a large positive number Γ which is a step to be taken in a randomly selected direction.

Next, randomly select a direction $d^i \in R^{\mathit{popsize}}$ and define a chromosome $V^i = V^0 + \Gamma * d^i$. This chromosome is added to the initial population if it represents a feasible solution; otherwise, randomly select another Γ in the interval $[0, \Gamma]$ until $V^0 + \Gamma * d^i$ is feasible. Repeat this process $\mathit{popsize}$ times and produce $\mathit{popsize}$ initial feasible solutions $V^1, V^2, \dots, V^{\mathit{popsize}}$.

Then, the algorithm undergo fitness value function. It evaluates the quality of each individual in the population at each iteration. The value of the objective functions was chosen as the fitness value for each individual. Afterward, an evaluation function, denoted by $eval(V^i)$, is defined to assign a probability of reproduction to each individual of the population. It is reasonable to assume the use of the order relationship among the $\mathit{popsize}$ chromosomes such that the $\mathit{popsize}$ chromosomes can be rearranged from good to bad. Let $a \in (0, 1)$ be a parameter in the genetic system. Next, define the rank-based evaluation function as follows:

$$eval(V^i) = a(1 - a)^{i-1}, \quad i = 1, 2, \dots, popsize.$$

Note that $i = 1$ means the best individual, $i = popsize$ the worst individual, and

$$\sum_{i=0}^{popsize} eval(V^i)n \approx 1.$$

After that, the algorithm go into the selection process. This process is based on spinning the roulette wheel $popsize$ times, each time selecting a single chromosome for an auxiliary population in the following way:

1. Calculate the cumulative probability q_i for each individual V^i ,
 $q_0 = 0,$

$$q_i = \sum_{j=1}^i eval(V^j), \quad i = 1, 2, \dots, popsize;$$

2. Generate a random real number \mathbf{r} in $[0, q_{popsize}]$;
3. Select the i th individual V^i , ($1 \leq i \leq popsize$) such that $q_{i-1} < r < q_i$;
4. Repeat steps 2 and 3 $popsize$ times and obtain $popsize$ individuals.

Then, in the crossover operator, the parameter P_c is defined to determine the probability of crossover. This probability gives us the expected number $P_c * popsize$ of chromosomes which undergo the operation. Denote the selected parents as F^1, F^2, \dots and divide them in pairs. At first, a random number, c is generated from the open internal $(0, 1)$, then we produce two children C^1 and C^2 using the crossover operator as follows:

$$C^1 = c * F^1 + (1 - c) * F^2,$$

$$C^2 = c * F^1 + (1 - c) * F^2.$$

Check the feasibility of each child. If both children are feasible, then replace the parents by them. If not, keep the feasible one if it exists, and then reply the crossover operator by regenerating the random number c until two feasible children are obtained or a given number of cycles is finished. In this case, we only replace the parents by the feasible children. The individuals that were not chosen to do the crossover operator will used in the population of the next generation.

While, in mutation operator, a parameter P_m is defined as the probability of mutation. This probability gives us the expected number of $P_m * popsize$ of chromosomes which undergo the mutation operations. For each selected parent, denoted by $V^i = (x_1, \dots, x_n)$, choose a mutation direction $d^i \in R^n$ randomly.

If $M^i = V^i + \Gamma * d^i$ is not feasible. Set Γ as a random number between 0 and Γ unit it is feasible. If the above process fails to find a feasible solution in a predetermined number of iterations, set $\Gamma = 0$. Based on the article by Ganesan, Vasant and Elamvazuthi (2012), the algorithm flow for the GA as below.

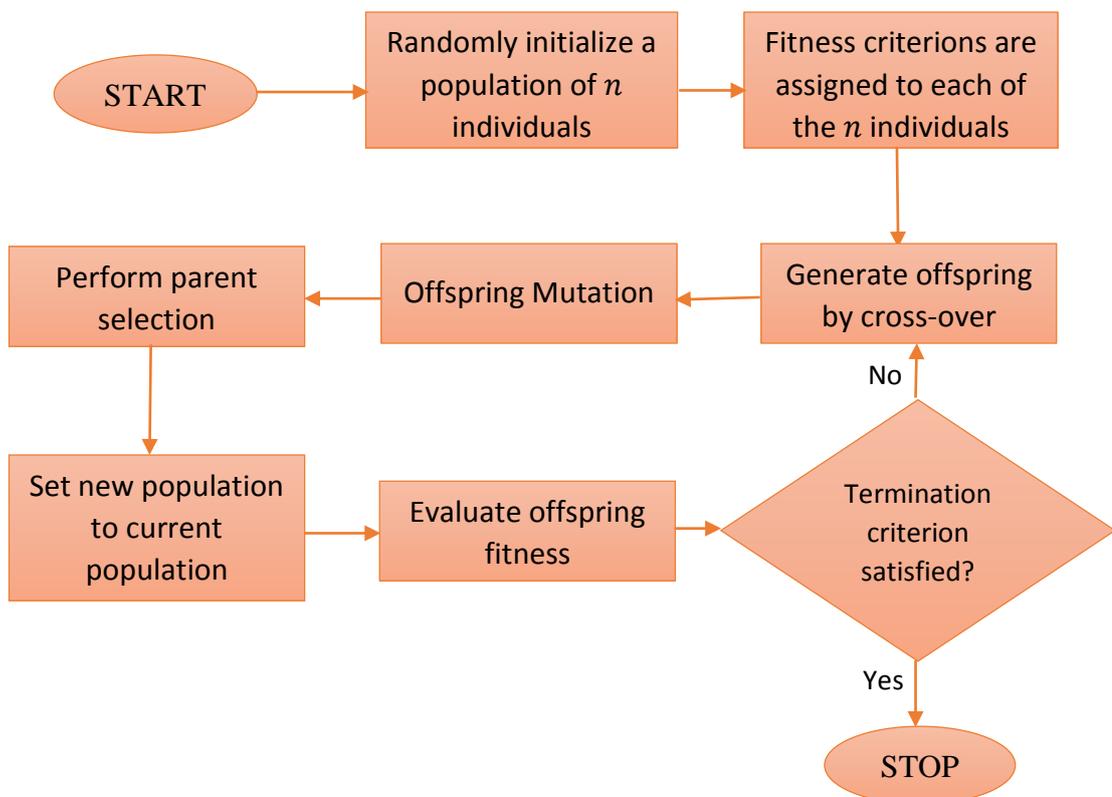


Figure 4: Flowchart GA algorithm

4.4 Discussion and comparison between the algorithm

After the algorithm testing, the result will be compared and discuss the difference between the result from two different optimization tools. The higher hydrogen yield algorithm will be highlighted can further discussion will be made to verify the result obtain for validation.

4.5 Report and Documentation

Finally, after the comparison with the two optimization tools, the algorithm that obtains the higher hydrogen gas produced is highlighted, the report and documentation then will be complete and submitted.

4.6 Gantt Chart FYP I

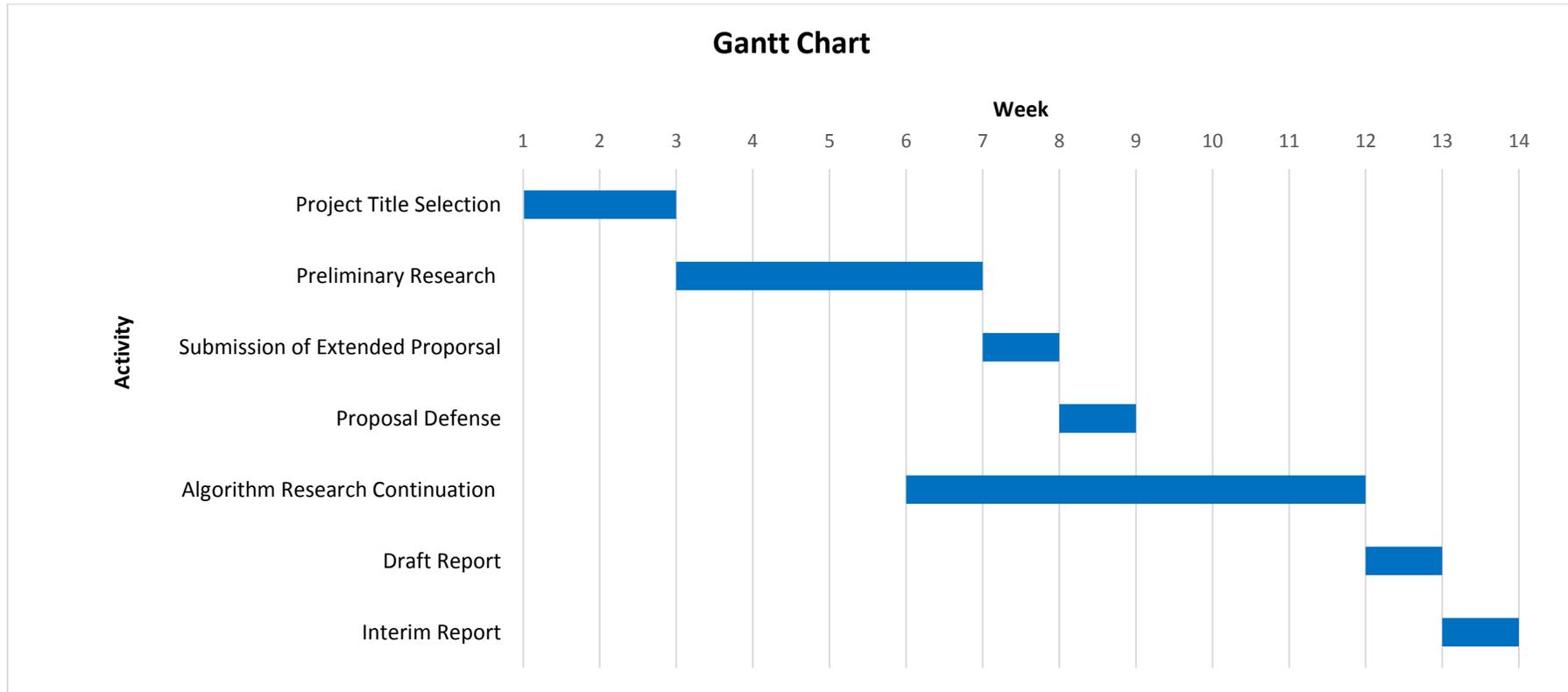


Figure 5 : Gantt Chart FYP I

4.7 Gantt Chart FYP II

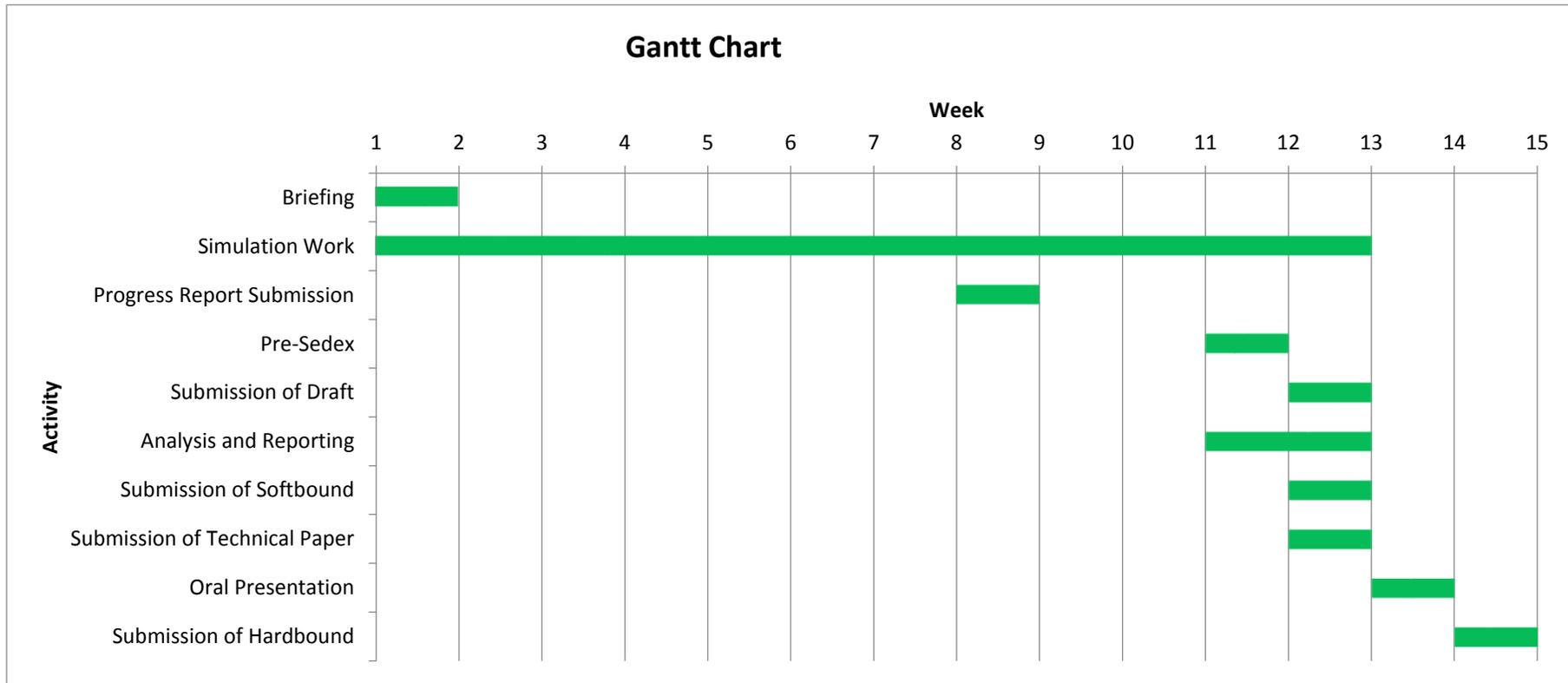


Figure 6: Gantt Chart FYP II

CHAPTER 5

Result and Discussion

By using the MATLAB, the regression equation is converted into a function name reg_fun which been save into a programme file. Using the Optimization Apps, the regression function is then optimize by setting all the tune by auto set by the MATLAB when the simulated annealing is choose in the solver option.

Below are the parameters constraint bounds which is used:

$$0.8 \leq X_1 \leq 1.2$$

$$5 \leq X_2 \leq 15$$

$$4 \leq X_3 \leq 8$$

*** X_1 = Initial glucose concentration (w/v)

X_2 = Inoculum age (h)

X_3 = Initial pH of the nutrient broth

5.1 Simulated Annealing (SA)

The annealing parameter set to linear temperature update with reannealing interval set at 1, 10 and 100. For each reannealing interval that have been set, 10 results is collected and the mean result is calculated and recorded. Stopping criteria is set to constant as the initial setting. The constraint bound is set to [0.8; 5; 4] for start point and the lower bound limit, and [1.2; 15; 8] for the upper bound limit. The negative is just sign to maximize the regression function as the optimization tool initial set to find the minimum value of the assign function.

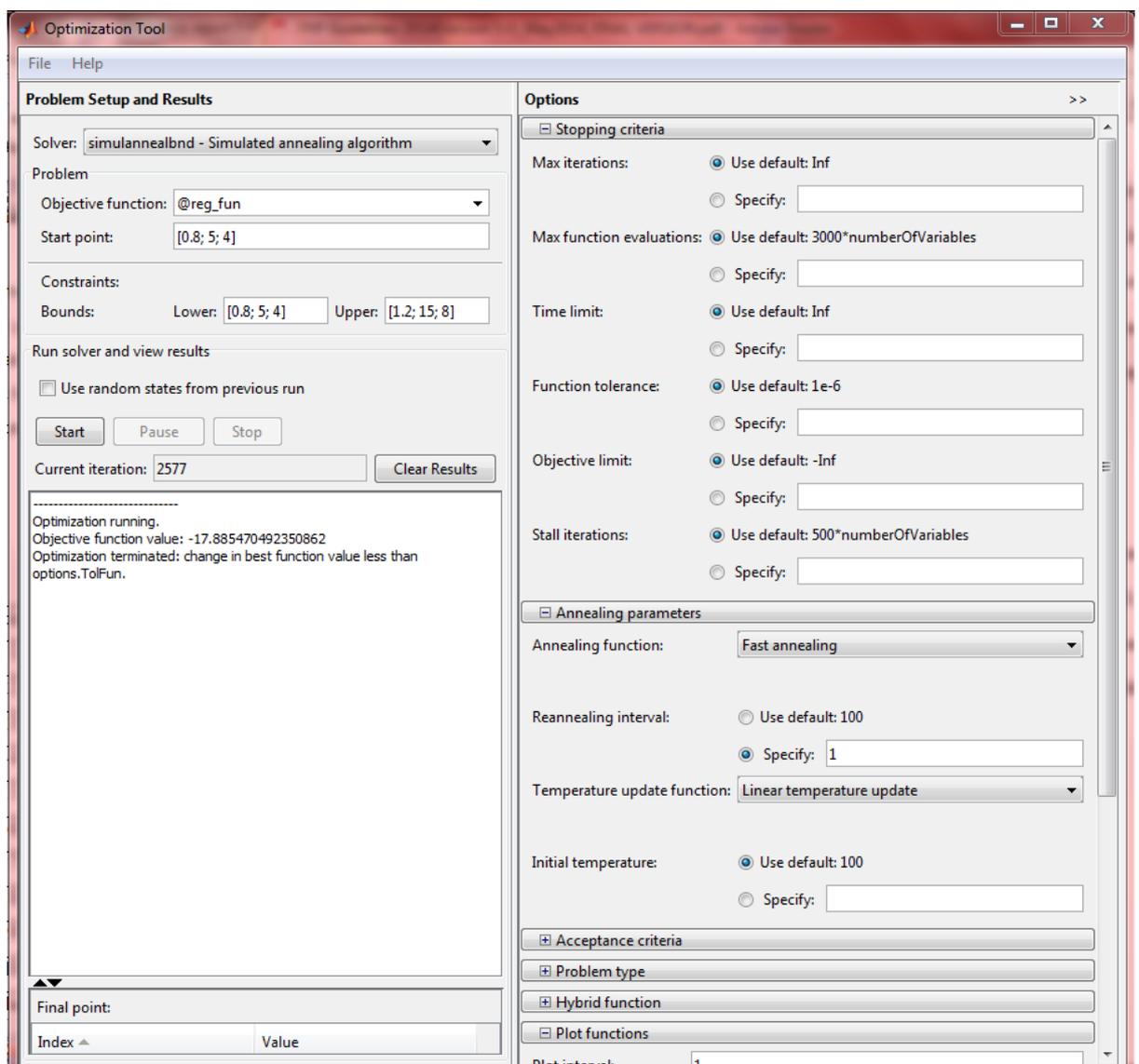


Figure 7: Optimization Tool Interface for Simulated Annealing.

The SA simulation results produce by the optimization tool is tabulated in Table 1, 2 and 3 as shown in the Appendix. Based on the data form Table 1, 2 and 3, the graph of results is plotted as shown below:

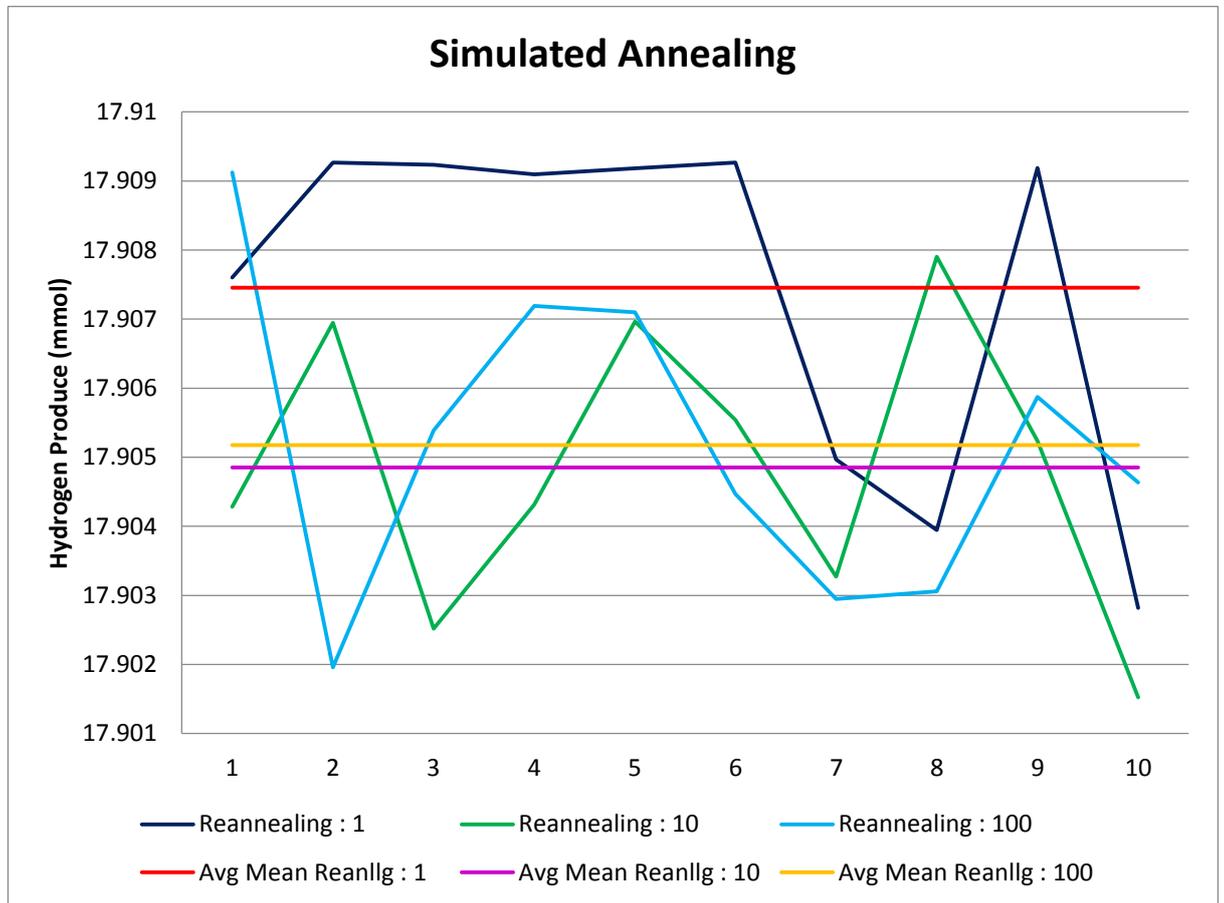


Figure 8: Simulated Annealing Result

Based on the graph above, it can be seen the trend by the SA simulation result by varying the reannealing factor in the SA algorithm. For the reannealing = 1, the hydrogen produce start at 17.907605 mmol and then going up the on the second trial until the sixth trial. After the sixth trial the hydrogen production rate decreases and increase back on the ninth trial and then decreases again. As we can see from the graph above, the trend of hydrogen produce for reannealing = 1 is quite stable.

For reannealing = 10, the graph start from 17.904285mmol, quite low from other reannealing factor. The trend of this reannealing factor, is not quite stable as

the reannealing = 1. The graph of hydrogen produce is going up and down, from first trial to the tenth trial.

For the factor, reannealing = 100, the graph start at a quite high value of the hydrogen produce about 17.909123 mmol on the first simulation trial. After that, the hydrogen produce is going down steeply on the second trial, and slowly increases again after a few trial before goes down again. Compare to the reannealing = 10, the graph for reannealing = 100 trend is more stable, but still less stable than the graph of reannealing = 1.

For the mean hydrogen produce, the highest mean simulation result is 17.907457 mmol, which from the reannealing interval = 1, with the parameter, $X_1 = 1.060$, $X_2 = 13.011$, and $X_3 = 6.046$. Follow by reannealing interval = 100, 17.905175 mmol and reannealing interval = 10, with 17.904851 mmol hydrogen produced.

Thus, the as the reannealing interval increases, the simulation result of SA becomes unstable. Nevertheless, after the reannealing internal increases further in the trial, the simulation result of SA will becomes stable again.

5.2 Pattern Search (PS)

The initial size and maximum size of the Mesh is set to the default, while the expansion factor is set at 100, 200 and 300. For each expansion factor that have been set, 10 results is collected and the mean result is calculated and recorded. Polling order is put to random, while other criteria such as contraction factor, poll method, stopping criteria and others are set to constant as the initial setting. The constraint bound is set to [0.8; 5; 4] for start point and the lower bound limit, and [1.2; 15; 8] for the upper bound limit. The negative is just sign to maximize the regression function as the optimization tool initial set to find the minimum value of the assign function.

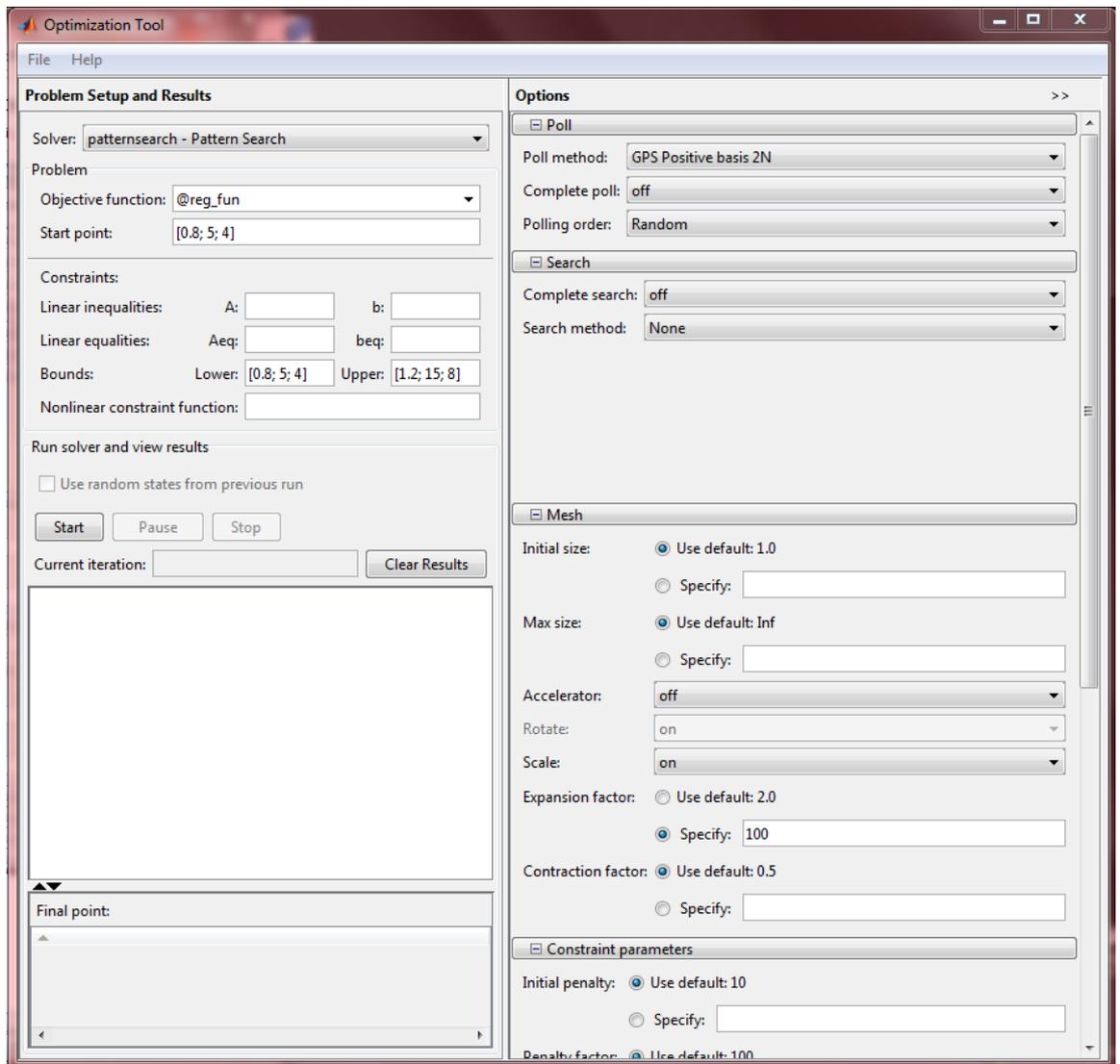


Figure 9: Optimization Tool Interface for Pattern Search.

The PS simulation results produce by the optimization tool is tabulated in Table 4, 5 and 6 as shown in the Appendix. Based on the data form Table 1, 2 and 3, the graph of results is plotted as shown below:

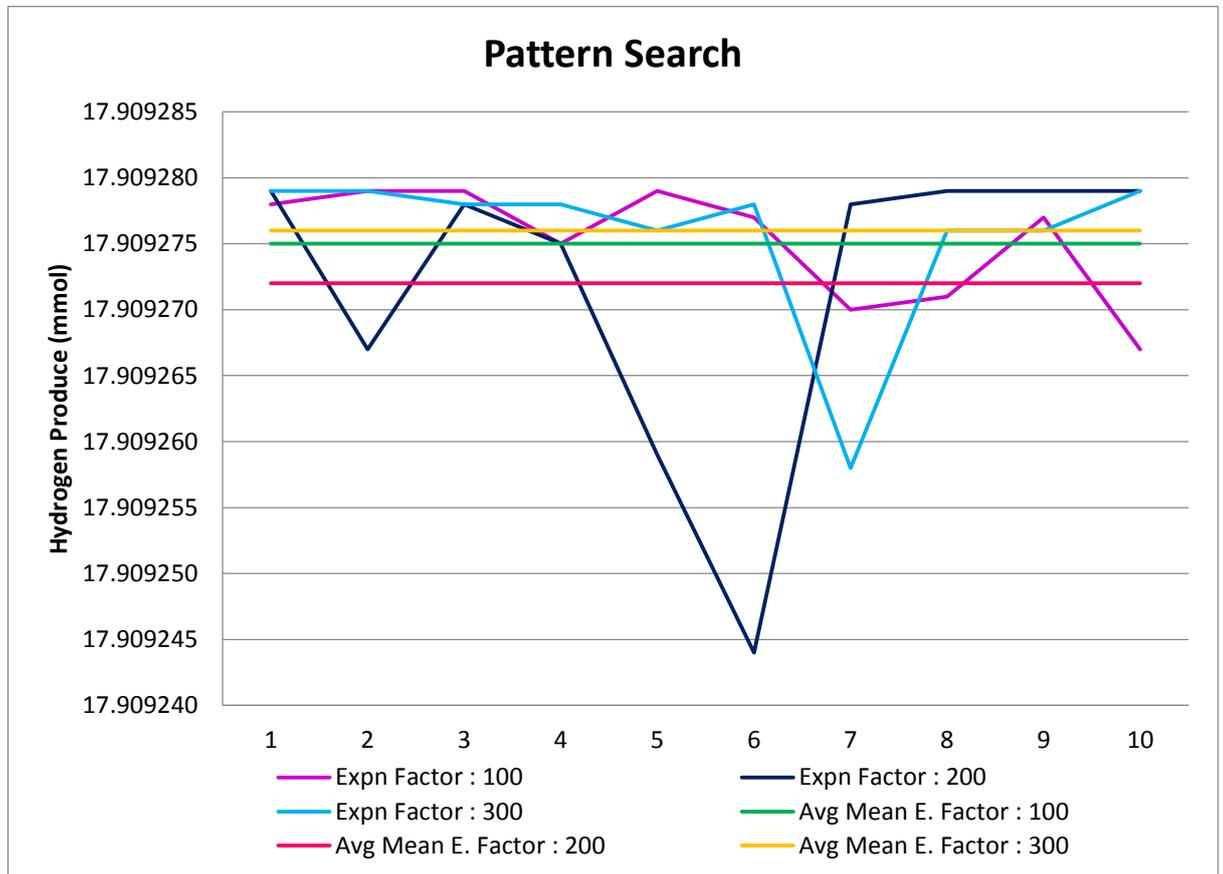


Figure 10: Pattern Search Result

Based on the graph above, it can be seen the trend by the PS simulation result by manipulating the expansion factor of the PS algorithm. For the expansion factor = 100 and 200, the graph trend is quite similar as the expansion factor = 100, start at 17.909278 mmol hydrogen produce, while the PS simulation expansion factor = 300, graph start at 17.909278 mmol hydrogen produce.

Both PS simulation graph, expansion factor = 100 and 300 are quite stable throughout the ten trial. For the seventh trial, the expansion factor = 300 graph rapidly decreases and then increases again back in the trial towards the end. In comparison, the expansion factor = 300 hydrogen produce value is slightly higher and stable than the value hydrogen produced by expansion factor = 100.

While, for expansion factor = 200, the simulation result start high at 17.909278 mmol hydrogen produce. The value decrease as the trial goes on, and rapidly goes down on the sixth trial about 17.909244 mmol hydrogen produce, and then increases back until the tenth trial.

Based on all the three expansion factor trend, the most stable variable is expansion factor = 300 with the mean Simulation Result 17.909276 mmol hydrogen produced, by the parameter, $X_1 = 1.060$, $X_2 = 12.967$, and $X_3 = 6.060$. Followed by 17.909275 mmol hydrogen produced by the expansion = 100 and 17.909272 mmol by expansion factor = 200.

Hence, it can be seen the trend that, as the expansion factor increases, the PS simulation result become more stable and mean simulation result also simultaneously becomes higher.

5.3 Genetic Algorithm (GA)

The fitness function is set as the regression function and the number variable is set at 3. The population size is set at 100, 200 and 300. For each population size that have been set, 10 results are collected and the mean result is calculated and recorded. The fitness scaling, selection, reproduction, mutation and other criteria are set to constant as the initial setting. The constraint bound is set to [0.8; 5; 4] the lower bound limit, and [1.2; 15; 8] for the upper bound limit. The negative is just sign to maximize the regression function as the optimization tool initial set to find the minimum value of the assign function.

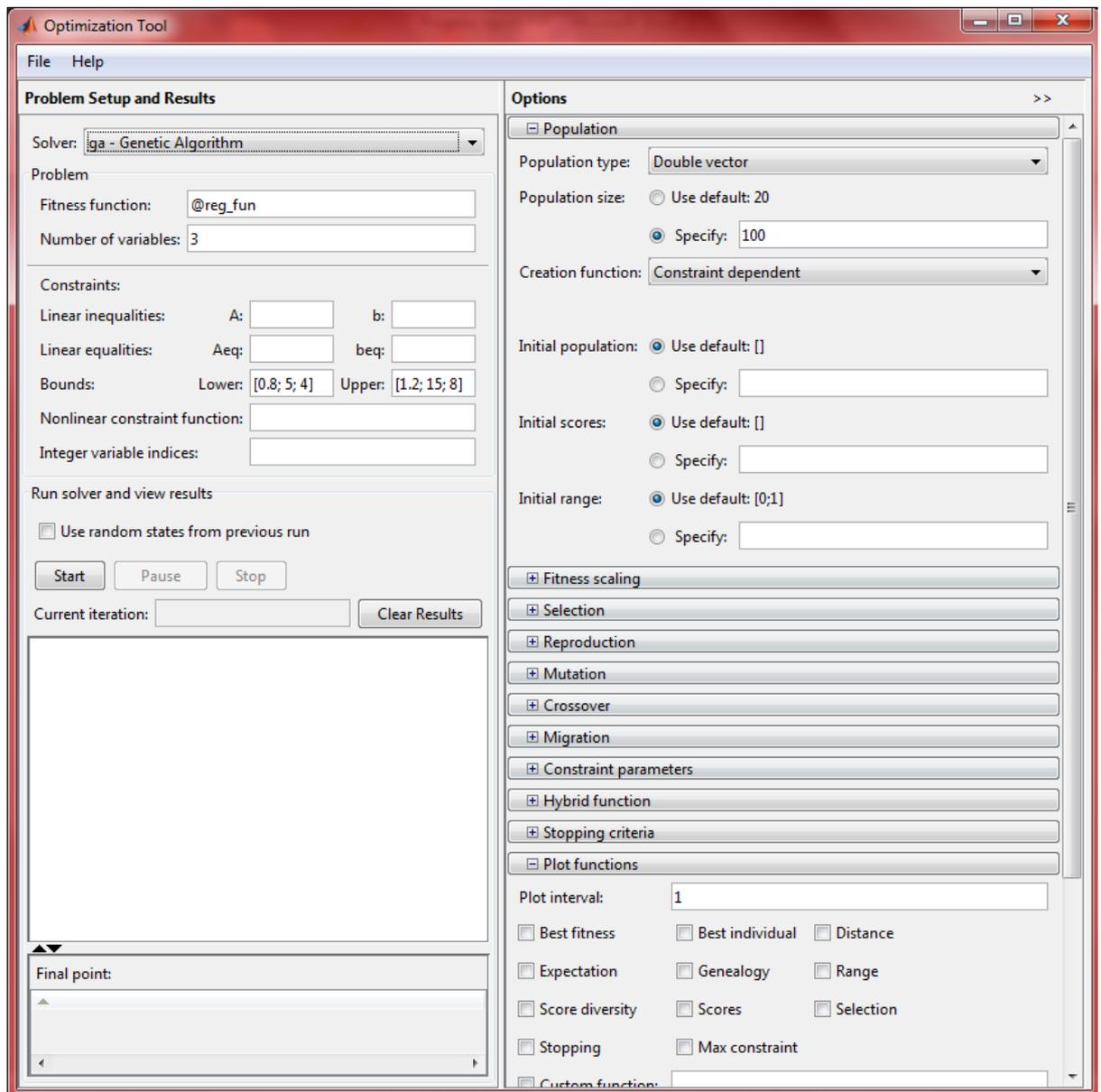


Figure 11: Optimization Tool Interface for Genetic Algorithm.

The PS simulation results produce by the optimization tool is tabulated in Table 4, 5 and 6 as shown in the Appendix. Based on the data form Table 1, 2 and 3, the graph of results is plotted as shown below:

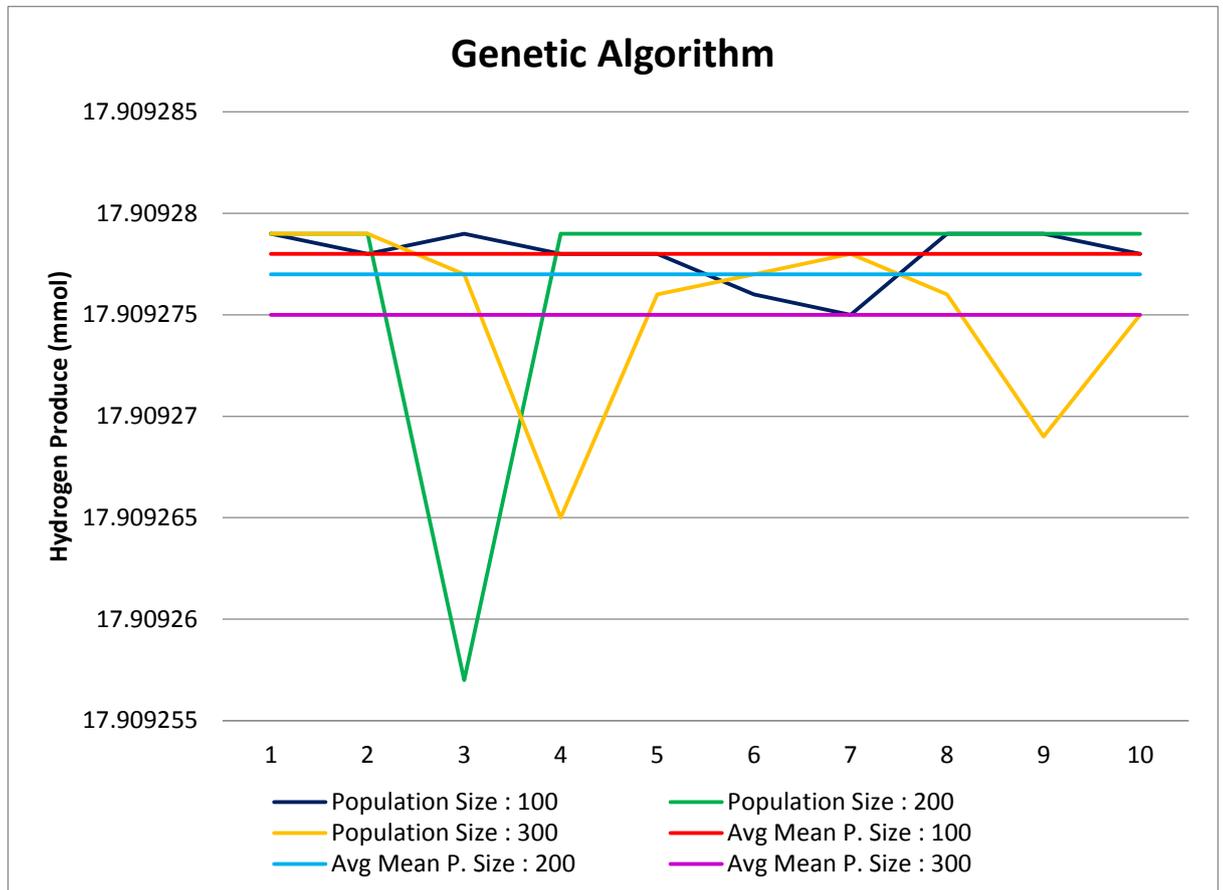


Figure 12: Genetic Algorithm Result

Based on the graph above, it can be seen that trend by the GA simulation result by varying the population size in the GA algorithm. For population size = 100, the graph start at high hydrogen produce with 17.909279 mmol. Its show quite stable trend throughout the ten simulation trial.

While for the population size = 200, the graph start at the same hydrogen value with population size = 100, 17.909279 mmol at the first simulation trial. However, at the third trial, the graph rapidly decreases to 17.909257 mmol and then increase back 17.909279 mmol hydrogen produce with constant value until to the tenth simulation trial.

The graph of population size = 300, also start with 17.909279 mmol hydrogen produce and then slow decreases until the fourth trial. After that, the value hydrogen produce increases again until the seventh trial, slowly decreases to the ninth trial and then rise back again on the last trial. The graph trend for this population size can be seen quite unstable.

For the mean hydrogen produce, the highest mean simulation Result is 17.909278 mmol, from the population size = 100, with the parameter, $X_1 = 1.060$, $X_2 = 12.966$, and $X_3 = 6.061$. Followed with population size = 200, 17.909277 mmol and then population size = 300, with 17.909275 mmol hydrogen produced.

Thus, from the graph trends, it can be conclude that, as the population size increases, the simulation result becomes unstable and the mean simulation at the same time will decreases.

5.4 Overall Discussion

Based on all three algorithm tested for optimization, the best algorithm is GA with the mean simulation of hydrogen produced, 17.909278 mmol. The second best algorithm is PS, with 17.909276 mmol hydrogen produced, followed by SA algorithm with 17.907457 mmol.

According to the result by the algorithm simulations, it can be seen in the graph that the more stable the simulation results, the more higher the mean value of the simulation results produced by the algorithm. In this case, GA is tends to give more stable simulations result compare with the PS and SA. Simultaneously, GA will give higher simulation results, compare to the PS and SA algorithm.

Basically, the GA algorithm is more stable than PS and SA because the algorithm it is more complex and comprehensive with the amount the parameters imbedded in the algorithms itself. The structural of the GA itself, shows the possibility that it can be used to solve the solution structure and solution of multi-parameters simultaneously.

Even though, the GA mean simulation result cannot exceed the value of hydrogen produce by the last research study value, 17.9093 mmol, but the value of hydrogen produce by GA still higher than the experimental value of the previous study which is around 17.8571 mmol.

Table 1: Percentage of Improvement

Algorithm	Hydrogen Produce (mmol)	Percentage of Improvement (%)
Previous Research	17.909300	0.29232
Simulated Annealing (SA)	17.907457	0.28200
Pattern Search (PS)	17.909276	0.29219
Genetic Algorithm (GA)	17.909278	0.29220

The percentage was calculated by comparing the simulation value with the previous experimental value, 17.8571 mmol. From the Table above, the percentage of improvement of GA is close to the previous research with the different of 1.2E-4 %. The PS is the second highest percentage of improvement with 0.29219 % and SA have the least percentage of improvement with 0.28200 %.

CHAPTER 6

CONCLUSION AND RECOMMENDATION

6.1 Conclusion

In line with the current advances in technology today, many optimization theory have been proven and tested its validation throughout numerous past researches and studies. A lot of these past studies and researches had proved that there are several numerical methods can be applied to obtain optimal parameters of their experiments and theories.

All the simulation results were inside the constraint parameter limitation. The three algorithms do not break any of the constraints in order to optimize the parameters in obtaining the maximum hydrogen produced. Thus, the constraints are feasible to be used in the optimization of the *Enterobacter cloacae* to obtain the maximum hydrogen production.

Even though the result obtained do not beat the maximum hydrogen produced by the previous study research, but it is definitely close to the value that the previous study had done and it is believed that the maximum hydrogen gas produced by the *Enterobacter Cloacae* can be increased further using other algorithm methods.

6.2 Recommendation

Based on this project, it is believed that the maximum hydrogen production can be increased more as the developments of numerical optimization method have been constantly evolving through the numerous breakouts of new technologies and theories nowadays.

Thus, it is recommended that other algorithms are used for next further research than the simulated annealing, pattern search and Genetic algorithm that have been analyzed. Thus, other new or hybrid numerical optimization method should be considered in the future research in order to get best result for the optimal parameters to produce maximum hydrogen by the *Enterobacter Cloacae* in the near future.

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APPENDICES

Table 1: Simulated Annealing Result, Reannealing Interval = 1

Simulation Run	Simulation Result	X_1	X_2	X_3
1	17.907605	1.062	13.136	6.025
2	17.909268	1.060	12.977	6.061
3	17.909234	1.059	12.982	6.054
4	17.909097	1.061	13.006	6.054
5	17.909182	1.059	13.007	6.052
6	17.909266	1.060	12.978	6.057
7	17.904966	1.059	13.397	6.023
8	17.903948	1.060	13.208	5.989
9	17.909186	1.059	12.968	6.068
10	17.902818	1.062	12.452	6.076
Mean Simulation Result	17.907457	1.060	13.011	6.046

Table 2: Simulated Annealing Result, Reannealing Interval = 10

Simulation Run	Simulation Result	X_1	X_2	X_3
1	17.904285	1.052	12.692	6.083
2	17.906947	1.064	13.029	6.022
3	17.902518	1.064	13.388	6.001
4	17.904316	1.066	13.184	6.014
5	17.906966	1.062	12.751	6.103
6	17.905542	1.064	12.836	6.024
7	17.903272	1.069	13.000	6.082
8	17.907904	1.059	12.936	6.031
9	17.905237	1.057	12.584	6.085
10	17.901524	1.050	13.397	6.009
Mean Simulation Result	17.904851	1.061	12.980	6.045

Table 3: Simulated Annealing Result, Reannealing Interval = 100

Simulation Run	Simulation Result	X_1	X_2	X_3
1	17.909123	1.060	12.967	6.07
2	17.901960	1.051	12.828	6.121
3	17.905388	1.051	13.007	6.084
4	17.907191	1.059	13.068	6.016
5	17.907101	1.053	12.995	6.053
6	17.904470	1.058	13.300	5.996
7	17.902948	1.051	12.905	6.114
8	17.903061	1.063	12.475	6.114
9	17.905875	1.055	13.034	6.099
10	17.904633	1.068	12.870	6.089
Mean Simulation Result	17.905175	1.057	12.945	6.076

Table 4: Pattern Search Result, Expansion factor = 100

Simulation Run	Simulation Result	X_1	X_2	X_3
1	17.909278	1.060	12.962	6.061
2	17.909279	1.060	12.968	6.060
3	17.909279	1.060	12.967	6.060
4	17.909275	1.060	12.959	6.061
5	17.909279	1.060	12.967	6.060
6	17.909277	1.059	12.967	6.061
7	17.909270	1.060	12.980	6.058
8	17.909271	1.060	12.970	6.058
9	17.909277	1.059	12.964	6.060
10	17.909267	1.059	12.962	6.063
Mean Simulation Result	17.909275	1.060	12.967	6.060

Table 5: Pattern Search Result, Expansion factor = 200

Simulation Run	Simulation Result	X_1	X_2	X_3
1	17.909279	1.060	12.967	6.060
2	17.909267	1.060	12.950	6.059
3	17.909278	1.059	12.965	6.061
4	17.909275	1.060	12.972	6.062
5	17.909259	1.060	12.978	6.059
6	17.909244	1.060	12.941	6.060
7	17.909278	1.059	12.965	6.061
8	17.909279	1.060	12.966	6.060
9	17.909279	1.060	12.967	6.060
10	17.909279	1.060	12.967	6.060
Mean Simulation Result	17.909272	1.060	12.964	6.060

Table 6: Pattern Search Result, Expansion factor = 300

Simulation Run	Simulation Result	X_1	X_2	X_3
1	17.909279	1.060	12.967	6.060
2	17.909279	1.060	12.968	6.060
3	17.909278	1.060	12.969	6.059
4	17.909278	1.059	12.969	6.060
5	17.909276	1.059	12.964	6.059
6	17.909278	1.060	12.970	6.059
7	17.909258	1.059	12.952	6.062
8	17.909276	1.059	12.969	6.059
9	17.909276	1.059	12.969	6.059
10	17.909279	1.060	12.968	6.060
Mean Simulation Result	17.909276	1.060	12.967	6.060

Table 7: Genetic Algorithm Result, Population size = 100

Simulation Run	Simulation Result	X_1	X_2	X_3
1	17.909279	1.060	12.964	6.061
2	17.909278	1.060	12.963	6.060
3	17.909279	1.060	12.965	6.061
4	17.909278	1.060	12.966	6.060
5	17.909278	1.060	12.963	6.061
6	17.909276	1.060	12.963	6.062
7	17.909275	1.059	12.972	6.060
8	17.909279	1.060	12.967	6.060
9	17.909279	1.060	12.967	6.060
10	17.909278	1.060	12.965	6.060
Mean Simulation Result	17.909278	1.060	12.966	6.061

Table 8: Genetic Algorithm Result, Population size = 200

Simulation Run	Simulation Result	X_1	X_2	X_3
1	17.909279	1.060	12.967	6.060
2	17.909279	1.060	12.967	6.060
3	17.909257	1.060	12.974	6.063
4	17.909279	1.060	12.967	6.061
5	17.909279	1.060	12.966	6.060
6	17.909279	1.059	12.966	6.060
7	17.909279	1.060	12.967	6.060
8	17.909279	1.060	12.966	6.060
9	17.909279	1.059	12.966	6.060
10	17.909279	1.060	12.967	6.060
Mean Simulation Result	17.909277	1.060	12.967	6.060

Table 9: Genetic Algorithm Result, Population size = 300

Simulation Run	Simulation Result	X_1	X_2	X_3
1	17.909279	1.060	12.965	6.060
2	17.909279	1.060	12.968	6.060
3	17.909277	1.060	12.961	6.061
4	17.909265	1.060	12.964	6.061
5	17.909276	1.060	12.964	6.061
6	17.909277	1.060	12.965	6.060
7	17.909278	1.060	12.966	6.060
8	17.909276	1.060	12.964	6.061
9	17.909269	1.060	12.962	6.061
10	17.909275	1.059	12.968	6.060
Mean Simulation Result	17.909275	1.060	12.965	6.061