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# Algorithm in the Fluidized-Bed Reactor for the Polymerization of Propylene

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***Abstract:** A modified artificial bee optimization is proposed in this study. The algorithm is based on the colony behavior of certain bee species to achieve optimal solution in the bounded environment. The proposed algorithm is designed by improving the exploration knowledge of onlooker bee from meta-heuristic concept in search space. The multiple searches is proposed in the exploration phase to evaluate the multi objective functions. The performance of the proposed algorithm is tested on the typical benchmark equations and complex case of the polymerization of propylene in fluidized bed reactor. The proposed technique is able to provide an optimal solutions and it shows a good performance in term of convergence, accuracy and computational load.*

***Keywords:** Polymerization, fluidized bed reactor, optimal solutions*

## I. INTRODUCTION

Process modelling and solve multi optimization problems by implementing natural metaphors or colony-based optimization is a method in the scientific community as well as engineering field. Since the conventional optimization algorithms that provides solution for the larger scales combinational and/or highly non-linear problem is inefficient, therefore, a new knowledge or a new concept of optimization which is known as swarm intelligence isemphasized on insect's behaviour is required to create and develop some meta-heuristics which can demonstrate insect's problem solution abilities.

The situation is small different if integer and/or discrete variables are required in most of the linear optimization models as well. There are few types of swarm intelligence optimization such as Ant Colony Algorithm (ACA) and Artificial Bee Colony (ABC) algorithms. Furthermore, social insect colonies can be known as dynamical system collecting information from environment and rearrange its behaviour in accordance to it. During gathering information and adjustment process, individual insect does not perform all the tasks because of their characteristics. Basically, all social insect colonies behave according to their own division labours related to their morphology [1].

A relative new idea of meta-heuristic algorithm based on swarm intelligence is Artificial Bee Colony (ABC) [2]. Based on nature inspired interacting agent, population are sued in swarm based optimization. The activity of the honey bees food searching is the main concept of ABC algorithm. The ABC algorithm is developed by Karaboga [2] which is based on the food foraging characteristic of honey bees. It is simple and strong algorithm which is able to solve complex combinatorial optimization problem [3]. Thus, ABC algorithm has a strong searching ability which incorporates the exploitation and exploration of the search space [4].

Furthermore, ABC consists of three main types of bee which are employed bee, onlooker bee and scout bee. There are two main processes are required to carry out for the whole ABC algorithm which are exploitation process and exploration process. Exploration is the ability of bees to enlarge the search space whereas exploitation is the ability of bees to determine the optima from the good solution. Employed bee phase and onlooker bee phase execute the exploitation process and scout bee phase executes the exploration process. The triple search capability of the ABC algorithm based on the search phases of three types of bees prevent obstructing of solution and further enhance the search process in defining the optimum value [5].

Polymerization is a complicated process with complex chemical kinetics and physical mechanisms, and modeling polymerization process and control is a very challenging task [6]. It consist of several reaction that bonds all the monomer together within a straight line or a branch chemical structure. The reactions of polypropylene and other monomers can form a wide range of important co-polymers. The different structure of polymer has different chemical properties and physical properties, so the desired structure will be considered in order to produce the desired product to suit certain specific application. For instant, the polypropylene with isotactic sequence structure (commercial polypropylene) is usually obtained in an intermediate level of crystallinity between low density polyethylene and high density polyethylene. In order to manufacture the desired sequence of polypropylene, the operating conditions have to be determined accurately.

In this study, a specific target of polymer production is used as a case study, namely a production of Bi-axially Oriented Polypropylene, BOPP film which it requires to have a MFI of 2.6 to 3.3 g per 10 minutes. In this production, the high value of 3.3 g per 10 minutes is desired to achieve good quality of polymer whereas at this desire value, low production rate of polymer is reported. Therefore, the multi objective optimisation is must to minimise the trade-off effect between production rate and quality of the polymer. Thus, two objectives are formulated and used in this study to test the proposed metaheuristic optimisation.

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## II. META-HEURISTIC ARTIFICIAL BEE COLONY ALGORITHM

Artificial Bee Colony (ABC) is an optimisation technique that based on swarm intelligence. ABC demonstrates the behaviour of real honey bees in searching a food for the colony. During the food source searching, several mechanisms can be studied *i.e* access, evaluate and search by employed bee, onlooker bee and scout bee respectively. Basically, employed bee is responsible to access initial food source and determine the availability of the food and pass the information to onlooker bee. Then the onlooker bee will evaluate the amount of food that based on colony needs. This stage is critical which is could guaranty the sustainability of honey collection. If the availability of food less the desired target, then scout bee will search for a new food source location and the previous location is abandon and employed bee will access new location and the mechanism is repeated until these it satisfy onlooker bee objective. This makes the ABC a good candidate in developing an optimization intelligence algorithms. Nevertheless, ABC algorithm is also known to solve a deterministic non-polynomial problem where the bee's behaviour provides a feedback, fluctuation and density of tolerant for every individual bee. This behaviour can be evaluated at the proposed algorithm in next subsection. The algorithm consists of five major steps; initialization, employed bee phase, onlooker bee phase, scout bee phase and termination

### Initialization

Initialization is to create a landscape of food source for ACO case study. The food source is defined as in (Eq. 1) and it is formulated as:

$$X = C_{min} + (C_{max} - C_{min}) \times r(N, D) \quad (1)$$

Where $X$ is set of food source $\in \{x_{ij}, x_{kj}\}$, $N$ is size of bee's population, $D$ is dimension of the colony and $C_{max}$ and $C_{min}$ is a maximum and minimum limit of the food source respectively. Random number, $r(N, D)$ is introduced in the Eq. to make sure the searching activities are within the reach of colony.

### Employed Bee Phase

Each of the employed bees is send to the food source that generated in initialization step in order to collect the information of the food source and decide the nectar quality. Employed bee will generate a new food source and compare with the previous food source by using Eq. 2 and it will be applied to update the new food source, $v_{ij}$ .

$$v_{ij} = x_{ij} + \varphi_{ij}(x_{ij} - x_{kj}) \quad (2)$$

Where $\varphi_{ij}(x_{ij} - x_{kj})$ is known as step size, $k$ = {1,…,N} and $j$ = {1,…,D} are two random selected index. $k \neq i$ is to make sure that step size has some problem-solving upgrading.

$$J_i = \begin{cases} \dfrac{1}{1+f_i} if f_i \geq 0 \\ 1 + abs(f_i) else \end{cases} \quad (3)$$

where $f_i$ is the value of objective function of $i^{th}$ element. If the food source can be improved, remain the $J_i$ value as zero otherwise increase the $J_i$ value by one.

### Onlooker Bee Phase

The information of the food source that evaluated by the employed bee will share with onlooker bee. Onlooker bee needs to decide on the food source subsequent to gathering information from the employed bee and deciding the nectar eminence. Onlooker bee will decide which food source to evaluate first based on the probability of the food source. The probability, $P_i$ expression is shown as:

$$P_i = \frac{J_i}{\sum_{i=1}^{N} J_i} \quad (4)$$

where $P_i$ is the probability of ith food source, $J_i$ is the fitness of $i^{th}$ food source and $\sum_{i=1}^{N} J_i$ summation of the fitness of all food source. After that, onlooker bee will generate a new food source and apply greedy selection as in employed bee phase.

The proposed method improve on the onlooker bee's mechanism which the study propose two new solutions of finding new food source. Then, these solution are used to determine the best food source as a candidate at certain point. The searching process can be expressed as Eq. 5 and Eq. 6. These are equation to evaluate the food source probability. The better food sources that selected based on the probability are used to compete with the upper, $Ub$ or lower, $Lb$ boundary of the constraint.

$$v_{ij}^2 = x_{ij} + 2(\phi_{ij}^2 - 0.5)(x_{ij} - x_{kj}) + \varphi_{ij}^2(y_i - x_{ij}) \quad (5)$$

$$v_{ij} = \begin{cases} v_{ij}^1 ; J(v_{ij}^1) \geq \max\{J(x_{ij})\} \\ UborLb; \quad J(v_{ij}^1) \geq J(UborLb) \end{cases} \quad (6)$$

where $\phi_{ij}$ is a positive parameter that control the maximum step size during searching process and $y_i$ is the $j^{th}$ element of the global best solution

### Scout Bee Phase

If the locality of a food source is not improved for a predefined number of iterations, then the food source is considered as obsoleted and scout bee phase is engaged. During scout bee phase, the bee coupled with the obsoleted food source transformed into scout bee and the abandoned food source is replaced by randomly chosen food source inside the search space which is generated by Eq. 7:

$$x_{ij} = x_{minj} + (x_{maxj} - x_{minj}) \times r(N, D) \quad (7)$$

### Termination Phase

The algorithm will be terminated when there is better than the previous best solution. The new best solution will be recorded and memorized as solution. Besides that, if the termination requirement is met, the best solution will be announced otherwise will proceed back to employed phase.

## III. CATALYTIC POLYMERIZATION OF PROPYLENE IN FLUIDIZED BED REACTOR

Modelling of polymerization process can be divided mostly into 2: kinetic modelling and polymer properties modelling.

Both modelling are important because it play vital role in design, product development, control system, and plant optimization. This study, two phases (solid and gas) polymerization of propylene phenomena has been considered in the modelling development. The mathematical model has been derived based on the elementary reaction (active side, monomer insertion, polymer chain, chain reaction, and deactivation of catalyst). The extensive model derivation can be referred to Shamiri [7] and Harshe [8] while general modelling for polymerization can be refers to Alizadeh [9], McKenna and Soares [10], and Kiparissides [11]. In polymerization modelling, reaction kinetic is the most difficult part to describe, especially when the reaction condition and phenomena are unexplainable. In conjunction to this matter, there are several assumptions that should be considered in development of propylene polymerization. The assumptions are listed as follows.1.The kinetic reactions are in homogenous whereof two phase reaction states (bubble and emulsion) are involved [12].2.The mixing is ideal with bubbles state contain only a solid particle.3.The polymerization of propylene occur at emulsion state only where the emulsion for fluidization level is not minimum.4.Reaction must occurs in both bubble and emulsion state.5. The reaction process must deal with small particle size. Thus, the heat and the mass transfer resistance between the gases and the polymer particles can be neglected [13].6.The bubble size is constant through the whole reactor column. 7.Gas only in 1 direction which is up flow.

Polymerization kinetics, or moments, is important to the model as it introduces the polymerization process that takes place. Soares [10] presented their study with admitance that the presence of multiple sites on the Ziegler-Natta catalyst is the leading factor as to why the heterogeneous catalyst has the tendency to create polymers with wide molecular weight distributions. The single-site kinetic has failed to provide satisfactory information on the kinetic behavior, production rate and molecular weight distribution of propylene polymerization. Thus, the polymerization kinetics were produced by involvement of the Ziegler-Natta catalyst with multiple actives sites, where each type possesses its unique relative reactivity. The moment of polymerization is developed first by understanding the synthesis that takes place in polymerization process. Following that, the ODEs required for modelling can be retrieved. In this study, the type of active site is indicated by the index, *j*, whereby *j* = 1, 2.

## IV. PERFORMANCE ANALYSIS

In general, the multi objective functions can be formulated as Eq 8:

$$\textbf{Maximize}\ \mathrm{AND/OR}\ \textbf{Minimise}:\ \mathrm{J} \in \{f_1(x_1, x_2, \ldots x_n)\,, f_2(x_1, x_2, \ldots x_n) \ldots f_n(x_i, x_{i+1}, \ldots x_n)\ \} \quad (8)$$

$$\boldsymbol{Subjectto}: X \epsilon \prod_{i=1}^{n} [lb_i, Ub_i] \quad (9)$$

where$J$ consist of several objective functions in case study and these objectives are subjected to the set of $X$ for every bounded or non-equalities constraint condition.

**Case study 1: Test function**

Table 1, tabulate the reference benchmark for two objective functions and both are solved simultaneously by the proposed algorithm. The algorithm is to determine the optimal solution as per in the reference solution.

**Table. 1 Typical test functions**

| | Reference Benchmark | | | | |
|---|---|---|---|---|---|
| $i$ | Objective Function, $J_i$ | Interval | Reference | | |
| | | | $x_i$ | $y_i$ | $J_i$ |
| 1 | $0.5 + \left( sin\left( \sqrt{(x_1^2 + y_1^2)} \right)^2 \right) - \frac{0.5}{1 + 0.001(x_1^2 + y_1^2)^2}$ | [100, - 100] | 0 | 0 | 0 |
| 2 | $(x_2 - y_2)^2 + \left( \frac{x_2 + y_2 - 10}{3} \right)^2$ | [10, 0] | 5 | 5 | 0 |

In Table 2, the results are shown for population of 50 number of population and 100. For N = 50, the time taken for the iteration is shorter compare to N = 100. For N=100, the values for design variables are closer to the benchmark results and more accurate. This is because the number of population decides the quantity of design variable generated in the initiation stage. Higher quantity of design variable generated will cause the artificial bee takes longer time to evaluate each of the design variable value. Nevertheless, high quantity of design variable generated will create a wide range of better selection option for the artificial bee to evaluate the design variable value.

**Table. 2 Result Multi objective functions for Proposed Algorithm**

| N | Computational time (s) | $x_1$ | $y_1$ | $x_2$ | $y_2$ | $J_1$ | $J_2$ |
|---|---|---|---|---|---|---|---|
| 50 | 553.6886 | -0.0032 | -0.0246 | 5 | 4.9995 | 4.200E-3 | 2.3822E-8 |
| 100 | 715.9163 | -0.0409 | -0.0500 | 5 | 4.9997 | 6.173E-5 | 1.2316E-8 |

### Case Study 2: Operating conditions optimisation of Fluidized Bed reactor for Polymerisation of Polypropylene

As the commercial polypropylene is very high market demand, the advance modelling simulation analysis of polypropylene reaction is very important. Basically, polypropylene has 3 types of stereo-configuration sequence such as isotactic, syndiotactic and atactic. Each of the configuration sequence has their very own unique physical and chemical properties. This structure can be represented by melt flow index (MFI) number which in this study, the maximum value is desired to produce isotactic type of polymer. The increase of melt flow index results the crease of molecular weight which will cause the crystallinity of the polypropylene increase. The increase of crystallinity will provide more isotactic stereo configuration of the polypropylene due to the decrease of molecular weight will cause the polymer chains become shorter and it is easy for all regions along adjacent chains to align so as to produce an ordered atomic array.

In the other hand, the production rate of the polymerisation is another motivation of the simulation. The production rate will influence the feasibility of the process and attractive attribute to be considered. Therefore, 2 objective functions are used in the complex engineering application to test the performance of the proposed algorithm. Moreover, these objectives are subjected to temperature, pressure, superficial gas velocity and concentration of propylene of the polymerisation in fluidized bed reactor.

**Maximize**: $J_1 = f_1(x_1, x_2)$ **AND** $J_2 = f_2(x_3, x_4)$

$$f_1(x_1,x_2) = 2.662E6 - 37.23\,x_1 + 1076\,x_2 + 0.02476\,x_{12} + 0.1451\,x_1x_2 + (5.636E-5)x_{22} - (3.325E-3)x_{12}x_2 - 0.003325\,x_1x_{22} + 0.3347\,x_{23}$$

$$f_2(x_3,x_4) = -1.122 + 41.01\,x_3 - 3.261\,x_4 - 171.5\,x_{32} + 17.24\,x_3x_4 + 0.3853\,x_{42} + 330.3\,x_3 - 34.91\,x_{32}x_4 - 1.622\,x_3x_{42} - 240\,x_{34} + 24.27\,x_{33}x_4 + 2.024\,x_{32}x_{42}$$

**Subject to:**

$70°C \leq x_1 \leq 80°C$

$18\text{ bar} \leq x_2 \leq 30\text{bar}$

$0.2\text{m/s} \leq x_3 \leq 0.8\text{m/s}$

$x_4 \leq 1 mol/L$

Where the objective function, $f_1$and $f_2$is a production rate and melt flow index of polymer respectively. While, the optimisation constraints;$x_1$ is emulsion phase temperature, $x_2$ is FBR pressure, $x_3$ is superficial gas velocity and $x_4$ is propylene concentration. Other dependent parameters like$x_{12}$,$x_{22}$, $x_{23}$, $x_{32}$,$x_{33}$, $x_{34}$ and $x_{42}$ are dynamically changed with the polymerisation process in time series as explained in modelling section.

In order to reduce the calculation complexity and computational time, let the number of population for this optimization is three. To note, the range of limitation for pressure and temperature are chose based on the favour of Ziegler Natta catalyst activation conditions. After Optimization, the production rate and melt flow index for production of polypropylene are improved and shown in Table 4. The operating conditions are improved to more safety and cost effectively for the production. The operating temperature is from 345 K increase to 347 K. This temperature is very close to the temperature of maximum activity of the catalyst. If catalyst activate under the activation temperature, it will produce Ti4.DBP (DibutyPhthalate) residue whereas if activate over the activation temperature will cause the formation of carbonyl halides. Both of the scenarios clearly show that result in reduction in polymerization activity of propylene. Melt flow index is improved from 2.3863 to 2.7650 g per 10 min, the degree of crystallization of polypropylene is decrease due to decrease of softening temperature and melt viscosity. The melt flow rate between 2.6 to 3.3 g per 10 min is a premium grade of polypropylene for the BOPP film application. Furthermore, superficial gas velocity is reduced from 0.35 to 0.20 m/s which provides longer monomer mean residence time which leads to higher monomer conversion. Nevertheless, concentration of propylene is reduced from 1 mol/L to 0.2 mol/L which able to reduce the raw material cost for the polymer plant. At the end of the multi objective ABC algorithm, the optimum operating conditions for polypropylene production are shown in Table 3.

**Table. 3 Performance test comparison**

| $i$ | Objective Function, $J_i$ | Initial | ABC |
|---|---|---|---|
| 1 | Production Rate, kg/year | 2.6664E6 | 4.8811E6 |
| 2 | Melt Flow Index, g/10min | 2.3863 | 2.7650 |
| $i$ | Constraint, $x_i$ | Initial | ABC |
| 1 | Temperature, ˚C | 72 | 74 |
| 2 | Pressure, bar | 25 | 22 |
| 3 | Superficial gas velocity, m/s | 0.35 | 0.20 |
| 4 | Propylene concentration, mol/L | 1.00 | 0.2 |

Figure 1 is representing the production rate versus number of iteration. Based on the observation, the ABC algorithm is operated until 50th iteration in order to obtain the optimum operating condition to improve production rate. During iteration, there is a fluctuation of the production rate approximate on 4.5E6 kg/year. This is because the artificial bees are recognized a set point of maximum production rate by controlling design variables. Every time the artificial bees reach the maximum production rate they will try to seek for an optimum production rate and improve the operating condition from the optimum production rate. The scout bee will engage for every end of the iteration when the solution does not meet the termination requirement. Scout bee generates a new set of food source based on the current food source that obtained from onlooker bee. The reason of improvement throughout the ABC algorithm is because the scout bee generate new food source based on the current best solution which minimize the range of best food source from time to time and allow the employ bee and onlooker bee to evaluate and choose the better food source to obtain the optimal solution. Figure 1 shows the improvement of production rate from the beginning to the end of iteration.

Figure 2 is representing the melt flow index versus number of iteration. Based on the observation, the ABC algorithm is operated until 50th iteration in order to obtain the optimum operating condition to improve melt flow index. During iteration, there is a fluctuation of the melt flow index approximate on 1.6 g per 10 min This is because the artificial bees are recognized a set point of minimum melt flow index by controlling design variables. Every time the artificial bees reach the minimum melt flow index they will try to seek for a higher melt flow index and improve the operating condition. Figure 2 shows the data after filtered out the fluctuation; it presents the improvement of melt flow index from the beginning to the end of iteration. At the end of the iteration, melt flow index is improved and maintain in the range of 2.6 to 3.0 g per 10 min. In polymer industry, melt flow index is the easier guideline to make decision for the selection of polymer. Polypropylene which categorised in the premium grade is when the melt flow index at the range of 2.6 to 3.3 g per 10 min.

Pareto front is a set of solution possess a property that choosing a better value of any one objective function. It would cause a worse value of other objective function in order to satisfy the objective function. Pareto front is used to observe the performance optimization that performed by the ABC algorithm. The Pareto front of design parameters for objective function 1 and objective function 2 are plotted and show in Figure 3 and Figure 4 whereas the Pareto front of objective function 1 versus objective function 2 is plotted and show in Figure 5. The Pareto front is generated based on the constraint of the objective functions that mentioned.

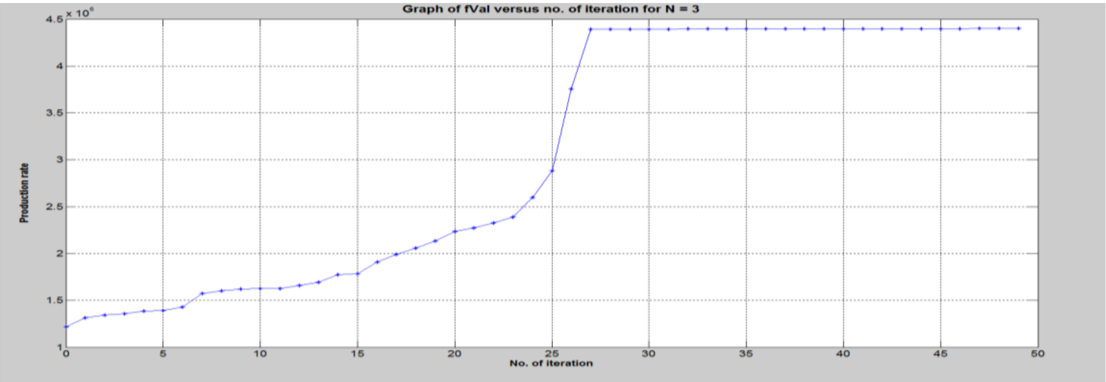

**Fig. 1 Production Rate optimisation performance for N = 3**

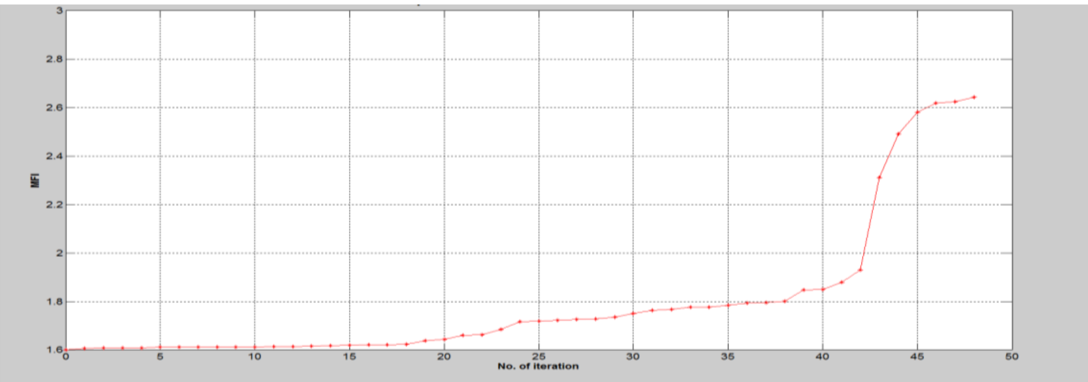

**Fig. 2 Melt Flow Index optimisation performance for N = 3**

Based on Figure 3 the optimum temperature range is obtained from the graph which is from 343 K to 353 K where the optimum pressure range is from approximate 18 to 30 bar. The Pareto front separate the graph into two regions which are feasible region and not feasible region, feasible region is above the Pareto front whereas not feasible region is located at below the Pareto front. The point that registered in the feasible region is the solution that obtained from ABC algorithm which is temperature is equal to 347 K and pressure is equal to 22 bar.

Figure 4 is representing the Pareto front of design parameters for objective function 2. The optimum superficial gas velocity range is obtained from the graph which is from 0.15 m/s to 0.205 m/s where the optimum propylene concentration range is from approximate 0.1 mol/L to 1 mol/L. The Pareto front separate the profile into two regions which are feasible region and not feasible region, feasible region is above the Pareto front whereas not feasible region is located at below the Pareto front.

The point that registered at very close to the Pareto front is the solution that obtained from ABC algorithm which is superficial gas is equal to 0.2 m/s and propylene concentration is equal to 0.2 mol/L. In this case, the solution can be considered as Pareto optimal solution. From Figure 3 and Figure 4 show that the temperature and pressure are sacrificed in order to satisfy the superficial gas velocity and concentration propylene.

Figure 5 is representing the Pareto front of objective function 1 and objective function 2. The two objective functions are optimized by the ABC algorithm. The objective 1 is to maximize the production rate and it is being maximize from 2.6664E6kg/hourto 4.8811E6 kg/hour whereas objective 2 is to maximize the melt flow index of polypropylene and it is being maximize from 2.3863 g per 10 min to 2.785 g per 10 min.

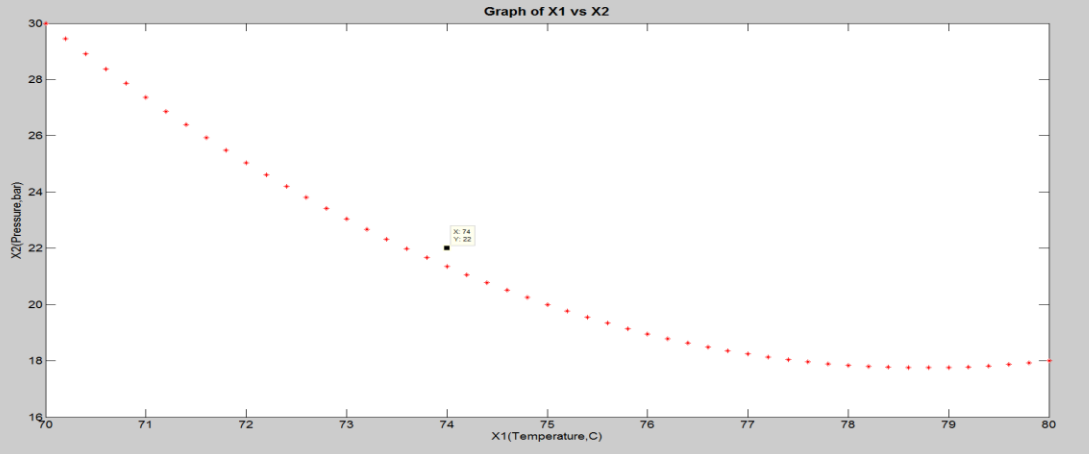

Fig. 3 Pareto Front of $X_2$ vs $X_1$

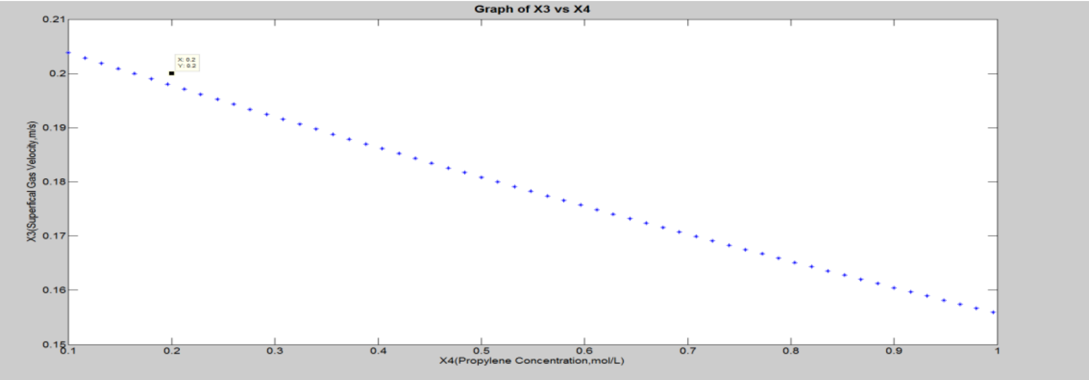

Fig. 4 Pareto Front of $X_3$ vs $X_4$

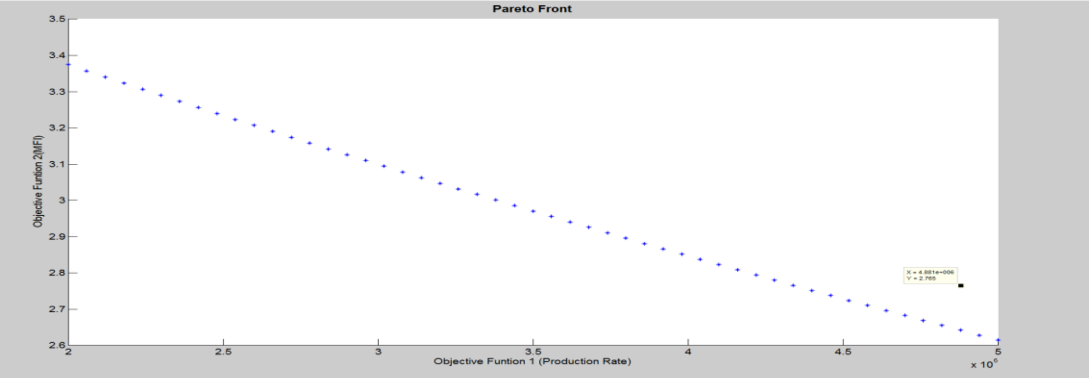

Fig. 5 Pareto Front of Objective 1 versus Objective 2

## V. CONCLUSION

The meta-heuristic colony based optimization algorithm is performed to find the optimal operating condition for specific targeted production for polypropylene derivative. The simulation is highly complex and multi-phase process where is challenging to find good trade-off for multi objective optimisation application. In this study the onlooker bee phase of the ABC algorithm is modified and improved in order to obtain more accurate and shorten the optimization time. There two parts for onlooker bee phase, the first part will be the usual evaluation of the current value with the random pick neighbour value to determine the better solution, second part is apply the better solution from first part to compete maximum or minimum constraint. Besides that, the polypropylene reaction in multi-phase system is developed in time series with Runge–Kutta ODE's solver and few assumptions are made in order to solve the model. The optimization for the polypropylene reaction is carried out by the multi objective functions ABC algorithm, and the objective functions are maximum production rate and melt flow index by controlling operating temperature and pressure, superficial gas velocity, and concentration of feed propylene. In summary, the optimal operating temperature and pressure, superficial gas velocity, and concentration of feed propylene are 347 K, 22 bar, 0.2 m/s and 0.2 mol/L respectively. The optimal operating conditions are able to maximize the production rate and melt flow index to 4.8811E6kg/year and 2.785 g per 10 min respectively.

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