Simulation and Optimization of a Continuous Biochemical Reactor

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Abstract

The present work focused on the dynamic and optimization of a continuous biochemical reactor using the glucose as a substrate. Simulated model provides the development of the process and reducing the risk of experimental runs. The selected process variables are; dilution rate (D), feed substrate concentration (Si), pH and temperature (T).The major effect of D was observed at Si below 20 g/L. pH and T are affecting within Si of 60 g/L.Si is the effective process variable on the dynamic characteristics of the reactor. Reasonable agreement has found when compared the simulated results with that obtained by the previous work .Optimization technique guides the decision maker to select the best operating conditions.Stochastic genetic algorithm has found suitable for the nonlinear reactor.Optimal results indicate that the maximum biomass concentration (X) is 80.57 g/L at Si of 197.56 g/L and low D of 0.1(1/hr).Si was the sensitive variable for changing of the objective X.

Keywords: Biochemical reactor; Dynamic model; Optimization; Simulation.

1. Introduction

Lee [1] and Kapadia *etal.* [2] described the concept and applications of the biochemical reactors.The stirred-tank bioreactor is one of the most commonly used types for large scale production in industrial applications such as food, pharmaceuticals, various commodity and specialty chemicals .It is used mainly in two modes: the continuous mode and the fed-batch mode.In the continuous mode, the limiting substrates are constantly added to the reactor, while the output stream is simultaneously removed at the same rate, to keep the reactor volume constant.The continuous stirred biochemical reactor is widely used in the treatment of liquid wastes.Its process kinetic can be characterized by the following reaction scheme:

$$\text{Substrate} \rightarrow \text{Biomass} + \text{Gas}$$

Nomenclatures

D: Dilution rate, [1/hr]

F: Flow rate, [L/hr]

Km: Saturation constant, [g/L]

PH: Acidity [-]

r1: Rate of cell generation,[g/L.hr]

r2: Rate of substrate consumption,[g/L.hr]

S: Substrate concentration in the reactor,[g/L]

Si: Feed substrate concentration,[g/L]

T: Temperature, [C°].

t: Time, [hr]

V: Volume of the reactor,[L]

X: Biomass concentration in the reactor,[g/L]

Y: Yield, [-]

Greek Symbols

μmax: Maximum specific growth rate coefficient,[1/hr].

μ(s): Local specific growth rate coefficient, [1/hr].

Henson [3] explained that as compared to conventional chemical reactors, bioreactors present unique modeling and control challenges due to complexity of the underlying biochemical reactions.

Karadag and Puhakka [4] and Garhyan *etal*.[5] studied the bioreactor performance using mixed cultures influenced by several operational parameters which affect its static and dynamic behavior such as: dilution rate, feed substrate concentration pH, hydraulic retention time, organic loading rate and temperature. In particular, the role of pH seems the most important parameter in the regulation of enzymes pool production. Ruggeri etal. [6] indicated that the pH adjustments validated the dynamics of the system.Charoenchai, *et al.* [7] concluded that the temperature is a variable that directly affects the growth rate of organisms.
Annamalai and Doble [8] had found the mathematical modeling of fermentation process helps to; elucidate the mechanism of production process, estimate kinetic parameters such as specific growth rate of biomass and product formation rate develop the understanding between effects of operational conditions on production, and reduce laboratory experiments thereby saving time and resources.

Alhumaizi and Ajbar [9] and Shimizu [10] proved the biological processes are inherently very nonlinear and had frequently been changing optimum operating conditions. Many available mathematical models for biological reactions were not suitable for a control design since no accurate biological law had been proposed.

Kapadia *etal.*[11] proposed a novel robust controller for a continuous stirred biochemical reactor that controls the culture dilution rate into the reactor in order to maximize a cost function representing the biomass yield.

Genetic algorithm (GA) is global stochastic search based on mechanics of natural selection and natural genetics.GA is based on Darwin's theory of 'survival of the fittest'. There are several genetic operators. Such as; selection, crossover and mutation…etc.Gupta and Srivastova [12] concluded that the deterministic algorithms for function optimization are generally limited to convex regular functions. However, many functions are either not differentiable or needed a lot of difficult mathematical treatment: decomposition, sensitivity computing…etc.

2. Scope of the Work

The present work focuses on the simulation and optimization of the continuous biochemical reactor using glucose as the substrate. Study the effect of the process variables on the dynamic behavior of the reactor .The selected process variables are; feed substrate concentration, dilution rate, pH and temperature. The reliable simulated model can be used to generate the desirable data for formulating the optimization equation. The objective is to maximize the biomass concentration in the reactor. Stochastic globe genetic algorithm search is implementing to select the best operating conditions of the reactor.

3. Dynamic model

Dynamic modeling for optimization and control requires models that describe the essential dynamic characteristics of the process under study. In the present work, the following assumptions have been adopted for the model:

1. Homogenous liquid-phase system.
2. Non-isothermal conditions.
3. Acidity of liquid is changed.
4. First order irreversible reaction.
5. Constant hold-up.
6. Follow the Monod law.

The component material balances for biomass(X) and substrate(S) are:

$$dX/dt = r1-(F/V)\ X \tag{1}$$

$$dS/dt = (F/V)\ Si - (F/V)\ S- r2 \tag{2}$$

In addition, the reaction rate equations are:

$$r1=\mu(s)\,X1 \qquad (3)$$

And, $Y = r1/r2$ (4)

For Monod law;
$$\mu(s) = (\mu max * S)/(Km+S) \qquad (5)$$

$$\mu max = -40.5 + 11.78pH - 0.0691pH^2 + 1.65T + 0.003T^2 - 0.468pH.T \qquad (6)$$

Equations (1&2) can be simplified to:

$$dX/dt = (\mu(s) - D)X \qquad (7)$$

$$dS/dt = D\,(Si - S) - (X/Y)\mu(s) \qquad (8)$$

Where $D=F/V$

Equation (6) was correlated depended on the experimental data of Lopez etal. [13].

The simulated model will implement for the wastewater contains glucose with different concentrations from 6.0 to 200.0 gm/L.Temperature of water are varied from 20 to 30 C° and the acidity are from pH2 to pH4.The kinetic parameters of the biological reaction are; maximum specific growth rate coefficient ($\mu max=0.3\ hr^{-1}$), saturation constant (Km=1.0 g/L) and yield (Y=0.4) depended on the results of Lopez *etal.*[13] ,Cutlip and Shacham[14].

4. Results and Discussion

4.1. Optimal operating Conditions

The initial optimal operating conditions of the system (Table 1) were estimated by the nonlinear Levenberg-Marquardt method with the aid of the MATLAB computer program.

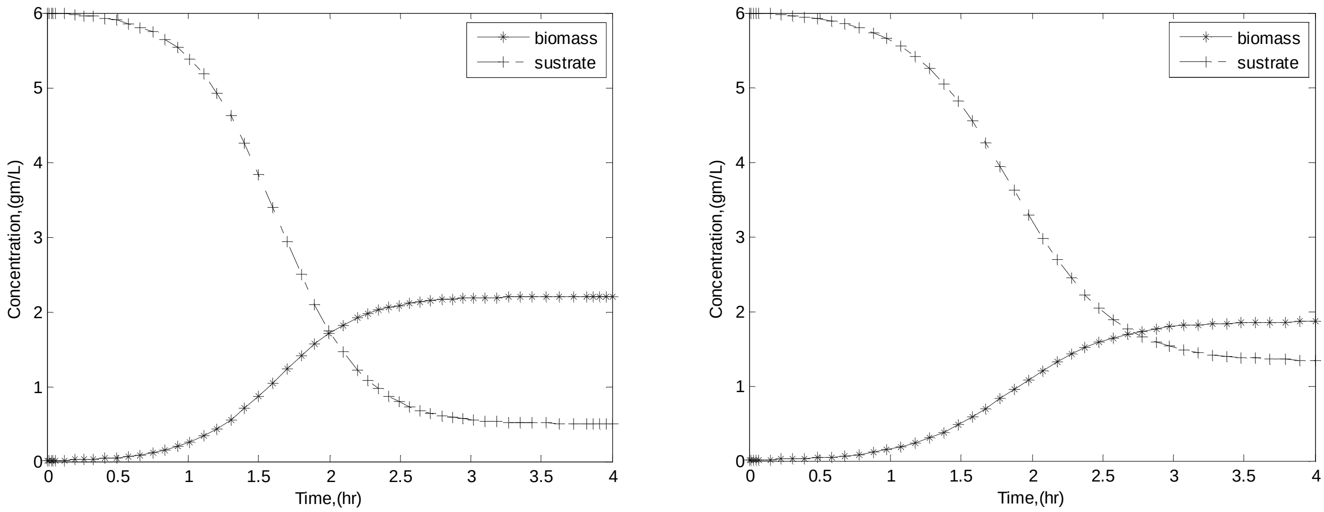
Table 1. Optimum initial operating conditions

X(gm/l)	Si(gm/l)	D(hr^{-1})	Y(-)	μ(1/hr)
0.001	6.0	0.3	0.4	0.4

4.2. Unsteady State Conditions:

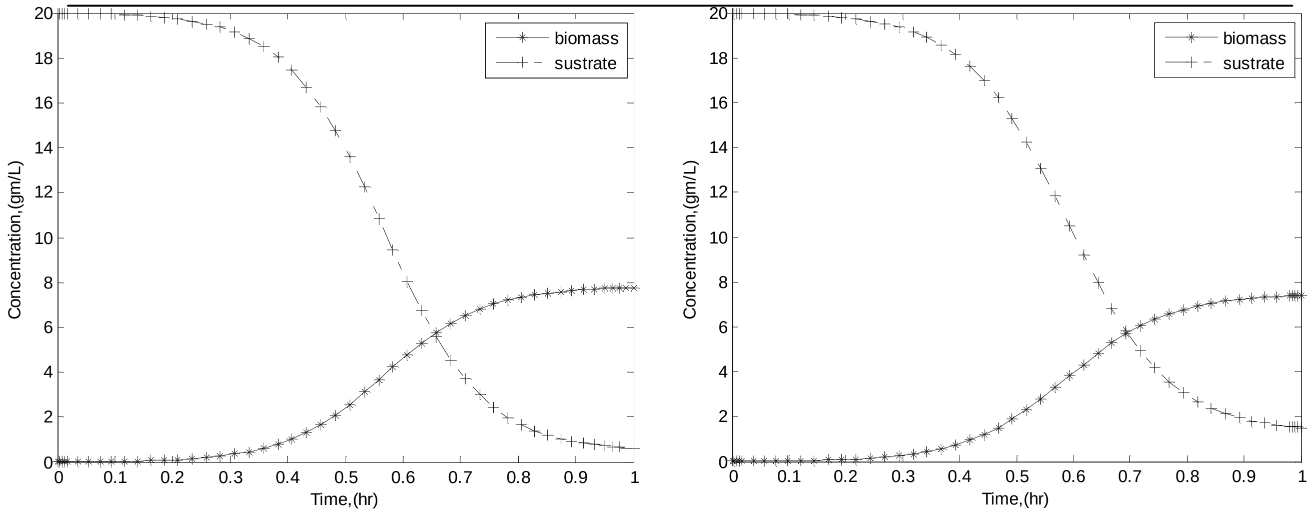
The present bioreactor can be viewed as nonlinear dynamic system and the simulation is very useful tool for model validation .The unsteady- state model (Equations 7 and 8) are solved numerically using 4th order Runge-Kutta method with the aid of the MATLAB program, starting from steady- state operating conditions (Table1). Figures (1-7) explain the behaviors of the biochemical process under different operating conditions.

Dynamically, the system behaves as the first- order lag system. The dynamic model appears that the biomass concentration curves have S-shape and more sluggish when compared with the substrate curves, which have an exponential shape because of the rate of consumed substrate is more than the rate of biomass cell generation in the reactor. The response speed of the biomass and substrate curves increase with Si and decreases with D as shown in Figures (1-3).The intersection point between two curves indicates to the local optimal point of the system, where the concentration of the biomass equal to that of the substrate. These points are various depended on the operating conditions.



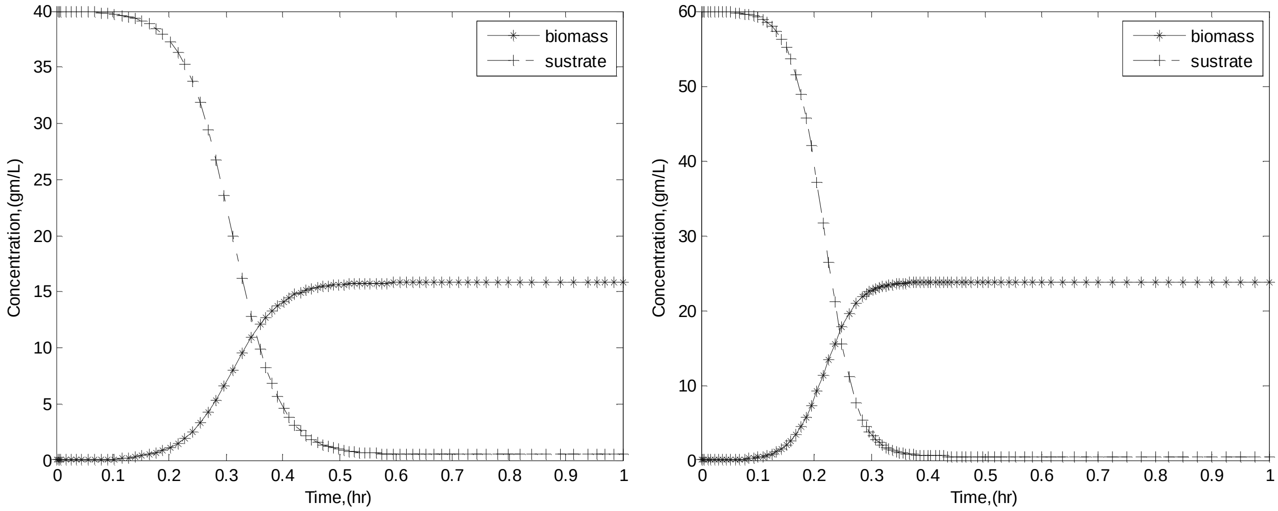
(a) (b)

Fig.1. Unsteady state concentration of biomass and substrate at Si=6 for :(a)D=0.3, (b) D=0.8.



(a) (b)

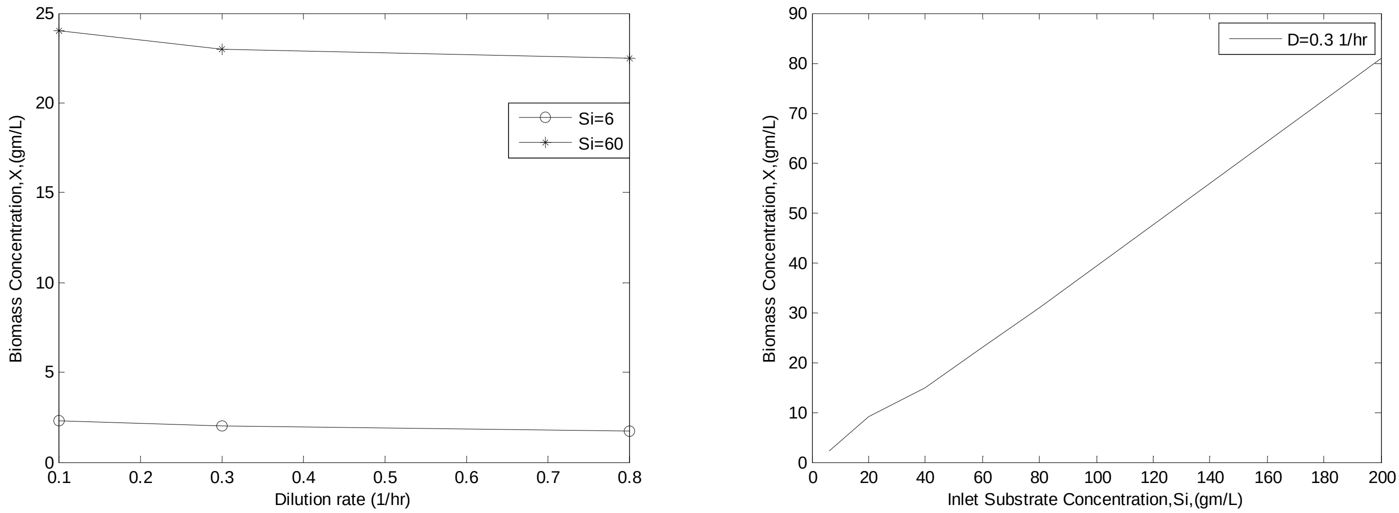
Fig. 2. Unsteady state concentration of biomass and substrate at Si=20 for ;(a) D=0.3, (b) D=0.8.



(a) (b)

Fig. 3. Unsteady state concentration of biomass and substrate at D=0.3for; (a) Si=40, (b) Si=60.

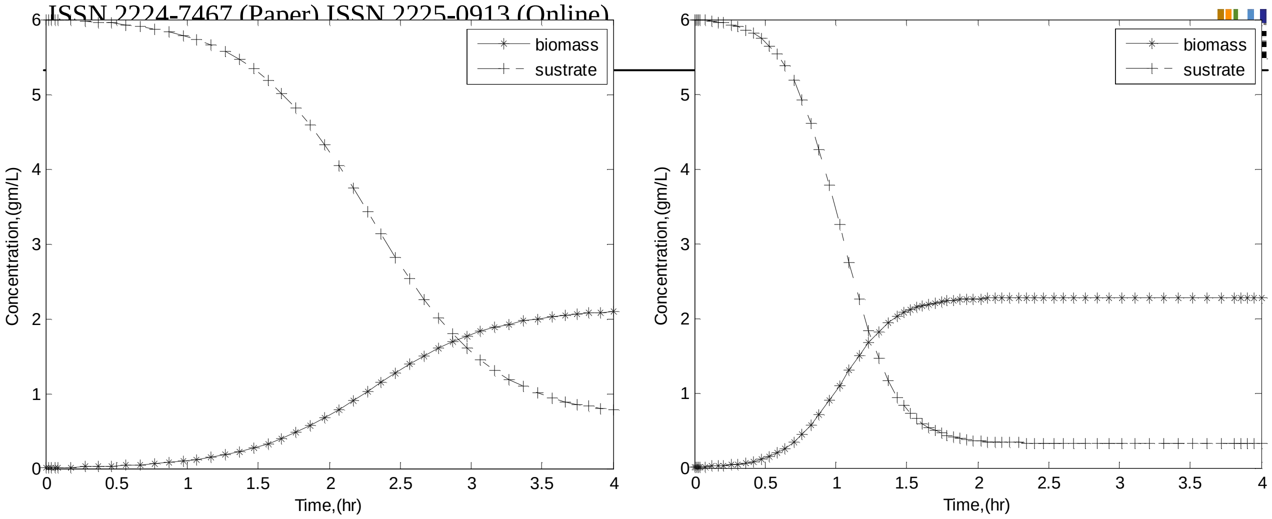
The concentration of the biomass in the reactor decreases with increasing D (Figure 4a) for low and high Si. In the contrast, the increasing of Si increases the concentration of biomass in the reactor as shown in Figure 4b.This is due to the fact; that Si has a positive effect on the specific growth rate constant (μ) regarding to the Monod law (Equation 5).While the increasing of D tends to increase the dilution of the substrate which could moderate the growth rate then reduces the concentration of the biomass in the biochemical reactor .The sensitivity of the process (steady- state gain) against Si (Figure 4b) is more than that with D (Figure 4a).The effect of Si is more pronounced at low D as shown in Figure 4. Jarzebski [15] also concluded these behaviors.



(a) (b)

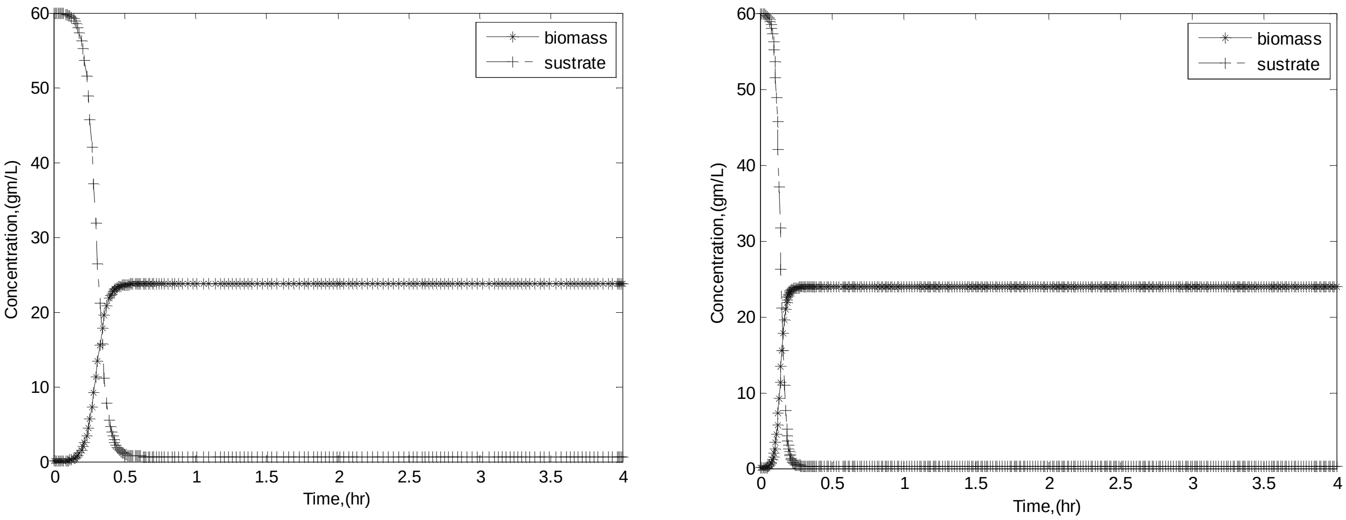
Fig.4. Biomass concentration as a function of (a) Dilution rate, (b) Inlet substrate concentration.

The effect of temperature on the biomass growth rate appears in Figures (5 and 6) at the temperature range from 15 to 30 ^{o}C.The simulated results explain that the increasing of temperature enhances the growth rate of the biomass at low and high Si. This increases the response speed of the biomass concentration. The steady- state value of the biomass concentration was unaffected with the rising of temperature as shown in Figures (5and 6).



(a) (b)

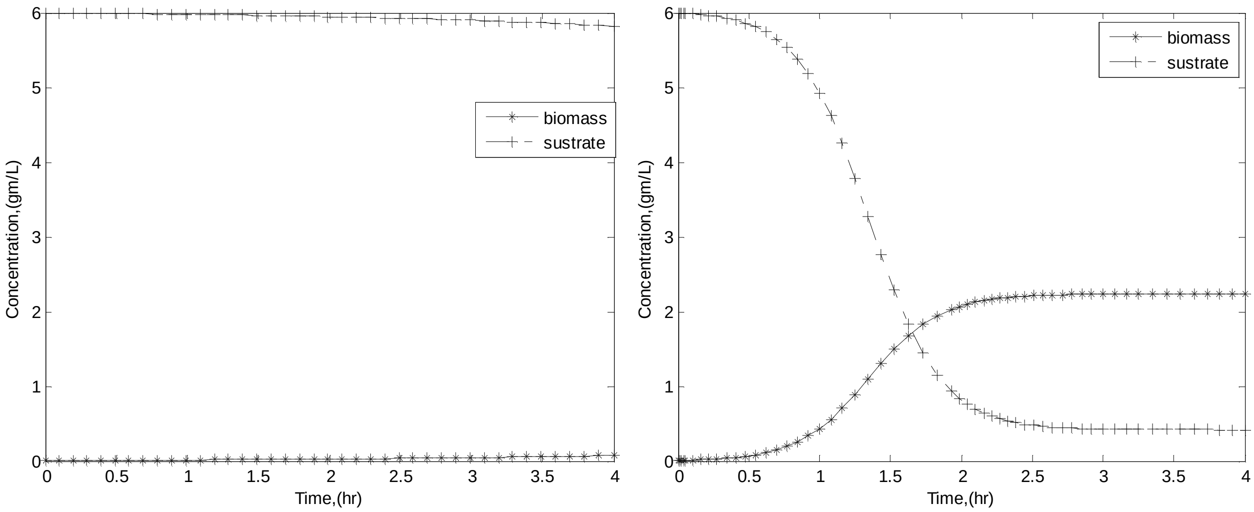
Fig.5.Effect of temperature on the process at D=0.3 and Si=6 for (a) T=20, (b) T=30.



(a) (b)

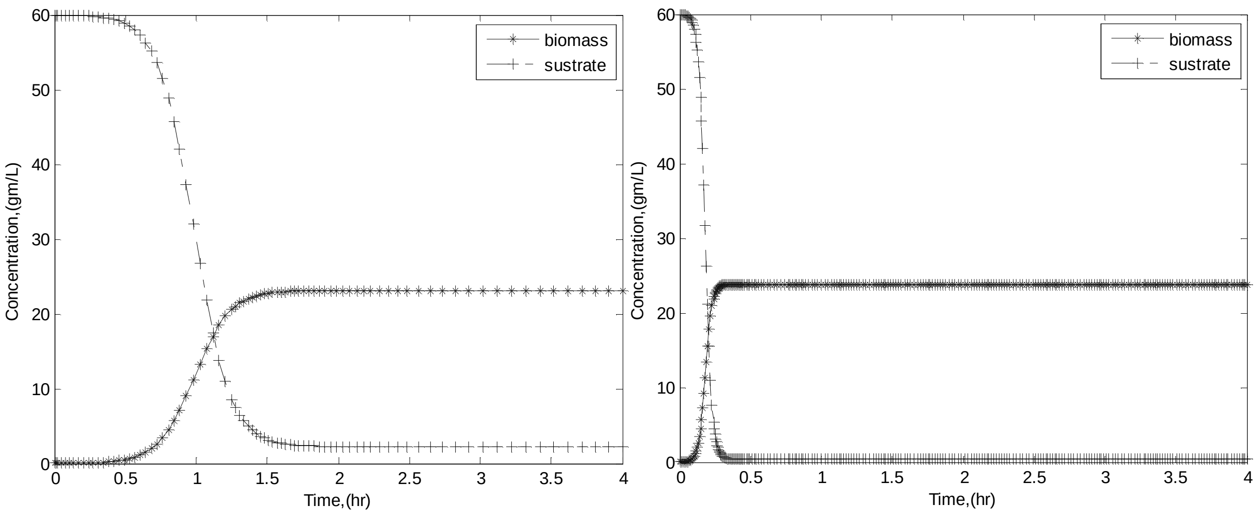
Fig.6 .Effect of temperature on the process at D=0.3 and Si=60 for (a) T=20, (b) T=30.

Figures (7 and 8) explain the effect of the water acidity (pH) on biomass growth. The effect studied for the available data ranged between pH 2 to pH 4.The biomass growth is very slow at low acidity (pH 2) and increased with increasing to pH 4 as shown in Figures (7a and b).The concentration of the biomass in the reactor is very low with the lower feed substrate concentration(Si=6) and pH 2 of water as shown in the Figure 7a.At high substrate feed concentration(Si=60) ,the growth of biomass cell would enhanced at low acidity(pH=2) when compared Figure 7a with Figure 8 a. Si regarding to the Monod law directly affects the growth rate coefficient (μ). The final steady- state concentration of biomass is unaffected by the increasing of pH at high Si as shown in Figure 8.



(a) (b)

Fig. 7 .Effect of pH on the process at D=0.3 and Si=6 for; (a) pH=2, (b) pH=4.



(a) (b)

Fig. 8. Effect of pH on the process at D=0.3 and Si=60 for; (a) pH=2, (b) pH=4.

Reasonable result can observe when compared the simulated results with these obtained by Cutlip and Shacham [14] as shown in the Figure 9 .The deviation is about 8%.This indicates that the proposed simulated model is agreed for the present biochemical reactor. Therefore, the reliable model could use to generate the desirable data for formulating the optimization equation.

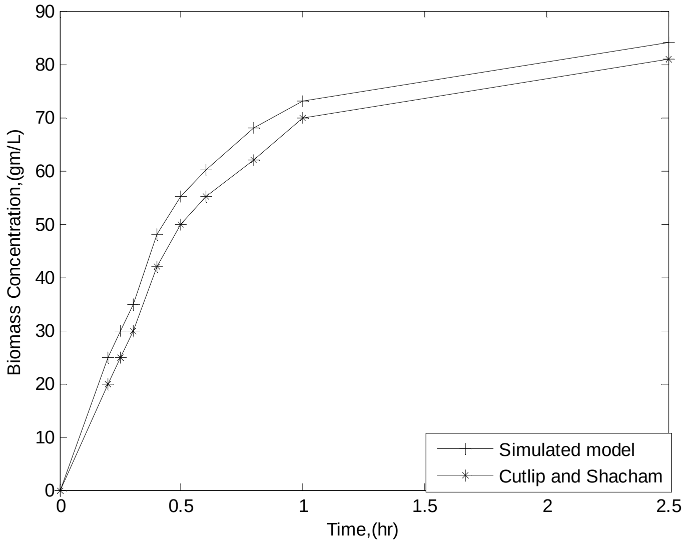


Fig.9.Comparison with previous work

4.3. *Optimization problem*

The available simulated data have been used to correlate the objective (concentration of biomass) with the decision variables to facilitate the optimization scheme. The selected effective decision variables are; dilution rate (D) and inlet concentration of substrate (Si). Nonlinear regression (Levenberg-Marquardt) method was implemented with the aid of the computer program (Statistica version10).

The optimization equation is:

$$X=0.409\ Si\ -0.575D-0.028DSi\ +0.02 \tag{9}$$

Subject to inequality constraints:

$$6.0 \leq Si \leq 200 \tag{10}$$
$$0.1 \leq D \leq 0.8$$

Equation 9 indicates that the dilution rate (D) has negative effect on the biomass concentration while the inlet concentration of substrate (Si) has positive effect.

4.4. *Optimization Technique*

The objective is to maximize the biomass concentration in the reactor. The optimization equation (Equation 9) is interacted and nonlinear, so that the deterministic search is unsuccessful. GA has been found suitable for the present biochemical process. GA is stochastic global search based on mechanics of natural selection. Figure 9 illustrates the results/solution of the algorithm scheme. The parameters of the GA were adapted, and the selected operators are suitable for solving the problem to obtain the best optimal values. Hybrid function implemented as the combined search between genetic algorithm and pattern search to refine the values of decision variables. 51 generations occurred regarding to the nonlinearity of the process. The adapted operators of GA are explained in the Table 2.

Table 2.Adapted parameters of GA.

Population type	Double vector
Population size	80
Creation function	Feasible population
Scaling function	Rank
Selection function	Roulette
Crossover function	Scattered
Crossover fraction	0.8
Mutation function	Adaptive feasible
Migration direction	Forward
Migration fraction	0.1
Hybrid function	Pattern search
Number of generation	51
Function tolerance	1.0E-6

Table 2 explains the best operators of the genetic algorithms. Figure 10 illustrates the outputs of the algorithms solutions/operators of genetic algorithm.GA is implemented with the pattern search by using the hybrid function as shown in Table 2 to refine the decision variables .The best fitness, best function and score histogram as shown in Figure 10 illustrate that the maximum biomass concentration is 80.57 g/L.The histogram of decision variables indicates that the optimal values are; Si=197.56 g/L (variable 1) and D=0.1hr^{-1} (variable 2), which are within the limit of inequality constraints (Equation 10). The histogram of the variables in Figure 10 indicate that Si (variable 1) is the effective variable on X.Due to the nonlinearity of the bioreactor process, the optimization equation(equation 9) was solved by (51) generations as shown in Figure 10.

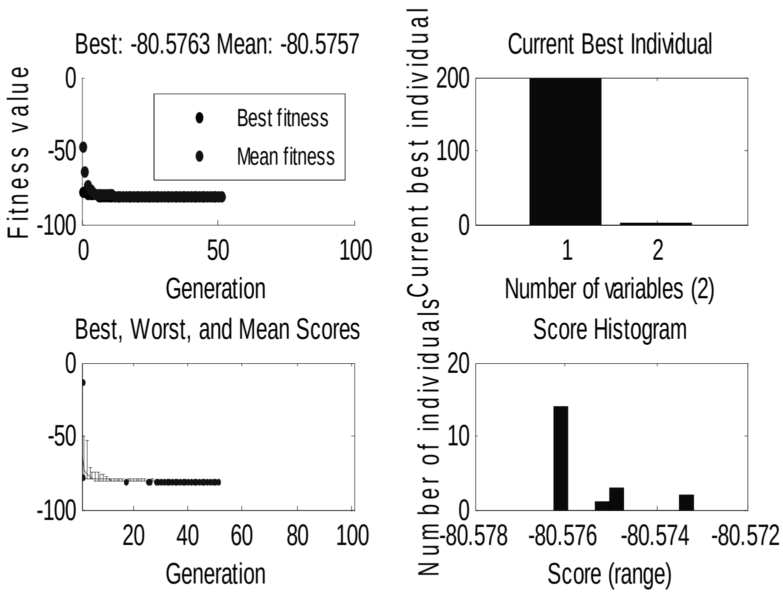
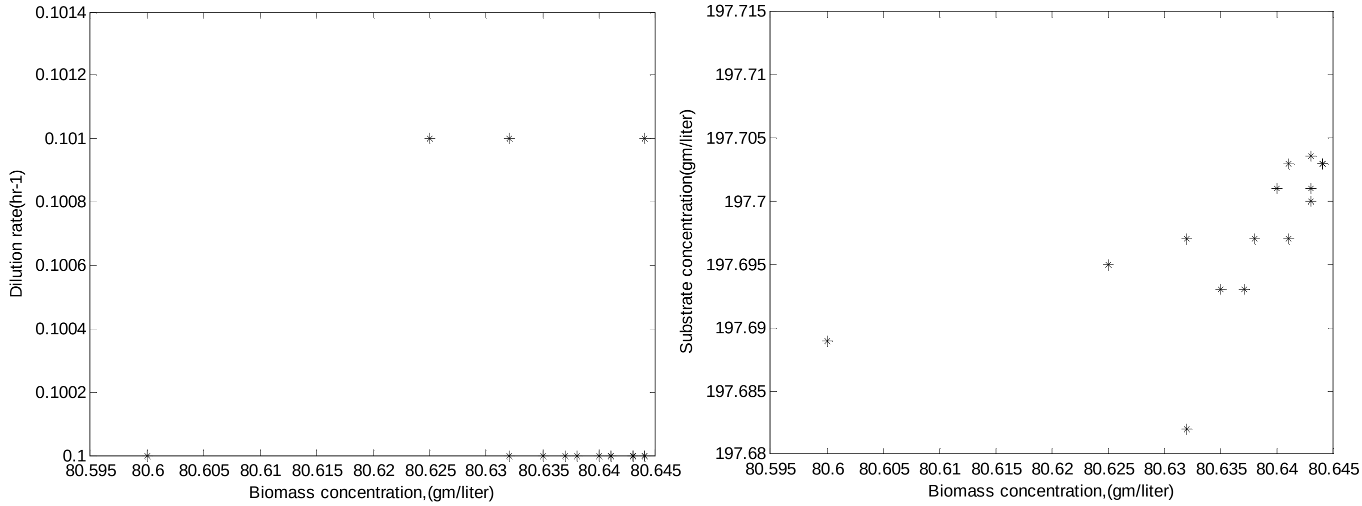


Fig.10. Solution/results of GA search.

The optimal sets of the decision variables are illustrated in Figures (11a, and 11b) corresponding to the objective X.The scattering and stochastic of the results are appeared in these figures as a results of natural selection by GA .It is found that the optimal values
of the dilution rate (D) is approximately constant within its lower bound as explained in Figure 11a.Inlet substrate concentration (Si) is more sensitive to the optimal objective change(X) as shown in Figure 11b .This is because of that Si is the effective variable on X as shown in Figure 10.Si is changed within its upper bound (Figure11b).These behaviors are because of Si has positive effect while D has negative effect on X as shown in the Equation 9. Optimal values of the two decision variables are stayed within optimal value of X, which equal to 80.57 g/L as shown in Figure 11.



(a) (b)

Fig.11.Optimal values of decision variables corresponding to objective X.

Optimization technique is a powerful tool to obtain the desired operating conditions that improves the performance of the reactor. This reduces the risk of experimental runs and cost consumed for design and operation. However, the reliability of the search depends on; the best selection of decision variables, formulation of the objective function and the selection of the proper optimization technique.Palonen, *etal.* [16] was indicated to this conclusion.

5. Conclusions

1. Simulated model helps the study of dynamic characteristics of the biochemical reactor. Reliable model could use to generate extra data in the case of unavailable experimental results.
2. Effect of dilution rate was observed at low feed substrate concentration that is below 20 g/L. The effect of pH and temperatures were appeared within the concentration of 60 g/L.
3. Feed substrate concentration was found the effective process variable on the growth rate of the biomass cell in the reactor.

4. Maximum concentration of the biomass cell could be obtained at high concentration of substrate and low dilution rate. Optimal feed substrate was more sensitive to the variations of the objective biomass concentration.
5. Reasonable agreement was obtained when compared the simulated results with that obtained by the previous work.
6. Simulation and optimization provide the development of the process, and reducing the risk of experimental runs and consumed cost for design and operation.
7. Stochastic genetic algorithm has found the suitable search for the nonlinear biochemical reactor process.

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