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A Study On the Mathematical Model of Chemostat with Incomplete Mixing

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Abstract: This study aims to investigate the mathematical model of incomplete mixing in a continuously stirred tank reactor (CSTR) and to study the impact of the size of a stagnant area on the steady-state. The chemical model used is a quadratic autocatalysis scheme with linear decay of autocatalyst, and these reactors represent the 'highly agitated' and 'stagnant' regions. The effect of incomplete mixing in a chemostat is analyzed by adjusting the size values in the stagnant region, while the stability of the mathematical model of incomplete mixing is determined by identifying the stability analysis and stability diagrams such as phase plane and time series plot. The study of the chemostat model with incomplete mixing is done by obtaining the dimensionless equations, steady-states, Jacobian Matrix, trace, and determinant. From the stability analysis, the obtained washout is stable while the no-washout has no physically meaningful solutions. For the steady-state diagrams, it shows that the size of the stagnant region (ε) does not affect much on the steady-state diagram, but there is a "poor mixing" region for extremely small values of the mixing parameter (δ). Therefore, the mixing parameter does affect the steady-state diagrams more than size of the stagnant region.

Keywords: Chemostat Model, Incomplete Mixing, Stability Analysis

1. Introduction

According to [1], a chemostat or continuous stirred-tank reactor (CSTR) is a basic piece of laboratory apparatus, that plays an important role in mathematical ecology. A study of chemostats has always been investigated by many researchers to improve the microbial production in the chemostat. The chemostat was first presented by [2] as a mechanism to culture a microbial population at a consistent rate for an unknown period under regulated environmental circumstances. Based on [3], the ability to control the growth rate of microbial experimentally is one of the major benefits of culturing microbial in a chemostat. However, there is less review on the imperfect mixing models. The imperfect mixing or non-ideal mixing models have been introduced by [4] and further mentioned in [5]. The concept of incomplete mixing in the chemostat is when the moment a new fluid flow through the reactor, it is not effectively dispersed throughout the system. According to [6], when the mixing parameter

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approaches zero ($\delta \rightarrow 0$), ε becomes a dead volume as the stagnant area uncouples from the highly agitated area and when the mixing parameter becomes infinitely large, that approaches infinity $\delta \rightarrow \infty$, the model is in perfect mixing as the concentration of the reactants in the couple areas of the reactor become the same.

The main objectives of this study are to investigate the mathematical model of chemostat with incomplete mixing and to analyze the effect of size of stagnant region in the chemostat with incomplete mixing. The equation used is from a quadratic autocatalytic scheme with linear decay of the autocatalyst invented by [7]. The mathematical model contains the reactant concentration in the feed, the autocatalyst concentration, the rate constant for the autocatalytic step, flow rate through the reactor, the decay rate, time, and volume of the reactor with the residence time. For the incomplete mixing model, the parameter of mixing between two areas and the fraction of the total volume belonging to the stagnant area was introduced. The problem statement of this study are imperfect mixing in chemostat is obtained from the factors such as the increase of size of the reactors or the availability of cells that may grow on solid surfaces, such as the reactor walls or the surface of probes. These factors contribute to the difficulty of achieving the ideal perfect mixing. Therefore, in this study we apply the mathematical model from [7] to investigate the stability of the mathematical model of incomplete mixing and to analyze the effect of size of the stagnant region in chemostat. The stability diagrams and steady-state diagrams of the model are visualized using Maple software to determine their stability and to analyze effect of size of the stagnant region towards the steady-states.

2. Materials and Methods

2.1 Mathematical Model of Incomplete Mixing

This research considered the mathematical model equation from [7] which is a chemical process regulated by quadratic autocatalytic kinetics with imperfect mixing. The dimensional model equations for the case of imperfect mixing are as follow

Equations in the highly agitated region

$$V(1-\varepsilon)\frac{da_1}{dt} = q(a_0 - a_1) - V(1-\varepsilon)k_1 a_1 b_1 - q\delta(a_1 - a_2), \qquad Eq.1$$

$$V(1-\varepsilon)\frac{db_1}{dt} = q(a_0 - a_1) - V(1-\varepsilon)k_1 a_1 b_1 - V(1-\varepsilon)k_2 b_1 - q\delta(a_1 - a_2), \qquad Eq.2$$

Equations in the stagnant region

$$V\varepsilon\frac{da_2}{dt} = q\delta(a_1 - a_2) - V_\varepsilon k_1 a_2 b_2, \qquad Eq.3$$

$$V\varepsilon\frac{db_2}{dt} = q\delta(b_1 - b_2) + V_\varepsilon k_1 a_2 b_2 - V_\varepsilon k_2 b_2. \qquad Eq.4$$

The variables and parameters in Equation (1 – 4) are a_0 is the reactant concentration in the feed ($mol\ m^{-3}$), a_1 is the reactant concentration in the agitating area ($mol\ m^{-3}$), a_2 is the reactant concentration in the stagnant area ($mol\ m^{-3}$), b_0 is the autocatalyst concentration in the feed ($mol\ m^{-3}$), b_1 is the autocatalyst concentration in the agitating area ($mol\ m^{-3}$), b_2 is the autocatalyst concentration in the stagnant area ($mol\ m^{-3}$), k_1 is the rate constant for the autocatalytic step, ($m^3 mol^{-1} s^{-1}$), k_2 is the decay rate (s^{-1}), q is the flow rate through the reactor ($m^3 s^{-1}$), t is the time (s); V is the volume (m^3), δ is the parameter of mixing between the couple of areas and ε, $0 \leq \varepsilon < 1$, is the fraction of the total volume belong to the stagnant area.

The dimensionless equations for imperfect mixing are obtained by reducing the number of parameters in equations by using the dimensional analysis method. To get the dimensionless equation, [7] introduced the dimensionless groups: $\alpha_1 = \frac{a_1}{a_0}$, $\alpha_2 = \frac{a_2}{a_0}$, $\beta_1 = \frac{b_1}{a_0}$, $\beta_2 = \frac{b_2}{a_0}$, $t^* = k_1 a_0 t$.

Equations in the highly agitated region

$$\frac{d\alpha_1}{dt^*} = \frac{1-\alpha_1}{(1-\varepsilon)\tau^*} + \alpha_1\beta_1 - \frac{\delta(\alpha_1-\alpha_2)}{(1-\varepsilon)\tau^*}, \qquad Eq.5$$

$$\frac{d\beta_1}{dt^*} = \frac{\beta_0-\beta_1}{(1-\varepsilon)\tau^*} + \alpha_1\beta_1 - \kappa_2\beta_1 - \frac{\delta(\beta_1-\beta_2)}{(1-\varepsilon)\tau^*}. \qquad Eq.6$$

Equations in the stagnant region

$$\frac{d\alpha_2}{dt^*} = \frac{\delta(\alpha_1-\alpha_2)}{\varepsilon\tau^*} - \alpha_2\beta_2, \qquad Eq.7$$

$$\frac{d\beta_2}{dt^*} = \frac{\delta(\beta_1-\beta_2)}{\varepsilon\tau^*} + \alpha_2\beta_2 - \kappa_2\beta_2. \qquad Eq.8$$

The non-dimensional concentration of autocatalyst in the feed, $\beta_0 = \frac{b_0}{a_0}$ the non-dimensional decay rate, $\kappa_2 = \frac{k_2}{k_1 a_0}$; and the non-dimensional residence time $\tau^* = \frac{Vk_1a_0}{q}$ are the parameter groups.

2.2 Steady-State Solutions

After obtaining the dimensionless equation, the steady-state solutions need to be introduced. According to [8], a steady-state is a situation in which the system does not undergo any changes. Therefore, the derivatives must equal to zero to find the solutions.

$$\frac{d\alpha_1}{dt} = 0, \frac{d\beta_1}{dt} = 0, \frac{d\alpha_2}{dt} = 0, \frac{d\beta_2}{dt} = 0. \qquad Eq.9$$

Then, there are two steady-state solutions branches for the incomplete mixing in chemostat. The washout solution obtained is

$$(\alpha_1, \beta_1, \alpha_2, \beta_2) = (1,0,1,0). \qquad Eq.10$$

While, the no-washout solution obtained is

$$(\alpha_1, \beta_1, \alpha_2, \beta_2) = (\widehat{\alpha_1}, \widehat{\beta_1}, \widehat{\alpha_2}, \widehat{\beta_2}). \qquad Eq.11$$

Where

$$\widehat{\beta_1} = \frac{\delta\beta_2}{1+\delta+(\kappa_2-\alpha_1)(1-\varepsilon)\tau^*}, \qquad Eq.12$$

$$\widehat{\alpha_2} = \frac{\delta\alpha_1}{\delta+\beta_2\varepsilon\tau^*}, \qquad Eq.13$$

$$\widehat{\beta_2} = \frac{\delta\left[-(\alpha_1-\kappa_2)^2(1-\varepsilon)\varepsilon\tau^{*2} + (\varepsilon+\delta)(\alpha_1-\kappa_2)\tau^* - \delta\right]}{\tau^*\varepsilon\left[-(1-\varepsilon)(\alpha_1-\kappa_2)\varepsilon\kappa_2\tau^{*2} - [(1-\varepsilon)\delta\alpha_1 - \kappa_2(\varepsilon+\delta)]\tau^* + \delta\right]}, \qquad Eq.14$$

The cubic equation obtained for $\widehat{\alpha_1}$ is

$$G(\widehat{\alpha_1}) = A_3{\tau^*}^3{\alpha_1}^3 + A_2{\tau^*}^2{\alpha_1}^2 + A_1\tau^*\alpha_1 + A_0. \qquad Eq.15$$

Where the coefficients A_i are

$$A_3 = (1-\varepsilon)^2\varepsilon[\tau\varepsilon\kappa_2(1+\delta)+\delta],$$

$$A_2 = -(1-\varepsilon)\varepsilon\{(2\kappa_2+3\kappa_2\delta+1)(1-\varepsilon)\varepsilon\kappa_2\tau^2 + [(1-\varepsilon)\delta + 2(1+\delta)\kappa_2(\varepsilon+\delta)]\tau + 2\delta(1+\delta)\},$$

$$A_1 = \varepsilon^2{\kappa_2}^2(1-\varepsilon)^2(2+\kappa_2+3\kappa_2\delta)\tau^3 + \varepsilon\kappa_2(1-\varepsilon)\{5\varepsilon\kappa_2\delta + 2\varepsilon(1+\kappa_2) + 2\varepsilon(1+\kappa_2) + \delta[\kappa_2(1+4\delta)+2]\}\tau^2 + \{\delta\varepsilon(1-\varepsilon)(\delta+2) + [\delta^3 + \varepsilon(3(2-\varepsilon)\delta^2 + (\varepsilon+2)\delta+\varepsilon)]\kappa_2\}\tau + \delta(\delta^2+\varepsilon+2\delta\varepsilon), \qquad Eq.16$$

$$A_0 = -\{\delta\varepsilon\tau^2(1-\varepsilon){\kappa_2}^2 + [\delta(\varepsilon+\delta)+\tau\varepsilon(1-\varepsilon)]\tau\kappa_2 + \varepsilon\tau(1+\delta)+\delta^2\} .\{\delta + [(1-\varepsilon)\varepsilon\kappa_2\tau + \varepsilon + \delta]\tau\kappa_2\}.$$

By using Descartes' Rule of Signs, shows that there are three changes and the series of coefficients of the cubic $G(\alpha_1)$ have one or three positive roots exist. When we assume, $G(-\alpha_1)$, shows that there are no signs changes in the sequence and the equation has no negative roots.

Then, by assuming $G(\alpha_1 = 0) = A_0 < 0$ and substitute $G(\alpha_1 = \kappa_2)$ we obtain

$$G(\alpha_1 = \kappa_2) = -\left\{\varepsilon^2(1+\delta)^2(1-\kappa_2)\kappa_2{\tau^*}^2 + [\varepsilon(1+\delta-\kappa_2)+\kappa_2\delta^2]\delta\tau^* + \delta^3\right\} < 0, \qquad Eq.17$$

as $0 < \kappa_2 < 1$. Substitute $\left(\alpha_1 = \frac{1+\delta}{(1-\varepsilon)\tau} + \kappa_2\right)$ into equation (17) we obtain

$$G\left(\alpha_1 = \frac{1+\delta}{(1-\varepsilon)\tau} + \kappa_2\right) = \delta^4[1+\tau^*\kappa_2(1-\varepsilon)] > 0. \qquad Eq.18$$

Therefore, there is always a solution when

$$\kappa_2 < \alpha_1 < \kappa_2 + \frac{1+\delta}{(1-\varepsilon)\tau^*}. \qquad Eq.19$$

According to [7], they conjecture that when the no-washout solution is physically meaningful it is uniquely defined and it does not seem possible to obtain any more useful results regarding the no-washout solution branch.

2.3 Stability Analysis

The stability of the steady-state solutions needs to be studied to obtain the stability of the mathematical model of incomplete mixing and it is important to explore the dynamical systems of the model. According to [8], the steady-state will be stable provided that the following condition is satisfied. The Jacobian matrix along the washout branch (1,0,1,0) are as follow

$$J(1,0,1,0) = \begin{pmatrix} -\frac{(1+\delta)}{(1-\varepsilon)\tau^*} & -1 & \frac{\delta}{(1-\varepsilon)\tau^*} & 0 \\ \beta_1 & -\frac{(1+\delta)}{(1-\varepsilon)\tau^{*2}} + 1 - \kappa_2 & 0 & \frac{\delta}{(1-\varepsilon)\tau^{*2}} \\ \frac{\delta}{\varepsilon\tau^*} & 0 & -\frac{\delta}{\varepsilon\tau^*} & -1 \\ 0 & \frac{\delta}{\varepsilon\tau^*} & 0 & -\frac{\delta}{\varepsilon\tau^*} + 1 - \kappa_2 \end{pmatrix}. \quad Eq.20$$

The determinant and trace for the Jacobian matrix along the washout branch (1,0,1,0) are as follow

$$|J| = \frac{\delta\left(\varepsilon^2\tau^{*2}{\kappa_2}^2 - \varepsilon\tau^{*2}{\kappa_2}^2 - \delta\kappa_2\tau^{*2} + \varepsilon\kappa_2\tau^{*2} - \varepsilon^2\tau^{*2} - \delta\tau^{*2} + \varepsilon\tau^{*2} - \tau^{*2} + \delta\right)}{(-1+\varepsilon)^2\tau^{*4}\varepsilon^2}. \quad Eq.21$$

$$Trace(J) = -\frac{2(1-\delta)}{(1-\varepsilon)\tau^*} + 2 - 2\kappa_2 - \frac{2\delta}{\varepsilon\tau^*}. \quad Eq.22$$

Since the determinant and trace obtained follows the condition which is the system will be stable provided the trace is always negative and determinant always positive, therefore the system of the Jacobian matrix along the washout branch is stable while the system of the Jacobian matrix along the no-washout branch has no physically meaningful solution.

3. Results and Discussion

3.1 Stability Diagram

The phase plane diagram of the reactant concentration against autocatalysis concentration in highly agitated region and the phase plane diagram of the reactant concentration against autocatalysis concentration in stagnant region will be visualized using Maple. The time series plot of the reactant concentration in highly agitated region (α_1), the autocatalysis reactant concentration in highly agitated region (β_1), the reactant concentration in stagnant region (α_2) and time series plot of the autocatalysis reactant concentration in stagnant region (β_2) also will be plotted using Maple Software.

3.1.1 Phase Plane Analysis

Figure 1 shows the phase plane diagram of the concentration in highly agitated region. It is shown that the arrows approaching the washout point and obtain $(\alpha_1, \beta_1) = (1,0)$ and the graph is in stable node. By using Maple Software, the corresponding eigenvalues for highly agitated region obtained are $\lambda_1 = -0.4565714290$ and $\lambda_2 = -1.428571429$, where both of the eigenvalues is negative. Since the eigenvalues obtain is negative and the graph in a stable node, the washout steady-state for (1,0) is stable.

Figure 2 shows the phase plane diagram of the concentration in stagnant region. Based on the graph, it shows that the graph is in unstable saddle point because the arrow did not approach any point. By using Maple Software, the corresponding eigenvalues obtain for stagnant region are $\lambda_1 = 0$ and $\lambda_2 = 0.927$ respectively. Since both of the eigenvalues are real and always positive, the fixed point at (1,0) for stagnant region is unstable.

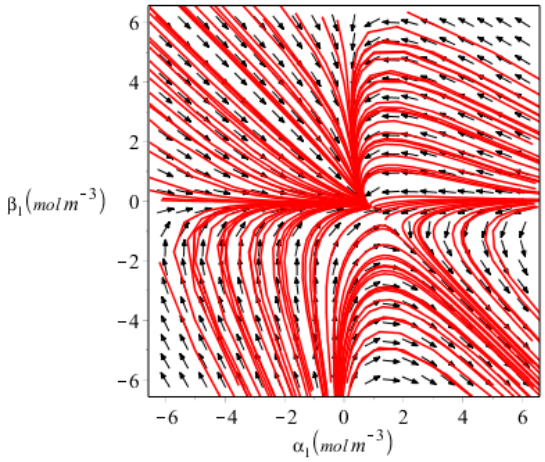

Figure 1: Concentration in Highly Agitated Region

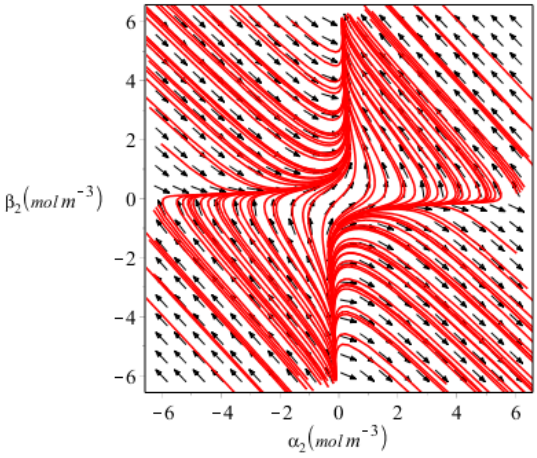

Figure 2: Concentration in Stagnant Region

3.1.2 Time Series Plot

Based on Figure 3, provides a time series plot of the reactant concentration in highly agitated region against residence time. It shows that the reactant concentration in highly agitated region decreases with increasing residence time. The maximum value for the reactant concentration occurs when the residence time is zero which is the concentration of reactant entering the reactor. There is an extreme decrease from $\tau^* = 0$ to $\tau^* = 4$ and become constant at $\alpha_1 = 0.6$, which means that the reactant concentration of the chemical is always decreased through the certain residence time and constant as the reactant concentration is achieved through the infinite residence time.

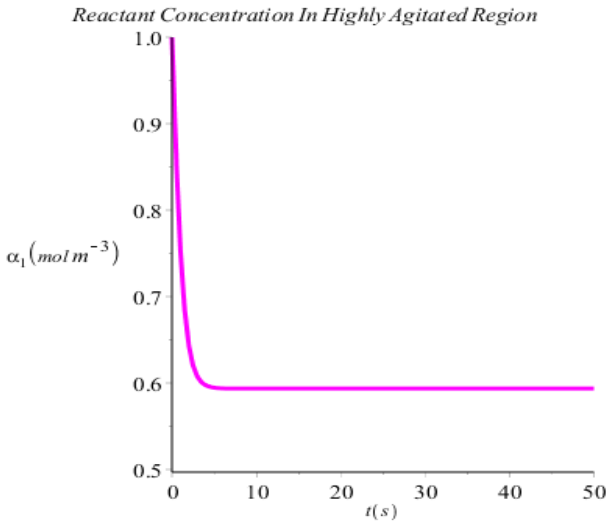

Figure 3: Reactant Concentration in Highly Agitated Region

Figure 4 shows the autocatalysis reactant concentration in the highly agitated region against residence time with initial condition $\kappa_2 = 0.028, \varepsilon = 0.3, \delta = 0.2$ and $\tau^* = 1$. It shows that the autocatalysis reactant concentration in highly agitated region increases with the increase of residence time. The maximum value of the autocatalysis concentration is 0.49 respectively and becomes constant throughout the infinite of residence time. The value of the residence time at the maximum value for the autocatalytic concentration is called the maximum residence time [9]. Therefore, the incomplete mixing

has a larger effect upon the required value of the residence time rather than the maximum value of the autocatalyst.

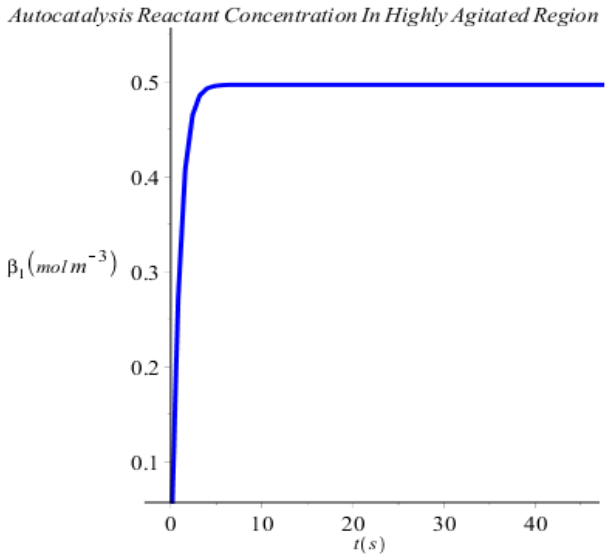

Figure 4: Autocatalysis Concentration in Highly Agitated Region

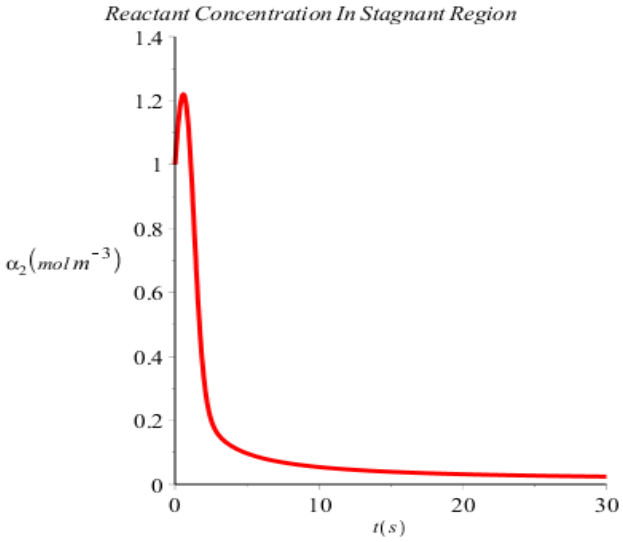

Figure 5: Reactant Concentration in Stagnant Region

For Figure 5, the reactant concentration in stagnant region slightly increases from $\tau^* = 0$ to $\tau^* = 0.55$ and become decreases with the increase of the residence time. The maximum value for reactant concentration in stagnant region is 1.21 respectively with the values of 0.55 for residence time. This shows that the maximum values of reactant concentration in stagnant region slightly affect the residence time. Based on Figure 6, shows that the time series plot of autocatalyst concentration against residence time with initial values $\kappa_2 = 0.028, \varepsilon = 0.3, \delta = 0.2$ and $\tau^* = 1$. The trend of the graph is increasing from $\tau^* = 0$ to $\tau^* = 350$ and constant at $\beta_2 = 47$ throughout the residence time. It means that when the concentration of autocatalyst increase the residence time become increase.

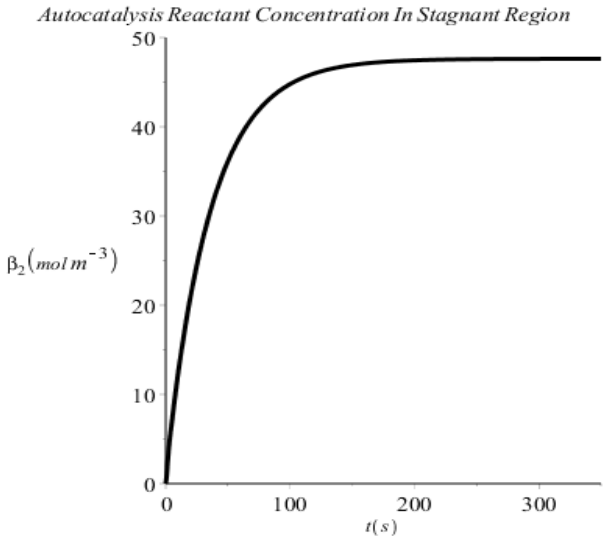

Figure 6: Autocatalysis Concentration in Stagnant Region

3.2 Steady-State Diagram

The steady-state diagrams for dimensionless reactant concentration for imperfect mixing in highly agitated and in stagnant region are plotted with different values of size of the stagnant regions. The values are $\varepsilon = 0.3, \varepsilon = 0.2, \varepsilon = 0.1$ with a same initial condition which are $\kappa_2 = 0.028, \delta = 0.2$ and $\tau^* = 1$.

3.2.1 Reactant Concentration in Highly Agitated Region

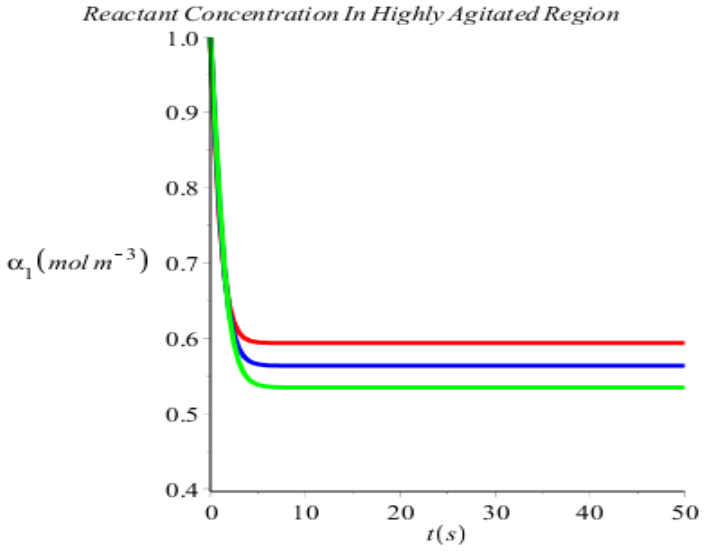

Figure 7: Steady-state diagram of reactant concentration in highly agitated region

Based on Figure 7, shows the steady state curve for the dimensionless reactant concentration as a function of the dimensionless residence time. We consider three different values for the size of the stagnant region from [7] which is $\varepsilon = 0.3$ (red line), $\varepsilon = 0.2$ (blue line) and $\varepsilon = 0.1$ (green line). From the graph we will obtain the critical value for the residence time that occurs when the size of stagnant region is sufficiently small. For $\varepsilon = 0.3$, we obtain $(\tau^*, \alpha_1) = (4.5,0.54)$. For $\varepsilon = 0.2$, we obtain $(\tau^*, \alpha_1) = (4.0,0.57)$ and for $\varepsilon = 0.1$, we obtain $(\tau^*, \alpha_1) = (3.5,0.60)$. As the value of size of the region

decrease, the residence time becomes increase. It shows that the effects of incomplete mixing are greater at lower reactant concentration.

3.2.2 AutocatalyticReactant Concentration in Highly Agitated Region

Figure 8 shows the steady-state curve for the dimensionless autocatalysis reactant concentration as a function of the dimensionless residence time. We consider three values for the size of the stagnant region which is $\varepsilon = 0.3$ (red line), $\varepsilon = 0.2$ (blue line) and $\varepsilon = 0.1$ (green line). From the graph, we will obtain that there is a maximum value for the residence time that occurs when the size of stagnant region is sufficiently small. For $\varepsilon = 0.3$, we obtain $(\tau^*, \alpha_1) = (3.5,0.49)$. For $\varepsilon = 0.2$, we obtain $(\tau^*, \alpha_1) = (4.0,0.52)$ and for $\varepsilon = 0.1$, we obtain $(\tau^*, \alpha_1) = (5.0,0.55)$. When the size of stagnant region increase, the reactant concentration becomes increase throughout the residence time.

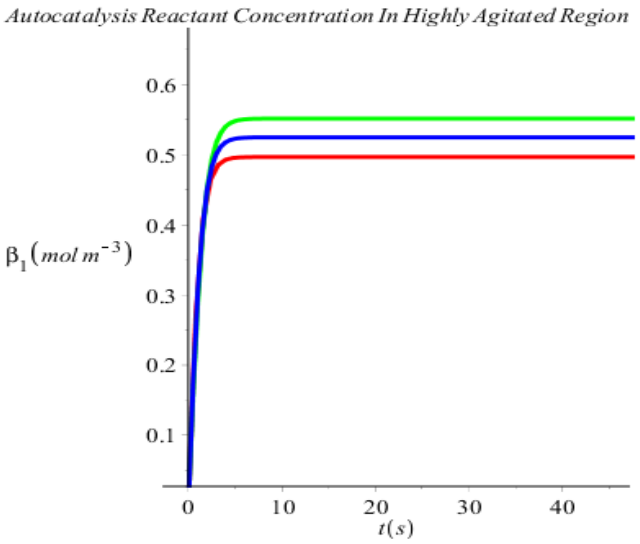

Figure 8: Steady-state diagram of autocatalysis reactant concentration in highly agitated region

4. Conclusion

In this paper, the stability analysis was conducted to investigate the mathematical model of incomplete mixing in chemostat.The dimensionless equations, steady-states, Jacobian Matrix, trace, and determinant are used to study the chemostat model with incomplete mixing.The obtained washout from the system is stable while the no-washout solution has no physically meaningful. The effect of size of stagnant region towards the steady-state is also discussed in this paper.The stability diagrams such as phase plane, time series plot and steady-state diagrams are visualized using Maple Software.

For future study, it is suggested that when investigating the mathematical modeling of incomplete mixing in Continuous Stirred Tank Reactor (CSTR), other factors such as the flow rate, volume of the reactor, the mixing parameter, the initial of the reactant concentration, the reactant concentration, and the autocatalyst concentration should be considered. This is because these characteristics are important factors that influence the formation and stabilization of the model in incomplete mixing chemostat.

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