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Optimal design of multistage chemostats in series using different microbial growth kinetics

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Abstract
In this paper, the optimum design of multistage chemostats (CSTRs) was investigated. The optimal design was based on the minimum overall reactor volume using different volume for each chemostat. The paper investigates three different microbial growth kinetics; Monod kinetics, Contois kinetics and the Logistic equation. The total dimensionless residence time (θ_{Total}) was set as the optimization objective function that was minimized by varying the intermediate dimensionless substrate concentration (α_i). The effect of inlet substrate concentration (S_0) to the first reactor on the optimized total dimensionless residence time was investigated at a constant conversion of 0.90. In addition, the effect of conversion on the optimized total dimensionless residence time was also investigated at constant inlet substrate concentration (S_0). For each case, optimization was done using up to five chemostats in series.

Keywords: Monod kinetics; Contois kinetics; Logistic kinetics; Chemostat.

1. Introduction

A chemostat is a simple continuous-flow apparatus used to study the growth of microorganisms and substrate consumption in an environment cultured by microorganisms [1]. Compared to the batch cultivation devices, chemostats are continuous culture devices in which growth and product formation can be maintained for prolonged periods. However, in some fermentation processes, particularly for secondary metabolite production, the growth and product formation phases need to be separated, as optimal conditions for each step are different. Conditions such as temperature, pH, and limiting nutrients may be varied in each stage, resulting in different cell physiology and cellular products in multi-stage chemostats [2]. As a result, optimization of chemostats in series is important to ensure proper microbial growth, product formation, and substrate consumption.

Multistage chemostats are also commonly used in biological waste water treatment [3]. However, the use of multistage chemostats in series requires optimal design. Multiple chemostats in series can be optimized by minimizing the total reactor volume required. Usually, a system of CSTRs in series approaches PFR behavior when the number of reactors is large (five or more) [2]. As a result, in this study, the number of chemostats in series was limited to five.

The objective of this paper is to optimize a system of N-CSTRs in series using three different microbial growth kinetics, namely, Monod, Contois, and the Logistic kinetics. The optimal design is based on the minimum overall reactor volume (dimensionless residence time) required for a certain degree of substrate conversion and the total number of reactors. The optimization parameters used are the intermediate substrate concentrations. Moreover, the paper also highlights the effect of inlet substrate

concentration (S_0), the conversion (X) and the number of reactors (N) on the total dimensionless residence time.

2. Theory

The general form of the specific growth rate for the three growth kinetics used in this study is given by the following equation:

$$\mu = \mu_{\max} \frac{d\,S + e\,S^2}{a + b\,S + C\,S^2} \tag{1}$$

where, S is the substrate concentration (g/L), μ_{max} is the maximum specific growth rate (h^{-1}). The values of a, b, c, d, and e vary depending on the type of growth kinetic equation. The following table shows the values of a, b, c, d, and e for three growth kinetics used in this study. In Table 1, $Y_{X/S}$ is the yield coefficient (g cell/g substrate), K_S is the saturation constant, S_0 is the inlet substrate concentration (g/L) to the first chemostat, and X_m is the maximum concentration (g/L) of the cells that corresponds to the cell concentration when the substrate is fully consumed.

Table 1. Kinetic constants for equation 1

	Monod Kinetics	Contois Kinetics	Logistic Equation
a	K_S	$K_S Y_{X/S} S_0$	0
b	1	$1 - K_S Y_{X/S}$	1
c	0	0	0
d	1	1	$1 - \frac{Y_{X/S} S_0}{X_m}$
e	0	0	$\frac{Y_{X/S}}{X_m}$

The maximum concentration of the cells (X_m) is given by the following equation:

$$X_m = Y_{X/S} S_0 + X_0 \tag{2}$$

Table 2 shows the values of the kinetics and stoichiometric coefficients used in the optimization procedure.

Table 2. Constants, kinetic parameters and the stoichiometric coefficients

K_S (Saturation Constant)	0.2 g/L
X_0 (Inlet Cell Concentration)	0.1 g/L
$Y_{X/S}$ (Yield Coefficient)	0.5 g/g

3. Optimization methodology

Figure 1 shows a schematic diagram of N chemostats (CSTRs) in series that needs to be optimized in order to achieve minimum total volume.

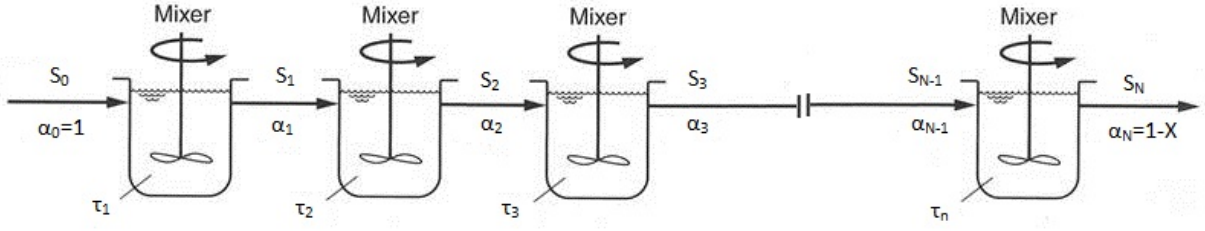

Figure 1. N chemostats in series

A substrate balance around the CSTR *i* gives the following equation:

$$FS_{i-1} - FS_i - \frac{V_{R,i}\mu_i X_i}{Y_{X/S}} = \frac{dS}{dt} \tag{3}$$

where, F is the feed volumetric flow rate (L/h), S_{i-1} and S_i are the substrate concentrations in and out of the CSTR respectively, and $V_{R,i}$ is the culture volume (L) of the CSTR *i*.
At steady state, equation 3 becomes the following:

$$\tau_i = \frac{S_{i-1} - S_i}{\mu_i \frac{X_i}{Y_{X/S}}} \tag{4}$$

where, τ_i is the residence time (h) given by the following equation:

$$\tau_i = \frac{V_{R,i}}{F} \tag{5}$$

Substituting equation 1 in to 5, we get the following:

$$\tau_i = \frac{S_{i-1} - S_i}{\mu_i \frac{X_i}{Y_{X/S}}} = \frac{(S_{i-1} - S_i)\, Y_{X/S}}{\mu_{max}\left(\frac{dS + eS^2}{a + bS + CS^2}\right) X_i} \tag{6}$$

In terms of dimensionless variables, the dimensionless residence time (θi) is given by the following equation:

$$\theta_i = \frac{(\alpha_{i-1} - \alpha_i)\left(a^* + b\alpha_i + c^*\alpha_i^{\,2}\right)}{\left(d\alpha_i + e^*\alpha_i^{\,2}\right)(A - \alpha_i)} \qquad i = 1, 2, 3, ... \tag{7}$$

where,

$$\theta_i = \tau_i \mu_{max} \tag{8}$$

$$\alpha_i = \frac{S_i}{S_0} \tag{9}$$

$$\alpha_{i-1} = \frac{S_{i-1}}{S_0} \tag{10}$$

$$a^* = \frac{a}{S_0} \tag{11}$$

$$c^* = cS_0 \tag{12}$$

$$e^* = eS_0 \tag{13}$$

$$A = \left[\frac{X_0}{Y_{X/S}S_0} + 1\right] \tag{14}$$

In equation 7, the dimensionless substrate concentrations (α_i) can be varied to obtain the minimum optimum total volume of the N CSTRs. Thus, the objective function is as follows:

$$\text{Objective Function} = \min\left(\sum_{i=1}^{N}\theta_i\right) = \min\left(\theta_{Total}\right) \tag{15}$$

Since, α_1=1 is fixed and α_N can be obtained from conversion (α_N=1-X), the variables to minimize the objective function are the following: $\text{Variables} = \alpha_i$, for $i = 2$ to $N-1$

Therefore, the optimization algorithm becomes the following:

$$\text{Find } \min\left(\sum_{i=1}^{N}\theta_i\right) \text{ by changing } \alpha_2, \alpha_3, ..., \alpha_{N-1} \tag{16}$$

Thus, to minimize the total volume for the N CSTRs in series, the total dimensionless residence time of the N CSTRs (θ_{Total}) can be minimized by varying the intermediate dimensionless substrate concentrations (α_i). In this study, optimization was done using Microsoft Excel's built-in Solver to find the optimum values of the intermediate dimensionless substrate concentrations.

4. Results and discussion

Figure 2 shows the optimized total dimensionless residence time as a function of number of CSTRs and the inlet substrate concentration S_0 for the case of Monod kinetics. The conversion was fixed at 0.90. As depicted in Figure 2, as S_0 increases (keeping the conversion and the number of CSTRs constant), θ_{Total} decreases. This means that less volume is required to achieve a certain conversion when a higher inlet substrate concentration is used for a given number of CSTRs in case of Monod kinetics.

Furthermore, keeping S_0 constant, more volume is required to achieve a certain conversion as fewer reactors are used in series. For Monod kinetics given by equation (1), it is beneficial to use more CSTRs in series since less total volume will be required. Moreover, high substrate inlet concentration S_0 must be used since the total reactor volume required will be smaller. Thus, for Monod kinetics, using higher inlet substrate concentration S_0 and using multiple reactors is preferred.

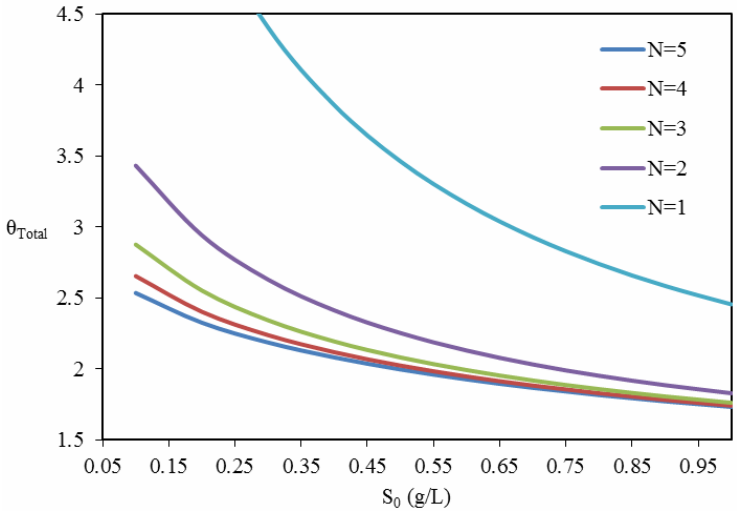

Figure 2. Variation of θ_{Total} with S_0 for Monod Kinetics, final conversion X = 0.90

Figures 3 and 4 show typical behavior that as the conversion is required, the volume of reactor required will be higher (both for S_0=0.1 and S_0=1 g/L). These figures again highlight the fact that using multiple reactors is better for Monod kinetics. As more reactors are added, the total volume required to achieve a given conversion decreases.

Figure 5 shows the optimized total dimensionless residence time as a function of number of CSTRs and the inlet substrate concentration S_0 for the case of Contois kinetics. Also, in this case, the conversion was fixed at 0.90. However, the trends observed for Contois kinetics was opposite to that of Monod kinetics.

For Contois kinetics, as depicted in Figure 5, as the inlet substrate concentration S_0 is increased, the required reactor volume also increases. However, as more reactors are added, the total required volume decreased. Switching from a single CSTR to two CSTRs in series, there is significant change in the total reactor volume required. However, using four or five reactors in series doesn't show a significant reduction in total reactor volume. Therefore, for Contois kinetics, for a conversion of 0.90, it is better to use low inlet substrate concentration S_0 and three reactors in series. Adding the fourth and the fifth reactor has no significant effect on the reduction in total reactor volume.

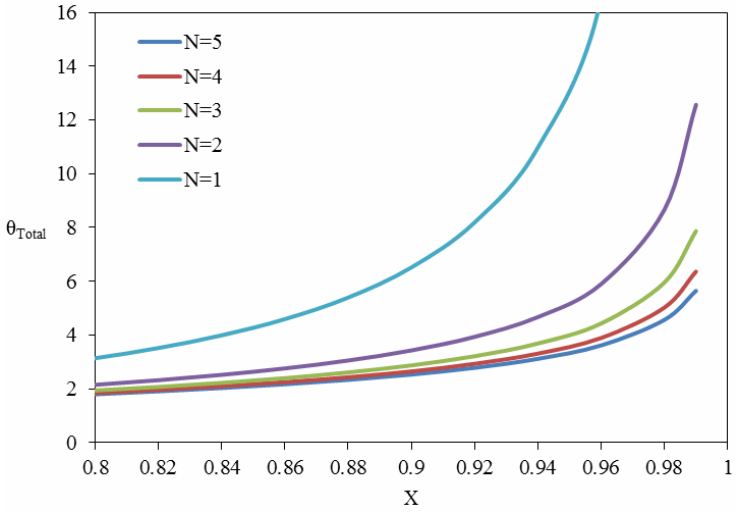

Figure 3. Variation of θ_{Total} with conversion for Monod Kinetics, S_0 = 0.1 g/L

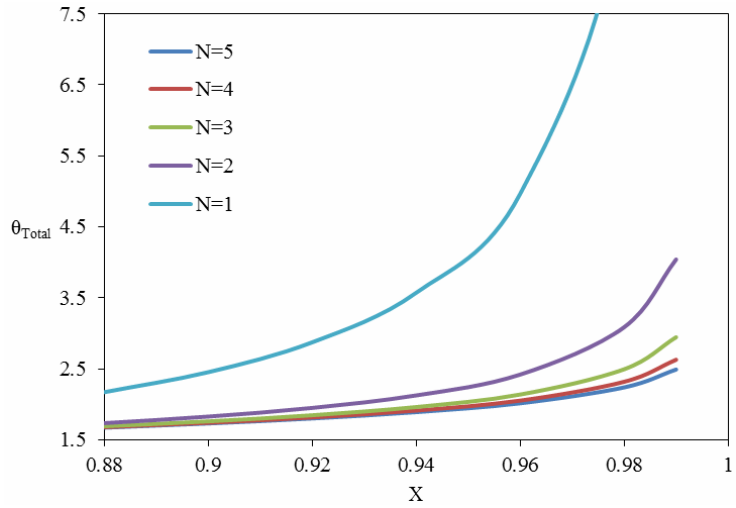

Figure 4. Variation of θ_{Total} with conversion for Monod Kinetics, S_0 = 1 g/L

Figures 6 and 7 show the variation of total dimensionless residence time with the level of conversion achieved at two different inlet substrate concentrations (S_0=0.1 and 0.5 g/L respectively) for Contois kinetics. Again, these figures show that using multiple reactors is also better in case of Contois kinetics. As more rectors are added, the total volume required to achieve a given conversion level increases.

Figure 8 shows the optimized total dimensionless residence time as a function of number of CSTRs and the inlet substrate concentration S_0 for the case when kinetics are described by the Logistic equation. The results obtained were similar to the case of Contois kinetics. That is, as the inlet substrate concentration is increased, more reactor volume is required to achieve a given conversion level. Also, using multiple reactors was found to be beneficial. Thus, for Logistic kinetics, it is beneficial to use lower inlet substrate concentration and multiple reactors.

Figures 9 and 10 show the variation of total dimensionless residence time with the level of conversion achieved at two different inlet substrate concentrations (S_0=10 and 5 g/L respectively) for the Logistic equation. Similar results can be observed as in the case of Monod and Contois kinetics, that is, as more

rectors are added, the total volume required to achieve a given conversion level increases. Also, more total reactor volume is required to achieve higher conversion levels.

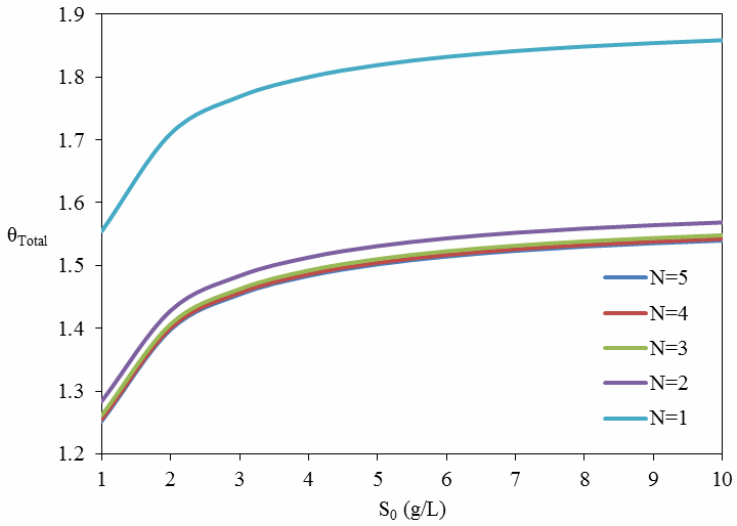

Figure 5. Variation of θ_{Total} with S_0 for Contois Kinetics, final conversion X = 0.90

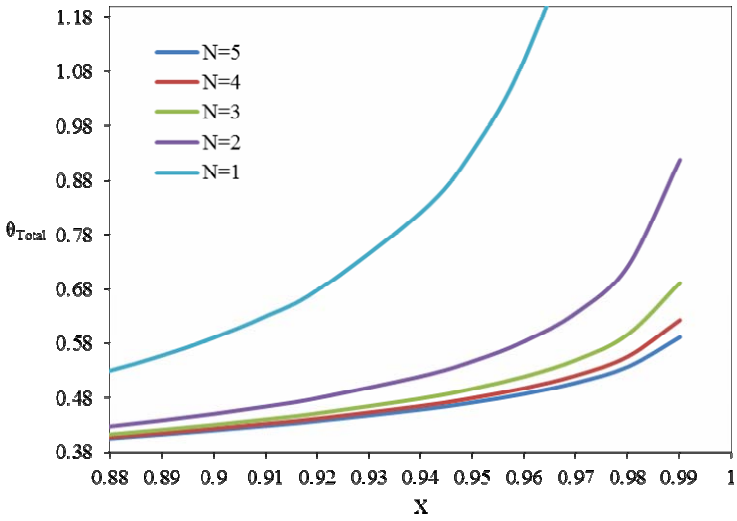

Figure 6. Variation of θ_{Total} with conversion for Contois Kinetics, S_0 = 0.1 g/L

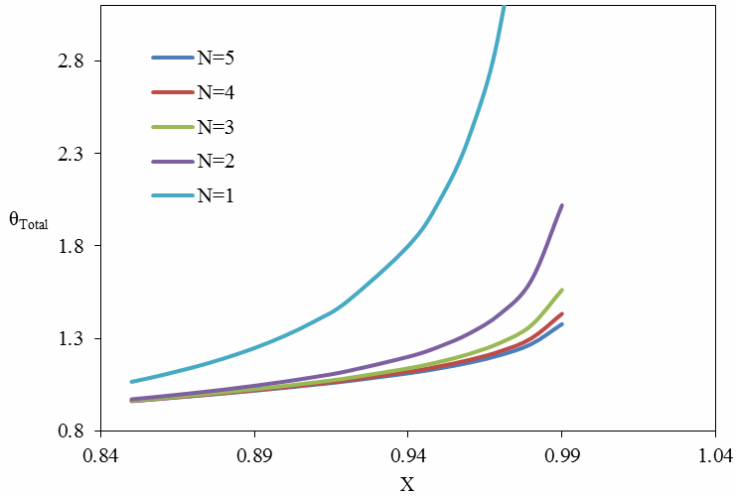

Figure 7. Variation of θ_{Total} with conversion for Contois Kinetics, S_0 = 0.5 g/L

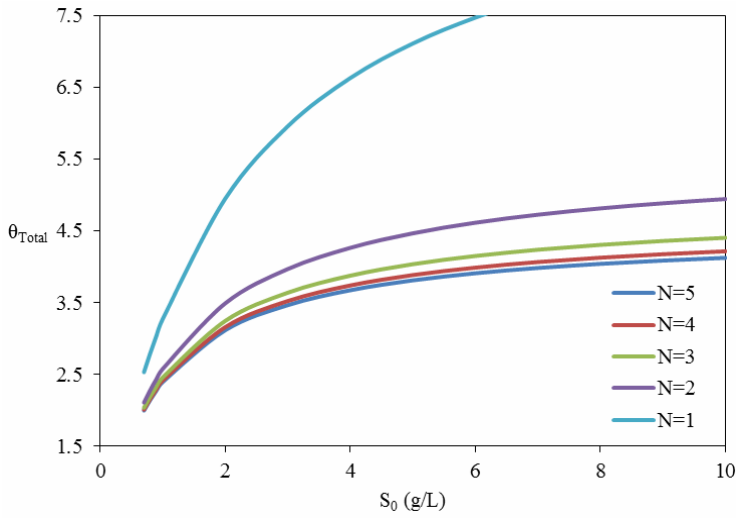

Figure 8. Variation of θ_{Total} with S_0 for Logistic Equation, final conversion X = 0.90

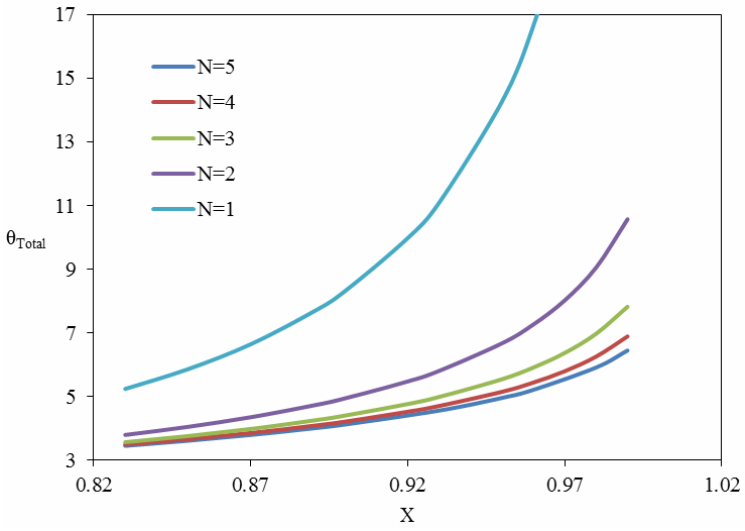

Figure 9. Variation of θ_{Total} with conversion for Logistic Equation, S_0 = 10 g/L

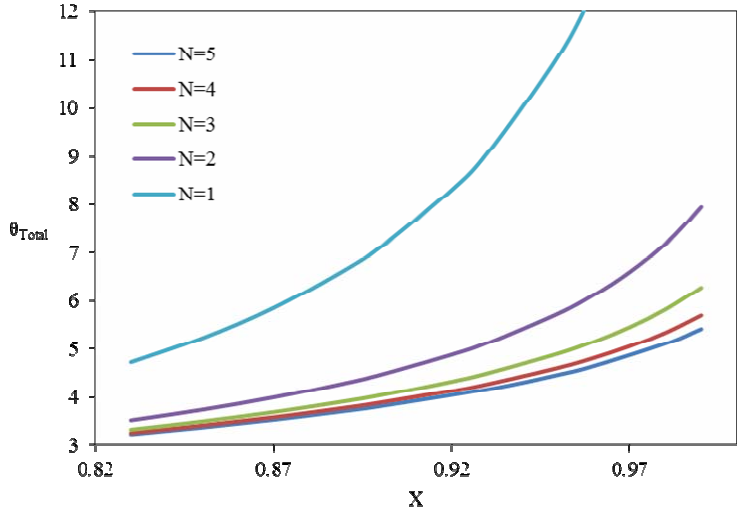

Figure 10. Variation of θ_{Total} with conversion for Logistic Equation, S_0 = 5 g/L

5. Conclusion

In this study, a system of N-CSTRs was optimized successfully by minimizing the total reactor volume using unequal volumes for each reactor. It was found that for the case of Monod, Contois, and Logistic kinetics, it was beneficial to use multiple reactors. For Monod kinetics, increasing S_0 decreases the total reactor volume required at a given number of reactors and conversion. However, for Contois and Logistic kinetics, more volume is required on increasing S_0. Therefore, the optimization results always depend on the type of kinetics used. For microbial cells following the Monod kinetics, using higher inlet substrate concentration S_0 and using multiple reactors is preferred. In case of kinetics described by Contois and Logistic equation, lower inlet substrate concentration S_0 is preferred. The optimal design of chemostats in series depends on the growth kinetics of the microbial cells employed.

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