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Chemical Engineering Department, Qatar University, P.O. Box 2713 Doha, Oatar

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Applications of Matlab optimization capabilities in the design of N-continuous stirred tank bioreactors connected in series

Ibrahim M. Abu-Reesh

ABSTRACT

The optimal design (variable volume) of continuous stirred tank reactors (CSTR's), in series, performing biological conversion of organic materials, was derived. The optimal design was based on the minimum overall reactor volume required for a certain degree of substrate conversion, and the number of reactors. In this study, it was assumed that cell growth kinetics follows the Contois model with endogenous decay. This unstructured kinetic model has been used by many researchers to describe biodegradation of organic materials, especially in the food industries and industrial wastewater treatment. The optimization problem was formulated as a nonlinear constrained mathematical programming problem, and solved using the Matlab function *"fmincon"*. The effect of operating parameters such as; substrate concentration in the feed to the first reactor, substrate conversion, and number of CSTR's in series for the optimum design was investigated. Using the optimum design is beneficial only at high substrate conversion. The substrate concentration in the feed to the first reactor has little effect on the total required reactor volume. Up to 5 CSTRs in series were used in this study.

Keywords: CSTRs in series, Matlab fmincon, bioreactor optimization, Contois model, constrained optimization

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1. INTRODUCTION

CSTR's in series are commonly used to achieve biological conversion in the treatment of industrial wastewater, using cascade-connected activated sludge basins. This arrangement of reactors offers a number of advantages for the biological degradation of wastewater, including an increased stability to the treatment plant when subjected to a pulse load of toxic materials, and also an enhanced degree of biodegradation by an adopted activated sludge recycle. Most studies have used the Monod kinetic equation to describe the dependence of a specific growth rate on the limiting substrate concentration. In recent years, the Contois model¹ has been used to describe the biodegradation of organic materials, especially in the food industries and for industrial wastewater treatment.²⁻⁴ In this study, kinetic constants were used for anaerobic digestion of ice-cream wastewater.⁵ A number of investigators have studied the optimum design of CSTR's in series performing different cell growth and enzyme kinetics.⁶⁻⁹ The objective of this work is to determine the optimum design of N-continuously stirred tank reactors in series, performing biological conversion of organic materials using the Contois model with decay term. The optimal design was based on the minimum overall reactor volume required for a certain degree of substrate conversion, and the number of reactors. The effect of biomass recycle, substrate conversion and concentration in the feed to the first reactor on the optimum design was determined.

2. METHODOLOGY

For N-CSTRs in series, substrate balance on the ith reactor assuming steady state, well-mixed reactors and Contois kinetics with cell death, the mean residence time in the ith reactor is given by:

$$\tau_{i} = \left[\frac{(S_{i-1} - S_{i})Y_{x}}{\mu_{\max}(X_{o} + Y_{x}(S_{o} - S_{i}))\left(\frac{S_{i}}{BX_{o} + BY_{x}(S_{o} - S_{i}) + S_{i}} - \frac{k_{d}}{\mu_{\max}}\right)}\right] \quad i = 1, 2, ..., N$$
(1)

Using dimensionless variables. The dimensionless residence time θ_i is given by:

$$\theta_{i} = \frac{(\alpha_{i-1} - \alpha_{i})}{(A - \alpha_{i})} \left[\frac{k_{x}^{\star}(A - \alpha_{i}) + \alpha_{i}}{\alpha_{i} - [k_{x}^{\star}(A - \alpha_{i}) + \alpha_{i}]K_{d}^{\star}} \right] \quad i = 1, 2, ..., N$$

$$(2)$$

Where $\alpha_i = \frac{S_i}{S_o}$, $k_x^* = BY_x$, $k_d^* = \frac{k_d}{\mu_{\max}}$, $\theta_i = \mu_{\max} \tau_i$, $A = \frac{X_o}{Y_x S_o} + 1$

The objective function of this optimization problem is to minimize the total dimensionless residence time. The numerical optimization was carried out using the Matlab function "*fmincon*". The optimization problem consists of

Ainimize
$$\theta_{tot} = \sum_{i=1}^{N} \theta_i$$
 (3)

Subject to
$$\theta_i = \frac{(\alpha_{i-1} - \alpha_i)}{(A - \alpha_i)} \left[\frac{k_x^*(A - \alpha_i) + \alpha_i}{\alpha_i - [k_x^*(A - \alpha_i) + \alpha_i]K_d^*} \right]$$
 $i = 1, 2, ..., N$ (4)

Constrains
$$\alpha_0 \rangle \alpha_1 \rangle \dots \rangle \alpha_{N-1} \rangle \alpha_N$$
 $i = 1, 2, \dots, N$ (5)
 $\alpha_0 = 1, \ \alpha_N = 1 - \delta$

3. RESULTS

From the design equations above, it is clear that the optimum configuration of N CSTRs in series depends on the substrate conversion, the inlet substrate concentration to the first reactor (for biomass recycle only), and the number of reactors in series. For no cell recycle, ($X_0 = 0$), Figure 1a

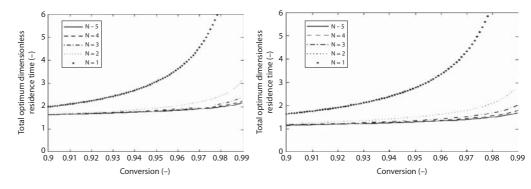


Figure 1. Effect of substrate conversion on the total optimum dimensionless residence time, So = o.1g/l No biomass recycle (a. left). Xo = o.01g/l (b. Right).

shows the effect of substrate conversion on the total optimum dimensionless residence time. It is clear that at high conversion, the higher the conversion, the higher the residence time needed to achieve this conversion. Also increasing the number of reactors has an advantage only at high substrate conversions. At low substrate conversion (data not shown), all reactors have almost similar residence time. At low conversion, the optimum configuration is one CSTR. With biomass recycle and $S_o = 0.1g/l$, similar trend was obtained (Figure 1b, $X_o = 0.01g/l$), It is clear from the Figures 1a, and b that increasing the biomass recycle reduces the residence time required to achieve substrate conversion. Figures 2a and 2b show the effect of inlet substrate concentration in the feed to the first reactor on the total optimum dimensionless residence time using 99% substrate conversion. With no biomass recycle (Figure 2a), the total optimum dimensionless residence time is independent of the inlet substrate concentration. With cell recycle, the total optimum dimensionless residence time is both Figures 2a and 2b, that at this high substrate conversion (99%), using multi-stage reactors is beneficial, compared to one CSTR, and two or three reactors are recommended for this case.

4. CONCLUSIONS

The optimum design for N-continuous stirred tank reactors in series performing biological conversion was determined assuming Contois kinetics with endogenous decay. The Matlab function "*fmincon*" was used to solve the nonlinear constrained optimization problem. Using multi-stage reactors is beneficial only at high substrate conversion. The inlet substrate concentration to the first reactor has little effect on the total optimum dimensionless residence time. Increasing the inlet substrate concentration to the first reactor increases the residence time. Up to five reactors in series were used in this study.

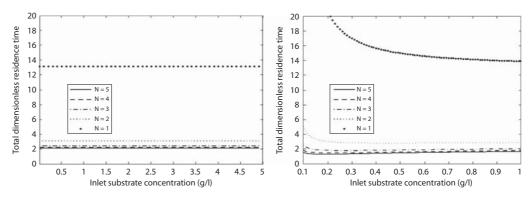


Figure 2. Effect of inlet substrate concentration in the feed to the first reactor on the total optimum dimensionless residence time (99% conversion). No biomass recycle (a. left). Xo = o. 1g/l, (b. Right).

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