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Abstract

We investigate a model for the production of ethanol through continuous fermentation using *Saccharomyces cerevisiae* in a single reactor and cascades of up to five reactors. Using path-following methods we investigate how the ethanol productivity varies with the residence time in each reactor of the cascade. With a substrate feed concentration of 160 g/l we find the optimal productivity is 3.80 g/l/h, 5.08 g/l/h, and 5.18 g/l/h in a single reactor, a double reactor cascade and a triple reactor cascade respectively. For the case of a cascade containing reactors of equal size we investigate reactor configurations of up to five reactors and find that the maximum productivity is obtained in a cascade containing three reactors.

KEYWORDS: ethanol, modelling, productivity, reactor cascade

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1 Introduction

The interest in biofuels has increased markedly since the Kyoto Protocol, where many industrialized countries agreed to reduce their carbon dioxide emissions and greenhouse gas production. Biofuels are not only environmentally friendly, but also have the potential to greatly reduce reliance on imported oil. One of the most promising biofuels is ethanol, which can be derived from renewable sources such as lignocellulosic waste/materials (Ward and Singh, 2002).

Ethanol has a number of attractive features as a fuel and ethanol blends are increasingly being used worldwide; more than 10 percent of all gasoline sold in the US in 2002 contained ethanol (United Sates Environmental Protection Agency, 2002). It is a much cleaner fuel than gasoline, being biodegradable without having harmful effects on the environment. It provides high octane at low cost, acting as an alternative to harmful fuel additives; ethanol blends can be used in gasoline engines without modifications. Ethanol's high oxygen content reduces carbon monoxide levels by 25-30% according to the US EPA and dramatically reduces emissions of hydrocarbons, a major contributor to the depletion of the ozone layer. Many car manufacturing companies (GM, Ford, Chrysler, Toyota, Honda) are now developing hybrid vehicle that run on an ethanol mix. The largest national ethanol fuel industries in the world exist in Brazil (Reel, 2006), where almost 50% of all cars are able to use 100% ethanol fuels and gasoline sold contains at least 20% ethanol. In the US the Energy Independence and Security Act of 2007 (EISA) required the use of 16 billion gallons of cellulosic biofuels by 2022 (U.S. Department of Energy, 2008). According to a study by the U.S. Department of Agriculture bioethanol generates 35% more energy than it takes to produce (Shapouri et al 2002). In addition, it is a renewable fuel as it may be made from plants.

The model used in this paper was developed by Jarzebski (1992) to explain oscillations observed during the continuous production of ethanol using cultures of *Saccharomyces cerevisiae*. This extended an earlier model proposed by Ghommidh et al (1989) which accounted for oscillations observed during continuous fermentation using *Zymononas mobilis*. Features of the model are described further in sections 1.1 & 2.1. Jarzebski estimated biochemical parameter values for this model using laboratory data obtained from the continuous fermentation of sugar-cane molasses at a temperature of 37^o C reported by Perego et al (1985).

Jarzebski (1992) analyzed the model using a selection of flow rates and substrate concentration in the feed using direct numerical integration. In Watt et al (2007) path following methods were used to investigate the dynamic behaviour of the model in more detail, identifying conditions for which periodic solutions occurred and establishing that the model exhibits a period-doubling route to chaos.

Our emphasis in this paper is to compare the productivity that can be obtained in a single reactor against that obtained in a cascade. Here we investigate reactor configurations of upto five reactors. Path following is a natural tool to investigate the productivity of a single reactor as a function of the residence time in the reactor. When investigating the behaviour of a cascade we fix the total residence time of the cascade and then consider two scenarios. In one scenario, the 'constrained' case, the residence time in each reactor takes the same value. Path-following is, again, the natural tool to use to investigate the productivity of a constrained reactor as a function of the total residence time in the cascade. The other scenario is the 'unconstrained' case, in which the residence time in each reactor can essentially take any value. Here we pose two questions.

1. For a given total residence time, which combination of residence times within each reactor in the cascade will result in the optimal ethanol productivity?
2. Does the graph of optimal ethanol productivity as a function of total residence time have a global maximum?

In general, these questions must be answered using the tools of optimization; the stability of the solution obtained in this way must still be determined. However, path-following techniques can be readily used for two scenarios. These are, firstly, a cascade containing either two reactors of unequal size and, secondly, a cascade containing n reactors of equal size.

In section 2 we investigate the performance of a single reactor. We find that, over a range of feed concentration, the reactor productivity is practically constant. We investigate cascades of two and three reactors in sections 3.2 & 3.3 respectively.

Steady-state diagrams were obtained using the path-following software AUTO (Doedel et al 1997). In these figures, the standard notation is used: solid and dashed lines represent stable and unstable steady states respectively, squares are Hopf points (i.e. points where oscillatory solution branches emanate from the steady state solution) and open and solid circles represent unstable and stable periodic solutions respectively. For periodic solutions, the measure chosen is the solution averaged, or integrated, over one period of oscillation.

1.1 Biochemical model

We use the biochemical mechanism for the production of ethanol given in (Jarzebski, 1992). The cell populations are broken into three groups: viable cells (X_v),

non-viable cells (X_{nv}) and dead cells (X_d). Non-viable cells are non-growing, but retain the ability to produce ethanol. The biological reactions are:

$$\begin{aligned} S &\rightarrow P, \\ X_v &\rightarrow 2X_v, \\ X_v &\rightarrow X_{nv}, \\ X_v &\rightarrow X_d, \\ X_{nv} &\rightarrow X_d, \end{aligned}$$

where S and P represent the substrate and ethanol respectively. The reaction rates for these processes, which are given in section 2.1, includes both substrate limitation and product inhibition.

2 Single reactor

In this section we investigate the behaviour of a single reactor. The model equations are given in section 2.1. In section 2.2 we establish a critical value of the residence time, such that if the residence time is smaller (larger) than this value then the washout solution is stable (unstable). In section 2.3 we obtained steady-state diagrams showing the system behaviour as a function of the residence time for various feed concentrations.

2.1 Governing equations

It is assumed that the tank is well mixed, that there is only substrate in the feed and that there is no recycle. The model equations are:

$$V\frac{dX_v}{dt} = -FX_v + V(\mu_v - \mu_{nv} - \mu_d)X_v, \tag{1}$$

$$V\frac{dX_{nv}}{dt} = -FX_{nv} + V(\mu_{nv}X_v - \mu_d X_{nv}), \tag{2}$$

$$V\frac{dX_d}{dt} = -FX_d + V\mu_d(X_v + X_{nv}), \tag{3}$$

$$V\frac{dP}{dt} = -FP + V\left(\frac{\mu_v X_v}{Y_{x|p}} + m_p X_{nv}\right), \tag{4}$$

$$V\frac{dS}{dt} = F(S_0 - S) - V\left(\frac{\mu_v X_v}{Y_{x|s}} + m_s X_{nv}\right), \tag{5}$$

where F is the flow rate into the tank, V is the volume of the tank, m is the maintenance factor, Y is the yield coefficient and S_0 is the substrate concentration in the feed. All other parameters are defined in the nomenclature. Note that the maintenance terms (involving m_p and m_s in (4) and (5)) do not appear in (2) as this process does not consume or produce non-viable cells. The formulation of the growth rates includes both substrate limitation and product inhibition:

$$\begin{aligned}
\mu_v &= \mu_{max}\frac{S}{K_1+S}\left(1-\frac{P}{P_c}\frac{S}{K_2+S}\right),\\
\mu_d &= -\mu_{max}\frac{S}{K_1+S}\left(1-\frac{P}{P_c}\frac{S}{K_2+S}\right),\\
\mu_{nv} &= \mu'_{max}\frac{S}{K_1+S}\left(1-\frac{P}{P'_c}\frac{S}{K_2+S}\right)-\mu_v.
\end{aligned}$$

All reaction rates are assumed to be non-negative. If the concentrations of the chemical species are such that a reaction rate is negative, that rate is then reset to zero (Ghommidh et al, 1989).

We investigate the steady-state behaviour of the system (1)–(5) and the reactor productivity, (Pr), defined by

$$Pr = \frac{P}{\tau},$$

as a function of the residence time ($\tau = V/F$) and the substrate concentration in the feed (S_0).

2.2 Washout conditions

In any biochemical system washout must be avoided. Washout corresponds to a steady-state where concentration of substrate in the influent is equal to that in the effluent. The washout steady-state solution to (1) - (5) is given by

$$X_v = X_{nv} = X_d = P = 0 \quad \text{and} \quad S = S_0.$$

The stability of the washout steady-state solution is determined by the eigenvalues of the corresponding Jacobian matrix. At the washout state the values of the reaction rates are given by

$$\mu_v = \frac{\mu_{max}S_0}{K_1+S_0}, \quad \mu_d = -\frac{\mu_{max}S_0}{K_1+S_0}, \quad \mu_{nv} = \frac{S_0}{K_1+S_0}(\mu'_{max}-\mu_{max}).$$

As μ_{max}, S_0 and K_1 are all positive we see that μ_d is negative. As all reaction rates are assumed to be positive, μ_d is set to zero. The value of μ_{nv} depends on μ'_{max} and

μ_{max}. From the experimental values given (Perego et al, 1985), we have $\mu_{max} > \mu'_{max}$ and so μ_{nv} is also set to zero. The Jacobian matrix for the washout solution is

$$\begin{bmatrix} \mu_{max}\mathscr{F} - 1/\tau & 0 & 0 & 0 & 0 \\ 0 & -1/\tau & 0 & 0 & 0 \\ 0 & 0 & -1/\tau & 0 & 0 \\ \mu_{max}\mathscr{F} & 0 & 0 & -1/\tau & 0 \\ -\mu_{max}\mathscr{F} & 0 & 0 & 0 & -1/\tau \end{bmatrix},$$

where $\mathscr{F} = S_0/(K_1 + S_0)$. The eigenvalues of this matrix are $\lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = -1/\tau < 0$ and $\lambda_5 = \mu_{max}\mathscr{F} - 1/\tau$. The washout state is therefore stable when $\lambda_5 < 0$, i.e., when

$$\tau < \frac{1}{\mu_{max}\mathscr{F}} = \frac{1}{\mu_{max}}\left(1 + \frac{K_1}{S_0}\right). \tag{6}$$

Since washout is undesirable, equation (6) defines the minimum residence time that can be used to run a single reactor. The critical value of the residence time, below which washout occurs, decreases from 4.12 hours to 4.075 hours as the substrate concentration is increased from 100 gl^{-1} to 160 gl^{-1}.

2.3 Numerical results

In this section our primary objective is to investigate how the maximum productivity of a single reactor depends upon the concentration of the substrate in the feed. Our secondary objective is to confirm some observations made by Jarzebski (1992). Unless otherwise stated the parameter values used in our investigation are given in the nomenclature. By direct integration of equations (1)–(5) Jarzebski found that the system exhibited both steady-state and oscillatory behaviour at a residence time $\tau = 20$ hours and a feed substrate concentration of 160 gl^{-1}. However, only steady-state solutions were obtained at a residence time $\tau = 20$ hours and a feed substrate concentration of 100 gl^{-1}.

Figure 1 shows a steady-state diagram for four of the process variables (the concentration of dead cells is not shown) when the feed substrate concentration is 100 gl^{-1}. Starting from a zero residence time, the system is in the washout state until a residence time of 4.12 hours is reached. For a residence time greater than 4.12 hours, viable cells and ethanol are produced and the substrate is consumed. When the residence time is increased to 6 hours, non-viable cells start to be produced, which decreases the number of viable cells. There is a region of bistability for residence times between 10.8 and 13.93 hours, where the viable cells are in abundance.

The largest ethanol concentration is $P = 45.25$ gl^{-1}, which occurs when the residence time is $\tau = 13.93$ hours (see Figure 1c). Significantly, there are no Hopf bifurcations and no periodic solutions at this feed concentration.

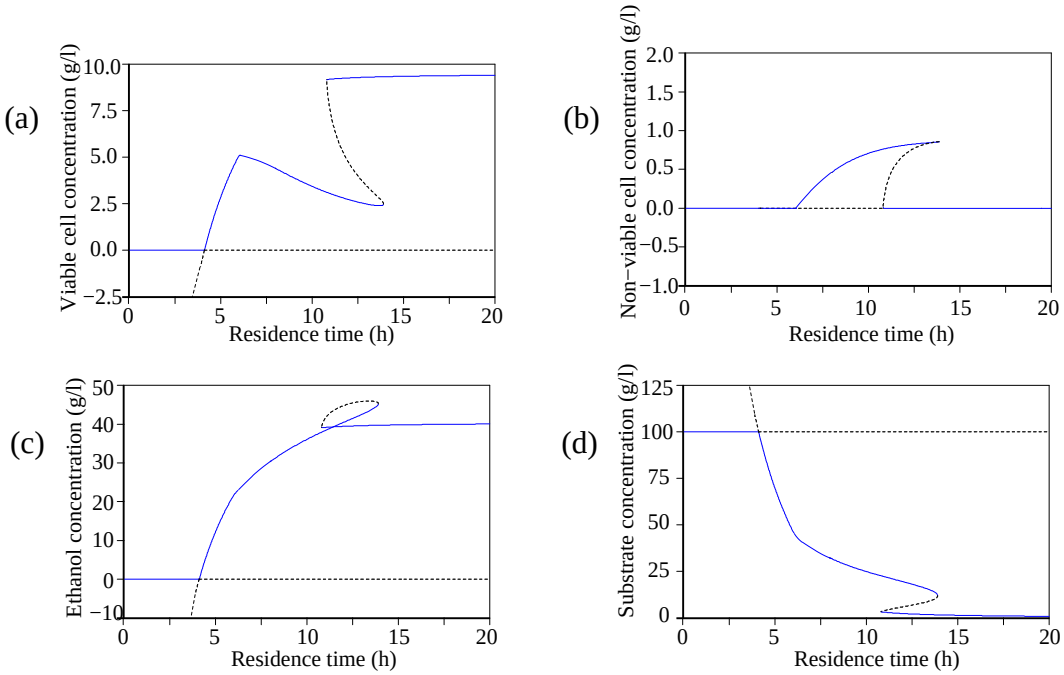

Figure 1: Steady-state diagrams for a single tank when the feed substrate of concentration is 100 gl^{-1} (a) viable cell concentration (b) non-viable cell concentration (c) ethanol concentration and (d) substrate concentration versus residence time.

Figure 2 shows the reactor productivity as a function of the residence time. The optimal productivity is given by $Pr = 3.8$ gl^{-1}h^{-1} which occurs at a residence time $\tau = 7.47$ hours. Although the maximum ethanol concentration is given by $P = 45.25$ gl^{-1}, when $\tau = 13.93$ hours, the productivity obtained at this residence time is only 3.25 gl^{-1}, about 15% less than the maximum value.

We now investigate what happens when the feed substrate concentration is increased to 160 gl^{-1}. The corresponding steady-state diagram for reactor productivity is shown in figure 3. The notable feature of this figure is that a Hopf bifurcation occurs at a residence time 10.62 hours and that this generates periodic solutions. A limit-point bifurcation occurs on a disjoin solution branch at a residence time of 17.15 hours. The system exhibits bistability with stable periodic solutions and stable steady-state solutions coexisting, as identified by direct numerical simulation by Jarzebski (1992). The optimal productivity in figure 3 is $Pr = 3.8$ gl^{-1}

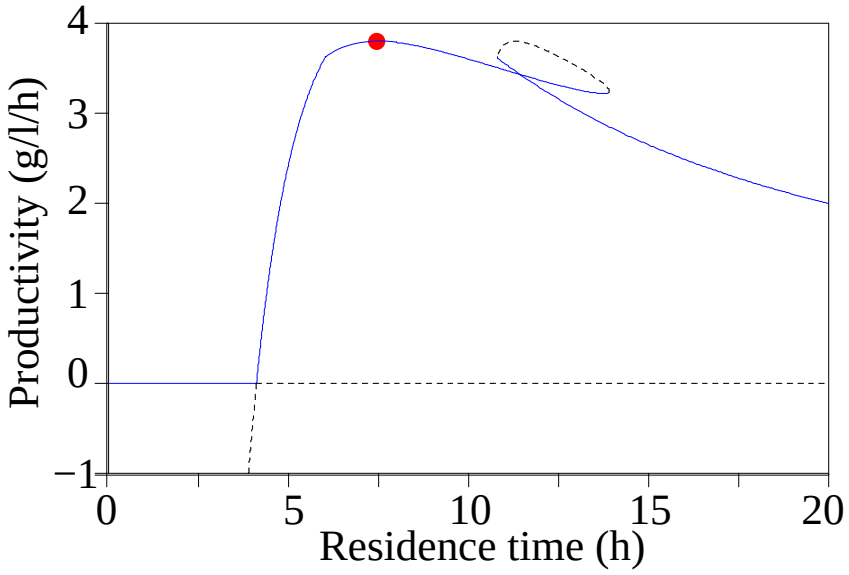

Figure 2: Steady-state diagram for the productivity of a single tank. The optimal productivity is denoted by the bold circle. Parameter value: feed substrate concentration, $S_0 = 100$ gl^{-1}.

which occurs at a residence time of $\tau = 7.11$ hours. Thus the optimal productivity is the same for feed concentrations of 100 gl^{-1} and 160 gl^{-1}.

A very similar steady-state diagram to figure 3 is obtained when the feed substrate concentration is decreased to 138 gl^{-1}, and for brevity it is not included. The optimal productivity in this case is again 3.8 gl^{-1}h^{-1}, occurring at a residence time of $\tau = 7.167$ hours. For feed substrate concentrations in the range 100 gl$^{-1} \leq S_0 \leq 160$ gl^{-1}, the optimal productivity was practically constant with an average value of 3.8039 gl^{-1}h^{-1} and a standard deviation of 9.8738×10^{-5} gl^{-1}h^{-1}. In every case we investigated, the reactor productivity was maximised when the system was operated at a steady-state.

Watt et al (2007) showed that for feed substrate concentrations greater than 122 gl^{-1} the steady-state diagram contains one Hopf point, for $108 < S_0\left(\text{gl}^{-1}\right) < 122$ there are two Hopf points and for $S_0 < 108$ gl^{-1}, there are no Hopf points on the steady-state diagram. Thus there are no natural oscillations in the system if the substrate concentration in the feed (S_0) is sufficiently low ($S_0 < 108$ gl^{-1}).

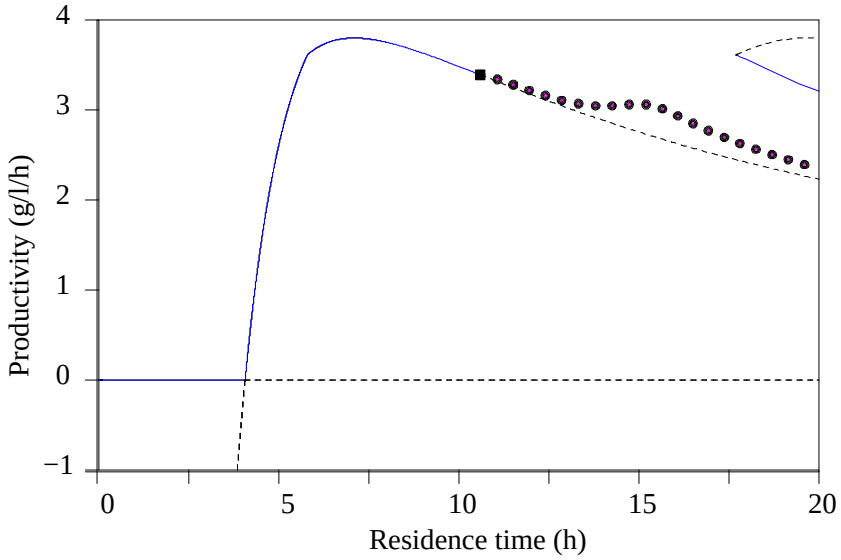

Figure 3: The productivity in a single tank with a feed substrate concentration of 160 gl^{-1}.

3 Multiple reactor cascade

In this section we investigate the reactor productivity that can be achieved by using a cascade of two or three reactors. The results presented in section 2.3 regarding the maximum productivity that can be obtained in a single reactor provide the necessary benchmark to correctly assess the performance of a reactor cascade (Nelson and Sidhu, 2006).

The equations for the reactor cascade model are given in section 3.1. The results for cascades containing two and three reactors are discussed in sections 3.2 & 3.3 respectively.

3.1 Governing equations

We assume that: the output from tank i is fed straight into the tank $i+1$; there is no recycle; and the concentrations and cell populations do not change while in transit from one tank to the next.

For each reactor, there are five ordinary differential equations describing the biochemical species. These equations are given by:

$$\frac{dX_{v,i}}{dt} = \frac{1}{\tau_i}(X_{v,i-1} - X_{v,i}) + (\mu_{v,i} - \mu_{nv,i} - \mu_{d,i})X_{v,i}, \tag{7}$$

$$\frac{dX_{nv,i}}{dt} = \frac{1}{\tau_i}(X_{nv,i-1} - X_{nv,i}) + (\mu_{nv,i}X_{v,i} - \mu_{d,i}X_{nv,i}), \tag{8}$$

$$\frac{dX_{d,i}}{dt} = \frac{1}{\tau_i}(X_{d,i-1} - X_{d,i}) + \mu_{d,i}(X_{v,i} + X_{nv,i}), \tag{9}$$

$$\frac{dP_i}{dt} = \frac{1}{\tau_i}(P_{i-1} - P) + \left(\frac{\mu_{v,i}X_{v,i}}{Y_{x|p}} + m_p X_{nv,i}\right), \tag{10}$$

$$\frac{dS_i}{dt} = \frac{1}{\tau_i}(S_{i-1} - S_i) - \left(\frac{\mu_{v,i}X_{v,i}}{Y_{x|s}} + m_s X_{nv,i}\right), \tag{11}$$

where the subscript i denotes the i^{th} tank. The residence time in the ith reactor is given by $\tau_i = V_i/F$. As was the case for the single reactor we assume that we only have substrate in the feed: i.e., $X_{v,0} = X_{nv,0} = X_{d,0} = P_0 = 0$ gl^{-1}. In this section we fix the substrate in the feed to $S_0 = 160$ gl^{-1}. Note that since there is no recycle, the behaviour of the first tank is independent of the second.

We characterize the performance of the cascade system by its reactor productivity. For the two- and three-reactor cascades these are given by

$$\mathrm{Pr}_2 = \frac{P_2}{\tau_1 + \tau_2} \quad \& \quad \mathrm{Pr}_3 = \frac{P_3}{\tau 1 + \tau_2 + \tau_3}.$$

3.2 Results for a double reactor cascade

In this section we investigate how the productivity of the a reactor cascade containing two tanks depends upon the total residence time of the cascade and the residence time in each reactor of the cascade. In section 3.2.1 we consider the the 'unconstrained' case, in which the residence time in each reactor may differ, while in section 3.2.2 we consider the 'constrained' case, in which the residence times of the two reactors are equal.

3.2.1 'Unconstrained' cascade performance

The total residence time of a double reactor cascade is given by $\tau_{total} = \tau_1 + \tau_2$. The limits $\tau_1 = 0$ and $\tau_2 = 0$ represent degenerate cases in which the 'cascade' consists of a single reactor. Unless otherwise stated, when we refer to a cascade we do not

include these limiting degenerate cases. In what follows, we fix the total residence time (τ_{total}) in the cascade and take the residence time in the first reactor (τ_1) as the primary bifurcation (or design) parameter.

For a sufficiently low total residence time the productivity of a two-reactor cascade is always lower than that of the optimized single reactor. Figure 4 shows the reactor productivity as a function of the design parameter (τ_1) when the total residence time is five hours. The productivity is zero over the design range $0.92 < \tau_1 < 4.08$ since for these residence times there is washout in both reactors. The productivity of the cascade is a decreasing (increasing) function of the residence time in the first reactor provided that $\tau_1 < 0.92$ ($\tau_1 > 4.08$). The maximum productivity of the cascade, $\mathrm{Pr}_2 = 2.60\,\mathrm{g\,l^{-1}h^{-1}}$ is given by either of the degenerate limits in which the cascade "becomes" a single reactor.

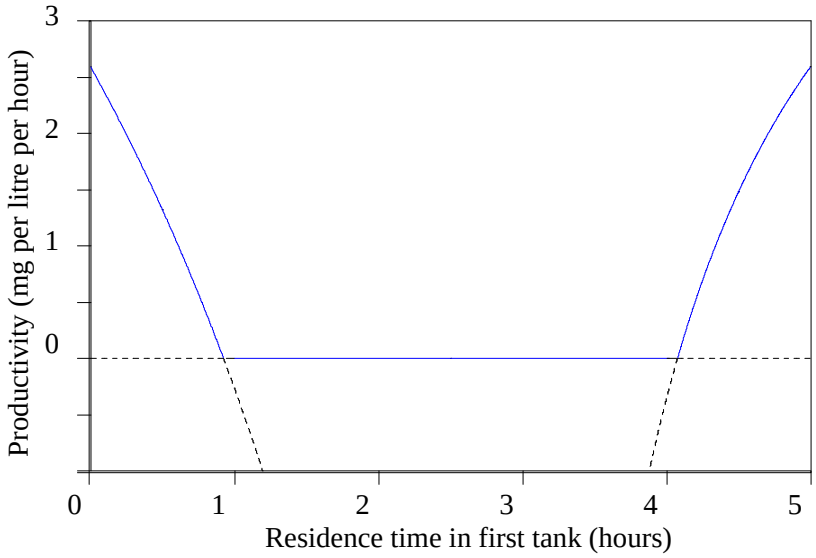

Figure 4: The dependence of the productivity for the two-reactor cascade upon the residence time in the first reactor. Parameter values: feed substrate concentration, $S_0 = 160\,(\mathrm{g\,l^{-1}})$; total residence time, $\tau_t = 5\,(\mathrm{hours})$.

When the total residence time is sufficiently high then the optimal performance of the two tank system does not occur at the degenerate limits ($\tau_1 = \tau_t$ and $\tau_2 = \tau_t$) but at an intermediate value of the design parameter (τ_1). Thus in figure 5, when the total residence time is ten hours, the optimal productivity, $\mathrm{Pr}_2 = 4.38$ $\mathrm{g\,l^{-1}h^{-1}}$, occurs when $\tau_1 = 5.81$ hours (with $\tau_2 = 4.19$ hours). As the optimal performance of a single tank is 3.8 $\mathrm{g\,l^{-1}h^{-1}}$, with a residence time of 7.167 hours, this cascade design increases the optimal productivity by 15%.

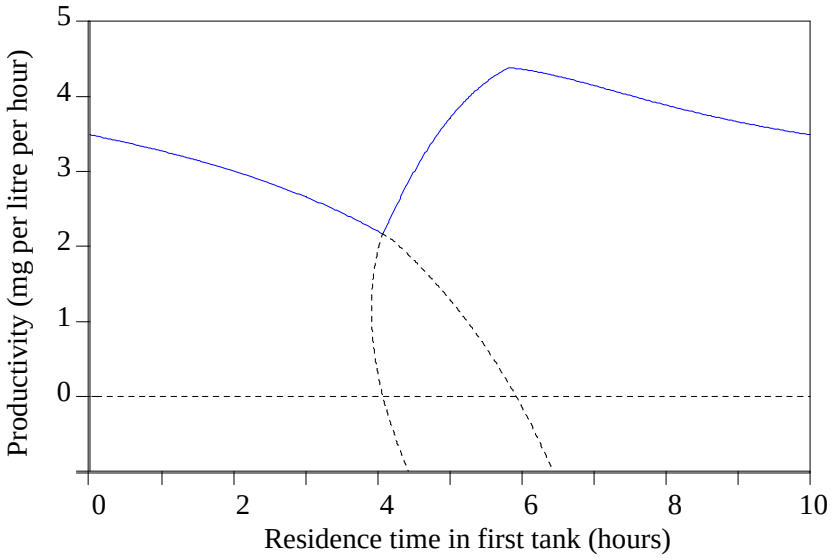

Figure 5: The dependence of the productivity for the two-reactor cascade upon the residence time in the first reactor. Parameter values: feed substrate concentration, $S_0 = 160\,(\mathrm{g\,l^{-1}})$; total residence time, $\tau_t = 10\,(\mathrm{hours})$.

For a two-reactor cascade figures 4 & 5 indicate that path-following methods are an efficient tool to determine the value of the design parameter (τ_1) that optimizes the reactor productivity. These figures represent the cases when the total residence time is five and ten hours respectively. Figure 6 shows the optimal productivity for a two-reactor cascade as a function of the total residence time ($0 \leq \tau_t \leq 20$) — the horizontal line shows the optimal productivity that can be achieved in a single reactor. We see that an optimally designed cascade only outperforms the single reactor when the total residence time is above eight hours. The maximum productivity that can be achieved using a two-reactor cascade occurs when the total residence time is 15 hours with residence times of 6.03 and 8.97 hours in the first and second reactors respectively. This yields a maximum productivity $\mathrm{Pr}_2 = 5.08\mathrm{g\,l^{-1}h^{-1}}$, which is an increase of 34% in productivity over the optimal single tank system.

Table 1 shows the variation in the optimal productivity of an unconstrained two reactor cascade as a function of the substrate concentration in the feed. Recall that for a single reactor the optimal productivity is insensitive to the value of the substrate concentration over the range $100 \leq S_0\left(\mathrm{g\,l^{-1}}\right) \leq 160$: $\mathrm{Pr} = 3.80\mathrm{g\,l^{-1}h^{-1}}$. Thus the improvement in performance that can be achieved by the cascade is an increasing function of the substrate concentration in the feed. Note that as the substrate concentration in the feed increases the design of the optimally designed

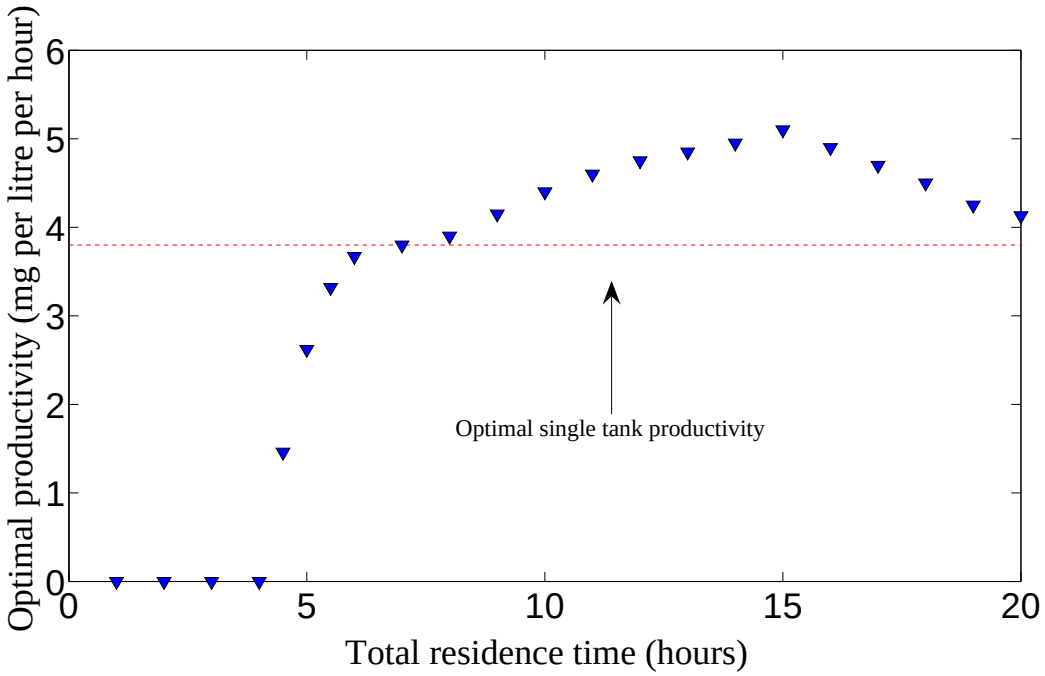

Figure 6: The dependence of the optimal productivity upon the total residence time in a two-reactor cascade (triangles). The horizontal dotted line shows the optimal productivity of 3.8 $gl^{-1}h^{-1}$ obtained in the single reactor.

reactor switches from having the higher residence time in the first reactor to having it in the second reactor.

3.2.2 Constrained cascade performance

The productivity of a cascade of two reactors in which the residence time in each tank is equal, i.e. $\tau_1 = \tau_2 = \tau_t/2$, is shown in Figure 7. The corresponding figure for the one-tank system was presented in Figure 3. The maximum productivity of a constrained double reactor cascade is 4.82 $gl^{-1}h^{-1}$. This is achieved using a total residence time of 13.83 hours. This productivity is lower than the best designed two-reactor cascade which had a productivity of 5.08 $gl^{-1}h^{-1}$.

Feed concentration $(\mathrm{g l^{-1}})$	Optimal productivity $(\mathrm{g l^{-1} h^{-1}})$	τ_1 (h)	τ_2 (h)	Total residence time (h)
100	3.99	6.62	2.98	9.60
120	4.41	6.00	4.91	10.91
140	4.83	5.89	5.41	11.30
160	5.08	6.03	6.91	12.94

Table 1: Operating conditions for the optimal productivity of an unconstrained cascade of two unequal reactors as a function of the substrate concentration in the feed.

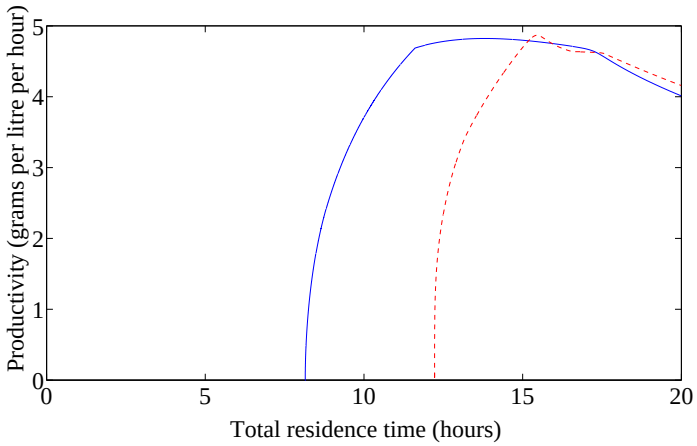

Figure 7: The dependence of the productivities of cascades with two-equal tanks (solid line) and three-equal tanks (dashed line) upon the total residence time. The corresponding figure for the one-tank system is presented in Figure 3. Parameter value: feed substrate concentration, $S_0 = 160\,(\mathrm{g l^{-1}})$.

3.3 Results for a three reactor cascade

In the earlier sections, we investigated the design parameters to determine the optimal two-reactor system. This was a straight-forward procedure as there were only two parameters to be varied (the total residence time τ_{total} and the residence time in the first reactor τ_1). For an unconstrained three-reactor system we used a two-step procedure to determine the optimal design. In the first step numerical integration of the governing equations was undertaken for residence times between 0 and 10 hours in each tank in steps of 0.1 hours. In the second step, the path following software Auto was used to investigate the behaviour more closely around the prospective global maximum.

Using this procedure, the optimal three-reactor cascade was found to have residence times of 5.82 h, 5.31 and 3.34 h in the first, second and third reactors respectively. This design of the cascade results in a productivity of 5.181 $gl^{-1}h^{-1}$, which is an improvement of 36% over that of the single reactor system and 2% over the optimal two-reactor cascade.

The productivity of a constrained cascade of three reactors, i.e. $\tau_1 = \tau_2 = \tau_3 = \tau_t/3$, is shown in Figure 7. The maximum productivity of the 'constrained' three reactor cascade is 4.87 $gl^{-1}h^{-1}$ which is achieved using a total residence time of 15.45 hours. This productivity is only slightly higher than the best productivity that can be achieved in a cascade of two reactors with equal residence times, 4.82 $gl^{-1}h^{-1}$, and is lower than the best designed two-reactor cascade which had a productivity of 5.08 $gl^{-1}h^{-1}$, at a total residence time of 15 hours.

4 Conclusions

We have investigated the productivity of ethanol production through continuous fermentation in a single tank and in a cascade of two and three reactors. For the single reactor we established the conditions for washout to occur and showed that the maximum productivity was essentially constant over a range of feed substrate concentrations. At low total residence times a single tank can outperform any cascade. For larger total residence times, we found that the cascade can outperform the single tank system by up to 34% with two (unequal) reactors and 36% with three (unequal) reactors. Considering two- and three-equal tank cascade systems we found that we could achieve an improvement of 27% in the two-tank system and 28% in the three-tank system over the best single tank productivity. The optimal configurations for the various reactor systems. investigated in this paper are summarized in Table 2. We have also included calculations for four and five constrained reactor cascades Increasing the number of tanks above three in fact reduces the maximum productivity that can be obtained.

The model we used is due to Jarzebski (1992), who determined biochemical parameter values using experimental data from Perego et al (1985). Jarzebski did not report any range of uncertainty in the fitted parameter values. It is likely that the small gain that can be achieved from going from a constrained cascade of two reactors to one of three reactors is not warranted given the uncertainty in the biochemical parameters. However, the principal contribution of this paper is not in determining the particular increases in productivity that can be gained from a cascade using this particular scheme. Instead, the main contribution is to show that path-following methods are efficient tools to investigate the performances of a single reactor, an 'unconstrained' double-reactor cascade and the 'constrained' *n*-reactor

Configuration	Optimal productivity ($gl^{-1}h^{-1}$)	τ_1 (h)	τ_2 (h)	τ_3 (h)	τ_4 (h)	τ_5 (h)	τ_t (h)
one reactor	3.80	7.47	-	-	-	-	7.47
two equal reactors	4.82	6.91	6.91	-	-	-	13.82
two unequal reactors	5.08	6.03	8.97	-	-	-	15
three equal reactors	4.87	7.73	7.73	7.73	-	-	15.46
three unequal reactors	5.18	5.82	5.31	3.34	-	-	14.47
four equal reactors	4.285	4.68	4.68	4.68	4.68	-	18.72
five equal reactors	3.776	4.19	4.19	4.19	4.19	4.19	20.95

Table 2: Operating conditions for optimal productivity for various system configurations.

cascade. This technique can be used to readily determine the effect of recycle upon productivity and to optimize productivity in more complicated reactor models. The latter might include a permselective membrane module and a cell/substrate separator which separates the cell and unused substrate from the exit stream to be recycled back into the first tank, as suggested by Garhyan & Elnashaie (2004).

Nomenclature

D	dilution rate (h^{-1})
F	flow rate into tank (lh^{-1})
K_1, K_2	saturation constants (gl^{-1})
m_p	maintenance factor of ethanol (h^{-1})
m_s	maintenance factor of substrate (h^{-1})
P	ethanol concentration (gl^{-1})
P_c	limiting ethanol concentration for viable cells (gl^{-1})
P_c'	limiting ethanol concentration for non-viable cells (gl^{-1})
Pr	productivity of ethanol ($gl^{-1}h^{-1}$)
S	substrate concentration (gl^{-1})
S_0	feed substrate concentration (gl^{-1})
t	time (h)
X_d	dead cell concentration (gl^{-1})
X_{nv}	non-viable cell concentration (gl^{-1})
X_v	viable cell concentration (gl^{-1})
V	volume of the reactor (l)

$Y_{x|p}$ yield coefficient in conversion from biomass to ethanol (-)
$Y_{x|s}$ yield coefficient in conversion from biomass to substrate (-)

Greek letters

μ_d growth rate of dead cells (h^{-1})
μ_{max} maximum growth rate of viable cells (h^{-1})
μ'_{max} maximum growth rate on non-viable cells (h^{-1})
μ_{nv} growth rate of non-viable cells (h^{-1})
μ_v growth rate of viable cells (h^{-1})
τ residence times (h)

The biochemical parameters in this model were estimated by Jarzebski (1992) from experimental data obtained by Perego et al (1985). Unless otherwise stated, the parameter values we use in this study are those given in Jarzebski (1992): $\mu_{max} = 0.25$ h^{-1}, $\mu'_{max} = 0.21$ h^{-1}, $P_c = 70$ gl^{-1}, $P'_c = 130$ gl^{-1}, $m_p = 2.6$ h^{-1}, $m_s = 4.42$ h^{-1}, $Y_{x|p} = 0.235$, $Y_{x|s} = 0.095$ and $K_1 = K_2 = 3$ gl^{-1}.

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