1-1-2011

The effect of incomplete mixing upon the performance of a membrane-coupled anaerobic fermentor

Ahmed Hussein Msmali
University of Wollongong, amsmali@uow.edu.au

Mark I. Nelson
University of Wollongong, mnelson@uow.edu.au

John M. Kavanagh
University of Sydney, jkavanagh@usyd.edu.au

The effect of incomplete mixing upon the performance of a membrane-coupled anaerobic fermentor

Abstract

We consider a model to describe the performance of a membrane-coupled anaerobic fermentor which was developed and calibrated using experimental data by Kim and Chung (2010). The model consists of six differential equations, modelling the concentration of five biochemical species and the rate of gasification. In the original work it was assumed that reactor is well-mixed. We use a two parameter mixing model to investigate the effect of incomplete mixing upon the performance of this process. The parameters in the mixing mode are the size of the stagnant region and a parameter controlling the degree of mixing between the regions. Perfect mixing corresponds to the limit in which delta approaches infinity. There are six differential equations in each region. We investigate how the concentration of volatile fatty acids in the agitated region depends upon the degree of mixing in the reactor and the size of the stagnant region.

Keywords

anaerobic, coupled, membrane, fermentor, performance, effect, upon, mixing, incomplete

Disciplines

Physical Sciences and Mathematics

Publication Details

Msmali, A., Nelson, M. I. & Kavanagh, J. M. (2011). The effect of incomplete mixing upon the performance of a membrane-coupled anaerobic fermentor. CHEMECA 2011: Proceedings of the Australasian Chemical Engineering Conference (pp. 1-12). (on USB drive): Engineers Australia.

THE EFFECT OF INCOMPLETE MIXING UPON THE PERFORMANCE OF A MEMBRANE-COUPLED ANAEROBIC FERMENTOR

Ahmed Hussein Msmali*[1], Mark I Nelson[1], and John Kavanagh[2]

1. School of Mathematics and Statistics, University of Wollongong, Wollongong, NSW 2522 Australia
*Email: ahom821@uowmail.edu.au

2. School of Chemical and Biomolecular Engineering The University of Sydney, NSW 2006.

ABSTRACT

We consider a model to describe the performance of a membrane-coupled anaerobic fermentor which was developed and calibrated using experimental data by Kim and Chung (2010). The model consists of six differential equations, modelling the concentration of five biochemical species and the rate of gasification. In the original work it was assumed that reactor is well-mixed. We use a two parameter mixing model to investigate the effect of incomplete mixing upon the performance of this process. The parameters in the mixing mode are the size of the stagnant region (ε) and a parameter controlling the degree of mixing between the regions (δ). Perfect mixing corresponds to the limit in which delta approaches infinity. There are six differential equations in each region.

We investigate how the concentration of volatile fatty acids in the agitated region depends upon the degree of mixing in the reactor and the size of the stagnant region.

INTRODUCTION

Anaerobic fermentation is routinely used for the treatment of both industrial and municipal wastewater, converting organic matter into a methane rich biogas and a small amount of sludge (Fleming, 2002, p.2). Although the overall process contains multiple steps in series and parallel, involving diverse groups of microorganisms, three stages are recognized as being important. In the first stage organic particulates are hydrolysed. In the second stage, the hydrolysis products are converted into volatile fatty acids. In the final stage the volatile fatty acids are converted into methane and carbon dioxide (Dinopoulou et al., 1988, p. 3). All three process are included in this model.

We use a mathematical model for the performance of a microfiltration membrane-coupled anaerobic fermentor due to Kim and Chung (2010). The biochemical model is described in section (2.1). Figure 1 shows a schematic diagram of the reactor. We extend the model of Kim and Chung to include incomplete mixing. In lab-scale experiments the use of small reactors ensures that mixing can be assumed to be perfect. However, as the size of the reactor increases it becomes increasingly unlikely that perfect mixing is achieved. In fact it is known to be difficult to maintain complete mixing in industrial-scale fermentation reactors (Fogler, 1999; Shuler & Kargi, 2002). Incomplete mixing is therefore the rule in such processes. In deed the assumption of perfect mixing has been shown to hinder accurate performance prediction and thus hinder the widespread deployment of the process (Fleming 2002, p. 4).

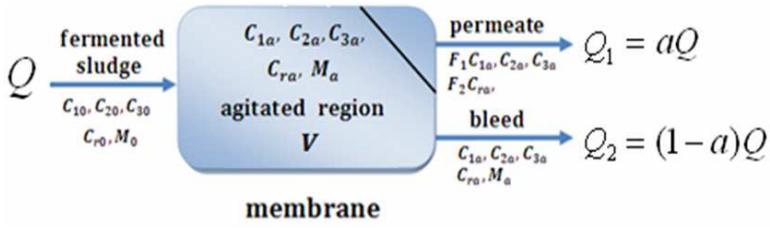

Figure 1. Schematic diagram for the membrane-coupled anaerobic fermentor assuming perfect mixing (Kim and Chung 2010).

We employ a two-parameter mixing model in which the membrane bioreactor is split into two compartments: one representing a highly agitated region and one representing a stagnant region. The agitated region and the stagnant region are both modelled as separate CSTRs with mass transfer between the two regions. This mixing process is illustrated schematically in figure 2. The agitation is the pump and the production of gas.

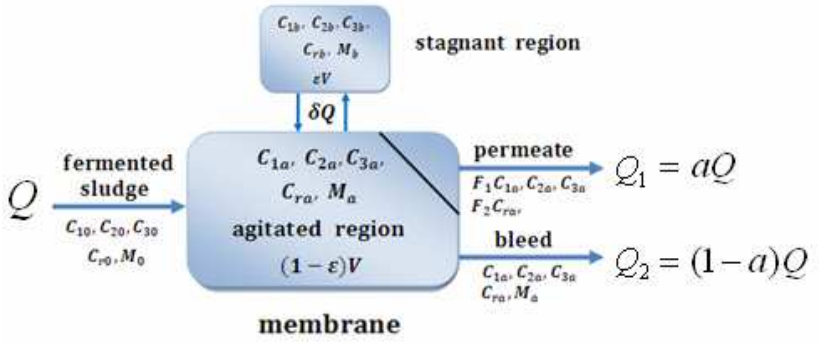

Figure 2. Schematic diagram for the membrane-coupled anaerobic fermentor assuming imperfect mixing. The mixing model parameters are the values for δ and ε.

MODEL EQUATIONS

In this section we detail the biochemical reactions, and provide the model equations for the cases of perfect mixing and imperfect mixing.

Biochemical model

The biochemical model consists of four biochemical reactions and the death of the bacteria (Kim and Chung, 2010). These processes are:

Hydrolysis of biodegradable organic solids

$$C_1 \xrightarrow{k_1} \alpha C_2 + C_r + Y_1 M + (1-\alpha-\gamma-Y_1)G. \quad (1)$$

Conversion of soluble organic to fatty acids

$$C_2 \xrightarrow{k_2} \beta C_3 + Y_2 M + (1-\beta-Y_2)G. \quad (2)$$

Conversion of volatile fatty acids to methane

$$C_3 \xrightarrow{k_3} EG. \quad (3)$$

Death of acid-forming bacteria

$$M \xrightarrow{kd} Y_M C_1 + \gamma_m C_r. \tag{4}$$

The model contains five state variables $(C_1, C_2, C_3, C_r,$ and $M)$.

Perfect mixing equations

The model equations for the case when the reaction is carried out in a well-stirred bioreactor are given below. In addition to the five state variables there is a sixth equation for the rate of gasification.

Biodegradable organic solids

$$V\frac{dC_{1a}}{dt} = QC_{10} - (Q - Q_1)C_{1a} - F_1 Q_1 C_{1a} - Vk_1 C_{1a} + VY_M k_d M_a. \tag{5}$$

Dissolved organic materials

$$V\frac{dC_{2a}}{dt} = Q(C_{20} - C_{2a}) + V\alpha k_1 C_{1a} - Vk_2 C_{2a}. \tag{6}$$

Volatile fatty acids

$$V\frac{dC_{3a}}{dt} = Q(C_{30} - C_{3a}) + V\beta k_2 C_{2a} - VEk_3 C_{3a}. \tag{7}$$

Refractory organic materials

$$V\frac{dC_{ra}}{dt} = QC_{r0} - (Q - Q_1)C_{ra} - F_2 Q_1 C_{ra} + V\gamma k_1 C_{1a} + V\gamma_m k_d M_a. \tag{8}$$

Acid-forming bacteria

$$V\frac{dM_a}{dt} = QM_0 (Q - Q_1)M_a + V\beta k_2 C_{2a} - VEk_3 C_{3a}. \tag{9}$$

Gasification rate

$$V\frac{dG_a}{dt} = V(1 - \alpha - Y_1 - \gamma)k_1 C_{1a} + V(1 - \beta - Y_2)k_2 C_{2a} + VEk_3 C_{3a}. \tag{10}$$

The permeate flow

$$Q_1 = aQ. \tag{11}$$

Residence-time

$$\tau = \frac{V}{Q}. \tag{12}$$

The total carbon content in the feed is given by

$$C_{T0} = C_{10} + C_{20} + C_{30} + C_{r0}. \tag{13}$$

In the system of equations (5-10) C_1 refers to degradable solids or polymer organic materials (mg C/l), C_2 refers to dissolved organic materials (mg C/l), C_3 refers to volatile fatty acids (VFA) (mg C/l), C_r refers to refractory organic concentration (mg C/l), E refers to VFAs consumption ratio by aeration, F refers to membrane passage ratio of C_1, F_2 refers to membrane passage ratio of C_r, G refers to gasification and mineralization ratio (%), M refers to hydrolysis by acid-forming bacteria (mg C/l), Q refers to input discharge (l/h), Q_1 refers to permeate flow rate (l/h), V refers to

bioreactor volume (l), Y_1 yield coefficient from C_1, Y_2 yield coefficient from C_2, Y_M yield coefficients from (M to C_1), a membrane filtration ratio, k_1 refers to hydrolysis rate coefficient (1/h), k_2 refers to acid-forming rate coefficient (1/h), k_3 refers to VFAs consumption rate coefficient (1/h), k_d refers to self-degradation rate coefficient for acid-forming bacteria (1/h), α yield coefficients from (C_1 to C_2), β yield coefficients from (C_2 to C_3), γ yield coefficients from (C_1 to C_r), and γ_m yield coefficients from (M to C_r).

Imperfect mixing equations

The model equations for an isothermal biochemical process with perfect mixing can be written in the generic manner.

$$\frac{dX}{dt} = \frac{X_0 - X}{\tau} + f(X). \tag{14}$$

In these equations $X_0 \in \Re^n$ is the concentration of the n biochemical species in the reactor feed, $X \in \Re^n$ is the concentration of the n biochemical species that take part in the process and τ is the residence time. The function $f(X)$ models the biochemical reactions.

A two-parameter mixing model for this system is given by Fogler (1999: Chapter 14)

$$\frac{dX_a}{dt} = \frac{(X_0 - X_a)}{(1-\varepsilon)\tau} + f(X_a) + \frac{\delta(X_a - X_b)}{(1-\varepsilon)\tau}. \tag{15}$$

$$\frac{dX_b}{dt} = f(X_b) - \frac{\delta(X_a - X_b)}{(1-\varepsilon)\tau}. \tag{16}$$

In these equations X_a and X_b are the concentrations of the n biochemical species in the aerated region and the stagnant region of the bioreactor respectively, δ is the mixing parameter and ε is the size of the stagnant region.

Parameter values

The parameter values used are given in Table 1.

Table 1: Values of kinetic and stoichiometric parameters (Kim & Chung, 2010).

Parameter	Value	Unit	Parameter	Value	Unit
C_{10}	1785	mg C/l	Y_M	0.3	-
C_{20}	50	mg C/l	a	0.1	-
C_{30}	5	mg C/l	α	0.85	-
C_{r0}	460	mg C/l	β	0.75	-
E	0.03	-	γ	0.01	-
F_1	0.04	-	γ_m	0.7	-
F_2	0.02	-	k_1	0.0122	1/h
M_0	0	-	k_2	0.1916	1/h

Y_1	0.01	-	k_3	0.0174	1/h
Y_2	0.022	-	k_d	0.0015	1/h

RESULTS

Characterising the performance of the reactor

Figure 3 shows the steady-state concentration of the volatile fatty acids (VFA) as a function of the residence time for both an ideal and a non-ideal reactor. The feature of interest in this figure is that there is a value of the residence time, $\tau = \tau_{\max}$, at which the concentration of volatile fatty acids is maximised, $C_{3a} = C_{3a,\max}$. For the ideal (non-ideal) reactor these values are $\tau_{\max} = 388.6$, ($\tau_{\max} = 421.7$) and $C_{3a,\max} = 821.2$, ($C_{3a,\max} = 795.7$). We refer to the value of $\tau_{\max}$ as the `maximum residence time'.

In what follows we sometimes characterize the performance of the reactor through the maximum carbon ratio ($R_{\max}$). $R_{\max}$ is the ratio of the maximum carbon content in the volatile fatty acids to the total inlet carbon ($R_{\max} = C_{3a,\max} / C_{T0}$).

Figure 4 shows how the maximum residence time ($\tau_{\max}$) and the maximum carbon ratio ($R_{\max}$) depend upon the value of the membrane filtration ratio (a) for an ideal and a non-ideal reactor.

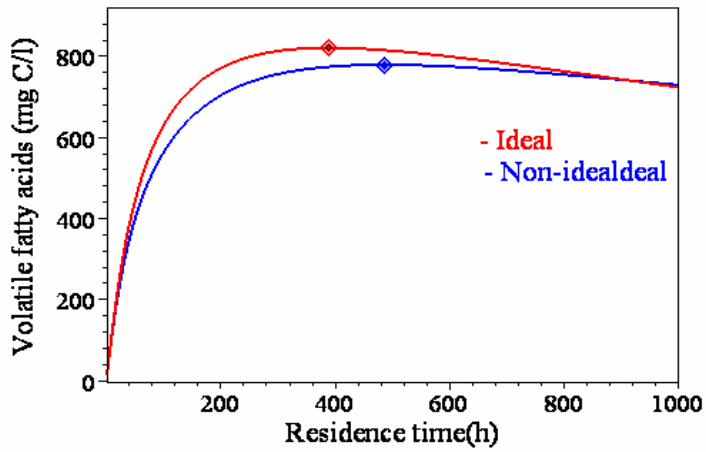

Figure 3. Steady-state diagram showing the concentration of volatile fatty acids as a function of the residence time. Parameter values: $a = 0.1$, $\delta = \varepsilon = 0$ (ideal); $\delta = 0.2$, $\varepsilon = 0.3$ (non-ideal).

Figure 4.a shows that the maximum residence time is an increasing function of the membrane filtration ratio (a). The value is lower for the reactor with perfect mixing. The difference between the reactors decreases as a increases: when $a = 1$ we have $\tau_{\max} = 128.9$ (perfect mixing) and $\tau_{\max} = 129.9$ (imperfect mixing).

Figure 4.b shows that the maximum carbon ratio ($R_{\max}$) increases as the membrane filtration ratio (a) increases. The value for the ideal reactor is slightly higher. However, at its maximum extent (when $a = 0$) the difference is only 0.011.

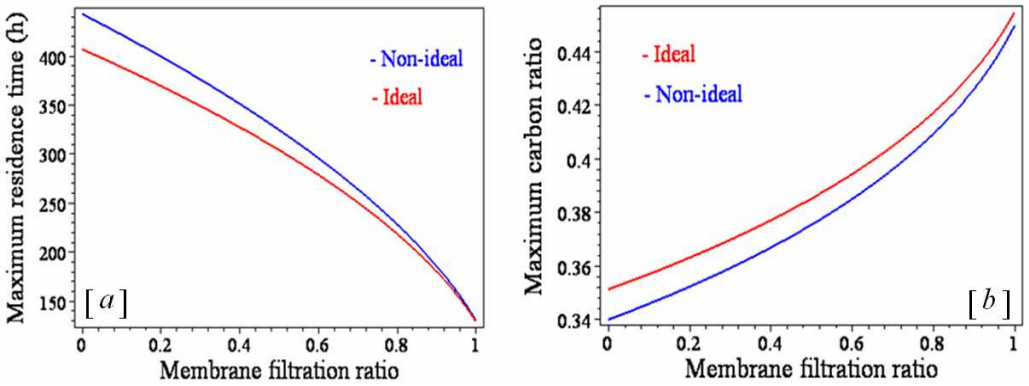

Figure 4. [a] The maximum residence time (h) and [b] the maximum carbon ratio as a function of the membrane filtration ratio. Parameter values: $\delta = \varepsilon = 0$ (ideal); $\delta = 0.2,\ \varepsilon = 0.3$ (non-ideal).

The limiting case of a dead-volume model

Figure 5 shows the steady-state diagram for the concentration of VFA in the limiting case of the mixing model in which $\delta = 0$. In this case the mixing model reduces to a `dead-volume' model (Fogler, 1999: Chapter 14). The steady-state diagram for the perfect mixing reactor is also shown. The important feature of this diagram is that the maximum VFA concentration is independent of the size of the dead-volume ($C_{3a,\max} = 886.02$). The value of the maximum residence time does depend upon the size of the dead volume. The maximum residence times are: $\tau_{\max}(\varepsilon = 0.0) = 304.12$; $\tau_{\max}(\varepsilon = 0.1) = 337.91$; $\tau_{\max}(\varepsilon = 0.2) = 380.15$; and $\tau_{\max}(\varepsilon = 0.3) = 434.45$. It follows from equation (1.15), in the case when $\delta = 0$, that: $\tau_{\max}(\varepsilon \neq 0.0) = \dfrac{\tau_{\max}(\varepsilon = 0.0)}{(1-\varepsilon)}$.

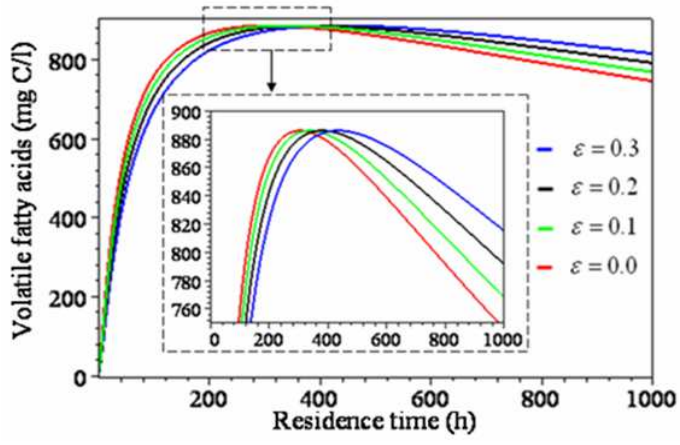

Figure 5. Steady-state diagram showing the concentration of volatile fatty acids (mg C/l) as a function of the residence time (h) for four values of stagnant region. Parameter values: $a = 0.5,\ \delta = \infty,\ \varepsilon = 0$ (ideal); $a = 0.5,\ \delta = 0.0,\ \varepsilon \neq 0.0$ (non-ideal).

The effect of the mixing parameter (δ)

In figure 6 we fix the size of the stagnant region (ε) and the value of the residence time (τ) and vary the mixing parameter (δ). The case $\delta = \infty$ corresponds to perfect mixing whilst the case $\delta = 0$ corresponds to the dead-volume model considered previously. Intuitively we might expect that the concentration of VFA will increase as delta increases from zero to infinity.

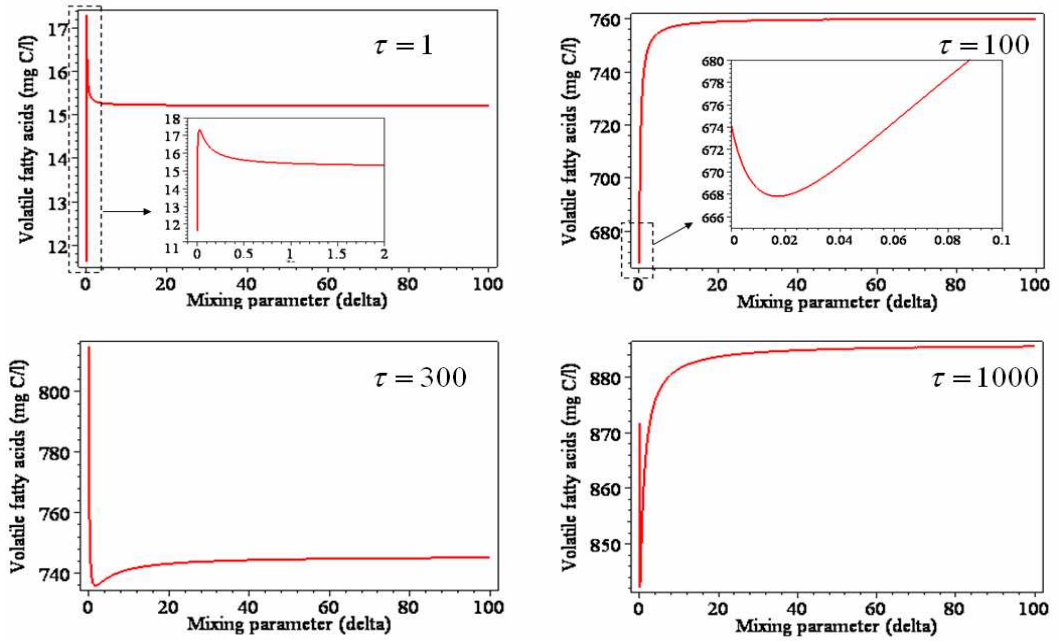

Figure 6 shows the concentration of volatile fatty acids (mg C/l) as a function of the mixing parameter (δ) for four values residence time. Parameter values: $a = 0.5$, $\varepsilon = 0.3$, [a] $\tau = 1$, [b] $\tau = 100$, [c] $\tau = 300$, and [d] $\tau = 1000$.

In figure 6 (a-b,d) we observe that the performance of the perfectly mixed reactor ($\delta = \infty$) is superior to the dead volume reactor ($\delta = 0$). However, the performance of the reactor does not always increase with increasing delta. For example, in figure 6 (a) the maximum VFA concentration ($C_{3a,\max} = 17.31$) occurs when ($\delta_{\max} = 0.02$). In figures 6 (b & c) the VFA concentration initially decreases. Thus there is a range of values for the mixing parameter over which a reactor with imperfect mixing between the agitated and stagnant regions gives a lower performance than a reactor with no mixing. In figure 6 (c) the minimum VFA concentration occurs when ($\delta_{\min} = 0.15$). The VFA concentration is only larger than the dead-volume value ($\delta = 0$) when ($\delta > \delta_{cr} = 2.64$).

Figure 6 (c) also exhibits very unexpected behavior. Namely the VFA concentration in a dead-volume reactor is superior to that in any reactor with a positive value for the mixing parameter ($\delta > 0$).

We can explain some of this unusual behaviour by considering the steady-state diagram, for perfect mixing. Figure 7 shows the steady-state diagram for the VFA concentration in more detail for two cases.

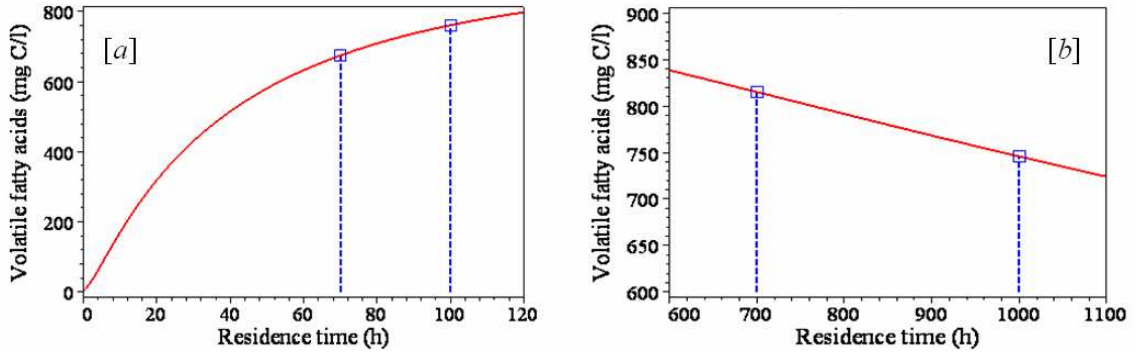

Figure7. Steady-state diagrams showing in a perfectly mixed reactor the concentration of volatile fatty acids (mg C/l) as a function of the residence time (h). Parameter values: $a = 0.5,\ \varepsilon = 0.0,\ \delta = \infty,\ \tau_1 = 70,\ \tau_2 = 100,\ \tau_3 = 700,$ and $\tau_4 = 1000$.

For a given residence time the steady-state value for a perfect reactor ($\delta = \infty$) is read-off the steady-state diagram. For example, when $\tau = 100$ (h) and $\tau = 1000$ (h) we have $C_{3a} = 674.07$ (mg C/l) and 815.07 (mg C/l) respectively. When $\delta = 0$ the generic model for any biochemical process becomes

$$\frac{dX}{dt} = \frac{X_0 - X}{\tau(1-\varepsilon)} + f(X),$$
$$= \frac{X_0 - X}{\tau_e} + f(X), \tag{17}$$

where we have defined an effective residence time

$$\tau_e = \tau(1-\varepsilon). \tag{18}$$

If $\varepsilon = 0.3$ and $\tau = 100$ then the effective residence time is 70. We see from figure 7[a] that $C_{3a}(\tau = 70) < C_{3a}(\tau = 100)$. Therefore in this case the performance of the ideal reactor ($\delta = \infty$) is better than that reactor with a dead-volume ($\delta = 0$).

If we take $\varepsilon = 0.3$ and $\tau = 1000$ then the effective residence time is 700. We see from figure 7[b] that $C_{3a}(\tau = 700) > C_{3a}(\tau = 1000)$. Therefore in this case the performance of the ideal reactor ($\delta = 1000$) is inferior to that of a reactor with a dead-volume ($\delta = 0, \varepsilon = 0.3$).

The effect of changing mixing parameter (δ) on the maximum residence time and the maximum VFA concentration for different values of membrane filtration ratio

Figure 3 shows a steady-state diagram for the VFA concentration as a function of the residence time for a non-ideal reactor. We see that the values for $C_{3a,\max}$ and $\tau_{\max}$ differ from these in an ideal bioreactor. In figure 8 we show how these quantities vary as the mixing parameter is increased from zero.

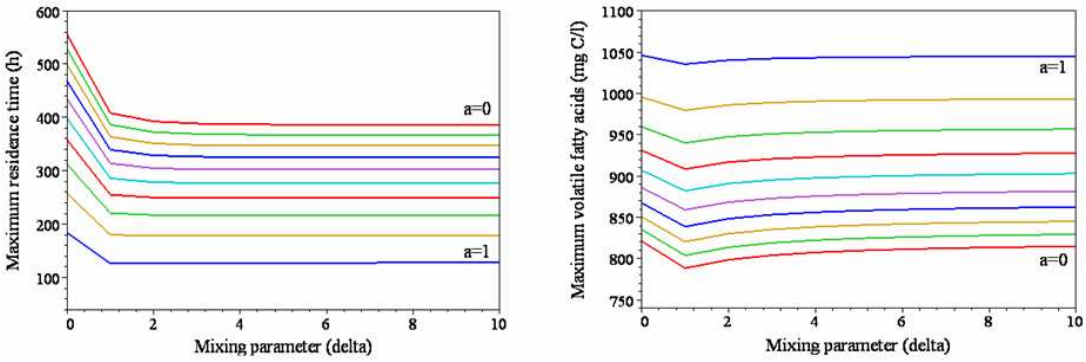

Figure 8 [a] The maximum residence time (h) and [b] the maximum ratio of VFA concentration as a function of the membrane filtration. Parameter: $\varepsilon = 0.3$.

Figure 8 [a] shows the maximum residence time ($\tau_{\max}$) as a function of the mixing parameter (δ) and the membrane filtration ratio (a). The value decreases sharply as the membrane filtration ratio is increased from zero, it quickly reaches a plateau in which the value decreases more gradually as the value for (a) increases. The highest value of the maximum residence time is located when there is no mixing. Figure 8 [b] shows the maximum VFA concentration ($C_{3a,\max}$) as a function of the mixing parameter (δ) and the membrane filtration ratio (a). There is a value of the mixing parameter ($\delta_{\min}$) at which the maximum VFA concentration is minimised. If the mixing parameter is in the region ($\delta < \delta_{\min}$) then the maximum VFA concentration decreases as δ is increased. If ($\delta > \delta_{\min}$) then the maximum VFA concentration increases as δ is increased. As noted earlier we have $C_{3a,\max}(\delta = 0) = C_{3a,\max}(\delta = \infty)$. As the filtration ratio (a) decreases the maximum VFA concentration decreases.

We use the value of the mixing parameter ($\delta_{\min}$) which minimizes the maximum VFA concentration (figure 8b) to define a reactor index for the maximum VFA concentration

$$RI = \frac{C_{3a,\max}(\delta = \delta_{\min})}{C_{3a,\max}(\delta = \infty)} \times 100.$$

The RI value gives the worst possible performance of a reactor due to incomplete mixing.

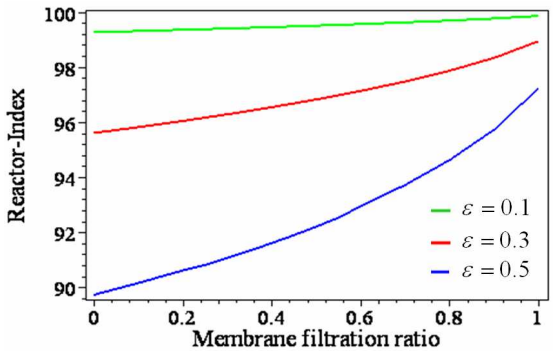

Figure 9. The dependence of the reactor index (RI) upon the membrane filtration (a).

Figure 9 **s**hows the relationship between the reactor-index and the filtration ratio (a) for three sizes of the stagnant region (ε). As the filtration ratio (a) increases the reactor-index increases, and as the stagnant region increases the reactor-index decreases. Thus, poor mixing is less important at high filtration ratio. In the case ($a = 0, \varepsilon = 0.5$) the minimum carbon content recovered is 90% of that recovered in an ideal reactor.

CONCLUSION

We have explored the behavior of a membrane-coupled anaerobic fermentor subject to non-ideal mixing. We investigated how the maximum VFA concentration depends upon the filtration ratio and the mixing parameters. As the filtration ratio increases the maximum residence time decreases and the maximum VFA increases. We observed that as the stagnant region increases the maximum residence time increases and the maximum VFA decreases. We are currently extending the work presented here by considering the effect of incomplete mixing upon the performance of a cascade of anaerobic fermentors and by undertaking a sensitivity analysis of the model parameters.

ACKNOWLEDGEMENT

Ahmed Msmali grateful acknowledges the Saudi government through the awarding of a PhD scholarship. We dedicate this paper to the memory of our colleague Dr. Grant Cox (passed away March 2011).

REFERENCES

Dinopoulou, R.M.S Lester, G and Lester, J.N 1988, 'Anaerobic acidogenesis of a complex wastewater: Ii. kinetics of growth, inhibition, and product formation', *Biotechnology and Bioengineering*, vol. 31, pp 969–978.

Fleming J.G 2002, 'Novel simulation of anaerobic digestion using computational fluid dynamics', PhD thesis, Mechanical Engineering, Faculty of North Carolina State University.

Fogler, H.S 1999, *Elements of Chemical Reaction Engineering*, Prentice Hall, 3rd ed.

Kim J and Chung J 2010. 'A mathematical and empirical model of the performance of a membrane-coupled anaerobic fermentor', *Biodegradation*, DOI 10.1007/s10532-010-9441-1.

Shuler, M.L and Kargi, F 2002, *Bioprocess Engineering Basic Concepts*, Prentice Hall, 2nd ed.

BRIEF BIOGRAPHY OF PRESENTER

Ahmed is a PhD student in the School of Mathematics and Applied Statistics at the University of Wollongong. In 2009 he gained a master degree in applied mathematics from UoW. In 2005 he gained a bachelor degree in mathematics of education with distinction from Jazan University (Saudi Arabia).