

## The Effect of Incomplete Mixing on a Cubic Autocatalytic Reaction Model

A.A. Yakubu<sup>1</sup>, M.Y. Yatim<sup>2</sup>, F. Sulayman<sup>1</sup> and A. Abubakar<sup>1</sup>

<sup>1</sup>Department of Mathematics Ibrahim Badamasi Babangida University, Lapai, Niger State, Nigeria

<sup>2</sup>School of Mathematical Sciences, Universiti Sains Malaysia, P.O.Box 11800, Penang, Malaysia

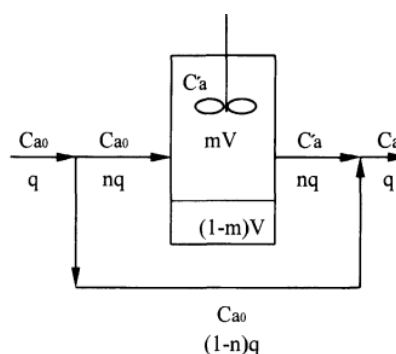
### ABSTRACT

The effect of incomplete mixing on a cubic autocatalytic reaction model with linear decay in a continuous stirred tank reactor (CSTR) is studied. The model comprises a system of nonlinear ordinary differential equation which describes the autocatalytic behavior of two chemicals (a reactant and an autocatalyst) flowing into the CSTR. When the system is affected by incomplete mixing, the concentration of the chemicals varies but then attains equilibrium state after a period of time. However, this depends on the adequate selection of resident time.

**Keywords:** Nonlinear ODE, Residence time, Continuous stirred tank reactor (CSTR)

### INTRODUCTION

The CSTR have been used widely to study the dynamic behavior of non-linear chemical systems according to bifurcation theory and singularity theory (Abasaheed,2000; Ariffin & Balasubramanian, 2013; Bishop & Locket, 2002; Crawford, 1991; King *et al.*, 2003, Logan, 2006). Though, these studies are generally based on ideal (complete) mixing (Gray & Scott, 1983; Gray & Scott, 1983; King *et al.*, 2003; Kogan, 2010). However, in most cases of reactor engineering models, the contents in the reactor are assumed to be perfectly mixed (Coker, 2001; Hayes & Mmbaga, 2012). When the reactor size is small, these assumptions may be good, but for a larger reactor, incomplete mixing is more likely to occur and therefore may affect the whole reaction process. Lo and Cholette (1983) investigated the multiplicity of a conversion in a cascade of incompletely mixing CSTR with an irreversible homogeneous exothermic first-order reaction. They concluded that for every parametric value, more than three steady states can exist. However, their study concentrated on the CSTR with only one feed while the CSTR with two feeds is mostly encountered in the chemical industry. Chien (2001) investigated the effect on by-passing the dead space of the Cholette's model represented in Fig 1.



**Fig 1** The schematic diagram of Cholette's model Chien (2001)

where  $C_{a0}$  is the inlet concentration from both influent and by-pass stream,  $m$  is the fraction of total volume in perfect mixing,  $n$  is the fraction of the feed entering the zone of perfect mixing  $V$  is the volume and  $q$  is the flow rate. The influence on the steady-state multiplicity and dynamic behavior of isothermal autocatalytic reaction but in the absence of the autocatalytic species was studied. Observation showed that the non-ideal parameters of the Cholette's model have a significant effect on the steady state stability. The study did not consider the probability of the autocatalyst decaying. In recent time, Msmali *et al.* (2012) studied the

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Address Correspondence to:

[aaishaty@ibbu.edu.ng](mailto:aaishaty@ibbu.edu.ng)

effect of incomplete mixing upon a quadratic autocatalytic reaction with the decay of the autocatalyst species and investigated how the reactor performance depends on upon the degree of mixing in the reactor. They noted that for very small values of the mixing parameter, the performance of the reactor is inferior to that of the reactor with no mixing between the two compartments.

In this paper, the effect of incomplete mixing of the CSTR is investigated on the cubic autocatalytic reaction model. Numerical simulations will be carried out in order to show the behavior of the chemicals in the reactor.

## THE MODEL FORMULATION

To analyse the model of a CSTR with an incomplete mixing, a two parameter mixing model will be considered. The reactor will be considered to have two well-mixed compartments. The compartments will be characterized by ‘a highly agitated’ region, where a complete mixing occurs and ‘a less agitated’ region where there is an incomplete mixing. The impeller is in the highly agitated region of the compartments (Scott Fogler, 1999). Fig 2 gives an illustration of reactor with both compartments.

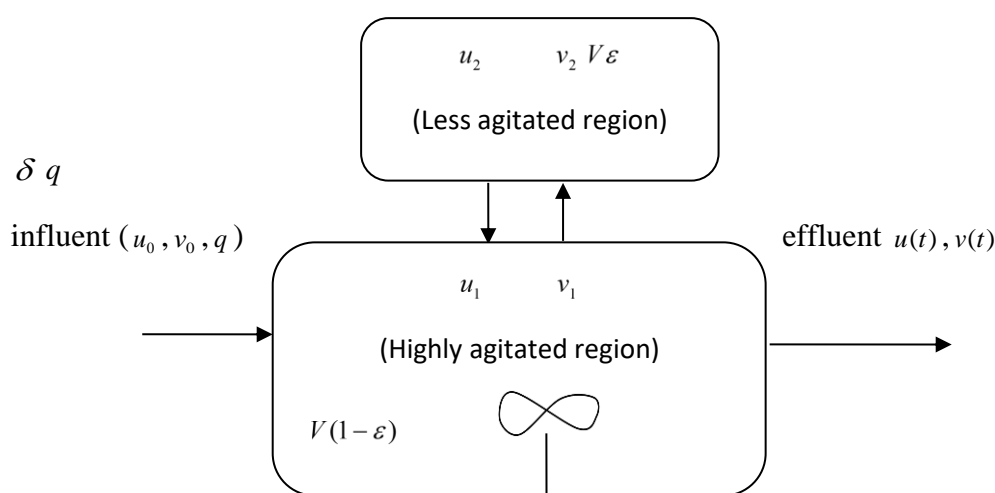


Fig2: Schematic diagram of a CSTR assuming incomplete mixing

where  $V$  is the volume of the reactor,  $q$  is the flow rate,  $u_1$  and  $v_1$  are the concentrations of the reactant and autocatalyst in the highly agitated region respectively,  $u_2$  and  $v_2$  are the concentrations of the reactant and autocatalyst in the less agitated region respectively,  $\delta$  is the strength of mixing and  $\varepsilon$  is the mixing parameter. The model is formulated using the law of conservation of mass balance which is mathematically expressed thus

$$V(1-\varepsilon)\frac{du_1}{dt} = q(u_0 - u_1) - V(1-\varepsilon)k_1u_1v_1^2 - q\delta(u_1 - u_2), \quad (1)$$

$$V(1-\varepsilon)\frac{dv_1}{dt} = q(v_0 - v_1) + V(1-\varepsilon)(k_1u_1v_1^2 - k_2v_1) - q\delta(v_1 - v_2), \quad (2)$$

Equation (1) and (2) are the system of ODE's representing the highly agitated region, while

(3) and (4) below represents that of the less agitated region.

$$V\varepsilon\frac{du_2}{dt} = q\delta(u_1 - u_2) - V\varepsilon k_1u_2v_2^2, \quad (3)$$

$$V\varepsilon\frac{dv_2}{dt} = q\delta(v_1 - v_2) + V\varepsilon(k_1u_2v_2^2 - k_2v_2). \quad (4)$$

where  $k_1$  and  $k_2$  are the reaction rate constant.

Dividing (1) and (2) by  $V(1-\varepsilon)$  and (3) and (4) by  $V\varepsilon$  gives

$$\frac{du_1}{dt} = \frac{q}{V(1-\varepsilon)}(u_0 - u_1) - k_1u_1v_1^2 - \frac{q}{V(1-\varepsilon)}\delta(u_1 - u_2), \quad (5)$$

$$\frac{dv_1}{dt} = \frac{q}{V(1-\varepsilon)}(v_0 - v_1) + k_1u_1v_1^2 - k_2v_1 - \frac{q}{V(1-\varepsilon)}\delta(v_1 - v_2), \quad (6)$$

$$\frac{du_2}{dt} = \frac{q}{V\varepsilon} \delta(u_1 - u_2) - k_1 u_2 v_2^2, \quad (7)$$

$$\frac{dv_2}{dt} = \frac{q}{V\varepsilon} \delta(v_1 - v_2) + k_1 u_2 v_2^2 - k_2 v_2. \quad (8)$$

$$x_i = \frac{u_i}{u_0}, \quad y_i = \frac{v_i}{u_0}, \quad \tau_{res} = k_1 u_0^2 t_{res}, \quad \tau = k_1 u_0^2 t,$$

$$\alpha = \frac{k_2}{k_1 u_0^2}, \quad \text{where } i = 0, 1, 2 \quad \text{and recall that } \frac{V}{q} = t_{res}.$$

**Non-Dimensional**

In this section the non-dimensional variables are defined in the form of

From the non-dimensional variables, it is seen that for  $u_i = u_0 x_i$  therefore  $\frac{du_i}{dt} = u_0 \frac{dx_i}{dt}$  and

also,  $v_i = u_0 y_i$  so that  $\frac{dv_i}{dt} = u_0 \frac{dy_i}{dt}$ .

Substitution of the non-dimensional variables into the equations (5)-(8) yields

$$u_0 \frac{dx_1}{dt} = u_0 \left( \frac{q}{V(1-\varepsilon)} (1-x_1) - k_1 x_1 u_0^2 y_1^2 - \frac{q}{V(1-\varepsilon)} \delta(x_1 - x_2) \right), \quad (9)$$

$$u_0 \frac{dy_1}{dt} = u_0 \left( \frac{q}{V(1-\varepsilon)} (y_0 - y_1) + k_1 x_1 u_0^2 y_1^2 - k_2 y_1 - \frac{q}{V(1-\varepsilon)} \delta(y_1 - y_2) \right) \quad (10)$$

$$u_0 \frac{dx_2}{dt} = u_0 \left( \frac{q}{V\varepsilon} \delta(x_1 - x_2) - k_1 x_2 u_0^2 y_2^2 \right) \quad (11)$$

$$u_0 \frac{dy_2}{dt} = u_0 \left( \frac{q}{V\varepsilon} \delta(y_1 - y_2) + k_1 x_2 u_0^2 y_2^2 - k_2 y_2 \right) \quad (12)$$

Applying chain rule to (9)-(12), i.e.,  $\frac{dx}{d\tau} = \frac{dx}{dt} \times \frac{dt}{d\tau}$ , where,  $t = \frac{\tau}{k_1 u_0^2}$  so that  $\frac{dt}{d\tau} = \frac{1}{k_1 u_0^2}$ . Thus, the system of ODE's containing the mixing parameter will be in the form of

$$\frac{dx_1}{d\tau} = \left( \frac{q}{V(1-\varepsilon)} (1-x_1) - k_1 x_1 u_0^2 y_1^2 - \frac{q}{V(1-\varepsilon)} \delta(x_1 - x_2) \right) \frac{1}{k_1 u_0^2},$$

$$\frac{dx_1}{d\tau} = \frac{(1-x_1)}{(1-\varepsilon)\tau_{res}} - x_1 y_1^2 - \frac{\delta(x_1 - x_2)}{(1-\varepsilon)\tau_{res}}. \quad (13)$$

$$\frac{dy_1}{d\tau} = \left( \frac{q}{V(1-\varepsilon)} (y_0 - y_1) + k_1 x_1 u_0^2 y_1^2 - k_2 y_1 - \frac{q}{V(1-\varepsilon)} \delta(y_1 - y_2) \right) \frac{1}{k_1 u_0^2},$$

$$\frac{dy_1}{d\tau} = \frac{(y_0 - y_1)}{(1-\varepsilon)\tau_{res}} + x_1 y_1^2 - \alpha y_1 - \frac{\delta(y_1 - y_2)}{(1-\varepsilon)\tau_{res}}. \quad (14)$$

$$\frac{dx_2}{d\tau} = \left( \frac{q}{V\varepsilon} \delta(x_1 - x_2) - k_1 x_2 u_0^2 y_2^2 \right) \frac{1}{k_1 u_0^2},$$

$$\frac{dx_2}{d\tau} = \frac{\delta(x_1 - x_2)}{\varepsilon\tau_{res}} - x_2y_2^2. \quad (15)$$

$$\frac{dy_2}{d\tau} = \left( \frac{q}{V\varepsilon} \delta(y_1 - y_2) + k_1x_2u_0^2y_2^2 - k_2y_2 \right) \frac{1}{k_1u_0^2},$$

$$\frac{dy_2}{d\tau} = \frac{\delta(y_1 - y_2)}{\varepsilon\tau_{res}} + x_2y_2^2 - \alpha y_2. \quad (16)$$

Equation (13) and (14) represents the system of ODE in the highly agitated region, while (15) and (16) is the system representing the less agitated region.

Taking this system at steady-state, i.e.,

$$\frac{dx_1}{d\tau} = \frac{dy_1}{d\tau} = \frac{dx_2}{d\tau} = \frac{dy_2}{d\tau} = 0, \text{ yield}$$

$$\frac{1-x_1}{(1-\varepsilon)\tau_{res}} - x_1y_1^2 - \frac{\delta(x_1-x_2)}{(1-\varepsilon)\tau_{res}} = 0, \quad (17)$$

$$\frac{y_0-y_1}{(1-\varepsilon)\tau_{res}} + x_1y_1^2 - \alpha y_1 - \frac{\delta(y_1-y_2)}{(1-\varepsilon)\tau_{res}} = 0, \quad (18)$$

$$\frac{\delta(x_1-x_2)}{\varepsilon\tau_{res}} - x_2y_2^2 = 0, \quad (19)$$

$$\frac{\delta(y_1-y_2)}{\varepsilon\tau_{res}} + x_2y_2^2 - \alpha y_2 = 0. \quad (20)$$

The dynamics of these equations will be studied to have an insight on the behavior of the system when affected with incomplete mixing.

### STABILITY ANALYSIS

At steady-state, the system (17)-(20) has two solution branches, the washout solution which is given by

$$(x_{1w}, y_{1w}, x_{2w}, y_{2w}) = (1, 0, 1, 0) \quad (21)$$

and the no-washout solution

$$(x_{1nw}, y_{1nw}, x_{2nw}, y_{2nw}) = (x_1, y_1, x_2, y_2) \quad (22)$$

where the subscript  $w$  and  $nw$  refer to washout and no washout respectively. For the steady-state which has the washout solution, it implies that there is a concentration of the reactant that will give an equilibrium solution and no concentration of the autocatalyst. That is at the inflow, the autocatalyst is absent. While for the no washout solution, the concentration of the reactant and autocatalyst is given by

$$x_1 = \frac{1+x_2\delta}{1+y_1\tau_{res}(1-\varepsilon)+\delta}$$

$$y_1 = \frac{y_0+y_2\delta}{1+(-1+\varepsilon)(x_1-\alpha)\tau_{res}+\delta}$$

$$x_2 = \frac{x_1\delta}{y_2\varepsilon\tau_{res}+\delta}$$

$$y_2 = -\frac{y_1\delta}{\varepsilon(x_2-\alpha)\tau_{res}-\delta}$$

However the stability of the system will be checked before proceeding to the simulation analysis, this is done by determining the nature of eigenvalues of the Jacobian matrix.

For the washout solution, the jacobian matrix is evaluated and this gives

$$J(1,0,1,0) = \begin{pmatrix} \frac{1+\delta}{(\varepsilon-1)\tau_{res}} & 0 & \frac{\delta}{\tau_{res}(1-\varepsilon)} & 0 \\ 0 & \frac{1+\alpha\tau_{res}(1-\varepsilon)+\delta}{(\varepsilon-1)\tau_{res}} & 0 & \frac{\delta}{\tau_{res}(1-\varepsilon)} \\ \frac{\delta}{\varepsilon\tau_{res}} & 0 & -\frac{\delta}{\varepsilon\tau_{res}} & -1 \\ 0 & \frac{\delta}{\varepsilon\tau_{res}} & 0 & 1-\alpha-\frac{\delta}{\varepsilon\tau_{res}} \end{pmatrix}.$$

The determinant is given by

$$\det(J) = \frac{\delta(-\varepsilon(\alpha-1)\tau_{res}(-1+(\varepsilon-1)\alpha\tau_{res})+\delta+(\alpha-\varepsilon)\tau_{res}\delta)}{(\varepsilon-1)^2\varepsilon^2\tau_{res}^4},$$

and the trace is given by

$$tr(J) = \frac{\varepsilon(2+(\varepsilon-1+2\alpha-2\varepsilon\alpha)\tau_{res})+2\delta}{(\varepsilon-1)\varepsilon\tau_{res}}.$$

The roots of the characteristic polynomial are given by the eigenvalues

$$\lambda_1 = -\frac{\varepsilon+\delta-\sqrt{\varepsilon^2-2\varepsilon\delta+4\varepsilon^2\delta+\delta^2}}{2\varepsilon\tau_{res}(1-\varepsilon)}$$

$$\lambda_2 = -\frac{\varepsilon+\delta+\sqrt{\varepsilon^2-2\varepsilon\delta+4\varepsilon^2\delta+\delta^2}}{2\varepsilon\tau_{res}(1-\varepsilon)}$$

$$\lambda_3 = -\frac{\varepsilon-(-1+\varepsilon)\varepsilon(-1+2\alpha)\tau_{res}+\delta-\sqrt{\varepsilon^2(1+\tau_{res}-\varepsilon\tau_{res})^2-2\varepsilon(-1+2\varepsilon)(-1+(-1+\varepsilon)\tau_{res})\delta+\delta^2}}{2\varepsilon\tau_{res}(1-\varepsilon)}$$

$$\lambda_4 = -\frac{\varepsilon-(-1+\varepsilon)\varepsilon(-1+2\alpha)\tau_{res}+\delta+\sqrt{\varepsilon^2(1+\tau_{res}-\varepsilon\tau_{res})^2-2\varepsilon(-1+2\varepsilon)(-1+(-1+\varepsilon)\tau_{res})\delta+\delta^2}}{2\varepsilon\tau_{res}(1-\varepsilon)}$$

The roots of the characteristics polynomial are negative, thus, it implies that the solution is stable. However, numerical computations on the stability of the eigenvalues was checked when complete mixing occurs at  $\varepsilon=0$  and when incomplete mixing occurs,  $0<\varepsilon<1$ . The state when complete mixing occurs  $\varepsilon=0$  implies that both the highly agitated and low agitated region respectively, are the same. The analysis shows that when there is complete mixing, the system is stable as  $\lambda_i < 0$ , with  $i=1,2,3,4$  and this is same as one of the equilibrium points  $P_1=(1,0)$  in (Yakubu&Yatim, 2015). However, for the

incomplete mixing case, the system is unstable because one of the eigenvalue of the characteristics polynomial is positive. However, when the washout solution is stable, it is not physically meaningful.

### Numerical Simulations In The Absence Of Autocatalyst ( $y_0=0$ ).

The numerical simulation of the reaction model without autocatalyst but with the mixing parameter will be discussed in this section. The analysis is will be carried out on the system using *Mathematica software*, considering when there is both complete ( $\varepsilon=0$ ) and incomplete mixing ( $0<\varepsilon<1$ ) (Msmaliet *al.*, 2012). For

this analysis, the residence time  $\tau_{res} = 5$ . The simulation results will be represented diagrammatically.

**Table1** Concentration values of reactants for complete mixing without autocatalyst, for (a)  $\tau_{res} = 5$  and (b)  $\tau_{res} = 10$ , when ( $\varepsilon = 0$  and  $\delta = 10^4$ )

(a)  $\tau_{res} = 5$

$\tau$	$x_1 = x_2$
0	0.6
10	0.945866
20	0.992674
30	0.999008
40	0.999866
50	0.999982
60	0.999998
70	1
80	1
90	1
100	1

(b)  $\tau_{res} = 10$

$\tau$	$x_1 = x_2$
0	0.6
15	0.910748
30	0.980085
45	0.995556
60	0.999008
75	0.999779
90	0.999951
105	0.999989
120	0.999998
135	0.999999
150	1

Table 1 presents the concentration values of the reactant for complete mixing without the autocatalyst. It is observed that there is an

**Table 2(a)** Concentration values of reactants for incomplete mixing without autocatalyst, for (a)  $\tau_{res} = 5$  and (b)  $\tau_{res} = 10$ , when ( $\varepsilon = 0.3$  and  $\delta = 0.2$ )

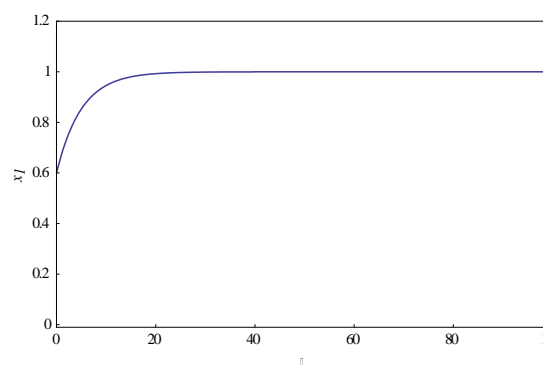
(a)  $\tau_{res} = 5$

$\tau$	$x_1$	$x_2$
0	0.6	0.6
15	0.970723	0.881144
30	0.993845	0.974045
45	0.998663	0.994357
60	0.999709	0.998773
75	0.999937	0.999733
90	0.999986	0.999942
105	0.999997	0.999987
120	0.999999	0.999997
135	1	0.999999
150	1	1

(b)  $\tau_{res} = 10$

$\tau$	$x_1$	$x_2$
0	0.6	0.6
25	0.961007	0.847407
50	0.989746	0.956844
75	0.997132	0.987897
100	0.999196	0.996607
125	0.999775	0.999049
150	0.999937	0.999733
175	0.999982	0.999925
200	0.999995	0.999979
225	0.999999	0.999994
250	1	0.999998

increase in the concentration of reactant which implies that a new product is formed. The table also shows that both concentration of reactants in the two different compartments of the reactor are the same, i.e.,  $x_1 = x_2$ . It is also observed that even with the introduction of the mixing parameter to the reaction model, the same result is yield as (Yakubu&Yatim, 2015). The graphical representation is seen in Fig 3.



**Fig 3** Behavior of reactant in the absence of autocatalyst with complete mixing ( $\varepsilon = 0$  and  $\delta = 10^4$ )

The analysis carried out for the incomplete mixing is shown in Tables 2 (a), (b) and (c), with different values of the mixing parameter. In this case, there is a difference in the concentration of reactants in the different compartments.

**Table 2(b)** Concentration values of reactants for incomplete mixing without autocatalyst, (a)  $\tau_{res} = 5$  and (b)  $\tau_{res} = 10$ , when ( $\varepsilon = 0.5$  and  $\delta = 0.2$ )

(a)  $\tau_{res} = 5$ 

$\tau$	$x_1$	$x_2$
0	0.6	0.6
25	0.982378	0.908501
50	0.996495	0.981799
75	0.999303	0.996379
100	0.999861	0.99928
125	0.999972	0.999857
150	0.999995	0.999972
175	0.999999	0.999994
200	1	0.999999
225	1	1
250	1	1

(b)  $\tau_{res} = 10$ 

$\tau$	$x_1$	$x_2$
0	0.6	0.6
40	0.975646	0.873622
80	0.993313	0.965276
120	0.998163	0.990459
160	0.999495	0.997379
200	0.999861	0.99928
240	0.999962	0.999802
280	0.99999	0.999946
320	0.999997	0.999985
360	0.999999	0.999996
400	1	0.999999

**Table 2(c)** Concentration values of reactants for incomplete mixing without autocatalyst, for (a)  $\tau_{res} = 5$  and (b)  $\tau_{res} = 10$ , when ( $\varepsilon = 0.9$  and  $\delta = 0.2$ )

(a)  $\tau_{res} = 5$ 

$\tau$	$x_1$	$x_2$
0	0.6	0
35	0.95903	0.76265
70	0.99037	0.94421
105	0.99774	0.98689
140	0.99947	0.99692
175	0.99988	0.99928
210	0.99997	0.99983
245	0.99999	0.99996
280	1	0.99999
315	1	1
350	1	1

(b)  $\tau_{res} = 10$ 

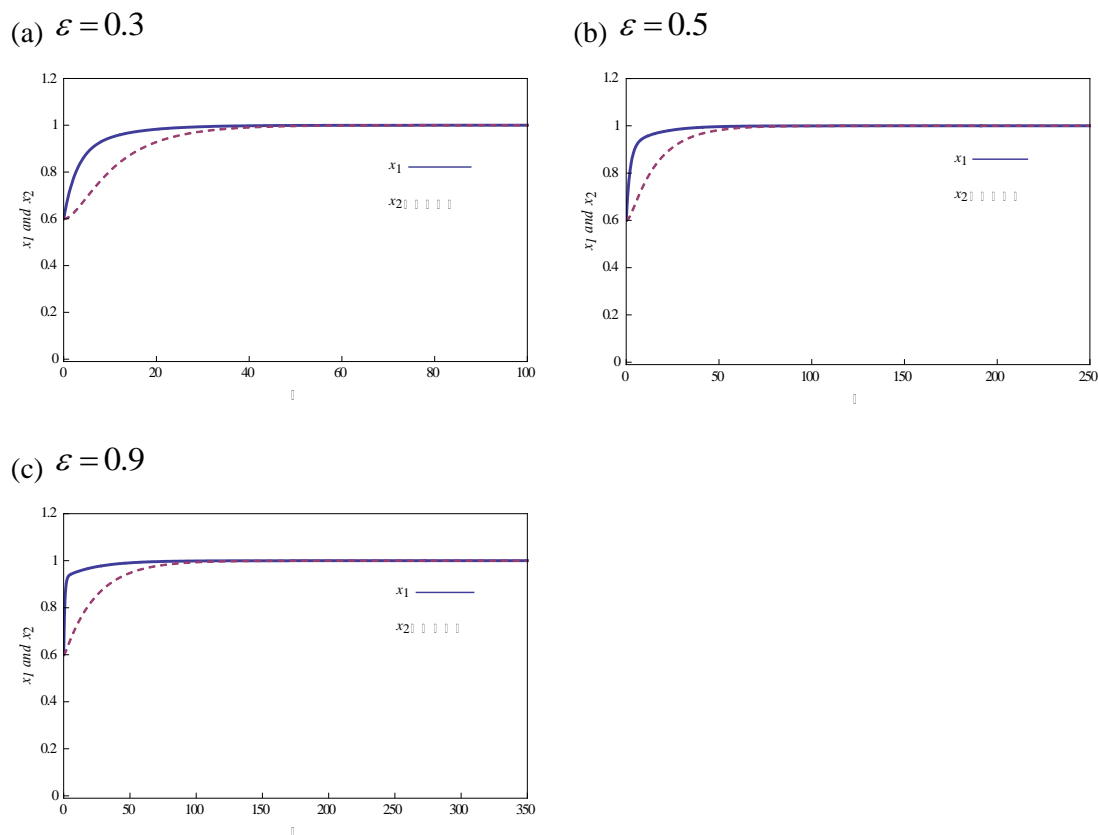
$\tau$	$x_1$	$x_2$
0	0.6	0.6
50	0.974584	0.85276
100	0.990965	0.947656
150	0.996788	0.981392
200	0.998858	0.993385
250	0.999594	0.997648
300	0.999856	0.999164
350	0.999949	0.999703
400	0.999982	0.999894
450	0.999994	0.999962
500	0.999998	0.999987

From the analysis, it is seen from the Tables that the concentration varies as  $x_1 > x_2$  for every given dimensionless time ( $\tau$ ). The table also reveals an interesting behavior of the concentration of the chemicals. When there is

an increase in the mixing parameter, the conversion of the reactants to reach an equilibrium state is been delayed. Also during the analysis, it is observed that concentration of the chemicals reach a state of equilibrium faster when the residence time selected is small. Considering the two cases of complete and

incomplete mixing, there is a smooth transition of the concentration until it reaches an equilibrium point, however, the slight difference in concentration of the reactant

makes the difference in the two cases as  $x_2$  takes a longer time before reaching equilibrium. Fig 4 displays the concentration difference of both reactants in the different compartments.



**Fig 4** Behavior of the reactants in the absence of autocatalyst for incomplete mixing with different mixing parameter values at (a)  $\epsilon = 0.3$ , (b)  $\epsilon = 0.5$  and (c)  $\epsilon = 0.9$  at  $\delta = 0.2$

**Numerical Simulations In The Presence Of Autocatalyst** ( $y_0 > 0$ ).

In the presence of autocatalyst the case becomes more interesting as the behavior of both chemicals is seen in Table 3 and Tables 4(a), (b) and (c). The Tables show the concentration values of both reactant and autocatalyst for complete and incomplete mixing (with different mixing parameter values). The behavior of both concentrations with complete mixing is illustrated in Figure 5. The simulation analysis is the same as in section 5 except for the inclusion of autocatalyst in this section.



**Table 3** Concentration values of reactants and autocatalyst for complete mixing with autocatalyst, for (a)  $\tau_{res} = 5$  and  $\tau_{res} = 10$ , when ( $\varepsilon = 0$  and  $\delta = 10^4$ )

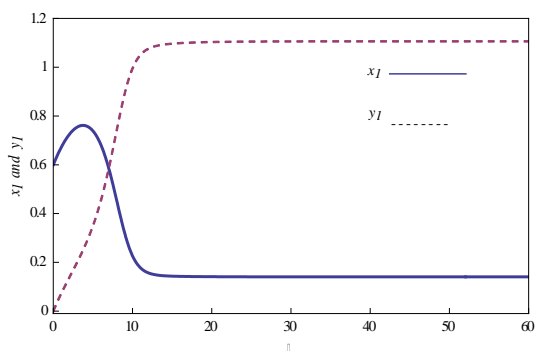
(a)  $\tau_{res} = 5$

$\tau$	$x_1 = x_2$	$y_1 = y_2$
0	0.6	0
5	0.738726	0.349608
10	0.226377	0.995257
15	0.143444	1.0963
20	0.141285	1.1031
25	0.140777	1.10501
30	0.140624	1.1056
35	0.140577	1.10577
40	0.140563	1.10583
45	0.140559	1.10585
50	0.140558	1.10585
55	0.140557	1.10585
60	0.140557	1.10585

(b)  $\tau_{res} = 10$

$\tau$	$x_1$	$x_2$
0	0.6	0
10	0.52219	0.539907
20	0.087823	1.02095
30	0.086761	1.0262
40	0.086529	1.02752
50	0.086469	1.02787
60	0.086453	1.02797
70	0.086448	1.02799
80	0.086447	1.028
90	0.086447	1.028
100	0.086447	1.028
110	0.086447	1.028
120	0.086447	1.028

The concentration of the reactant in both compartments are equal, same also for the autocatalyst in both compartments. However, the concentration of the reactant increases at a point in time then suddenly decreases to reach an equilibrium state. This is one of the characteristic of an autocatalytic reaction, thus, implying its total decomposition in the reaction. The autocatalyst concentration on the other hand increases with increase in time until it full decomposes there by reaching an equilibriumstate, the graphical illustration is seen in Fig 5.



**Fig5** Behavior of reactant and autocatalyst in the presence of autocatalyst with complete mixing ( $\varepsilon = 0$  and  $\delta = 10^4$ )

For the incomplete mixing, the values of the corresponding chemicals of both compartments vary as concentration of the chemicals in the highly agitated region is more than that of the less agitated region. This can be observed in Tables 4.4 (a),(b) and (c). Figure 4.5 (a),(b) and (c) reveals the behavior of the chemicals for the incomplete mixing.

**Table 4(a)** Concentration values of reactants and autocatalyst for complete mixing with autocatalyst when ( $\varepsilon = 0.3$  and  $\delta = 0.2$ )

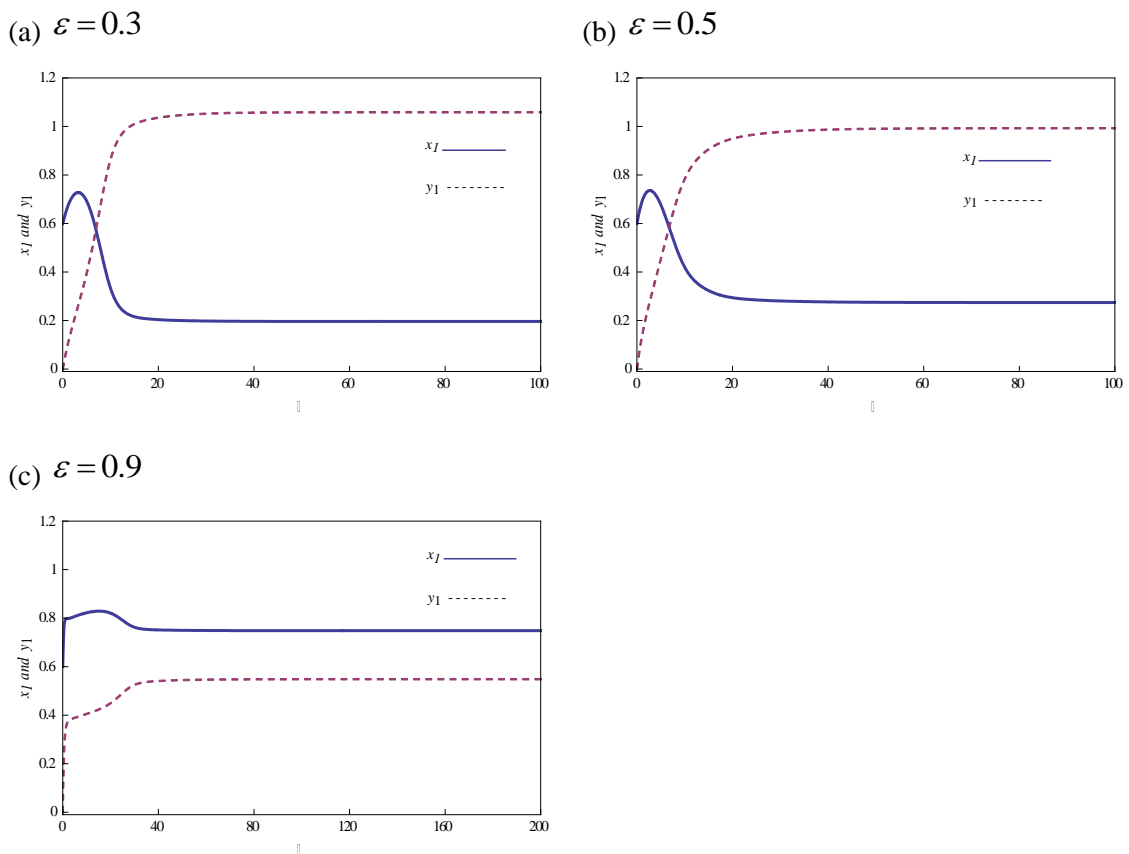
$\tau$	$x_1$	$y_1$	$x_2$	$y_2$
0	0.6	0	0	0
10	0.332473	0.864292	0.306262	0.460305
20	0.203625	1.03601	0.027207	0.948479
30	0.198043	1.05255	0.023387	1.00112
40	0.196639	1.0569	0.022571	1.01488
50	0.19627	1.05805	0.022362	1.01853
60	0.196172	1.05835	0.022307	1.01949
70	0.196146	1.05843	0.022292	1.01975
80	0.196139	1.05846	0.022288	1.01982
90	0.196138	1.05846	0.022287	1.01984
100	0.196137	1.05846	0.022287	1.01984

**Table 4(b)** Concentration values of reactants and autocatalyst for complete mixing with autocatalyst when ( $\varepsilon = 0.5$  and  $\delta = 0.2$ )

$\tau$	$x_1$	$y_1$	$x_2$	$y_2$
0	0.6	0	0	0
10	0.41954	0.78377	0.28584	0.29362
20	0.29404	0.94985	0.04305	0.77777
30	0.28065	0.97739	0.02726	0.87096
40	0.27665	0.98686	0.02487	0.90296
50	0.27516	0.99047	0.02404	0.91523
60	0.27458	0.99187	0.02373	0.91997
70	0.27436	0.9924	0.02362	0.9218
80	0.27428	0.99261	0.02357	0.92251
90	0.27424	0.99269	0.02355	0.92278
100	0.27423	0.99272	0.02355	0.92289

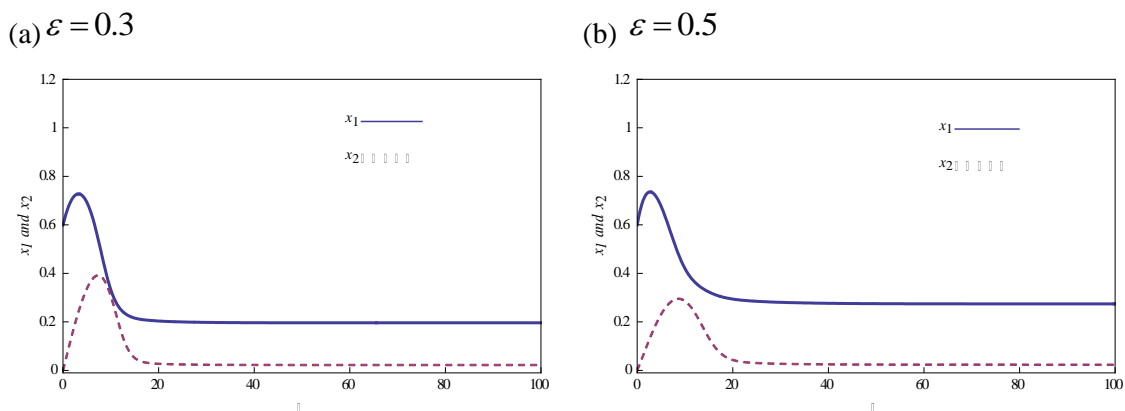
**Table 4(c)** Concentration values of reactants and autocatalyst for complete mixing with autocatalyst when ( $\varepsilon = 0.9$  and  $\delta = 0.2$ )

$\tau$	$x_1$	$y_1$	$x_2$	$y_2$
0	0.6	0	0	0
20	0.820696	0.449647	0.329615	0.331197
40	0.751507	0.540919	0.058089	0.734783
60	0.749105	0.546539	0.053905	0.758096
80	0.748555	0.547881	0.053038	0.763671
100	0.748419	0.548213	0.052828	0.765047
120	0.748386	0.548295	0.052776	0.765388
140	0.748377	0.548315	0.052763	0.765472
160	0.748375	0.54832	0.05276	0.765493
180	0.748375	0.548322	0.052759	0.765499
200	0.748375	0.548322	0.052759	0.7655

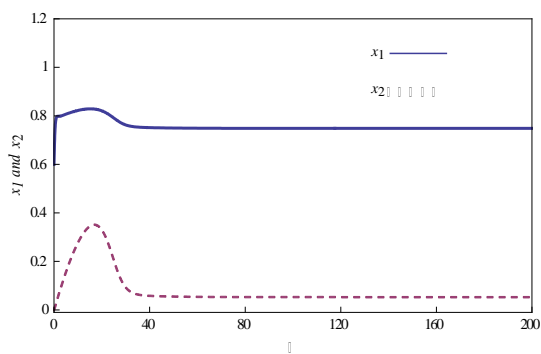


**Figure 6** Behavior of the reactants and autocatalyst in the presence of autocatalyst for incomplete mixing with different mixing parameter values at (a)  $\epsilon = 0.3$ , (b)  $\epsilon = 0.5$  and (c)  $\epsilon = 0.9$  at  $\delta = 0.2$

From the simulation carried out, it is observed that there is slight difference in the concentration of the chemicals and moreso, the diagrams show that the concentration of the reactant will always decrease until it reaches a state of equilibrium, while the autocatalyst will increase then later decrease so as to reach completion thereby forming the final product. This analysis is compared with the previous analysis carried out in (Yakubu&Yatim, 2015) were the mixing parameter is not included and it has the same characteristics. The behavior of the reactant and autocatalyst in each compartment with different mixing parameter value is illustrated in Fig 7 and Fig 8, respectively.

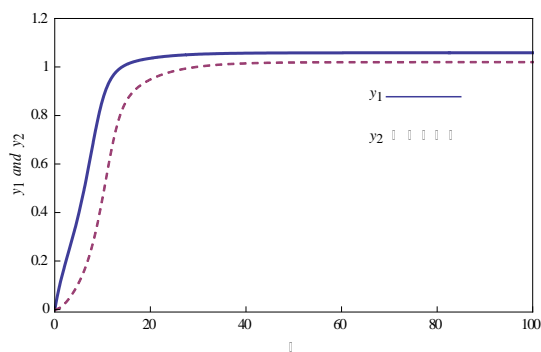


(c)  $\varepsilon = 0.9$

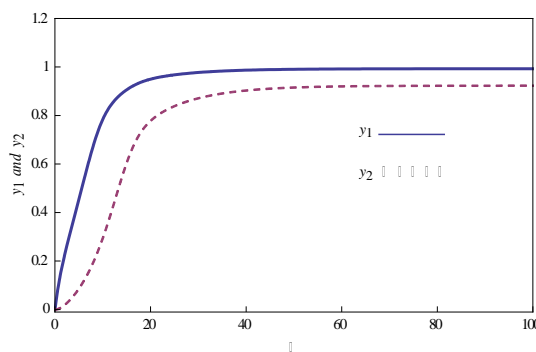


**Fig 7** Behavior of the reactants in the presence of autocatalyst for incomplete mixing with different mixing parameter values at (a)  $\varepsilon = 0.3$ , (b)  $\varepsilon = 0.5$  and (c)  $\varepsilon = 0.9$  at  $\delta = 0.2$

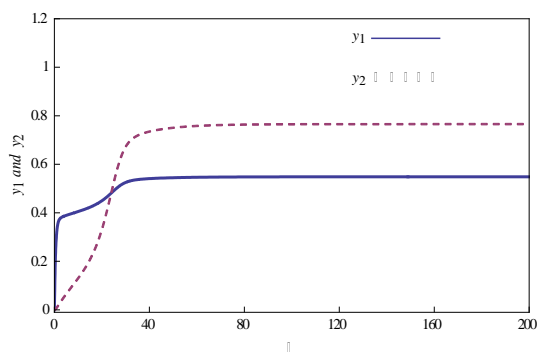
(a)  $\varepsilon = 0.3$



(b)  $\varepsilon = 0.5$



(c)  $\varepsilon = 0.9$



**Figure 8** Behavior of the autocatalyst in the presence of autocatalyst for incomplete mixing with different mixing parameter values at (a)  $\varepsilon = 0.3$ , (b)  $\varepsilon = 0.5$  and  $\varepsilon = 0.9$  at  $\delta = 0.2$

**Conclusion**

In this paper, a brief introduction was given about the reactor and its behavior as regards to mixing, a schematic diagram was also drawn to enable one understand the nature of movements of the reaction. Then the dynamics of the

reaction model was carried out were results were drawn based on the analysis. It is obvious that all concentration will reach an equilibrium point only that this will happen at various times as shown in the analysis. This has really proved

the characteristic of a continuous flow stirred tank reactor as concentration in the tank is equal to the out flow concentration. It was also noted during the course of analysis that when the residence time selected is high the longer it takes for the reaction to reach completion, but the smaller the residence time chosen, the faster the reaction, thus, saves time. The same also applies when the mixing parameter is large the faster it is for the reaction to reach completion but then considering a large reactor tank this might cause a breakdown of the impeller.

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