

MODELING OF CONTINUOUS OSCILLATORY BAFFLED REACTOR FOR BIODIESEL PRODUCTION FROM JATROPHA OIL

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ABSTRACT

The aim of this paper is model the continuous Oscillatory Baffled flow Reactor for biodiesel production from Jatropha oil. It presents the prediction of the number of serially arranged ideal stirred tank reactors (N), that will have an equivalent performance as an Oscillatory baffled flow reactor using Tanks –in-Series Model approach. The results show that the number of tanks in series was predicted to be 5.6 by the model which is almost equivalent to the experimental number of tanks in the oscillatory baffled reactor with a baffle number of seven and consequently having number of tanks to be six. The significance of 5.6 tanks, means that this non-ideal Oscillatory flow reactor under study could be represented by six ideal stirred tanks arranged in series with the same flow rate of 0.098m³ / hr. The combined volume (size) of the six tanks must however, be equal to that of the Oscillatory baffled flow reactor. From this analysis, it would be more economical to use a single OFR than using about six tanks of the CSTR for the given reaction because the average percentage error between the experimental and simulated results was about 5%.

Keywords: Modeling, Oscillatory Baffled Reactor, Biodiesel, Jatropha Oil.

INTRODUCTION

Oscillatory flow reactors (OFRs) consist of tubes fitted with equally spaced orifice plate baffles. A through flow is applied to the reactor, and an oscillatory fluid motion is superimposed on the entire volume of the fluid in the reactor, such that the interaction of the fluid with the baffle geometry generates highly effective mixing within each interbaffle cavity, as well as along the length of the reactor as a whole (Harvey et al,2003).

OFR offers a means to perform reactions which require long reaction times (of order hours) in a reactor of greatly reduced length-to-diameter ratio(Nasratun et al, 2010). This is achieved while maintaining plug-flow residence time distribution (RTD) characteristics, effective mixing, and high heat- and mass-transfer rates (Mackley and Stonestreet, 1995; Hewgil et al,1993). Such requirements are difficult to achieve (for long reaction time processes) in tubular reactors relying on throughput alone to achieve mixing (Stonestreet and Harvey,2002). These features make it possible to consider performing certain reactions continuously, which previously were only possible in batch(Harvey et al,2001). Oscillatory flow in baffled tubes has been studied for many years and much work have been done in areas related to fluid dynamics, heat and mass transfer and residence time distribution(Anh et al, 2011;Nasratun et al, 2011) . Many advantages have been characterized for oscillatory flow mixing, such as efficient dispersion for immiscible fluids, uniform particle suspension, gas-in-liquid dispersions and multiphase mixing (Mauri and Reinaldo,2003). Recent researches have indicated that oscillatory flow in a baffled tube has significant potential for process and product enhancement in a wide range of application. However, little have been done on

modeling and simulation of conversion in oscillatory baffled flow reactor. Hence, this paper presents the modeling and simulation of conversions in an oscillatory baffled flow reactor using Tanks –in-Series Model approach for biodiesel production.

MATERIALS AND METHODOLOGY

Equipment

The oscillatory baffled flow reactor (non-ideal) consist of six baffles and has a volume of 100 L (0.1m³). The volumetric flow rate of the combined streams of A and B was 0.098m³ / hr. A salt (KCl) tracer was injected at the inlet to the reactor, and the concentration-time behaviour was measured on-line at the outlet, using a flow cell, conductivity meter, and data logging system. The injection was assumed to approximate to a perfect pulse injection, which was reasonable given the time scale of experiment (>10min). Data on the residence time distribution (RTD) behaviour of the laboratory scale oscillatory flow reactor was collected as shown in Figure 1 to investigate and quantify the relative contributions of the oscillatory flow and bulk flow components in the baffled tube reactor (Anh et al,2011).

Modeling

To better understand the reactor behaviour and to be able to simulate reactor operation, a flow –conversion model has to be developed using the well established technique of combining reaction kinetics and Residence Time Distribution (RTD) information (Levenspiel, 1999). The model consists of two sections: a fluid mechanic model and chemistry model.

Fluid Mechanics Model

For the fluid-mechanics model, a standard tanks-in series approach was used as the basis for the reactor flow-conversion model. The main advantage of this approach is the simplicity with which the kinetics can be incorporated (Harvey et al, 2001). The premise of the model is to represent the baffled tube as a series of ideal CSTRs, the number of which defines the RTD characteristics.

In this model the RTD data otherwise known as tracer data, was obtained from a pulse tracer experiment carried out on OFR (Oscillatory Flow Reactor) from literature. The result was used to determine the number of equal sized ideal continuous stirred tank reactor (CSTR) arranged in series. The number of ideal stirred tanks that will fit the RTD data of the OFR simply means the number of ideal CSTR in series that will be equivalent to the OFR. This one parameter model, for specificity can be regarded as “tank in series model”. And, the only adjustable parameter to be extracted from the residence time distribution (RTD), data is the number of tanks in series (N) (Stonestreet and Vander, 1999).

Let consider three equal sized ideal CSTRs in series (Figure1). If a pulse tracer experiment is carried out on these three tanks in series, then from RTD function (Levenspiel 1999), the fraction of tracer material leaving the last tank between time t and t+Δt will be

$$E(t) = \frac{C_3(t)}{\int_0^{\infty} C_3(t) dt} \dots\dots\dots 1$$

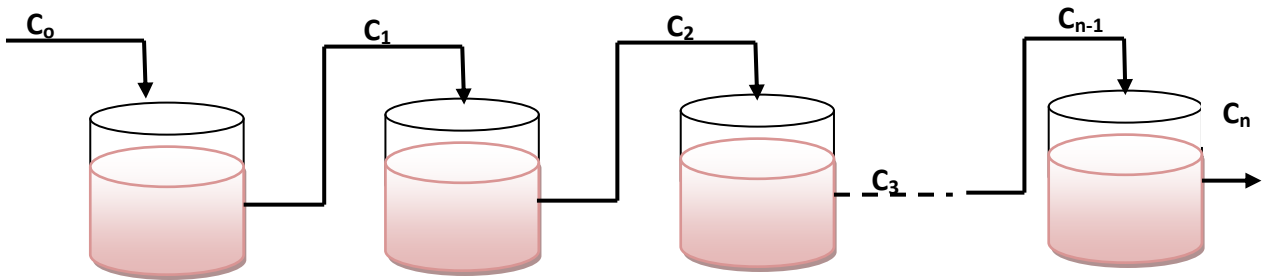


Figure 1: infinite Tank in series

where C_3 is the concentration of tracer material exiting the system (3^{rd} tank); $E(t)$ is the RTD function. The outlet concentration of tracer material, $C_3(t)$ as a function of time, can be obtained by carrying out material balance around each of the tanks. From the principle of conservation of mass;

$$Input = Output + Disappearance + Accumulation \dots\dots\dots 2$$

For a steady state system, there is no accumulation, therefore;

$$Input = Output + Disappearance \dots\dots\dots 3$$

Equation 3 can be expressed in rate form. Taking a material balance around a continuous stirred tank;

$$v_{in}C_{in} = v_{out}C_{out} + V \frac{dC_{out}}{dt} \dots\dots\dots 4$$

where V is the volume of the tank; v is the volumetric flow rate and C is the tracer concentration. From the three identical tanks in series, the volumetric flow rate v_1 is constant i.e. $v_{in}=v_{out}$ for each of the tanks. The volume V of each of the tanks is also identical i.e. $V_1=V_2=V_i$. Therefore, the space time τ_1 of the individual reactors is also identical, since the space time for ideal CSTR is the ratio of volume to volumetric flow rate, i.e. $\tau_1 = \tau_2 = \tau_i$.

Where the subscript 1,2 and i represents the first, second and i^{th} tank respectively. Taking the material balance round tank 1 (Fig. 2) gives;

$$vC_0 = vC_1 + V \frac{dC_1}{dt} \dots\dots\dots 5$$

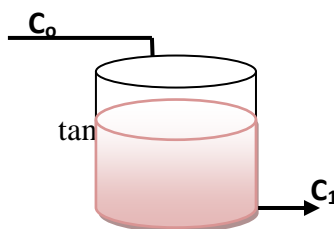


Figure 2:Material Balance over tank1

where C_o is the inlet concentration to tank 1; C_1 is the out let concentration from tank1. For a pulse tracer experiment, C_o as a function of time is zero. Therefore, equation 5 becomes;

$$-vC_1 = V_1 \frac{dC_1}{dt} \dots\dots\dots 6$$

$$C_1 = C_o e^{-vt/v_1} \dots\dots\dots 7$$

For ideal CSTR, the space time is given as;

$$\tau = \frac{V}{v} \text{ or } \tau_1 = V_1/v \dots\dots\dots 8$$

$$C_1 = C_o e^{-t/\tau_1} \dots\dots\dots 9$$

The material balance on tracer around tank 2 will be;

$$vC_1 = vC_2 + V_1 \frac{dC_2}{dt} \dots\dots\dots 10$$

Dividing through by V_i and then substituting equation 7 and 8 into equation 10 gives a first order ordinary differential equation;

$$\frac{dC_2}{dt} + \frac{C_2}{\tau_i} = \frac{C_o}{\tau_i} e^{-t/\tau_i} \dots\dots\dots 11$$

Using an integrating factor, e^{-t/τ_i} along with the initial condition $C_2=0$ ant $t=0$ gives;

$$C_2 = \frac{C_o t}{\tau_i} e^{-t/\tau_1} \dots\dots\dots 12$$

By taking material balance on tracer around tank 3, we have

$$vC_2 = vC_3 + V_i \frac{dC_3}{dt} \dots\dots\dots 13$$

Or

$$\frac{dC_3}{dt} + \frac{C_3}{\tau_i} = \frac{C_o}{\tau_i^2} e^{-t/\tau_i} \dots\dots\dots 14$$

or

$$C_3 = \frac{\frac{C_o t^2 e^{-t/\tau_1}}{2\tau_i^2}}{\int_0^\infty \frac{C_o t^2 e^{-t/\tau_1}}{2\tau_i^2}} \dots\dots\dots 15$$

Substituting equation 15 into 1 we obtain;

$$E(t) = \frac{\frac{C_o t^2 e^{-t/\tau_1}}{2\tau_i^2}}{\int_0^\infty \frac{C_o t^2 e^{-t/\tau_1}}{2\tau_i^2}} \dots\dots\dots 16a$$

$$E(t) = \frac{t^2 e^{-t/\tau_1}}{\int_0^\infty t^2 e^{-t/\tau_1} dt} \dots\dots\dots 16b$$

By applying integration by part (Stroud 1995), equation 16b becomes;

$$E(t) = \frac{t^2 e^{-t/\tau_1}}{2\tau_i^3} \dots\dots\dots 17$$

This is the RTD function for three tanks in series. Generalizing this method for a series of n CSTR gives the RTD function as;

$$E(t) = \frac{t^{n-1} e^{-t/\tau_1}}{(n-1)! \tau_i^n} \dots\dots\dots 18$$

The RTD function can be normalized by expressing in dimensionless time scale as (Levenspiel, 1999);

$$\theta = t/\tau \dots\dots\dots 19$$

Equation 18 becomes;

$$E(\theta) = \frac{n(n\theta)^{n-1} e^{-n\theta}}{(n-1)!} \dots\dots\dots 20$$

The variance, σ^2 , of the RTD data from tracer experiment is given by (Levenspiel 1999);

$$\sigma^2 = \int_0^\infty (t - tm)^2 E(t) dt \dots\dots\dots 21$$

Expressing this variance as dimensionless variance, $\sigma^2\theta$, gives;

$$\sigma^2\theta = \frac{\sigma^2}{\tau^2} = \int_0^\infty (\theta - 1)^2 E(\theta) d\theta \dots\dots\dots 22$$

Expanding equation 22 gives;

$$\sigma^2\theta = \int_0^\infty \theta^2 E(\theta) d\theta - 2 \int_0^\infty \theta E(\theta) d\theta + \int_0^\infty E(\theta) d\theta \dots\dots\dots 23$$

$$\int_0^\infty E(\theta) d\theta = 1 \dots\dots\dots 24$$

Since the fraction of all the materials that has resided for a period of time, t, in the reactor between t=0 and t = ω is 1 . Therefore;

$$\sigma^2\theta = \int_0^\infty \theta^2 E(\theta) d\theta - 1 \dots\dots\dots 25$$

Substituting equation 20 into 25 gives;

$$\sigma^2\theta = \int_0^\infty \theta^2 \frac{n(n\theta)^{n-1} e^{-n\theta}}{(n-1)!} d\theta - 1 \dots\dots\dots 26a$$

$$\sigma^2\theta = \frac{n^n}{(n-1)!} \int_0^\infty \theta^{n+1} e^{-n\theta} d\theta - 1 \dots\dots\dots 26b$$

Integrating will give;

$$\sigma^2\theta = \frac{n^n}{(n-1)!} \left[\frac{(n+1)!}{n^{n+2}} \right] - 1 \dots\dots\dots 27a$$

$$\sigma^2\theta = \frac{1}{n} \dots\dots\dots 27b$$

Taking the dimensionless variance back to time gives;

$$\frac{\sigma^2}{\tau^2} = \frac{1}{n} \dots\dots\dots 28$$

$$n = \frac{\tau^2}{\sigma^2} \dots\dots\dots 29$$

The number of tanks in series is given by n, where τ is the space-time in the combined tanks in series, but it is equivalent to the mean residence time, tm, in the OFR.

Chemical Reaction Model

This model is basically used for the chemical reaction taking place in the OFR. With this model it is possible to predict the outlet concentration, and then the conversion of a particular reactant taking part in the chemical reaction in the OFR. Unlike the first model, this model is not too general, because it is dependent on the order of reaction. But, its flexibility is that, it can be developed for any order of reaction depending on which reaction is taking place in the OFR (Harvey et al, 2001).

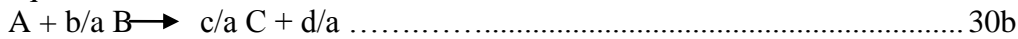
Having determined the number of tanks in a series performing a sequential mole balance around each of the tanks to obtain the outlet concentration. For a steady state ideal CSTR, there is no accumulation therefore, equation 3 will still hold for the material balance around the tanks (Luyben 1990; Aweh 2002). For a second order reaction, taking place in the n ideal tanks in series, of the form;



The rate expression is;

-r_A = K C_A C_B 31a

where a, b, c, and d are the stoichiometric coefficients, and if reactant A is taken as reference, equation 30 can be written as;



Taking a mole balance on reactant A around tank 1 will be;

$$F_{A0} = F_{A1} + V_1(-r_A)_1 \dots\dots\dots 32$$

Where F_{A0} is the molar flow rate of reactant A into the reactor, tank 1(moles/time); F_{A1} is the molar flow rate of reactant A out of tank 1(moles/time); V_1 is the volume of tank; $(-r_A)_1$ is the rate of disappearance of reactant A in tank 1 [moles/(volume x time)]; K is the specific rate constant; C_A , C_B are the concentrations of reactants A and B respectively (moles/volume); and $-r_A$ is the rate of disappearance of reactant A [moles/(volume x time)].

$$(-r_A)_1 = K C_{A1} C_{B1} \dots\dots\dots 31b$$

The molar flow rate is;

$$F_{A0} = vC_{A0} \text{ and } F_{A1} = vC_{A1} \dots\dots\dots 33$$

Substituting equation 31b and 33 into 32, we have;

$$vC_{A0} = vC_{A1} + V_1 K C_{A1} C_{B1} \dots\dots\dots 34$$

where v is the volumetric flow rate (volume/time) and C_{A1} , C_{B1} are the concentrations of reactants A and B respectively in tank 1 (moles/volume). Substituting equation 3.8 ($\tau_1 = V_1/v$) into 3.34 gives;

$$\tau_1 K C_{A1} C_{B1} = C_{A0} - C_{A1} \dots\dots\dots 35$$

From the principle of chemical engineering, conversion of reactant A, X_A , is given by (Himmelblau 1996);

$$X_A = (C_{A0} - C_A) / C_{A0} \dots\dots\dots 36$$

$$C_{A1} = C_{A0} - C_{A0} X_{A1} \dots\dots\dots 37$$

$$\text{and } C_{B1} = C_{B0} - b/a C_{A0} X_{A1} \dots\dots\dots 38$$

Where C_{A0} , C_{B0} are the inlet concentrations of A and B. equation 37 can be rearranged as;

$$C_{A0} X_{A1} = C_{A0} - C_{A1} \dots\dots\dots 39$$

Substituting equation 39 into 38 gives;

$$C_{B1} = C_{B0} - b/a C_{A0} + b/a C_{A1} \dots\dots\dots 40a$$

$$C_{B1} = \Delta C_o + b/a C_{A1} \dots\dots\dots 40b$$

$$\text{Where } \Delta C_o = C_{B0} - b/a C_{A0} \dots\dots\dots 41$$

Substituting equation 3.40b into 3.35 gives;

$$K \tau_1 C_{A1} (\Delta C_o + b/a C_{A1}) = C_{A0} - C_{A1} \dots\dots\dots 42a$$

$$b/a K \tau_1 C_{A1} + (K \tau_1 \Delta C_o + 1)C_{A1} - C_{A0} = 0 \dots\dots\dots 42b$$

Equation 42b is a quadratic equation of the form

$$ax^2 + bx + c = 0 \dots\dots\dots 43$$

This can be solved by the general formula;

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \dots\dots\dots 44$$

Therefore, C_{A1} , C_{A2} and C_{An} can be solved. It can be generalized that for n tanks in series, the outlet concentration of reactant A from the nth tank is;

$$C_{An} = \frac{-(K\tau_1\Delta C_o + 1) \pm \sqrt{(K\tau_1\Delta C_o + 1)^2 - 4(\frac{b}{a})k\tau_1 C_{An-1}}}{2(\frac{b}{a})k\tau_1} \dots\dots\dots 45$$

Using the overall conversion of reactant A in the n tanks in series (Himmelblau, 1996);

Equation 29 and combination of equations 45 to 46 forms the mathematical model of the Oscillatory Flow Reactor in which a second order reaction is taking place. The behaviour predicted for this model were analysed and the results were simulated .

RESULTS AND DISCUSSION

The mathematical model developed so far is for a second order liquid phase chemical reaction-taking place in an oscillatory flow reactor. To verify these model equations, the simulated result from the model was compared with practical / experimental data of a second order transesterification reaction of Jatropa oil taking place in a non-ideal oscillatory flow reactor of a biodiesel plant. The major reaction taking place in this reactor (as given in Eq. 2) involve the reaction of triglyceride with alcohol in the present of catalyst to give glycerol and methyl esters, this can simply be represented as:



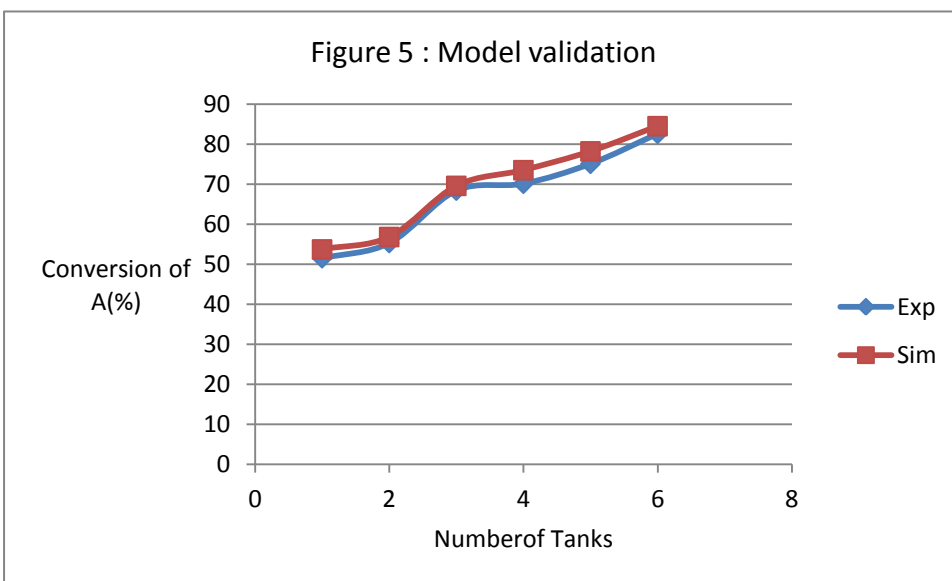
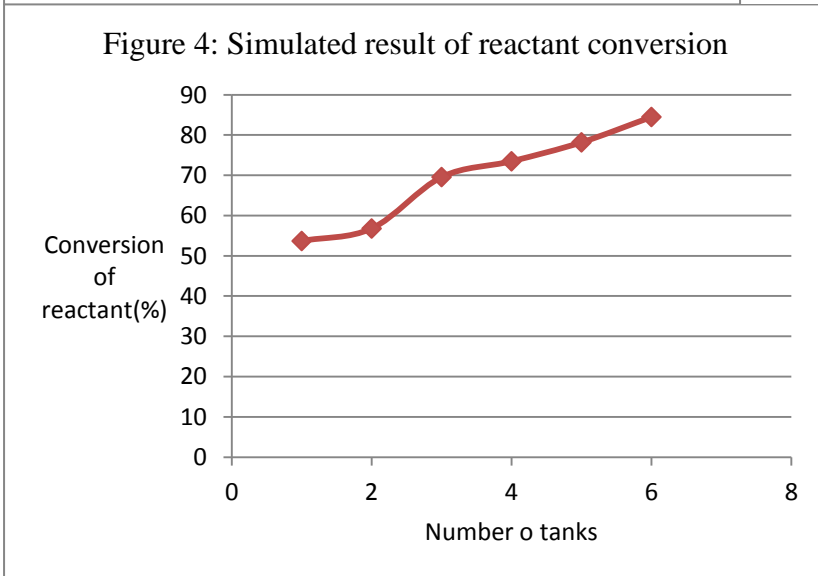
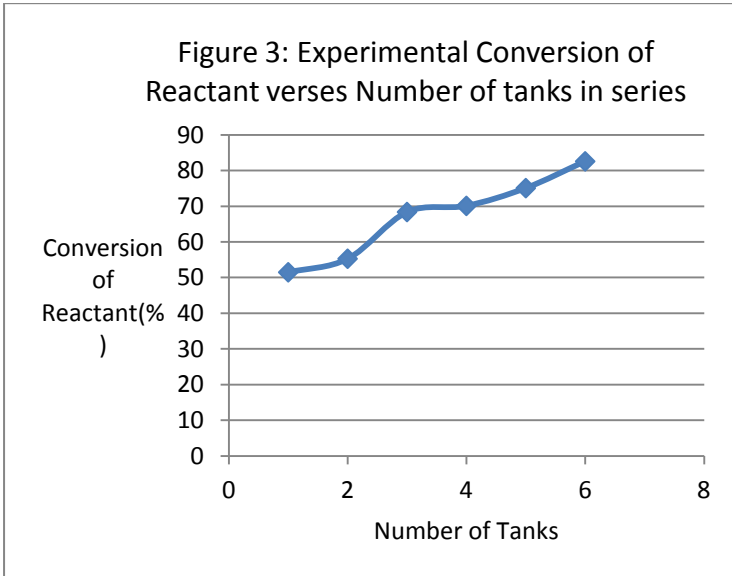
Where A= triglyceride (or $C_3H_5O_3(COR)_3$), B= alcohol (or C_2H_5OH), C = glycerol (or $C_3H_8O_3$) and D = methyl esters (or R_3COOH_3)

An iterative graphical procedure was used to perform the simulation, using Microsoft Excel for data processing and graph plotting. This involved generating the dimensionless E-curve for experimental concentration-time profiles of the experiment, and to compare these with predicted E-curve from tanks-in-series model. The number of tanks-in-series (N) which gave the best match by overlap on the E-curve to the experimental data was then taken as the model fit. An advantage of this method is that by comparing the span and height of the experimental and model E-curves it can be clearly seen if the tanks-in-series model is valid, whereas with calculation methods, a value of N can be obtained irrespective of whether the model is appropriate or not. The actual number of baffled cavities in the two pass reactor configuration is 6, which represents the ideal value for N assuming each baffle cavity behaves as a perfect stirred tank. In reality, it is expected that the experimentally determined values will all be less than ideal, but the closer to $N = 6$, the closer the system will be to ideal behaviour.

Table 1: Simulated result of the pulse traer Experiment

	Time (min)	CA ₃ (mol/m ³)	E(t)	tE(t)	(t-τ) ²	(t-τ) ² E(t)
	0	0	0	0	14.44	0
	1	10	0.05	0.05	7.84	0.392
	2	20	0.1	0.2	3.24	0.324
But	3	30	0.15	0.45	0.64	0.096
	4	15	0.075	0.3	0.04	0.003
Also	5	50	0.25	1.25	1.44	0.36
σ ² =	6	40	0.2	1.2	4.84	0.968
From	7	10	0.05	0.35	10.24	0.512
σ ² =	8	20	0.1	0.8	17.64	1.764
Thus	9	5	0.025	0.225	27.04	0.676
	10	0	0	0	38.44	0

From the simulated result of the RTD data, σ^2 was found to be 2.6



The comparison of the simulated and experimental results shows that the experimental outlet concentration and conversion of A were lower than those of the simulated. This deviation was consistent. The percentage error ranges from 5.25-11.41%. The causes of the observed errors might be associated with the fact that the model did not take into account the nature of the reactants, their concentration activeness, viscosity and other parameters that have effects on the reaction. The model developed also gives a prediction of the number of serially arranged ideal stirred tank reactors, n , that will have an equivalent performance as a Continuous Oscillatory Baffled flow reactor the size of which would be equal to that of the combined tanks. Simulation of equation 29 shows that the number of tanks in series would be 5.6. The significance of 5.6 tanks, means that this Continuous Oscillatory Baffled flow reactor under study could be represented by six ideal stirred tanks arranged in series with the same flow rate of $0.098 \text{ m}^3 / \text{hr}$. The first 5 tanks are of the same size (identical) and the 6th tank is 0.6 of the 5th tank in size (Aweh 2002; Luyben 1990). The combined volume (size) of the six tanks must however, be equal to that of the Oscillatory flow reactor. From this analysis it would be more economical to use a single OFR than using about six tanks of the CSTR for the given reaction.

CONCLUSION

The mathematical model for the operation of Continuous oscillatory flow reactor has been developed. The model was used to generate simulated results for a non-ideal oscillatory flow reactor of a biodiesel plant. In the process of simulation, it was found out that 5.6 identically sized ideal stirred tanks operating in series would have an equivalent performance with the non-ideal plug flow reactor.

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