Design and Development of Mathematical Model for Static Mixer

Rajamanickam, Akila*+

Department of Mathematics, Anna University, Guindy, Chennai – 600 025, Tamilnadu, INDIA

Balu, Krishnaswamy

A.C. College of Technology, Anna University, Chennai, Tamilnadu, INDIA

ABSTRACT: *A numerical model for simulating Residence Time Distribution (RTD) of turbulent flows in helical static mixers is proposed and developed to improve the understanding of static mixers. The results of this model is presented in terms of different volumetric flow rate to illustrate the complicated flow patterns that drive the mixing process in helical static mixers. The computed results are also used to predict the amount of mixing that occurs within a mixing device. Such theoretical estimates need, however, always to be thoroughly checked against observations in static mixer. To check the reliability of the theoretically estimated RTD from the simulation by the application of the model equation, a comparison of the same with those obtained from observed data experiments in static mixer using statistical characteristics is done. Comparison between RTD curves shows that motionless mixture can improve the performance of reactor.*

KEY WORDS: *Mathematical simulation; Mean residence time distribution; Static mixer.*

INTRODUCTION

Every industrial chemical process is designed to produce economically a desired product from a variety of starting raw materials through a succession of treatment steps. The products of chemical reaction undergo further physical treatment such as separating, purification etc., for the final desired product to be obtained. Chemical treatment steps are conducted in vessels known as reactors, which are stirred tank reactors (backmix reactors) and plug flow reactors. Actual reactors deviate from these idealised concepts. The deviation is due to non-uniform velocity profile, velocity fluctuation due to molecular or turbulent diffusion, short circuiting of fluid elements, bypassing and channelling, presence of stagnant regions due to reactor shape and internals, and recycling of fluid elements within the reactor as a result of agitation. The discrete (stagewise) backmixing model was considered as the best model representing residence time behaviour in the small-scale tube (*Chen*, 1971) [1]. Mathematical modelling coupled with rigorous statistical methods has been of great assistance in understanding and quantifying the flow in a reactor as it is critical for predicting performance of the reactor.

Motionless or static mixers are widely known and applied in process technologies for the mixing of liquids,

** To whom correspondence should be addressed.*

+ E-mail: akilarajamanikam@yahoo.com

1021-9986/16/1/109 8/$/2.08

especially for highly viscous materials, and to contact different phases to enhance heat and mass transfer. A list of commercial static mixers and their applications has been described by *Bor* (1971) [2], *Champernowne* (1956) [3], *Chandarana & Unverferth* (1996) [4], and *Charbel Habchi et al.*, (2010) [5]. Comparison of compared 12 different static mixer types has been made by *Pahl & Muschelknautz* (1982) [6], but considering only global properties, like pressure drop and overall mixing efficiency.

The fluid flow and RTD curves were solved using a commercial CFD code FLUENT 6.3(FLUENT Inc.). The results indicated that RTD was influenced by mass flow rate at inlet and stirring speed. The tubular reactor with a stirrer could improve the flow profile by narrowing the RTD curve, creating high Reynolds number, and avoiding back mixing (CAO *Xiao-Chang et al.* 2008) [7]. The turbulent chemical reactors as a network of stirred tanks and taking the interstage flows to be stationary Markov processes, *Krambeck et al.* (1967) [8] have developed the stochastic models of RTDs of turbulent flow and mixing systems based on the random walk assumption. Adoption of a broader class of Markov processes, birthdeath processes, has enabled *Shinnar & Naor* (1967) [9] to propose a more general method of calculating the residence-time distributions for systems with internal reflux. By introducing the concept of joint probability distribution for the number of recycles and the residence time, the total regional residence-time distribution for a continuous recycle system involving either a single unit or a cascade has been analyzed and characterized by *Mann et al.* (1979) [10], *Mann & Rubinovitch* (1981) [11]. *Rubinovitch & Mann* (1983a, b, 1985) [12,13] have presented Markov chain model for analyzing particulate processes. *Nauman* (1982) [14] has applied the theories of discrete and continuous random walks to the open systems governed by the dispersion equation. Fan and his colleagues have treated the arbitrary complex networks of stirred tanks by a general continuous-time compartmental model (*Fan et al*, 1996, 1995) [15,16] and by the master equation approach (*Fox & Fan* 1984) [17].

As the flow of fluids through a static mixer undergoes three types mechanisms, namely: (a). flow division, (b). flow reversal and (c). Flow combination. Due to continuous flow division, flow reversal and flow combination at every element of the mixer the parabolic velocity profile cannot get established and therefore ideal plug flow conditions are approached. Hence the static mixer can be utilised for any process application of tubular chemical reactors where the provision of narrow residence time is important. We also need efficient methods to estimate the RTD and the sole means of achieving this is through detailed mathematical modelling. Such theoretical estimates need, however, always to be thoroughly checked against observations in static mixer. This is a rather difficult task, since methods to estimate RTD from observations are not unique and can be subjected to strong criticism. The results of the model—the predicted RTD—are presented in terms of different volumetric flow rate to illustrate the complicated flow patterns that drive the mixing process in helical static mixers. The computed results are also used to estimate the amount of mixing that occurs within a mixing device. The Mathematical model presented in this paper is a part of a larger study on the use of static mixers for chemical reaction.

METHODOLOGY

The tubular flow reactor consists of an outer pyrex tube of 1210 mm in length and 35 mm inner diameter provided with two inlets at one end opposite to each other and inclined at 45˚ with the axis of the tube. The inlet is 15mm in diameter. Four intermediate outlets are provided at 212mm apart, along the length of the tube. These exits serve as manometer tappings for pressure drop experiments and would be used to turn out reactor effluent at intermediate length of the tube when conversion experiments are carried out. Alternatively, they would also be used to insert thermometer with slight modification, when the heat transfer experiments are conducted. Those exits not in use are normally kept closed by spring-type inch cocks on flexible rubber tube fitted on to the side exits. The Tubular flow reactor with helical mixing elements, as schematically shown Fig. 1.

Concentric with the outer pyrex tube is an inner tube of 22.4 mm outer diameter, 18.5mm inner diameter. A brass flange brazed to the tube is bolted to a corresponding perpex flange, fastened to the pyrex tube with an adhesive. To the brass tube the helical elements are brazed. Each element consists of two 0.8mm brass sheets 6.2mm wide, carefully cut and twisted to form part of a helix of 60mm pitch. The elements are of half a pitch in length i.e. 30mm. These are brazed to the outer

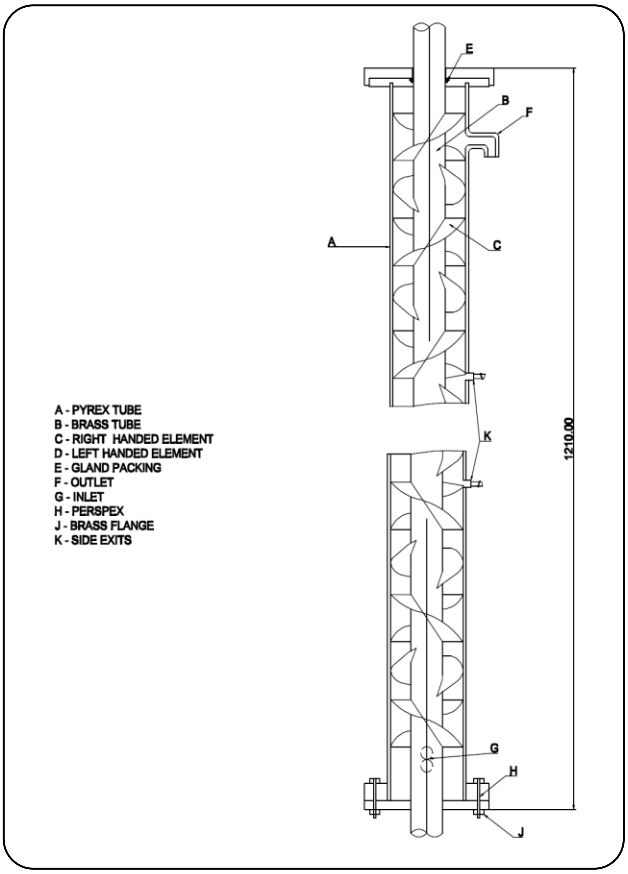

Fig.. 1. Tubular flow reactor with helical mixing elements with increasing flow rate.

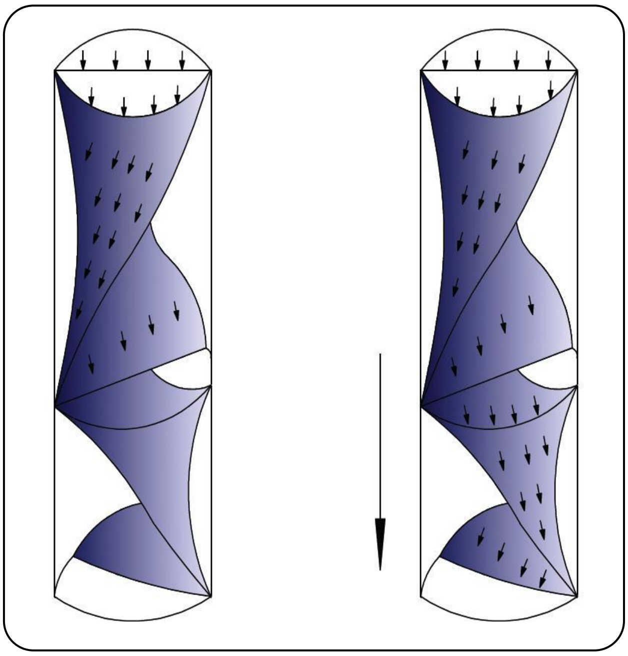

Fig. 2: Flow of fluid in the tubular reactor with helical element.

circumference of the tube 180˚ apart, alternative elements are right-handed and left-handed and each one is at right angles to the adjacent ones as shown in the Fig. .2. In all, the reactor contains thirty five elements, seventeen left-handed and eighteen right-handed. The cross-section of the flow channels on the two sides of a mixer element changes continuously along its length: the cross-sectional area on one side expands while on the other side it contracts as shown in the Fig. 3.

The Residence Time Distribution (RTD) for the unit is determined by measuring the response to a near pulse input. Water from the over head tank is allowed to flow through the unit. When the steady state is reached, the tracer is introduced into the reactor inlet. A hypodermic needle No.22 is used to inject 1 ml of tracer (nearly 5N sodium bicarbonate solution) in the reactor inlet. Samples of reactor effluent are collected at frequent intervals (of 5 seconds). From the quantity of sample collected, a small quantity of sample (10 mL) is titrated against a 0.05 N Aluminum sulfate solution. The volume of silver nitrate consumed is directly proportional to the concentration of sodium chloride solution in the outlet stream. The sample collection is done for sufficient time interval (for t>5E, where E is the average retention time). The above experiments are repeated until concordant litre values are obtained. The flow rate is then varied and the above mentioned procedure is repeated. For the annulus with mixing elements the flow rate range covered is 40-120 L/h, as above 120 L/h, the average retention time was very low to detect any appreciable change in concentration within the time intervals of collection period. The above experiments are conducted in a similar manner in the annulus without mixing elements.

In order to determine the RTD(E(θ)) for the static mixer, we consider a simpler situation where perfect mixing, constant density, steady state etc. prevails. We then look for the red tagged reactant in the out flow stream to determine residence time of the reactant in the tank.

NUMERICAL SIMULATION

The technique requires the use of an RTD model that best describes the behaviour of the flow within the reactor system; the model that best fits the experimental RTD data is obtained by determining the parameter values that minimize a suitable objective function. An objective

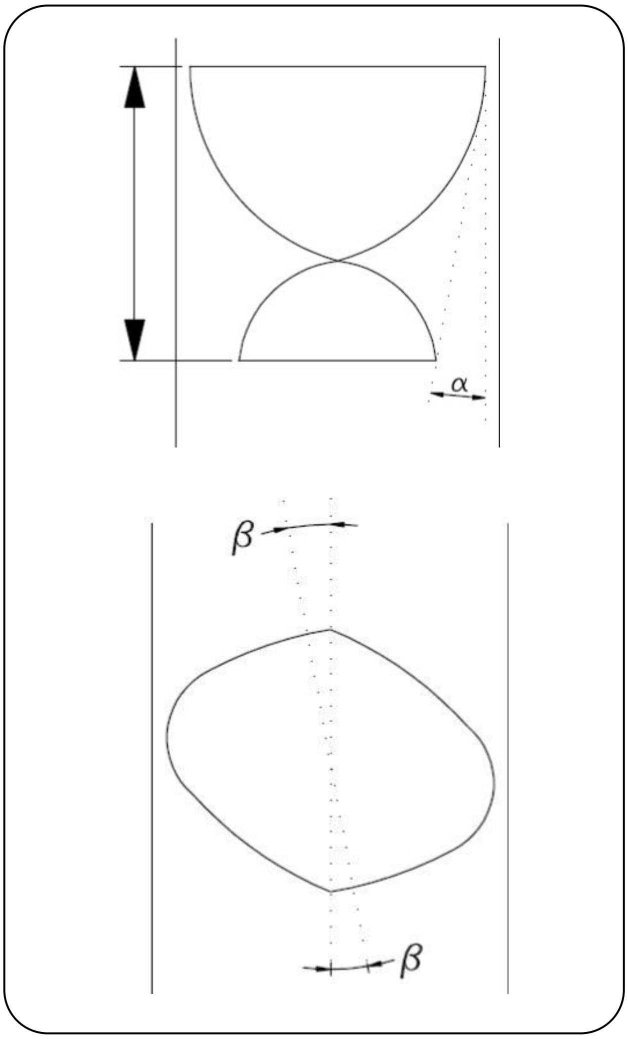

Fig. 3: The Fluid Flow Pattern in the Tubular Reactor with Helical Element (Parabolic Path/Exponential Path).

function would be one such as the minimization of the mean square deviation between the experimental and calculated values of the response curves. The value of the optimization function will be an indication of the quality of fit between the experimental data and model and can determine the choice of model to be used. This technique is more thorough, but if there are more than two parameters, the optimization techniques require complex, iterative computations and may give rise to indefinite solution (*Gianetto et al.*, 1978) [18].

The model formulated and developed is based on fluid flow pattern in the tubular reactor with helical element and takes into account mass transfer resistances across static mixer. The model also presents residence time distribution for all the major reactions.

As the flow of fluids through a static mixer undergoes three types mechanisms, namely: (a). flow division, (b). flow reversal and (c). Flow combination. Due to continuous flow division, flow reversal and flow combination at every element of the mixer the parabolic velocity profile cannot get established and therefore ideal plug flow conditions are approached. Accordingly by the above mechanism (shown in Figs. 2 and 3), in tubular reactor with brazed helical mixing elements (Fig. 1), the fluid flow pattern is assumed to be a combination of parabolic path $y_1(\theta)=\theta^2$ and exponential path $y_2(\theta) = e^{-\gamma\theta^2}$ (as shown in the Fig. 3). Taking both the path into account, the governing equations of exit age distribution for tubular flow reactor is stated as

$$E(\theta) = \beta\theta^2 e^{-\gamma\theta^2} \qquad (1)$$

where $\beta, \gamma > 0$, θ is the residence time and $E(\theta)$ is the residence time distribution. The RTD was calculated numerically by the governing equation.

To check the reliability and the quality of the theoretically estimated RTD from the simulation by the application of the Ricker equation, we compare them with those obtained from observed data using statistical characteristics.

The mean of $E(\theta)$ is given by

$$\mu = \frac{\beta}{2\gamma^2} \qquad (2)$$

Maximum value of $E(\theta)$ is attained at $\theta = \sqrt{\frac{1}{\gamma}}$ and the value of $E(\theta)$ at this point is

$$E\left(\sqrt{\frac{1}{\gamma}}\right) = \frac{\beta}{\gamma e} \qquad (3)$$

The variance of $E(\theta)$ is

$$\sigma^2 = \frac{\beta}{4\gamma^2}\left(\frac{3}{2\sqrt{\gamma}}\pi - \frac{\beta}{\gamma^2}\right) \qquad (4)$$

The prediction of RTD is based on the numerical solution of the β and γ values in the Equation (1). The variations of the β and γ values can give reliable results for turbulence flow, is also applied in flow predictions in plug flow reactors. The RTD was calculated numerically by the governing equation. The simulation of RTD

Table 1: Comparison between numerical and experimental data of mean residence time and variance.

Flow rate, l/hr	Mean residence time		Variance, σ^2	
	Experimental	Simulated	Experimental	Simulated
40 l/hr	1.800063	1.00009	0.04135	0.05483
60 l/hr	1.000098	0.87204	0.04513	0.03665
80 l/hr	0.999776	0.760715	0.062059	0.06191
100 l/hr	0.799557	0.675673	0.07536	0.08860
120 l/hr	0.699791	0.585346	0.08766	0.08150

has been carried out by injecting a pulse of a tracer at the inlet. To check the reliability and the quality of the theoretically estimated RTD from the simulation by the application of the governing equation, we compare them with those obtained from observed data using statistical characteristics.

The experimental concentration verses time curves were used to get information about the mean fluid residence time, the variance of distributions σ^2, and normalized form of residence time distribution functions $E(\theta)$ at the exit of tubular reactor with brazed helical static mixer. From the experimental values of $E(\theta)$, the Maximum point, mean μ and σ^2 of RTD are computed for different volumetric flow rate(40-120 L/h). These values were utilised to determine the β and γ values. The long-term behaviour of a RTD by governing equation is dependent on volumetric flow rate.

RESULTS AND DISCUSSION

Analysis of fluid field

Under the effect of static mixer, the distribution of residence time shows that the flow field is very turbulent. In the visualization of segmental system, the fluid flows along the axial and helical mixing. It is demonstrated that the residence time increases in the tubular reactor with Brazed Helical element. Different optimum residence time is obtained at different inlet flow rates. The optimum volumetric inlet flow rate is 40 L/h.

Characteristics and profiles of RTD functions

The experimental concentration verses time curves were used to get information about the mean fluid residence time, the variance of distributions, σ^2, and normalized form of residence time distribution functions $E(\theta)$ at the exit of tubular reactor with brazed helical static mixer. Fig. 4 shows the comparison of the RTD curves by simulations with experimental data for an amplification of different volumetric flow rates in tubular reactor with brazed helical element, in which the two are coincide, especially at low flow rate, indicating that the governing equation approach used in this work is reliable for simulating the RTD curves of the tubular reactor with brazed helical static mixer. From the graphs we can infer that the change in Residence Time Distribution (RTD) calculated using the simulated values and experimental values agree well.

Table 1 shows the comparison between experimental and simulated result of mean residence time and variance. From Table 1, the variance and mean residence time of residence time distribution decreases by increasing the fluid flow rate. The $E(\theta)$ curves show the presence of stagnant zones. When the maximum of $E(\theta)$ appears at $\theta < 1$, it indicates the presence of short-circuits; while the maximum of $E(\theta)$ appears at $\theta > 1$, it indicates the presence of the back mixing. The width of RTD curve is an appropriate measurement to determine the approach to plug flow (*Champernowne*, 1956 [4], *Chandarana*, 1996 [14] and *Charbel Habchi*, 2010 [5]). Standard Error Estimation between Experimental RTD and Calculated RTD obtained for tracer in a turbulent reactor with brazed helical elements with different volumetric flow rates are shown in Table 2.

Fig. 5 shows the numerical RTD curves at different volumetric flow rate. Only one maximum of the curve appear with Brazed Helical element by simulation prediction. The Residence time distribution curve is narrow with helical elements, where the flow is shown to approach to plug flow conditions. Although brazed helical static mixer can narrow the RTD curve and improve the performance of the reactor, increasing flow

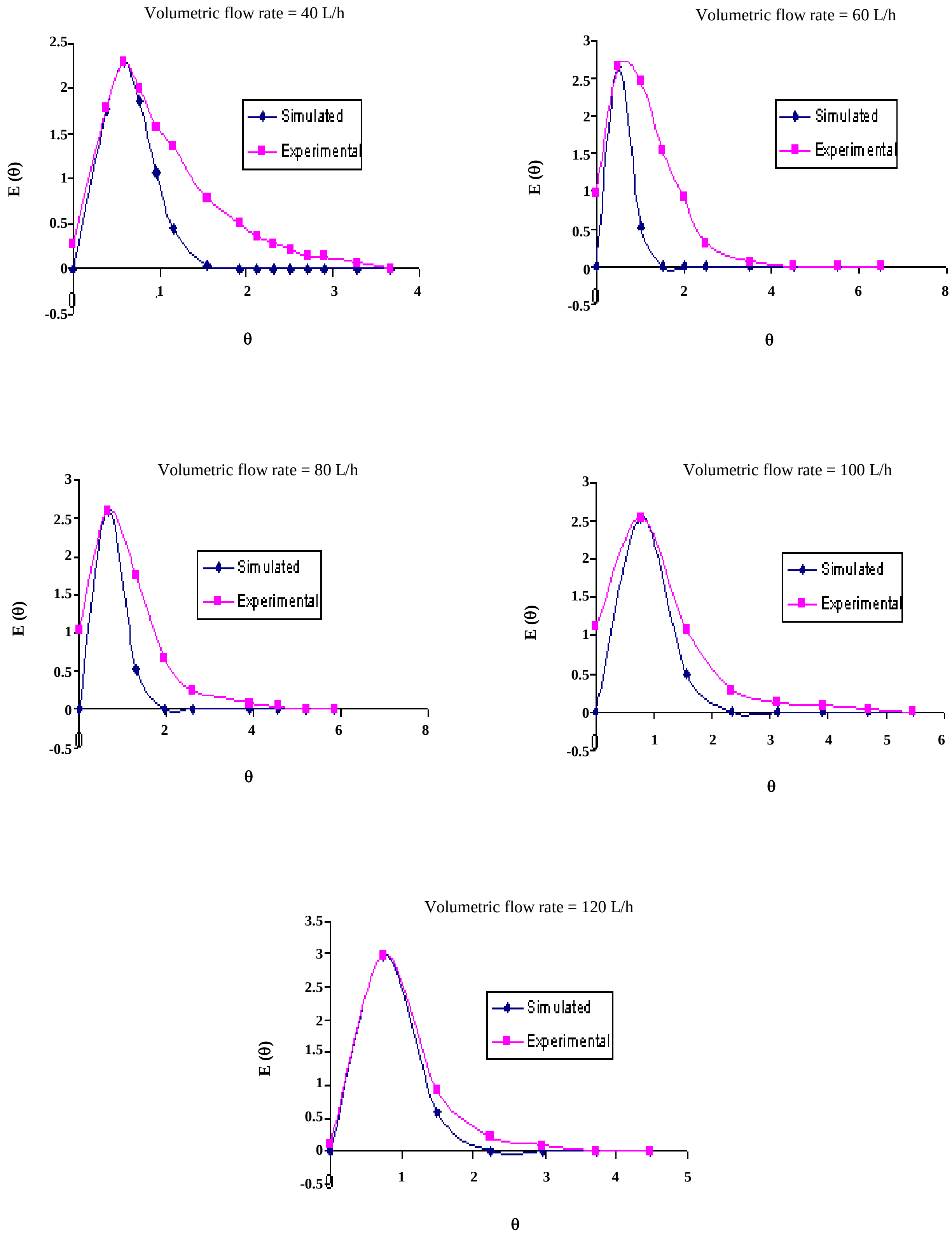

Fig. 4: Comparison of RTD curves between simulations and experimental data.

Table 2: Standard Error Estimation Between Experimental and Simulated Values of RTD for Tubular Reactor With Helical Element.

S. No	Volumetric Flow Rate L/h	Standard Error Estimation S*
1.	40	0.388395
2.	60	0.895968
3.	80	0.591645
4.	100	0.458954
5.	120	0.160487

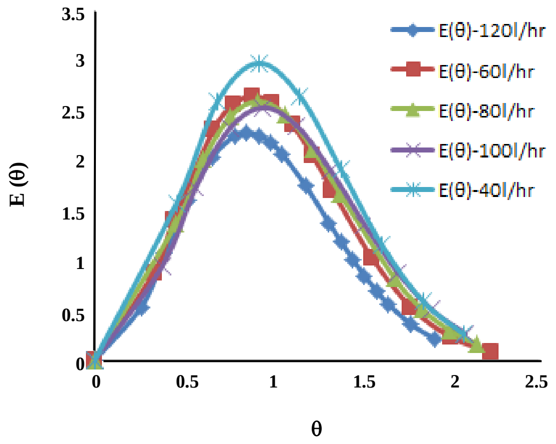

Fig. 5: Typical RTD curves at different volumetric flow rate.

rate widens the RTD curve. Maximum of E(θ) offsets to $\theta < 1$ at volumetric flow rate of 120 L/h, indicating the presence of the short- circuits. High volumetric flow rate can worsen reactor performance. The maximum of the curve E(θ) appears near θ=1 at Volumetric flow rate of 40 L/h, and flow pattern tends to ideal plug flow.

CONCLUSIONS

1- The RTD functions demonstrate that the profiles of flow approach to plug flow. As the flow rate increases, the mean residence time and the variance of residence time distribution decreases proportionally. The tubular reactor with Brazed Helical element can improve the flow profile by narrowing the RTD curve, decreasing mean residence time and avoiding back mixing.

2- The comparison is commonly scaled to the minimum standard error which yields the result that the Ricker equation simulated results are good fit to the experimental data. The comparison validates our synthetic modelling and shows that the Ricker equation is the best model to predict RTD for Static mixer. Also the experimental and computational evidence in relation to variance, mean and maxima scaled to minimum standard error yields the result that at the maximum value of RTD the errors between the experimental and calculated values are minimal. The fact proves that the model is best suited for our target applications.

3- Detailed comparisons of the predicted and measured RTD have been made and these comparisons show that the model captures the growth and evolution of the RTD and its subsequent distortion. The model also predicts a slower than measured recovery of the RTD. The agreement between the predicted and measured RTD is excellent. This work quantitatively measures the micromixing efficiency in a static mixer.

4- The distribution of Residence time shows that the flow field is very turbulent. The velocity magnitude increases by inserting brazed helical static mixer and larger the gradient of velocities magnitudes.

5- The tubular reactor with Brazed Helical element can improve the flow profile by narrowing the RTD curve, decreasing mean residence time and avoiding back mixing. The optimum inlet fluid flow rate is 40 L/h.

ACKNOWLEDGEMENTS

This research was made possible by my beloved guide Dr. K. Balu, Professor and Director, Department of Chemical Engineering, Anna University, Chennai and I would also like to thank Dr. K. Senthilkumar who worked and generously shared their ideas with me.

Received : Mar. 2, 2015 ; Accepted : Sep. 14, 2015

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