# CHAPTER 6

# RESULTS AND DISCUSSION

## 6.1 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 raw materials undergo a number of physical treatment steps to put them in the form in which they can be reacted chemically. The reactants then undergo a thermodynamically feasible chemical reaction in vessels known as 'REACTORS'. The products of chemical reaction undergo further physical treatment such as separating, purification etc., for the final desired product to be obtained. Figure 6.1 shows a typical situation.

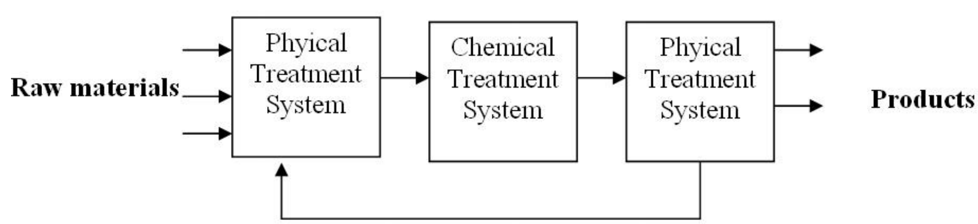


**Figure 6.1 Typical Chemical Process**

### 6.1.1. RTD Parameter Estimation Techniques

Residence time distributions are obtained at different operating conditions and physical properties of the reactor system; it is required to interpret the RTD curves and is an integral part in the success of tracing testing. RTD curves are approximated and thereby reduced to a number of parameter, in order to correlate reactor performance to operating conditions. There are a number of techniques in obtaining the RTD parameters:

- Method of moments. This technique obtains the solution of the differential equation of the RTD curves. The n-th moment obtained from an ideal stimulus is given by:

$$\mu_n = \int_0^\infty t^n E(t)dt, \qquad n = 0, 1, 2, 3\ldots \qquad (6.1)$$

The conditions of E(t) do not guarantee the existence of the moments greater than the second (n≥2) (Buffham and Mason 1993). However when an ideal stimulus is not obtainable the moments need to incorporate this. Mills and Dudukovic (1989) proposed the following for the n-th moments for a non-ideal stimulus:

$$\mu_n = \mu_{n,out} - \mu_{n,in} = \int_0^\infty t^n E(t)dt - \int_0^\infty t^n I(t)dt \qquad (6.2)$$

The appropriate moments of the RTD data provides an indication of various aspects of flow in the static mixer. The Zeroth moment is related to the amount of tracer injected and therefore the mass balance. For the mass balance to be satisfied the zeroth moment must equal one$(\mu_0 = 1)$. The first moment indicates the liquid holdup. The liquid holdup is then determined from equation (6.3).

$$H_L = \mu_1 \frac{Q}{V} \qquad (6.3)$$

The second moment is an indication to the deviation from plug flow. The determination of the second and higher moments from experimental RTD curves are sensitive to the measurement error in the tail of the E(t) curve as well as the value of time (t) chosen as the truncation point or upper limit of the integration as in equation (4.3) and (4.4) (Buffham and Mason 1993). Therefore the moments higher than the second are difficult to determine owing to the uncertainty of the RTD tails.

The method of moments is a means of testing models to match experimental data (Buffham and Mason 1993) by determining the moments from the RTD data as well as from the model. The theory and validity of the model is confirmed if the model and experimental moments agree.

- Numerical comparison of experimental and theoretical RTD response curves (curve fitting).

This 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 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).

- Graphical comparison of particular values of the theoretical and experimental RTD curve.
- Method of convolution/deconvolution. (Mills and Dudckovic 1989)

For these methods it is assumed that the experimental response data has been normalized to give the forcing function (i.e. the stimuli/input response) and the system output response. The forcing function represent the tracer response of the non-ideal tracer injection and sampling system, which for an ideal system would be described by the Dirac function. For the case of deconvolution, the impulse response of the static packed bed E(t) is determined by the inversion of the convolution integral operator using the input and output system responses. A more detailed description is provided in Mills and Dudukovic (1989).

The choice of method to be used to determine the RTD parameters is important as it influences the value of the various parameters. This influence was discussed in the work of Sicardi et al (1980), in the case of different RTD models. The parameter values are indeed very sensitive to the identification method as was reported by Sicardi et al (1980). In their work, the method of moments gave fairly good results, however moments greater than the first were sensitive to the cutting off of the response curves at low concentrations. Sicardi et al (1980) also investigated the curve fitting technique and it was found to perform considerably better than the method of moments. It must be added that the parameters were subject to the optimization function. From this it can be said that if a model exists that accurately describes the reactor system and the only reason for any discrepancies is due to experimental errors the method of curve fitting is the best option. The objective function can be chosen so as to suit the error range. In addition the nature of errors can be identified by the reproduction of experiments (Buffham and Mason 1993). On the other hand when the model does not accurately describe the experimental data a problem arises as the meaning of the parameters lie in the model description. For this reason it is better suited to opt for the graphical comparison of particular values of the theoretical and experimental RTD curve.

## 6.2 RESULTS

The flow in a tubular reactor with helical static mixter has been analyzed for a flow. The determination of Residence time distribution E(θ) for various values of experimental Residence time θs for turbulent reactor with brazed helical element involves the solution of Ricker equation (5.1) by assuming the values of γ and β. Plot for E(θ) versus θ for five different volumetric flow rates for a turbulent reactor with brazed helical element and without brazed helical element are shown in Figures 6.2 to 6.31. This gives the comparison of RTD curves between simulation values from the application of the Ricker model and experimental data for an amplification of different volumetric flow rates in tubular reactor with and without brazed helical element. Comparison of RTD curves between simulation and experimental data for an amplification of different volumetric flow rates in tubular reactor with brazed helical element are as given in Figures 6.2 to 6.6. (γ and β obtained by method I)

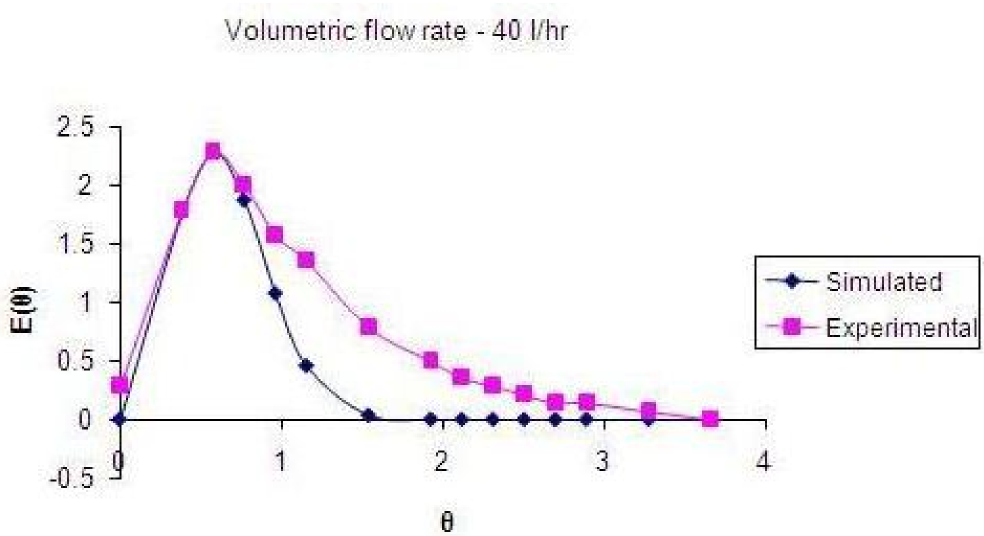


**Figure 6.2 Comparison of RTD Curves between Simulation (By Method I) and Experimental Data with BHE of Volumetric Flow Rate = 40 l/hr**

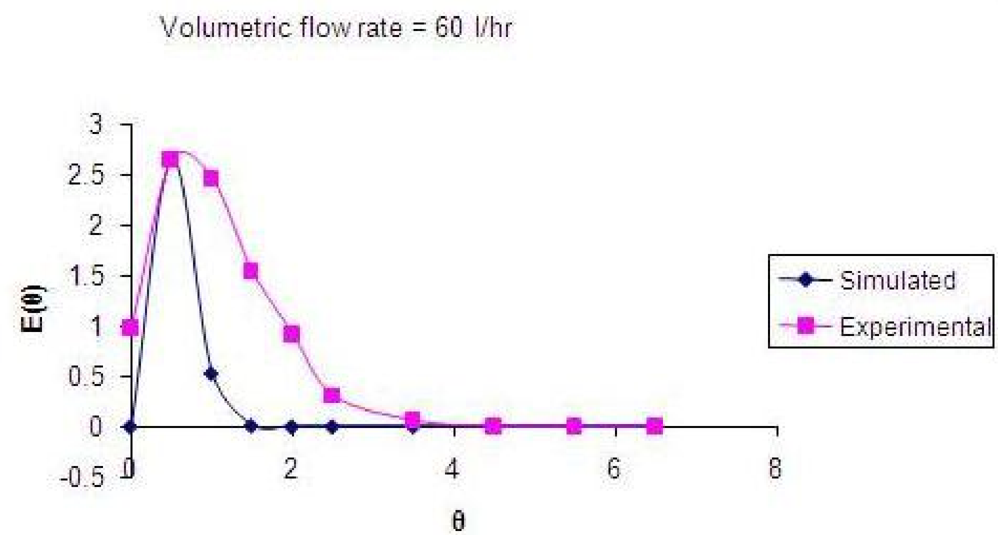


**Figure 6.3 Comparison of RTD Curves between Simulation (By Method I) and Experimental Data with BHE of Volumetric Flow Rate = 60 l/hr**

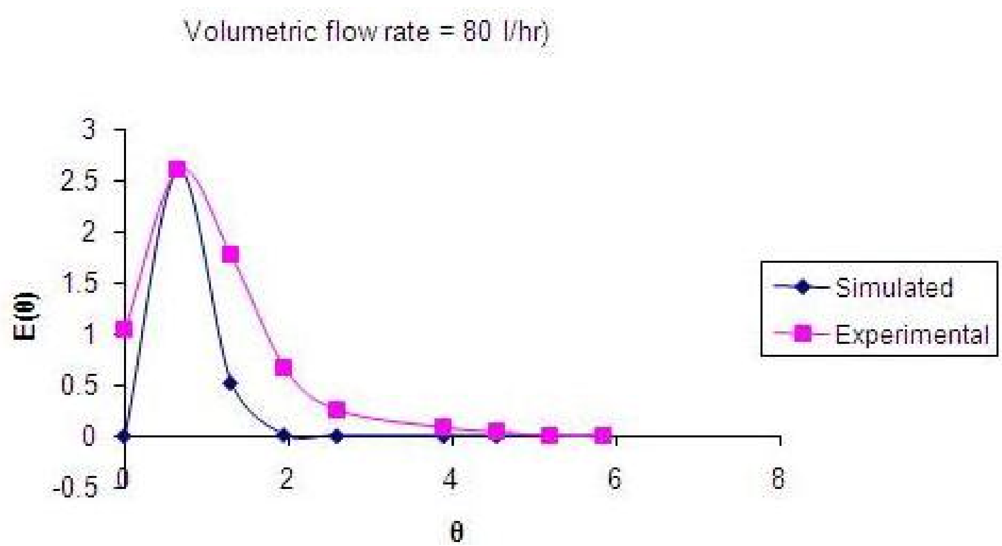


**Figure 6.4 Comparison of RTD Curves between Simulation (By Method I) and Experimental Data with BHE of Volumetric Flow Rate = 80 l/hr**

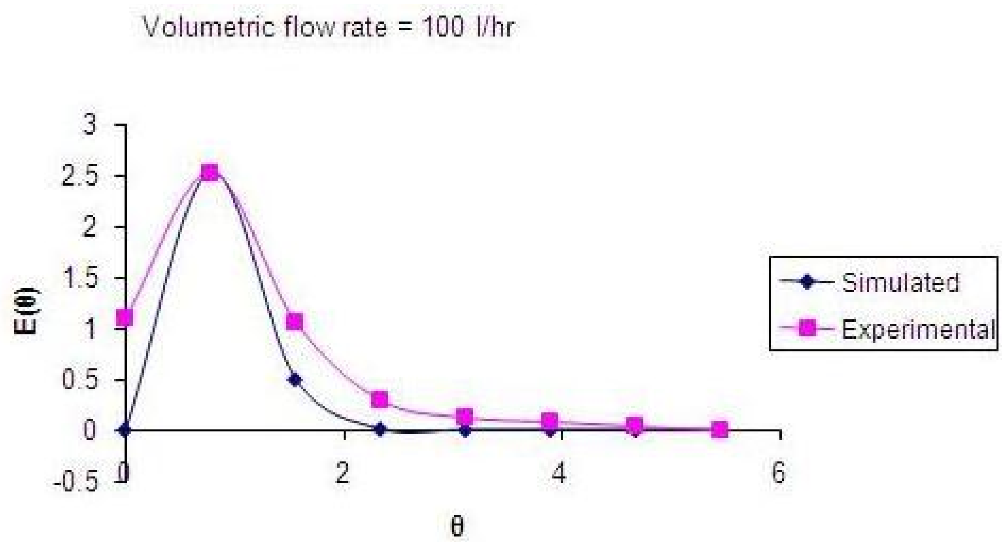


**Figure 6.5 Comparison of RTD Curves between Simulation (By Method I) and Experimental Data with BHE of Volumetric Flow Rate = 100 l/hr**

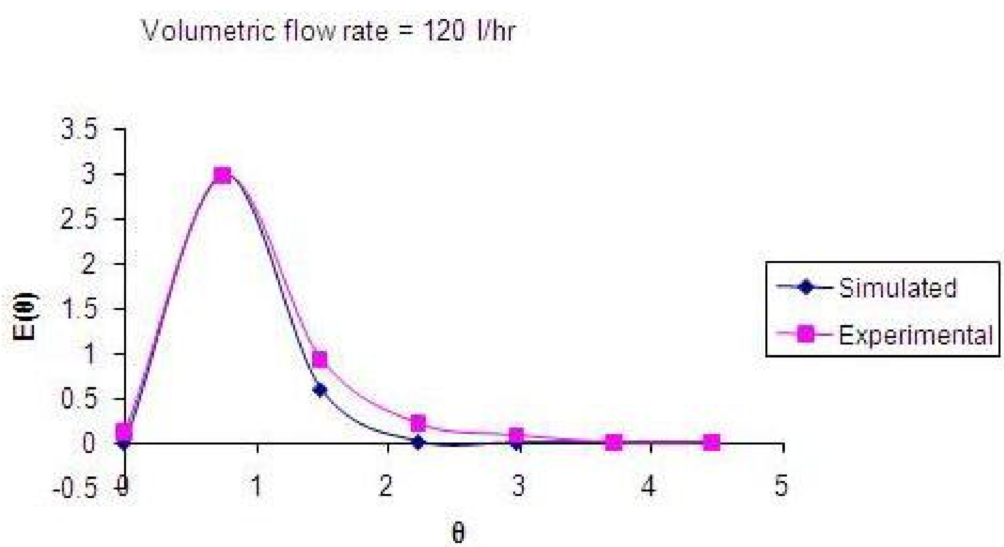


**Figure 6.6 Comparison of RTD Curves between Simulation (By Method I) and Experimental Data with BHE of Volumetric Flow Rate = 120 l/hr**

Comparison of RTD curves between simulation and experimental data for an amplification of different volumetric flow rates in a tubular reactor without brazed helical element are as given in Figures 6.7 to 6.11 ($\gamma$ and $\beta$ obtained by method I).

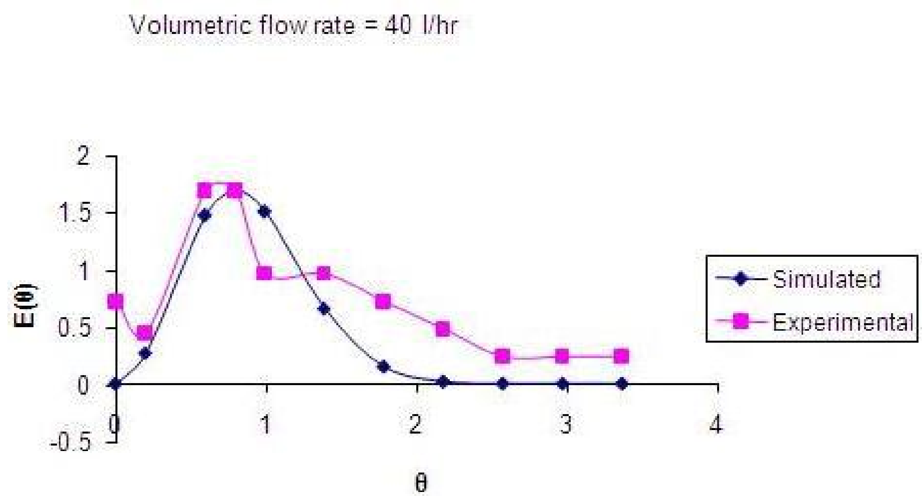


**Figure 6.7 Comparison of RTD Curves between Simulation (By Method I) and Experimental Data without BHE of Volumetric Flow Rate = 40 l/hr**

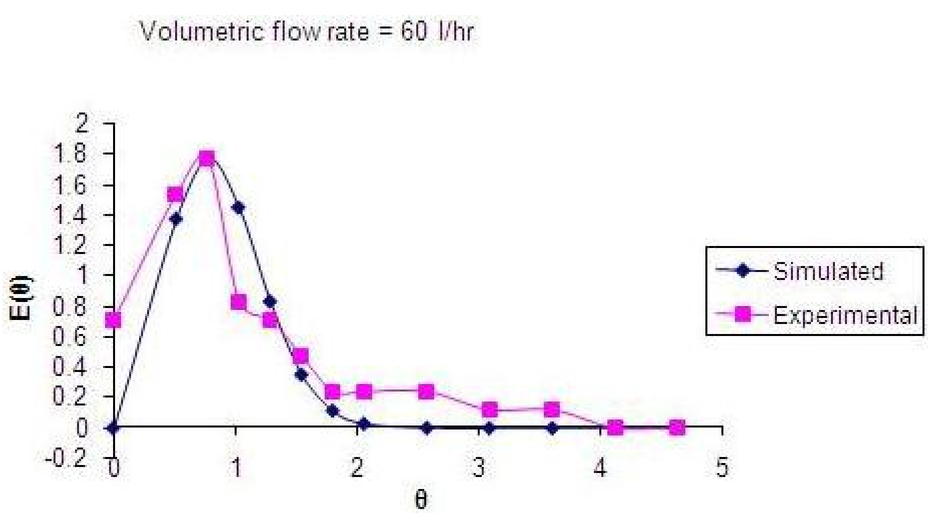


**Figure 6.8 Comparison of RTD Curves between Simulation (By Method I) and Experimental Data without BHE of Volumetric Flow Rate = 60 l/hr**

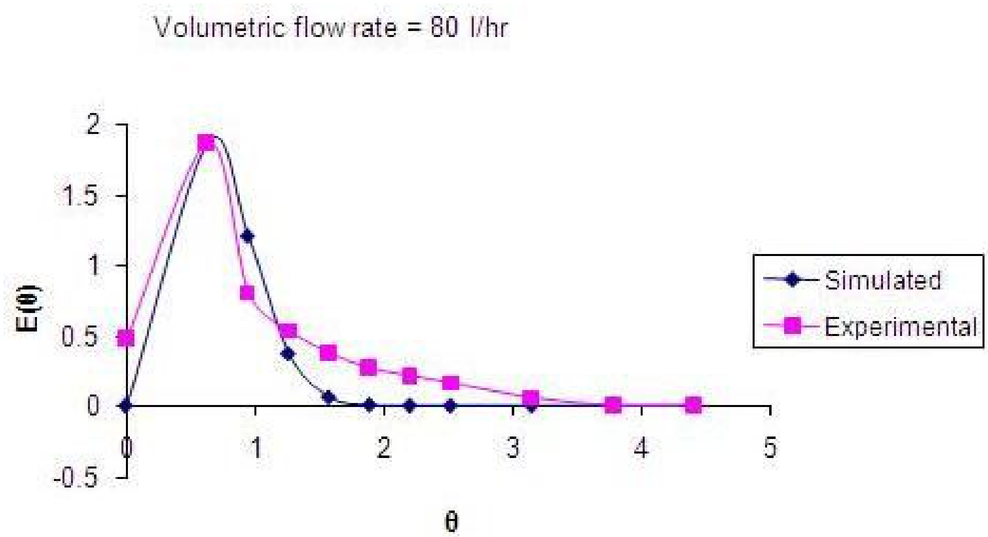


**Figure 6.9 Comparison of RTD Curves between Simulation (By Method I) and Experimental Data without BHE of Volumetric Flow Rate = 80 l/hr**

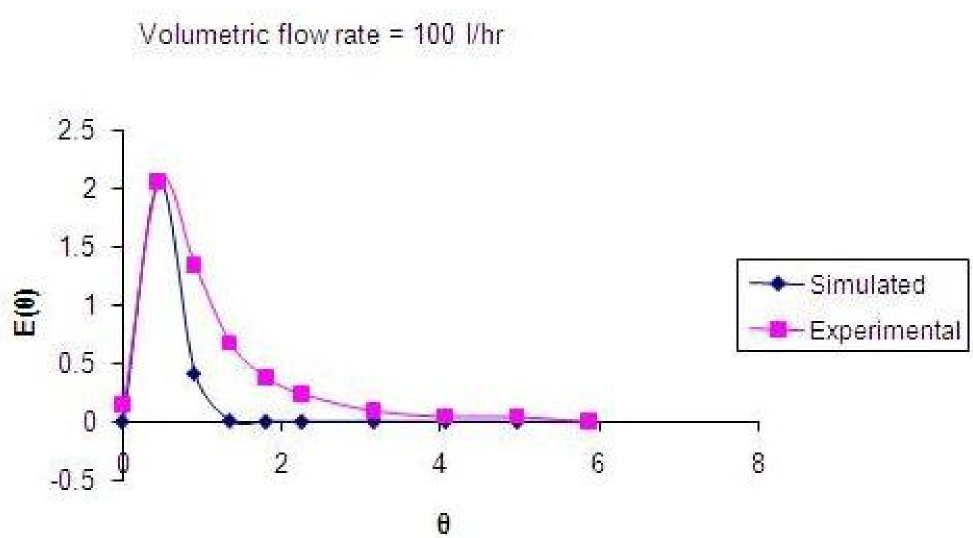


**Figure 6.10 Comparison of RTD Curves between Simulation (By Method I) and Experimental Data without BHE of Volumetric Flow Rate = 100 l/hr**

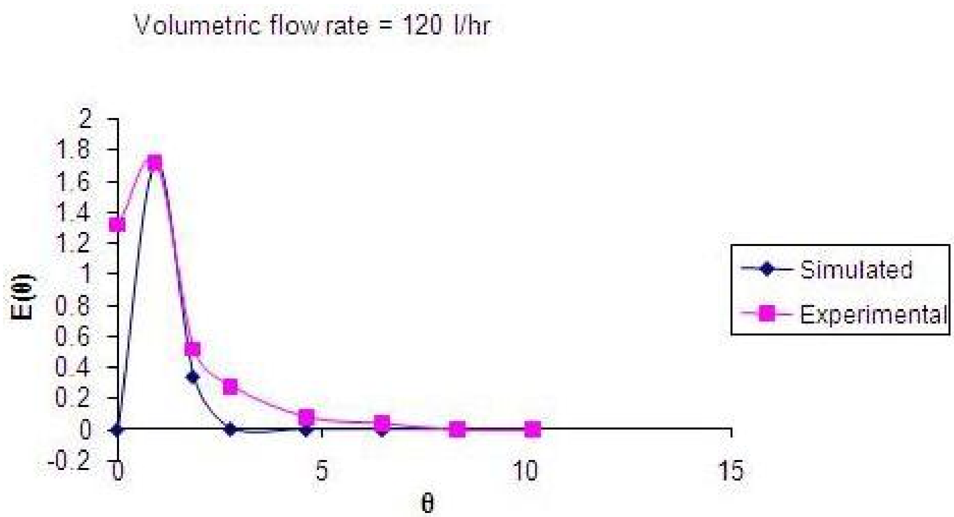


**Figure 6.11 Comparison of RTD Curves between Simulation (By Method I) and Experimental Data without BHE of Volumetric Flow Rate = 120 l/hr**

Comparison of RTD curves between simulation and experimental data for an amplification of different volumetric flow rates in a tubular reactor with brazed helical element are as given in Figures 6.12 to 6.16 ($\gamma$ and $\beta$ obtained by method II).

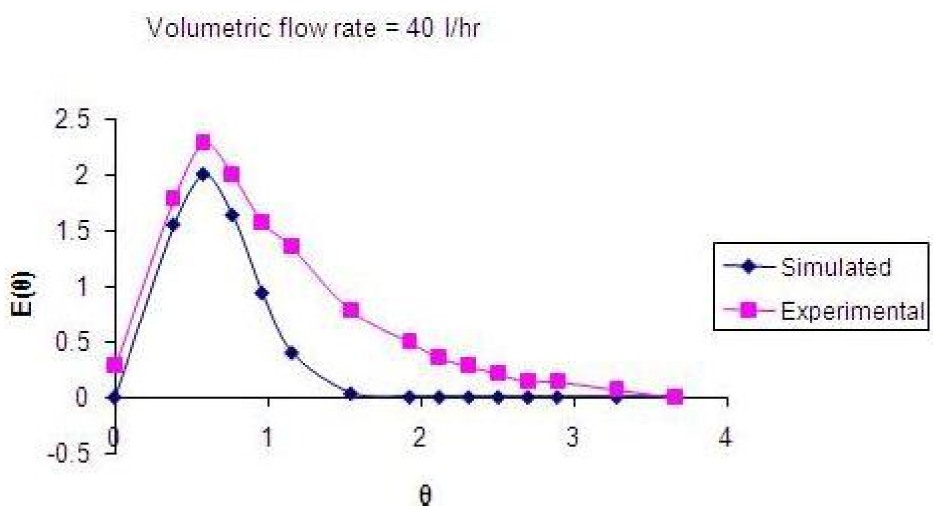


**Figure 6.12 Comparison of RTD Curves between Simulation (By Method II) and Experimental Data with BHE of Volumetric Flow Rate = 40 l/hr**

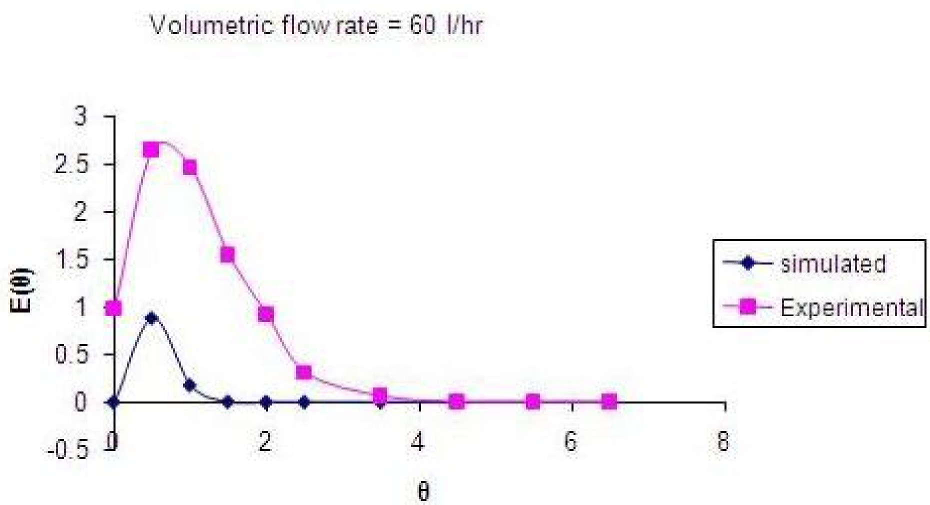


**Figure 6.13 Comparison of RTD Curves between Simulation (By Method II) and Experimental Data with BHE of Volumetric Flow Rate = 60 l/hr**

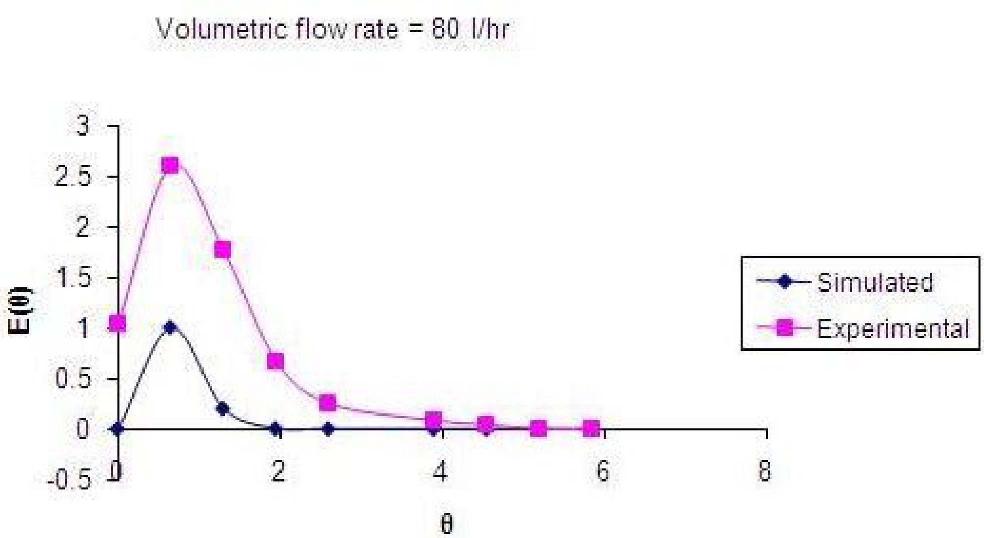


**Figure 6.14 Comparison of RTD Curves between Simulation (By Method II) and Experimental Data with BHE of Volumetric Flow Rate = 80 l/hr**

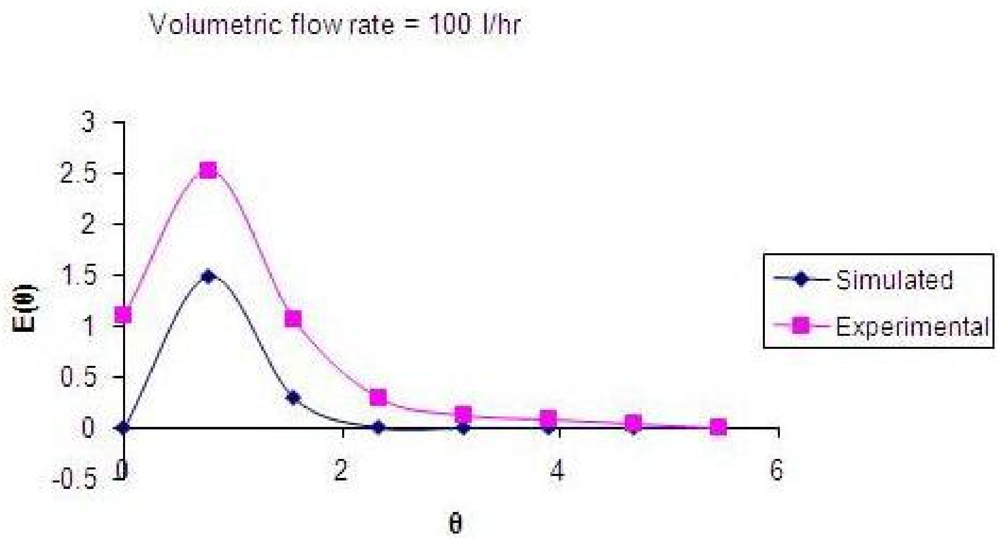


**Figure 6.15 Comparison of RTD Curves between Simulation (By Method II) and Experimental Data with BHE of Volumetric Flow Rate = 100 l/hr**

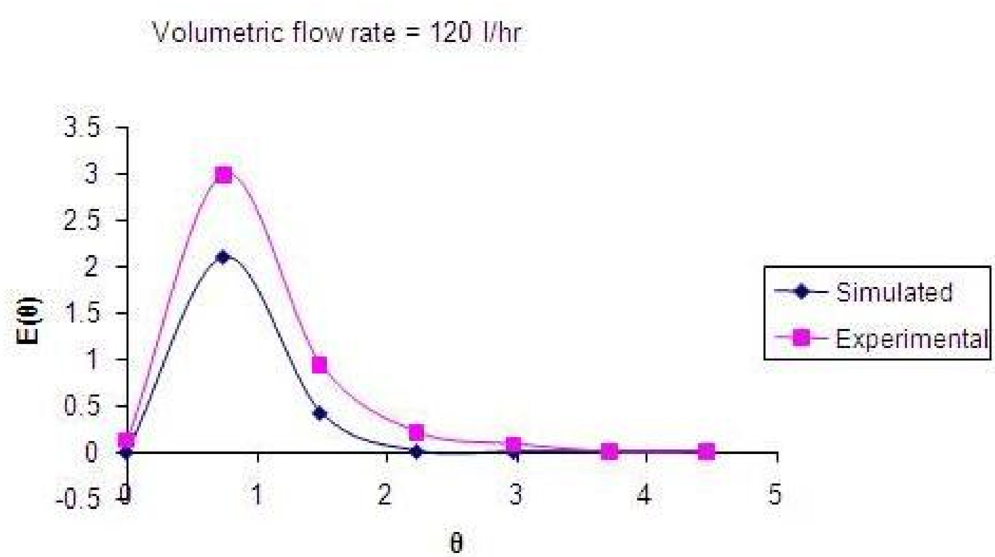


**Figure 6.16 Comparison of RTD Curves between Simulation (By Method II) and Experimental Data with BHE of Volumetric Flow Rate = 120 l/hr**

Comparison of RTD curves between simulation and experimental data for an amplification of different volumetric flow rates in a tubular reactor without brazed helical element are as given in Figures 6.17 to 6.21 ($\gamma$ and $\beta$ obtained by method II).

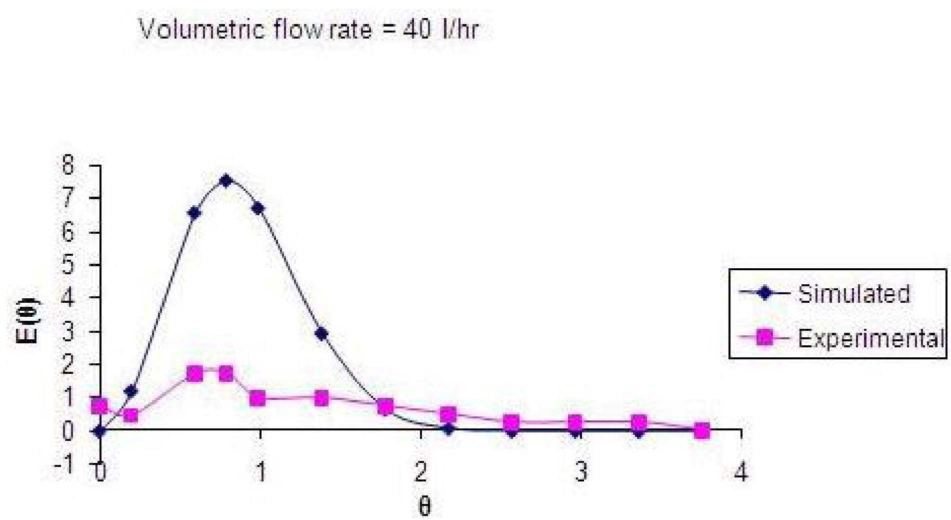


**Figure 6.17 Comparison of RTD Curves between Simulation (By Method II) and Experimental Data without BHE of Volumetric Flow Rate = 40 l/hr**

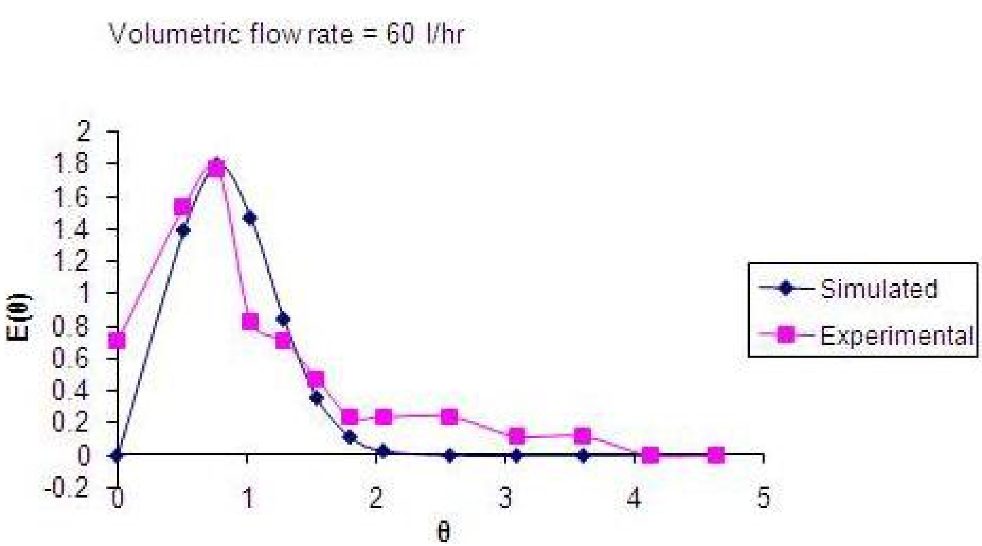


**Figure 6.18 Comparison of RTD Curves between Simulation (By Method II) and Experimental Data without BHE of Volumetric Flow Rate = 60 l/hr**

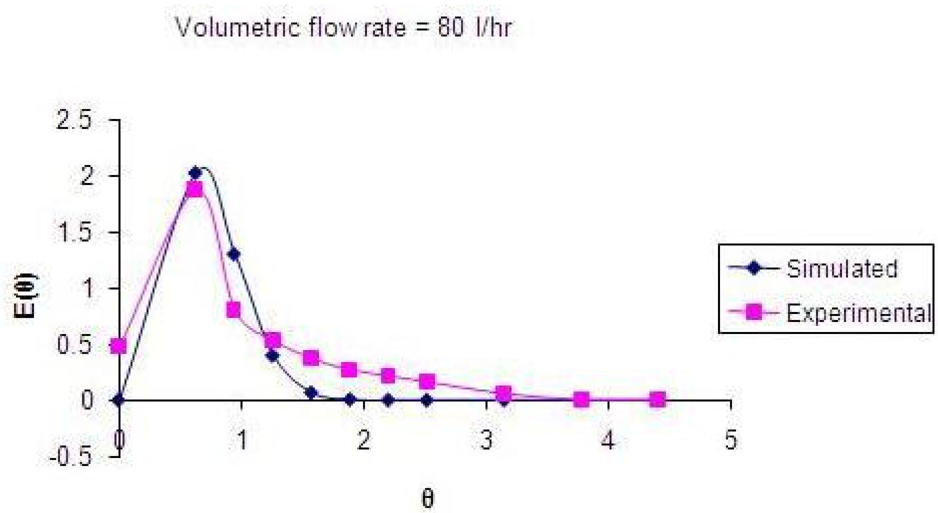


**Figure 6.19 Comparison of RTD Curves between Simulation (By Method II) and Experimental Data without BHE of Volumetric Flow Rate = 80 l/hr**

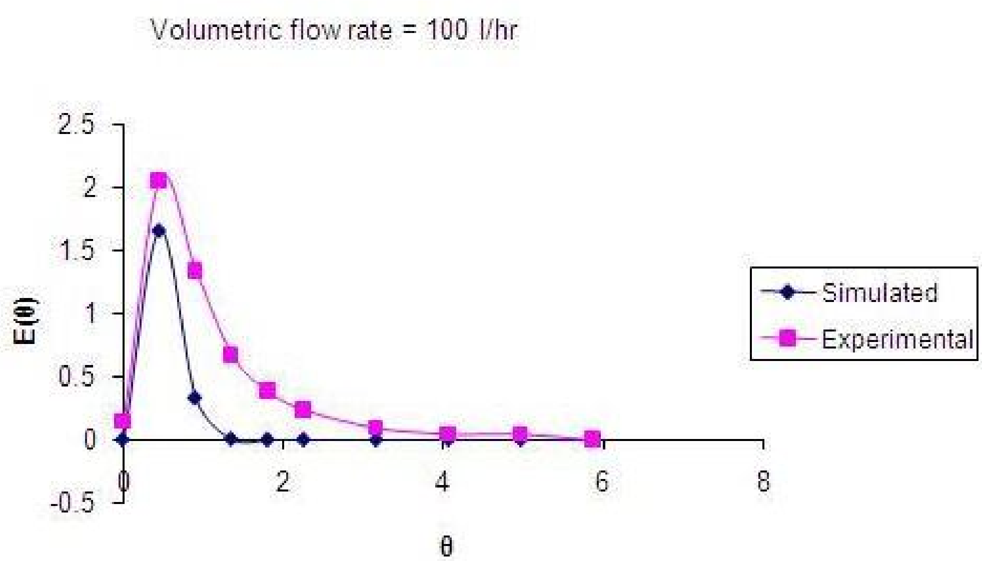


**Figure 6.20 Comparison of RTD Curves between Simulation (By Method II) and Experimental Data without BHE of Volumetric Flow Rate = 100 l/hr**

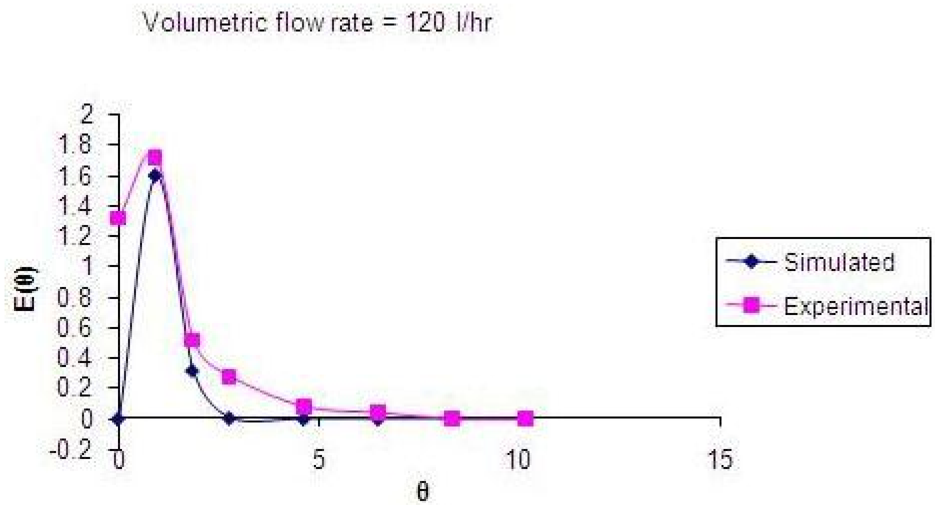


**Figure 6.21 Comparison of RTD Curves between Simulation (By Method II) and Experimental Data without BHE of Volumetric Flow Rate = 120 l/hr**

Comparison of RTD curves between simulation and experimental data for an amplification of different volumetric flow rates in a tubular reactor with brazed helical element are as given in Figure 6.22 to 6.26 ($\gamma$ and $\beta$ obtained by method III).

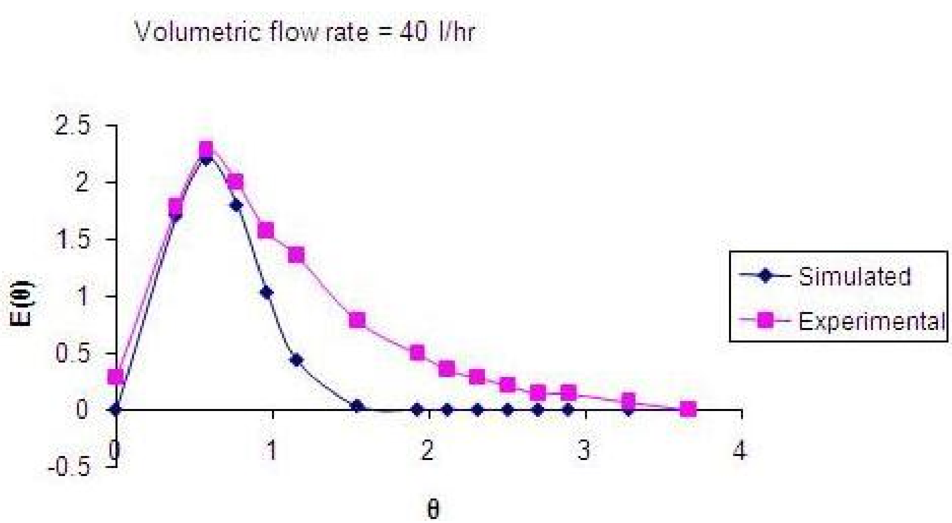


**Figure 6.22 Comparison of RTD Curves between Simulation (By Method III) and Experimental Data with BHE of Volumetric Flow Rate = 40 l/hr**

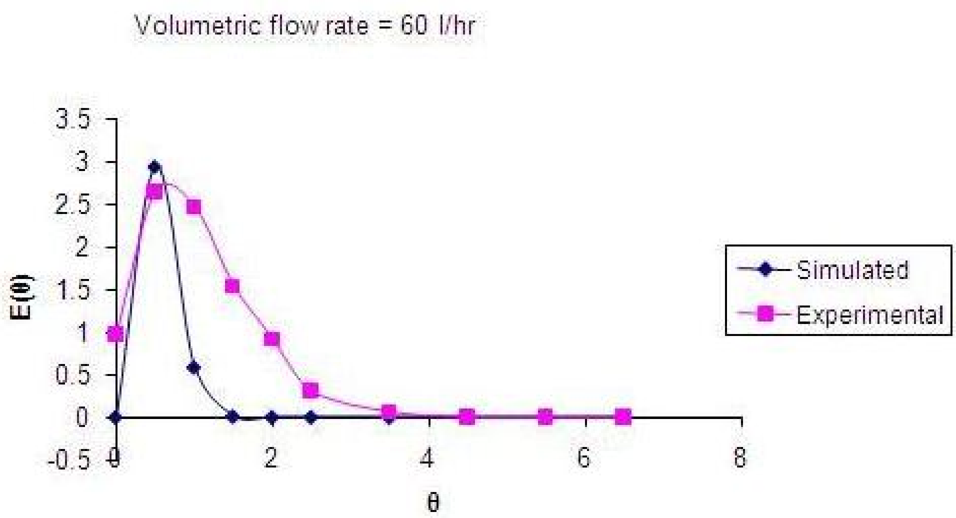


**Figure 6.23 Comparison of RTD Curves between Simulation (By Method III) and Experimental Data with BHE of Volumetric Flow Rate = 60 l/hr**

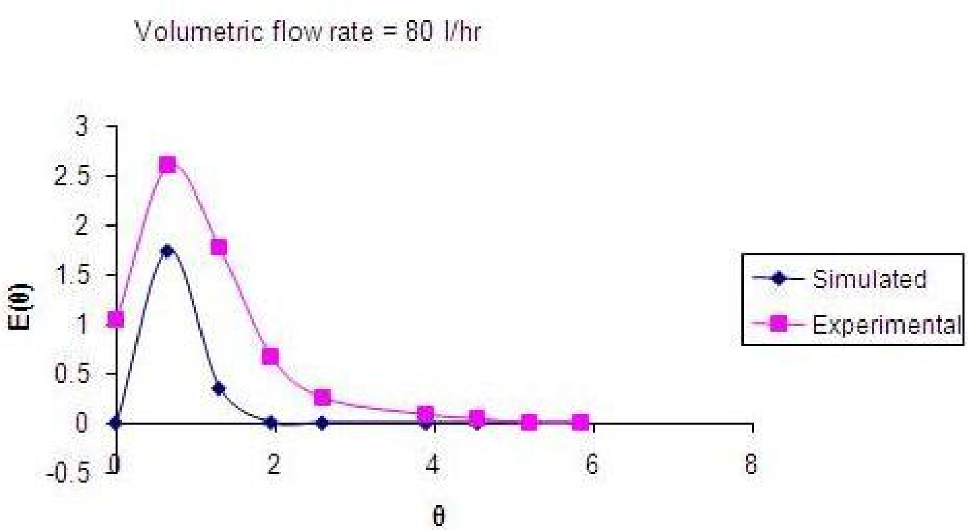


**Figure 6.24 Comparison of RTD Curves between Simulation (By Method III) and Experimental Data with BHE of Volumetric Flow Rate = 80 l/hr**

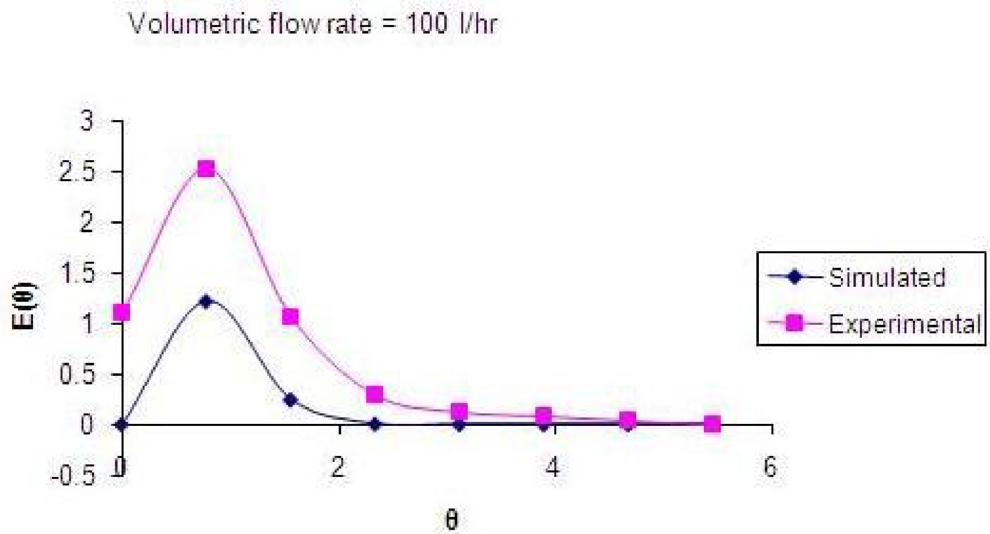


**Figure 6.25 Comparison of RTD Curves between Simulation (By Method III) and Experimental Data with BHE of Volumetric Flow Rate = 100 l/hr**

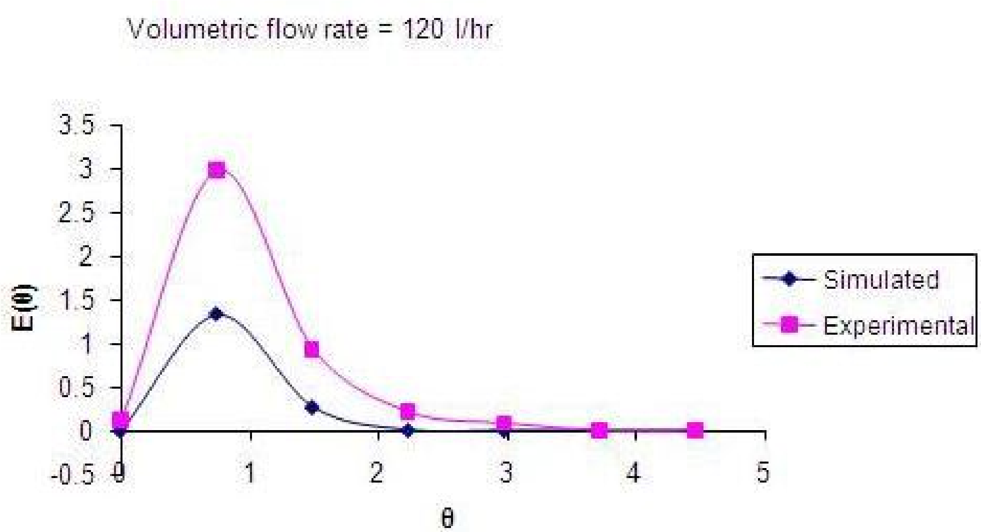


**Figure 6.26 Comparison of RTD Curves between Simulation (By Method III) and Experimental Data with BHE of Volumetric Flow Rate = 120 l/hr**

Comparison of RTD curves between simulation and experimental data for an amplification of different volumetric flow rates in a tubular reactor without brazed helical element are as given in Figures 6.27 to 6.31 ($\gamma$ and $\beta$ obtained by method III).

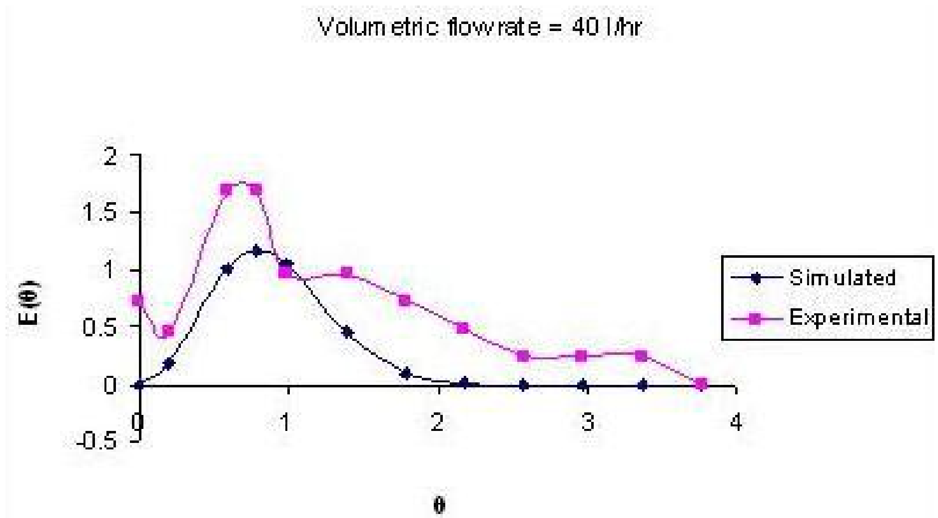


**Figure 6.27 Comparison of RTD Curves Between Simulation (By Method III) and Experimental Data without BHE of Volumetric Flow Rate = 40 l/hr**

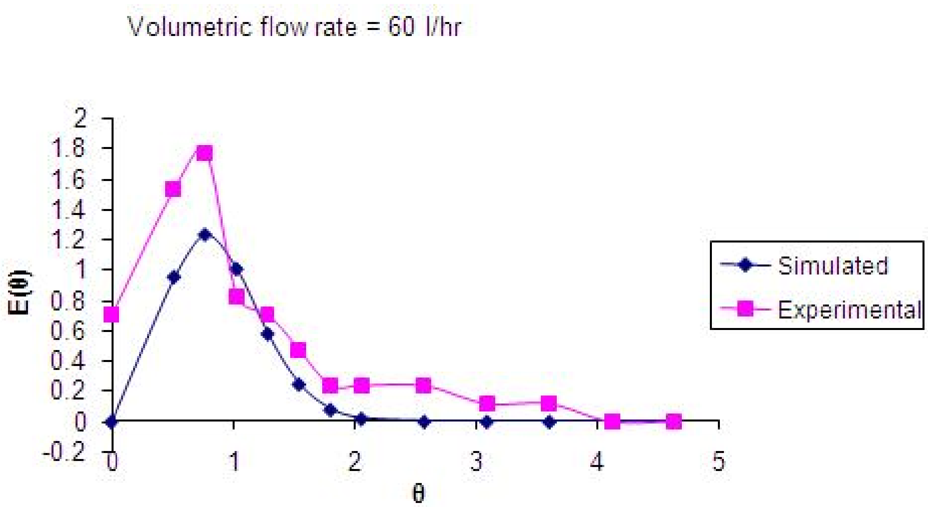


**Figure 6.28 Comparison of RTD Curves Between Simulation (By Method III) and Experimental Data without BHE of Volumetric Flow Rate = 60 l/hr**

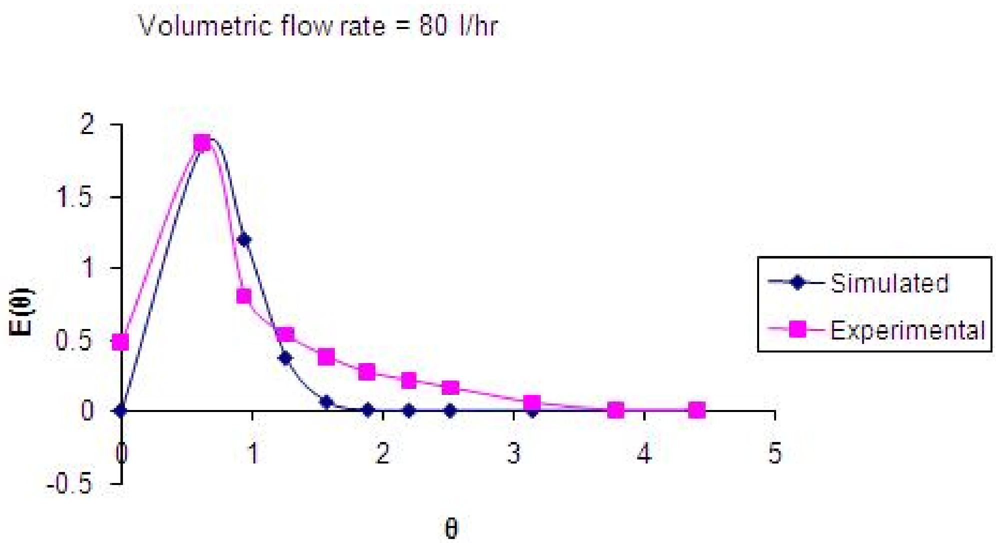


**Figure 6.29 Comparison of RTD Curves Between Simulation (By Method III) and Experimental Data without BHE of Volumetric Flow Rate = 80 l/hr**

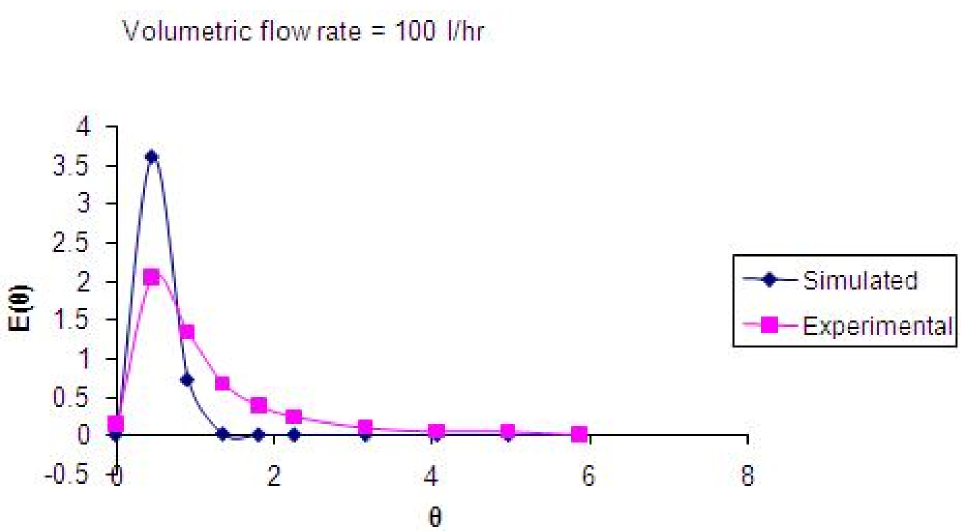


**Figure 6.30 Comparison of RTD Curves Between Simulation (By Method III) and Experimental Data without BHE of Volumetric Flow Rate = 100 l/hr**

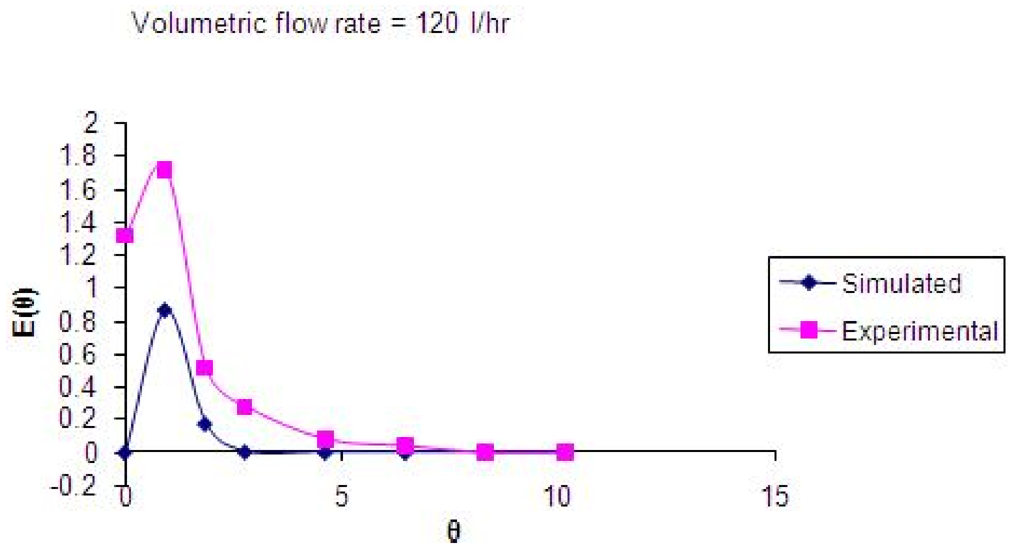


**Figure 6.31 Comparison of RTD Curves between Simulation (By Method III) and Experimental Data without BHE of Volumetric Flow Rate = 120 l/hr**

From these graphs we can infer that the RTD curves predicted with Ricker model show good agreement with experimental data. Dynamical behaviour of the RTD as a function of residence time is described by the Ricker equation (5.1) for various values of parameter $\gamma$ and $\beta$. Standard Error Estimation between Experimental RTD and Calculated RTD obtained using $\gamma$, $\beta$ values by various methods (I, II, III) for tracer in a turbulent reactor with and without brazed helical elements of different volumetric flow rates are shown in Table 6.1 and 6.2.

**Table 6.1 Standard Error Estimation between Experimental and Simulated Values of RTD for Tubular Reactor with Helical Element**

| S. No | Volumetric Flow Rate *l/hr* | Standard Error Estimation $S^*$ | Standard Error Estimation $S^+$ | Standard Error Estimation $S^{**}$ |
|---|---|---|---|---|
| 1. | 40 | 0.388395 | 0.430775 | 0.397132 |
| 2. | 60 | 0.895968 | 1.124858 | 0.888146 |
| 3. | 80 | 0.591645 | 0.858129 | 0.694277 |
| 4. | 100 | 0.458954 | 0.622184 | 0.68857 |
| 5. | 120 | 0.160487 | 0.399099 | 0.681788 |

$S^*$ Standard Error Estimation of experimental RTD and simulated values of RTD which is calculated using β and γ values by Method I of tracer in Tubular reactor with helical element.

$S^+$ Standard Error Estimation of experimental RTD and simulated values of RTD which is calculated using β and γ values by Method II of tracer in Tubular reactor with helical element.

$S^{**}$ Standard Error Estimation of experimental RTD and simulated values of RTD which is calculated using β and γ values by Method III of tracer in Tubular reactor with helical element.

Standard Error Estimation between Experimental RTD and Calculated RTD obtained using γ, β values by various methods (I, II, III) for tracer in a turbulent reactor without brazed helical elements with different volumetric flow rates are shown in Table 6.2.

**Table 6.2 Standard Error Estimation between Experimental and Simulated Values of RTD for Tubular Reactor without Helical Element**

| S. No | Volumetric Flow Rate *l/hr* | Standard Error Estimation $S^*$ | Standard Error Estimation $S^+$ | Standard Error Estimation $S^{**}$ |
|---|---|---|---|---|
| 1. | 40 | 0.378778 | 2.834499 | 0.445154 |
| 2. | 60 | 0.288631 | 0.291824 | 0.326225 |
| 3. | 80 | 0.245032 | 0.26293 | 0.24324 |
| 4. | 100 | 0.392197 | 0.430263 | 0.584707 |
| 5. | 120 | 0.481871 | 0.485317 | 0.57976 |

$S^*$ Standard Error Estimation of experimental RTD and simulated values of RTD which is calculated using β and γ values by Method I of tracer in Tubular reactor without helical element.

$S^+$ Standard Error Estimation of experimental RTD and simulated values of RTD which is calculated using β and γ values by Method II of tracer in Tubular reactor without helical element.

$S^{**}$ Standard Error Estimation of experimental RTD and simulated values of RTD which is calculated using β and γ values by Method III of tracer in Tubular reactor without helical element.

Detailed comparisons of the measured and predicted 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.

Tables 6.3 and 6.4 shows the comparison between simulated and experimental data of mean residence time and variance for the tubular reactor with and without brazed helical element by three methods with different volumetric flow rate respectively. For existing error and model simplification, numerical prediction is a little lower in mean residence time. But the result shows a good agreement in the whole trend, which provides positive reference significantly.

**Table 6.3 Comparison between Numerical and Experimental Data of Mean Residence Time and Variance Of RTD in Plug Flow Reactor with Brazed Helical Element( by Method I, II, III)**

| S. No. | Volumetric flow rate (l/hr) | Simulated Mean Residence time(θ) | | | Experimental Mean Residence Time(θ) | Simulated Variance($\sigma^2$) of RTD | | | Experimental Variance($\sigma^2$) of RTD |
|---|---|---|---|---|---|---|---|---|---|
| | | By method I | By Method II | By Method III | | By method I | By Method II | By Method III | |
| 1 | 40 l/hr | 0.675653 | 0.675653 | 0.675653 | 1.000098 | 0.054833 | 0.054833 | 0.054833 | 0.413583 |
| 2 | 60 l/hr | 0.585346 | 0.585346 | 0.585346 | 0.999776 | 0.056651 | 0.056651 | 0.056651 | 0.451259 |
| 3 | 80 l/hr | 0.760715 | 0.760715 | 0.760715 | 1.800063 | 0.061906 | 0.061906 | 0.061906 | 0.620588 |
| 4 | 100 l/hr | 0.910933 | 0.910933 | 0.910933 | 0.799557 | 0.088599 | 0.088599 | 0.088599 | 0.753585 |
| 5 | 120 l/hr | 0.87204 | 0.87204 | 0.87204 | 0.699791 | 0.081503 | 0.081503 | 0.081503 | 0.876626 |

**Table 6.4 Comparison between Numerical and Experimental Data of Mean Residence Time and Variance of RTD in Plug Flow Reactor without Brazed Helical Element (by Method I, II, III)**

| S.No | Volumetric flow rate (l/hr) | Simulated Mean Residence time(θ) | | | Experimental Mean Residence Time(θ) | Simulated Variance($\sigma^2$) of RTD | | | Experimental Variance($\sigma^2$) of RTD |
|---|---|---|---|---|---|---|---|---|---|
| | | By method I | By Method II | By Method III | | By method I | By Method II | By Method III | |
| 1 | 40 l/hr | 0.96316 | 0.96316 | 0.96316 | 1.09487 | 0.103814 | 0.103814 | 0.103814 | 0.644993 |
| 2 | 60 l/hr | 0.820807 | 0.820807 | 0.820807 | 1 | 0.09135 | 0.09135 | 0.09135 | 0.528975 |
| 3 | 80 l/hr | 0.72482 | 0.72482 | 0.72482 | 0.999298 | 0.05718 | 0.05718 | 0.05718 | 0.429488 |
| 4 | 100 l/hr | 0.629851 | 0.629851 | 0.629851 | 0.998416 | 0.030034 | 0.030034 | 0.030034 | 0.322517 |
| 5 | 120 l/hr | 0.582956 | 0.582956 | 0.582956 | 0.898274 | 0.025338 | 0.025338 | 0.025338 | 0.22229 |

Table 6.5 shows set of the comparison results of numerical (average value of three methods) and experimental data of mean residence time and variance of RTD in plug flow reactor with & without brazed helical element with different volumetric flow rate.

**Table 6.5 Residual Comparisons between Numerical and Experimental Data of Mean Residence Time and Variance of RTD in Plug Flow Reactor with & without Brazed Helical Element (BHE)**

| S.No. | Volumetric flow rate (l/hr) | Simulated Mean Residence time(θ) | | Experimental Mean Residence Time(θ) | | Simulated Variance($\sigma^2$) of RTD | | Experimental Variance($\sigma^2$) of RTD | |
|---|---|---|---|---|---|---|---|---|---|
| | | With BHE | Without BHE | With BHE | Without BHE | With BHE | Without BHE | With BHE | Without BHE |
| 1 | 40 l/hr | 0.675653 | 0.96316 | 1.000098 | 1.09487 | 0.054833 | 0.103814 | 0.413583 | 0.644993 |
| 2 | 60 l/hr | 0.585346 | 0.820807 | 0.999776 | 1 | 0.056651 | 0.09135 | 0.451259 | 0.528975 |
| 3 | 80 l/hr | 0.760715 | 0.72482 | 1.800063 | 0.999298 | 0.061906 | 0.05718 | 0.620588 | 0.429488 |
| 4 | 100 l/hr | 0.910933 | 0.629851 | 0.799557 | 0.998416 | 0.088599 | 0.030034 | 0.753585 | 0.322517 |
| 5 | 120 l/hr | 0.87204 | 0.582956 | 0.699791 | 0.898274 | 0.091503 | 0.025338 | 0.876626 | 0.22229 |