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CFD Simulation of Mixing Effect on a Continuous Stirred Tank Reactor

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***Abstract*—The continuous Stirred tank reactor (CSTR) is a process equipment frequently used in the chemical, food and pharmaceutical engineering related industries. The effect of fluid flow and impeller characteristics on the mixing behavior of the reactor via computational fluid dynamics has been studied. ANSYS FLUENT12.0 CFD software is used for the simulation of a reactive flow process involving of a second order reaction. The rate of reaction is determined by the impeller speed and its position from the bottom of the reactor and therefore on the mixing behavior during the steady state process. The presented mixing behavior data were compared with the available experimental values in the open literature. The Impeller produces boundary conditions that are important aspects significantly enriching the mathematical representation of the primary source of motion in tanks. The results obtained from the simulation are compared with experimental values and were found to be in agreement with the experimental data in open literature.**

Keywords—CFD, CSTR, Ansys fluent, impeller, mixing

I. Introduction

Continuous stirred-tank reactors (CSTRs) are widely applied in the chemical, food, and pharmaceutical and related industries, for their good mixing ability, efficient heat and mass transfer and good scale-up characteristics [1, 2].

Mixing operation in CSTRs has been the subject of many investigations. Under non-premixed conditions, reactants must first come in contact and then undergo reaction. Physical phenomena/processes like diffusion, fluid pumping in the reactor and mechanical agitation control the mixing [3]. Mixing due to diffusion depends on concentration or temperature gradients [2].

In larger reactors, mixing by diffusion is not practically acceptable because of low rate of mixing. In most cases, the continuous reactors use mechanical agitation for mixing. Because of agitation, efficient mixing can occur irrespective of production capacity and viscosity of the fluid. The mechanical agitator provides better performance of CSTR, giving more conversion of reactant to produce [4].

The limitations in lumping processes are avoided by using the distributed parameter models, based on the actual hydrodynamics inside the reactor. A huge amount of information about these hydrodynamics cannot be obtained via experimentations [5]. The continuing development of commercial codes for computational fluid dynamics applied to the case of mixing give accurate results [6].

Few studies have been done on the effect of mixing behavior on reactor performance. Brucato *et al*. [7] test two advanced modelling approaches using STAR-CD code. A k-ε model was used to analyze turbulence and the SIMPLE (Semi-Implicit Method for Pressure-Linked Equation) iterative algorithm and Guass-Seidel iterative method to solve pressure linked equations and proved that mixing depends on agitation rate and position of impellers. They extended the CFD three dimensional simulations to competitive reactions in a batch process and the results obtained are based on macro mixing assumption and they showed that there was a good agreement between simulation results and experimental values by using k-ε model with CFD flow 3D codes.

Forney and Nafia [8] worked on Eddy contact model using CFD to simulate liquid reactions in nearly homogeneous turbulence fluid flow. The results obtained showed that the model for parallel reactions between acid –base – ester in a nearly homogeneous turbulence is as accurate as Monte Carlo/PDF

methods and is comparable to a mixture fraction technique.

Kolthoff *et al*. [9] investigated a three dimensional hydrodynamic model of a mixing vessel for pitching blade turbines operating in laminar range of motion to account for the additional forces acting on the liquid in the impeller region using the Navier - Stokes equation. The model was verified by measuring the power consumption and axial forces acting on the bottom and wall of the vessel.

Yoon *et al*. [10] combined experimental and computational approach to simulate six different r – z planes locked at different angles from 0º to 50º and it was reported that the impeller induced flow is dominated by circumferential flow, tangential jet and pairs of tip velocity using ANSYS FLUENT at an impeller Reynolds Number of 4000. The computational values were validated with particle image velocimetry (PIV) data.

ANSYS FLUENT [11] presented a two compartment model for particle size distribution in polymerization reactors by taking into account the variations in turbulent kinetic energy and its dissipation rate in the vessel, using k-ε with ANSYS FLUENT and time evolution of the droplet distribution in the mixing vessel was also measured.

The effect of the impeller height and agitation speed giving rise to turbulence has not been investigated in previous studies known to us from open literatures. In the present research work, the reaction is modeled by Finite Rate/ Eddy dissipation volume mixed mesh model. The simulations were carried out using ANSYS FLUENT with the k-ε model for turbulence and multiple reference frame model for impeller induced flow, to analyze the reaction between Ethyl acetate and sodium hydroxide taking into consideration, the effect of the impeller height and agitation speed on turbulence.

II. MATERIALS AND METHOD

The computational fluid dynamics software, ANSYS FLUENT 12.0 was used in the simulation in order to investigate the effect of turbulence on the mixing behavior of CSTR in the reaction between ethyl acetate and sodium hydroxide, and the reaction is a second order reaction. The results of the simulation were validated with the experimental results of Rajavathsavai *et al*. [2].

The concentrations at the exit of the CSTR was simulated for different impeller speeds of 500, 750, 1000 and 2000 rpm and for different locations of the impeller such as 2 cm, 7cm and 11cm from the bottom of the reactor.

III. DEVELOPMENT OF GOVERNING EQUATIONS

The flow prediction is based on the numerical solution of the two dimensional reaction vessel for a single reaction with horizontal three blade impeller, which rotates along the horizontal direction.

The reactor was modeled with the following assumptions:

a) Constant density
b) Axi-symmetricity of the reactor with its inlet/outlet boundaries
c) The impeller is assumed as a disc

The general conservation of mass or continuity in the CSTR is given by [11, 12]

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho \vec{\upsilon}) = 0 \qquad (1)$$

where $\vec{\upsilon}$ is the velocity vector.

The momentum balance in the CSTR is given by the Navier Stokes equation [11, 13]:

$$\frac{\partial}{\partial t}(\rho \vec{\upsilon}) + \nabla.(\rho \vec{\upsilon}\vec{\upsilon}) = -\nabla p + \nabla.\left(\bar{\bar{\tau}}\right) + \rho \vec{g} + \vec{F} \qquad (2)$$

where p is the static pressure and $\bar{\bar{\tau}}$ is the stress tensor, $\vec{g}$ and $\vec{F}$ are the gravitational body force and external body forces respectively. The stress tensor $\bar{\bar{\tau}}$ is given by:

$$\bar{\bar{\tau}} = \mu\left[\left(\nabla \vec{\upsilon} + \nabla \vec{\upsilon}^{T}\right) - \frac{2}{3}\nabla.\vec{\upsilon} I\right] \qquad (3)$$

where μ is the molecular viscosity, I is the unit tensor, and the second term on the right hand side is the effect of volume dilatation.

The equation for the conservation of reacting mixture can be expressed in the following form [11, 13]:

$$\frac{\partial(\rho m_k)}{\partial t} + \frac{\partial(\rho u_j m_k)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D_{eff}\frac{\partial m_k}{\partial x_j}\right) + R_k \qquad (4)$$

where m_k is the mass fraction of k^{th} species, D_{eff} is the effective diffusivity of the species in the mixture and R_k is rate of reaction.

The turbulence influence on the reaction rate can be captured by employing the Finite rate/ Eddy dissipation model. The reaction rate, R_k is given by [11, 13]:

$$R_k = -v_k' M_i' AB\rho \frac{\varepsilon}{k} \sum \frac{Pm_P}{v_k' M_k'} \quad (5)$$

The concentration of species in the CSTR can be calculated by solving the scalar transport equations in 1-5.

IV. RESULTS AND DISCUSSION

The effect of the impeller speed and its height from the bottom are two important parameters on the performance of the CSTR. Here, ANSYS FLUENT version 12.0 was used to simulate the influence of the two parameters and therefore the influence of turbulence on the reaction between Ethyl acetate and sodium hydroxide. Both impeller speed and its position from bottom were varied keeping the flow rate constant. The stirrer speed was varied from 500 – 2000 rpm, whereas its position varied from 2-11 cm from the bottom of the reactor.

Several simulations of the reactive process under investigation were carried out, covering the experimental range of values of reactant concentrations, their dependence on agitation speeds and the position of impeller from the bottom of the reactor.

TABLE I. THE RESULTS OBTAINED IN EXPERIMENTS AND CFD SIMULATION VALUES.

S/No	Height of impeller from bottom	Speed of impeller	Experimental values		CFD Simulation	
			Exit mass fraction of NaOH m_A x 10^4	Conversion of NaOH X_A %	Exit mass fraction of NaOH m_A x 10^4	Conversion of NaOH X_A %
1	2 cm	500	6.335	36.65	6.21	37.93
2		750	5.813	41.95	6.06	39.41
3		1000	6.147	38.522	6.37	36.31
4		2000	6.7696	32.31	7.10	29.00
5	7 cm	500	6.822	31.86	6.89	31.21
6		750	6.102	39.08	6.191	38.19
7		1000	6.693	33.18	6.43	35.82
8		2000	7.203	28.07	7.51	24.06
9	11 cm	500	7.192	28.00	7.09	28.53
10		750	6.908	30.86	7.02	29.75
11		1000	7.396	25.97	7.72	22.84
12		2000	7.782	22.11	8.10	18.98

Table 1 - Comparison of Experimental values with CFD Simulation Results

The CFD simulation results obtained as shown in the Figures 1 to 13. Figure 1 shows the velocity contours inside the reactor for 500 rpm speed and 2 cm position from the bottom of the reactor.

Figures 2 to13 shows the concentration distribution of NaOH inside the reactor for different speeds of the stirrer and different positions of the stirrer from the bottom of the reactor. The contour values were viewed from color code. Simulation results of sodium hydroxide concentration do practically compared closely with experimental values. The deviation between experimental values and simulation results tends to increase at high agitation speeds, which implies some under estimation of mixing intensity. The simulation results of conversion of sodium hydroxide for different runs conducted for different impeller positions viz., 2 cm, 7 cm and 11 cm from bottom and for different speeds of impeller from 500 to 2000 rpm are compared with the experimentally observed trend.

From Figure 2, it is observed that the mass fraction of sodium hydroxide near the impeller region is somewhat higher than the other regions. This is observed for all impeller speeds for the impeller position of 2 cm from the bottom of the reactor. This may be due to the fact that when the impeller is located near the reactor inlet, there is a tendency for the impeller to pick-up reactant molecules and drop them in the vicinity of the impeller. The results obtained by CFD simulations are again in good trend with experimental data.

It is also observed that the speed has adverse effect on the reaction. As the speed increases, the conversion increases up to 750 rpm for all different impeller locations and then decreases 720.

Maximum conversion is obtained at 750rpm for all impeller locations. It can also be seen that, the conversion is high for 2 cm position of impeller from bottom than that at 11 cm position of impeller from

bottom and the same for 7 cm position of impeller is in between 2 cm and 11 cm height from the bottom of the reactor for all impeller speeds.

The good agreement obtained between simulated and experimental values can therefore be regarded as a proof of the fact that CFD technique is a powerful tool for proper accounting of such phenomena.

V. CONCLUSION

CFD based simulations of turbulence effect in a stirred tank reactor employed with a three blade impeller was carried out. The simulations were conducted for different positions of the impeller from bottom and various speeds of impeller in a 14.7 cm diameter and 26.5 cm height CSTR. A very good agreement between the experimental values and simulation results was found. The small deviation may be due to the assumption of axisymmetric of the reactor with its inlet and exit.

Simulations were carried out with ANSYS FLUENT using standard k-ε model, Finite Rate/ Eddy dissipation model and multiple reference frame model for turbulence, reaction and moving zone (impeller) respectively.

An approximate 2 Dimensional simulation with 39931, 40125, 41257 nodes for 2cm, 7 cm and11 cm impeller position respectively, was performed assuming axis-symmetry.

The observations led to conclusion that the impeller speed and its height affect the conversion. It is also concluded that the impeller positioned at 2 cm from the bottom and rotated at 750 rpm gives the maximum conversion.

The trend between simulated and experimental values substantiates the fact that CFD is a powerful technique for proper accounting of turbulence effect on reaction in stirred tank reactors.

GREEK LETTERS

k Turbulent kinetic energy, m^2/s^2
ε Turbulence dissipation rate, m^2/s^3
ρ Density, kg/m^3
μ Molecular viscosity, kg/ m.sec
$\bar{\bar{\tau}}$ Stress tensor
I Unit tenser

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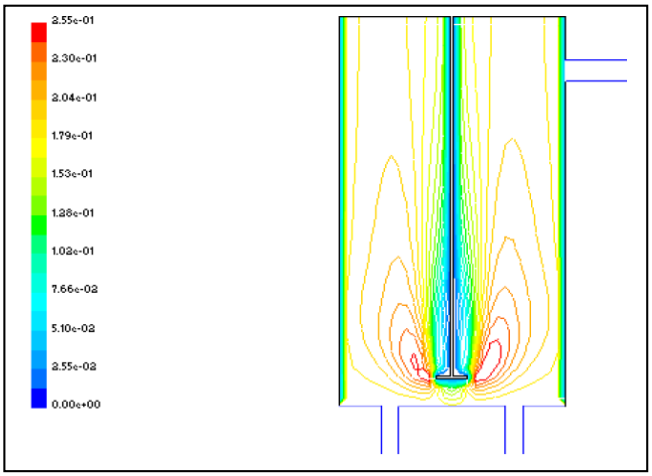

Figure 1. Velocity Profile for Impeller at 2 cm from Bottom for 500 rpm Speed

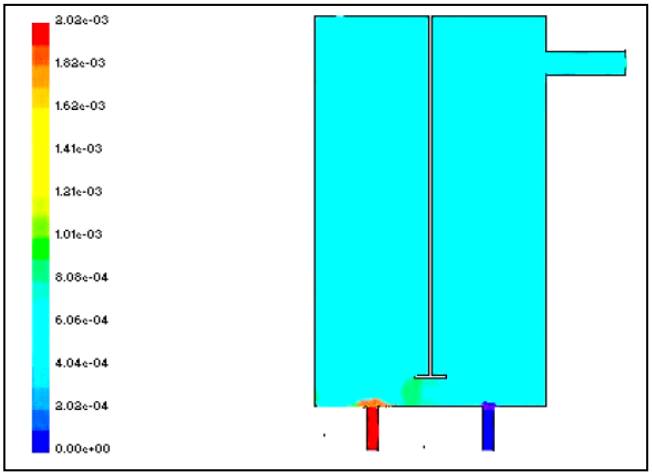

Figure 2. Mass Fraction of NaOH for 500 rpm Impeller Speed for Impeller at 2 cm from Bottom

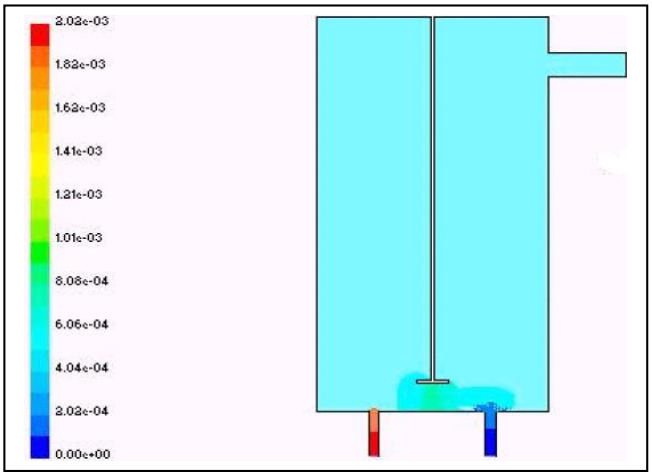

Figure 3. Mass Fraction of NaOH for 750 rpm Impeller Speed for Impeller at 2 cm from Bottom

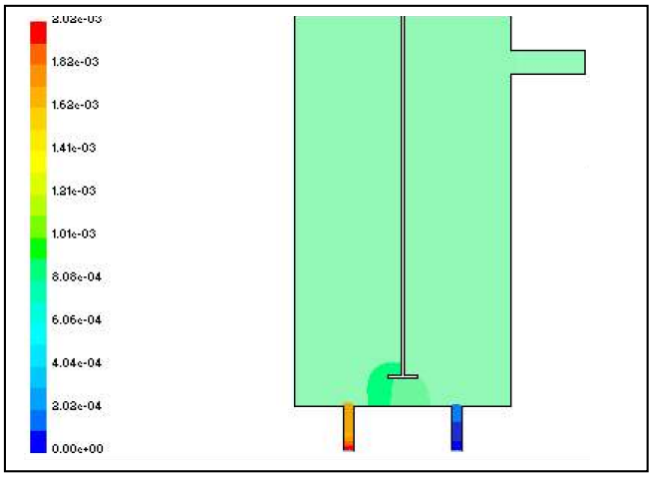

Figure 4. Mass Fraction of NaOH for 1000 rpm Impeller Speed for Impeller at 2 cm from Bottom

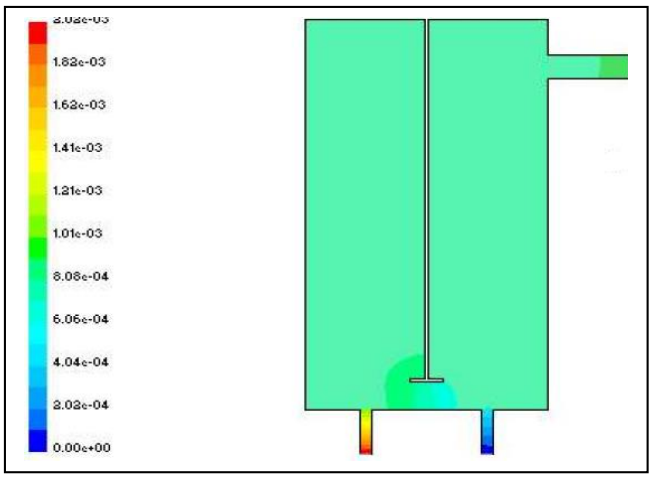

Figure 5. Mass Fraction of NaOH for 2000 rpm Impeller Speed for Impeller at 2 cm from Bottom

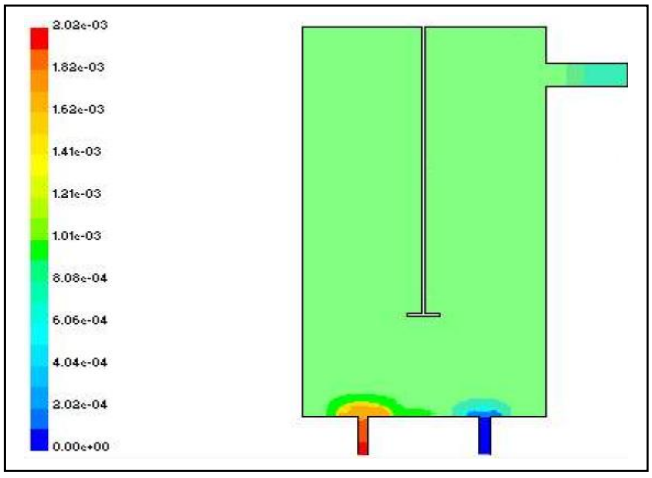

Figure 6. Mass Fraction of NaOH for 500 rpm Impeller Speed for Impeller at 7 cm from Bottom

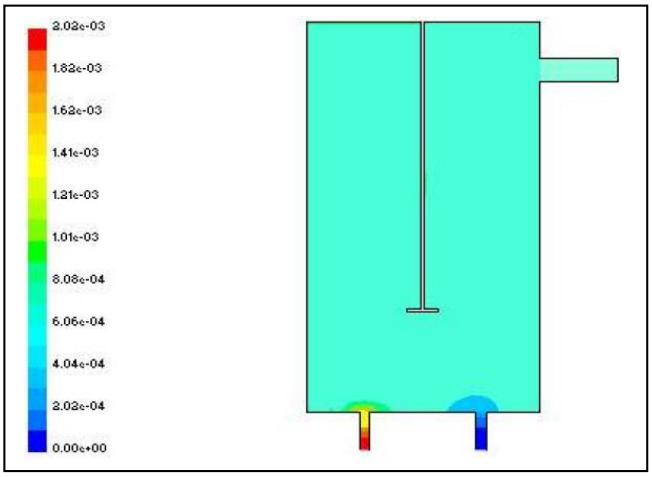

Figure 7. Mass Fraction of NaOH for 750 rpm Impeller Speed for Impeller at 7 cm from Bottom

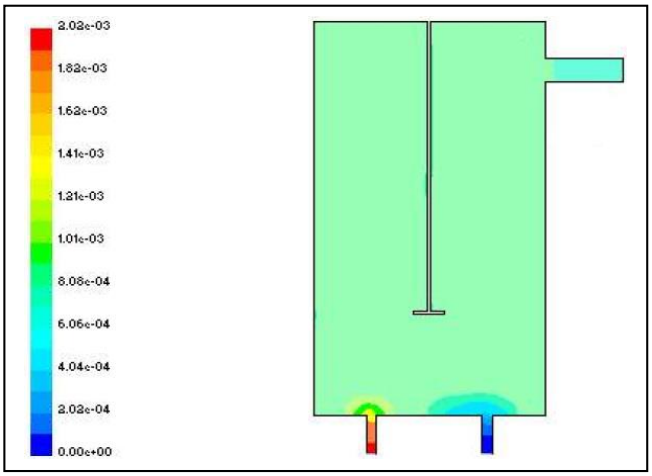

Figure 8. Mass Fraction of NaOH For 1000 rpm Impeller Speed for Impeller at 7 cm from Bottom

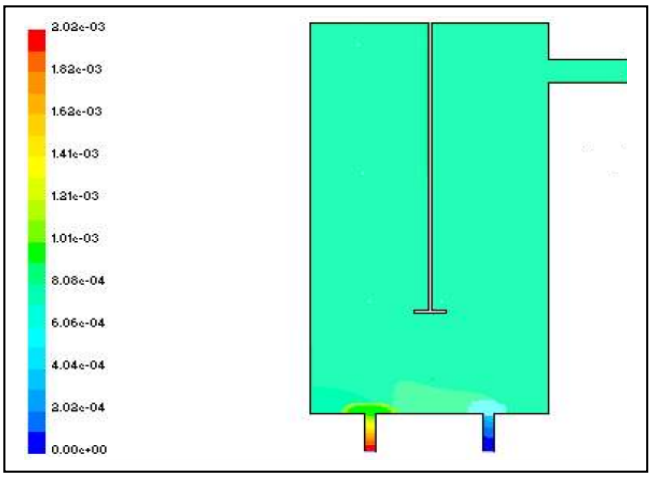

Figure 9. Mass Fraction of NaOH for 2000 rpm Impeller Speed for Impeller at 7 cm from Bottom

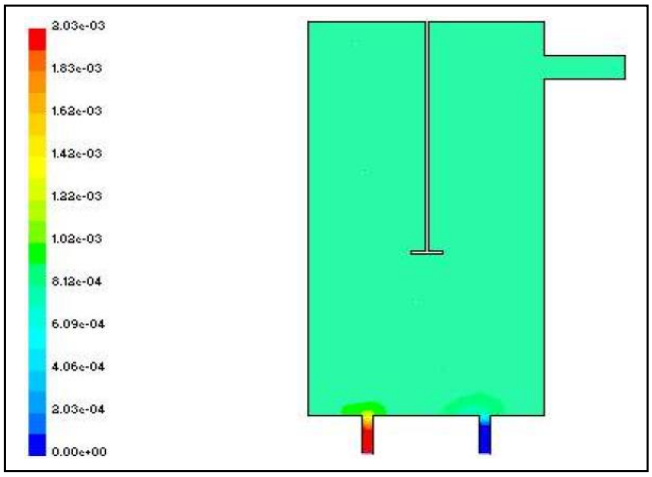

Figure 10. Mass Fraction of NaOH for 500 Rpm Impeller Speed for Impeller at 11 cm from Bottom

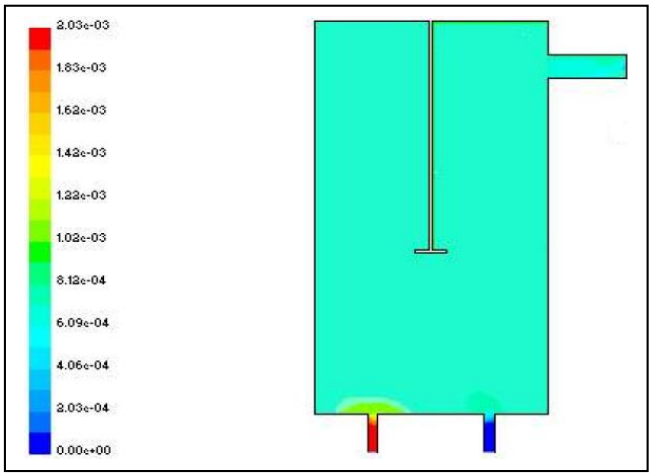

Figure 11. Mass Fraction of NaOH for 750 rpm Impeller Speed for Impeller at 11 cm from Bottom

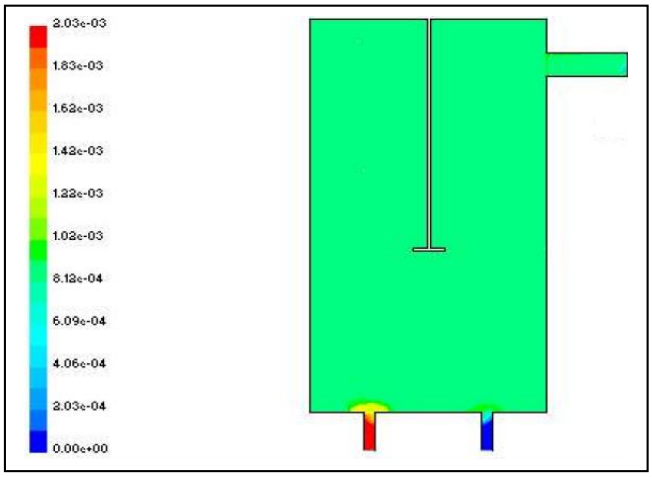

Figure 12. Mass Fraction of NaOH for 1000 rpm Impeller Speed for Impeller at 11 cm from Bottom

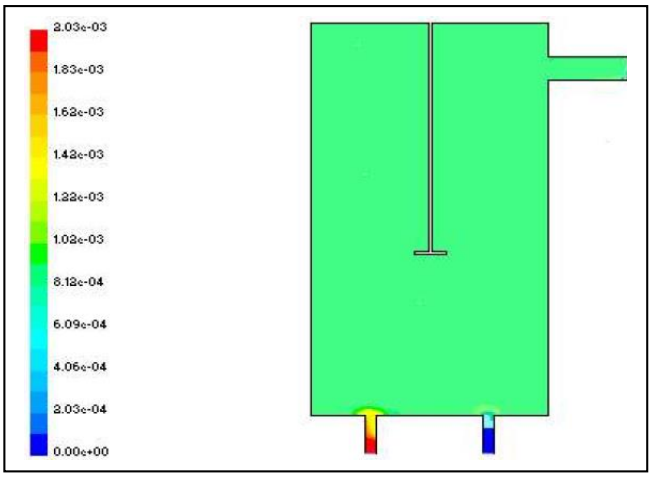

Figure 13. Mass Fraction of NaOH for 2000 rpm Impeller Speed for Impeller at 11 cm from Bottom

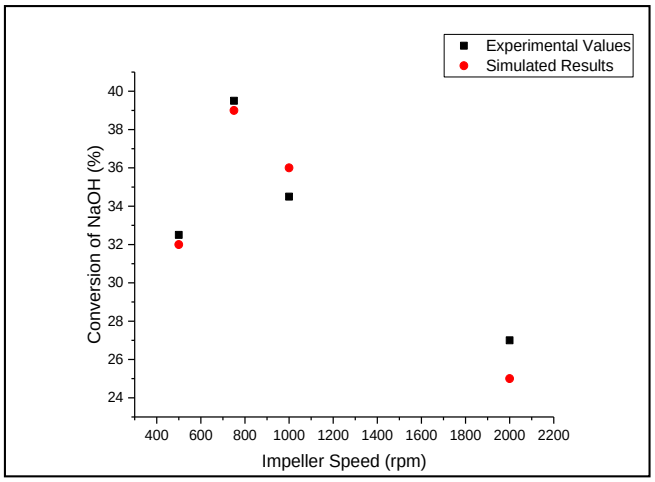

Figure 15. Effect of Impeller Speed on Conversion of NaOH for Impeller at 7 cm from Bottom

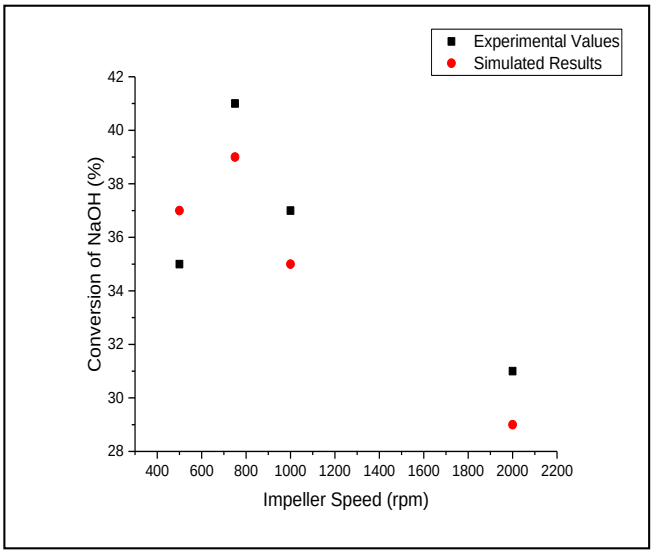

Figure14. Effect of Impeller Speed on Conversion of NaOH for Impeller at 2 cm from Bottom

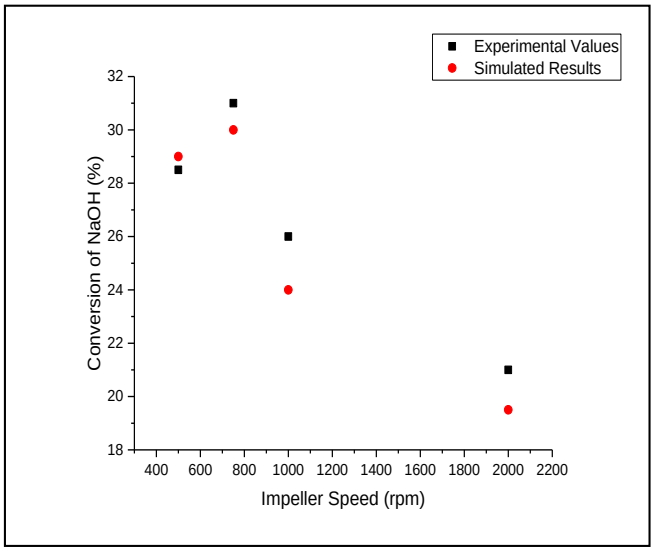

Figure 16. Effect of Impeller Speed on Conversion of NaOH for Impeller at 11 cm from Bottom