CFD ANALYSIS OF TURBULENCE EFFECT ON REACTION IN STIRRED TANK REACTORS

Udaya Bhaskar Reddy R*, Gopalakrishnan S, Ramasamy E
Department of Chemical Engineering, Coimbatore Institute of Technology, Coimbatore- 641014, INDIA.

ABSTRACT

Stirred tank reactors are one of the most commonly used equipments in industry for achieving mixing and reaction. Flow fields in a stirred reactor are obtained via computational fluid dynamics. In this work CFD is used for the simulation of a reactive flow process consisting of a second order reaction. The extent of reaction is found to depend on impeller speed and its position from the bottom of the reactor and therefore on the mixing behavior during the steady state process. The flow field based simulations performed led to predictions that are very well compared with the experimental data. These results are obtained by modeling through finite volume method using FLUENT (version 5.5). Impeller induced boundary conditions are important aspects that significantly enriches the mathematical representation of the primary source of motion in tanks. The results are compared with experimental values obtained from a laboratory stainless steel reactor employed with marine impeller.

KEY WORDS: Computational fluid dynamics, Stirred tank reactor, Marine impeller

---

* Corresponding author
C/O International Research centre, Akzo Nobel car refinishes (I) Pvt. Ltd., Plot no. 62P, Hoskote Industrial area, Bangalore -562114. INDIA. Ph: 91-80-7971941-3 Mobile: 91-98456 13630
E-mail address: to_baskar@hotmail.com

1. INTRODUCTION

Mixing is an important unit operation in many chemical engineering applications. Mixing operation has been the subject of many investigations.

The limitations associated with the lumping process are avoided by using the distributed parameter models, which are based on the actual hydrodynamics inside the tank. A huge amount of information about these hydrodynamics cannot be obtained via experimentations. The continuing development of commercial codes for computational fluid dynamics applied to the case of mixing give accurate results. Two advanced modeling approaches were tested by Brucato et. al., (1999) using STAR-CD code. A k-ε model was used to analyze turbulence and the SIMPLEC method to solve pressure linked equations and proved that mixing depends on agitation rate and position of impellers. Brucato et. al.,(2000) extended the CFD three dimensional simulations for 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 CFDS flow 3D code.

The results of Eddy contact model (Forney L J, and Nafia N, 2000) 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. A 2D hydrodynamic model of a mixing vessel for pitched blade turbines operating in laminar range of motion is presented (Kunnecewicz, pietzykowski, 2001) to account for the additional forces acting on 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.

A combined experimental and computational approach to simulation (Yoon H S et. al., 2001) was performed on six different r – z planes locked at different angles from 0^o to 50^o and it was reported that the impeller induced flow is dominated by circumferential flow, tangential jet and pairs of tip velocity using FLUENT at an impeller Reynolds Number of 4000. The computational values were verified with PIV. A two compartment model (Kiparissides et. al., 2002) 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 FLUENT and time evolution of the droplet distribution in the mixing vessel was also measured.

In the present work, k-ε model is used which accounts for the turbulent flow field in the possible manner. The reaction is modeled by Finite Rate/ Eddy dissipation volume mixed ness model. The simulations were carried out using FLUENT (version 5.5) 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. The following sections deals with the experimental procedure, governing equations and results obtained.

2. EXPERIMENTAL STUDIES

Experiments were carried out in a laboratory scale 306 stainless steel reactor of height 26.5 cm and 14.7 cm diameter, provided with a marine impeller of 2 cm diameter as shown in fig.1, stirred by universal motor. The experiments were conducted for the reaction between Ethyl acetate and Sodium hydroxide, which is a second order reaction. The reactor contains two inlets through which Ethyl acetate and Sodium hydroxide of 0.05 mol/lit concentration each were pumped using valve less metering pumps to maintain constant flow rate. The concentration at the exit of the reactor in a steady state process was measured using standard analytical technique (Kolthoff I M, Stenger V A, 1947). Concentration at the exit was measured for different impeller speeds of the viz. 500, 750, 1000 and 2000 rpm and for different locations of the impeller such as 2cm, 7cm and 11cm from the bottom of the reactor.

3. GOVERNING EQUATIONS

The reactor was modeled with the following assumptions

1. Constant density
2. Axi-symmetricity of the reactor with its inlet/outlet boundaries
3. The impeller is assumed as a disc

The paper discusses the 2D modeling and simulation of the reaction vessel for a single reaction with horizontal three blade marine impeller, which rotates along the horizontal direction. In this case, the equations solved for a CFD solution are continuity equation (both component and overall) and momentum equation. A turbulence model for the calculation of turbulent flows supplements these. A standard k-ε model is used, in which the species concentration associated with turbulent flow is calculated in terms of additional parameters namely, turbulent kinetic energy and its dissipation rate via Finite Rate/Eddy dissipation model. The concentration of species is calculated by solving the generalized scalar transport equation (Verstteeg H K, Malalasekera, 1998) given by the following equation

$$\frac{\partial(\rho m_i)}{\partial t} + \frac{\partial(\rho u_i m_i')}{\partial x_i} = \frac{\partial}{\partial x} j_i + R_i' + S_i'$$

The influence of turbulence of on the reaction rate is taken into account by employing the Finite rate/ Eddy dissipation model. The reaction rate is given by

$$R_{i,k} = -v'_{i,k} M'_i A B \rho \frac{\varepsilon}{k} \frac{\sum P m_P}{\sum_j v''_{j,k} M'_j}$$

4. RESULTS AND DISCUSSION

Impeller speed and its height from the bottom are two important parameters. Here, FLUENT 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 1 gives the results obtained in experiments and simulation values.

S. No	Height of impeller from bottom	Speed of impeller	Experimental values		CFD Simulation Results	
			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 Simulation Results

The CFD simulation results obtained as shown in the fig.2 to 14. Fig. 2 shows the velocity contours in side the reactor for 500 rpm speed and 2 cm position from the bottom of the reactor. Fig.3 to14 shows the concentration distribution of NaOH in side 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 coincide 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 fig. 3, it is observed that the mass fraction of sodium hydroxide near the impeller region is somewhat higher than the other regions. This is happened 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 pickup 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 observed that the speed has adverse effect on reaction. As the speed increases, the conversion increases up to 750 rpm for all different impeller locations and then decreases. Maximum conversion is obtained at 750rpm for all impeller locations. It is also observed 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 powerful tool for proper accounting of such phenomena.

CONCLUSION

CFD based simulations of turbulence effect in a stirred tank reactor employed with a three blade marine impeller was carried out. Experiments 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 laboratory scale stainless steel reactor. A very good agreement between the experimental values and simulation results was found. The small deviation may be due to the assumption of axi-symmetry of the reactor with its inlet and exit.

Simulations were carried out with FLUENT (version 5.5) using standard k-ε model, Finite Rate/ Eddy dissipation model and multiple reference frame model for turbulence, reaction and moving zone (impeller) respectively and the equations were discretized using first order up- wind scheme.

An approximate 2 Dimensional simulation with 39931, 40125, 41257 nodes for 2cm, 7 cm and11cm 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.

NOMENCLATURE

A	Constant for Finite Rate/Eddy dissipation model
B	Constant for Finite Rate/Eddy dissipation model
$C_{1\mu}$, $C_{2\mu}$,C_{μ}	Constants for k- ε model
D_{il}'	Diffusivity of i^{th} species, m^2/sec
E_{ij}	Reynolds Stresses
$j_{i,i}$	Flux of i^{th} species
m_A	Exit mass fraction of Sodium hydroxide
m_i	Mass fraction of i^{th} species
m_p	Mass fraction of product
M_i'	Mass fraction of Reactant
N_{Re}	Reynolds number
P	Product, moles
$R_{i,k}$	Rate of production of i^{th} species, moles /time
R_p	Residual of flow property
Sc_t	Schmidt Number
S_i	Source term for i^{th} species
t	Time
U	Velocity vector
x	Direction
X_A	Conversion of Sodium hydroxide
Y_i	Mole fraction of i^{th} species

GREEK LETTERS

k	Turbulent kinetic energy, m^2/s^2
ε	Turbulence dissipation rate, m^2/s^3
ρ	Density, kg/m^3
μ	Viscosity, kg/ m sec
μ_t	Turbulent Viscosity, kg/ m sec
σ_k , σ_ε	Constants for k- ε model
v'	Stoichiometric Co-efficient for reactant
v''	Stoichiometric Co-efficient for product

BIBLIOGRAPHY

[1] Ranade V V (1997) *Computational Flow Modeling for Chemical Reactor Engineering*, 1st ed.

[2] Giorgio Micale et. al.,(*March 1999*) Predictions of flow fields in a dual- impeller stirred vessel, *AIChEJ*, *Volume 45, Issue3, P*ages 445- 464

[3] Brucato et. al., (*January 2000*)On the Simulation of Stirred tank Reactors via Computational

Fluid Dynamics, Chemical Engineering Science, Volume 55, Issue 2, Pages291 - 302

[4] Forney L J, Nafia N (*December 2000)* Eddy Contact model: CFD simulations of Liquid reactions in nearly homogeneous turbulence *Chemical Engineering Science, Volume 55, Issue24, Pages 6049 – 6058*

[5] Lamberto D J, Alvarez M M, Muzzio F J (*August 2001*), Computational Analysis of regular and chaotic mixing in Stirred tank reactor, *Chemical Engineering Science, Volume 56, Issue 16 , Pages 4887- 4899*

[6] Yoon H S et. al., (*December 2001*)Integrated experimental and Computational approach to simulation of flow in a stirred tank, *Chemical Engineering Science, Volume 57, Issue 23, , Pages 6635 – 6649*

[7] Stephen Bugay et. al.,(March 2002) Experimental analysis of Hydrodynamics in axially agitatedTank,*AICHEJ, Volume 48, Issue 3, Pages 463-475*

[8] Alexo Poulos A H, (May 2002) CFD analysis of turbulence non- homogeneity in mixing vessels, A two – Compartment model, *Chemical Engineering Science, Volume 57, Issue 10, Pages 1735- 1752*

[9] Versteeg H K MalalaSekera W (1995) *An Introduction to Computational Fluid Dynamics- The Finite Volume Method*, Longman group Limited,

[10] FLUENT users Manual (1998), Fluent Inc.,

[11] FLUENT SOLVER (2002) – Training Lecture Notes, Fluent India Pvt. Ltd.,

[12] Kolthoff I M, Stenger V A (1947), *Volumetric analysis, Volume I & II*, Inter science Publishers, Inc., New York,

[13] Keith J Laidler, (1987) *Chemical kinetics*, Harper& Row Publishers, Newyork,

[14] John D Anderson Jr. (1995) *Computational Fluid Dynamics – The basics with applications*, McGraw- Hill, Inc.,

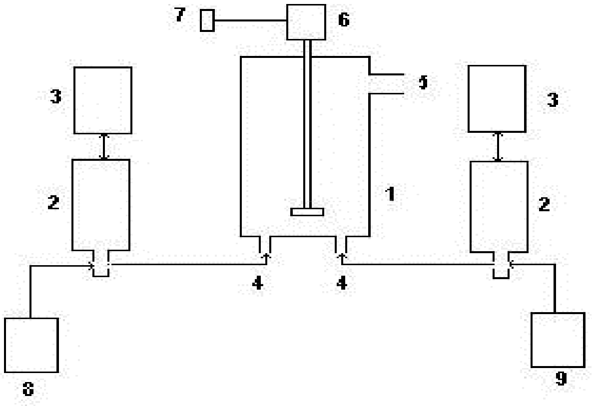

Fig.1 Experimental set up

LEGEND KEY:

1. Reactor 2. Valve less metering pumps 3. FMI Stroke rate Controller 4. Reactor Inlets 5. Reactor Outlet 6. Universal motor 7. Speed Regulator 8. Sodium hydroxide storage tank 9. Ethyl acetate storage tank

SIMULATION RESULTS

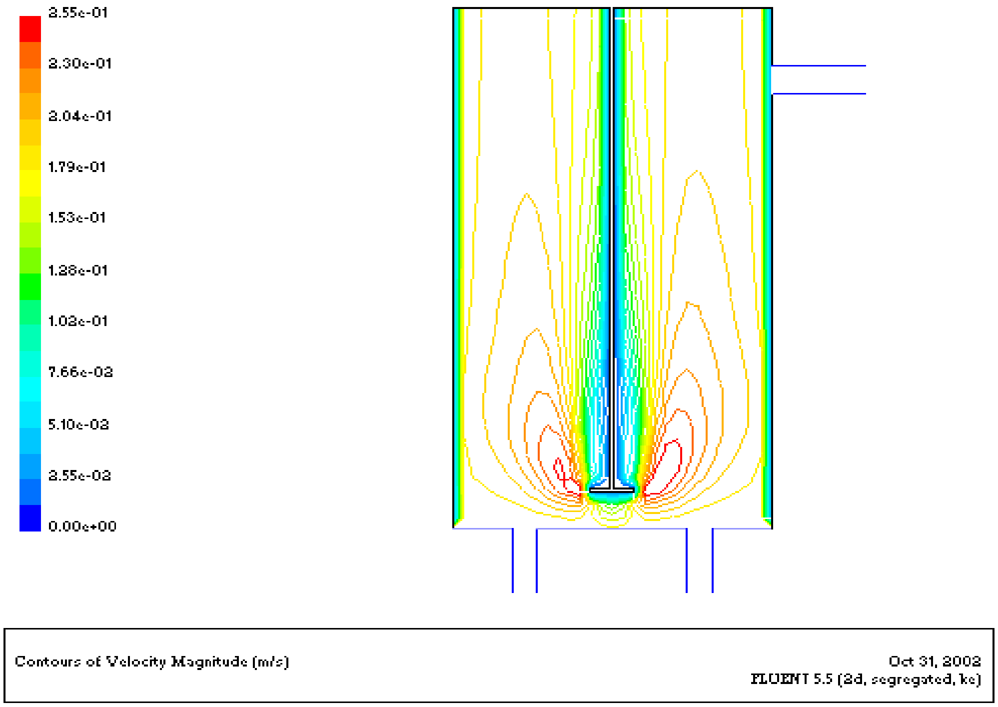

Fig.2 Velocity profile for impeller at 2 cm from bottom for 500 rpm speed

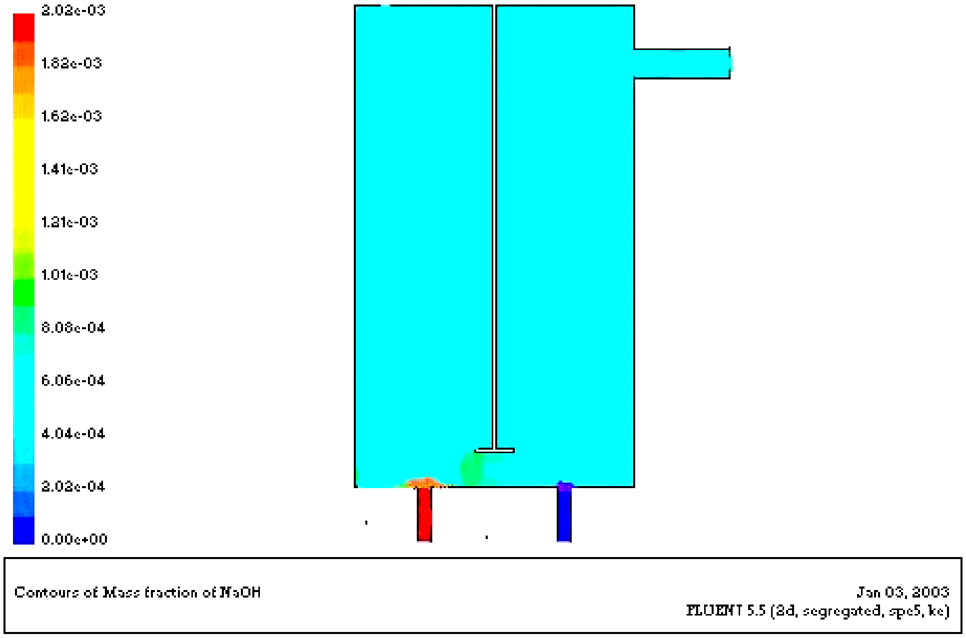

Fig. 3 MASS FRACTION OF NaOH FOR 500 rpm IMPELLER SPEED FOR IMPELLER AT 2 cm FROM BOTTOM

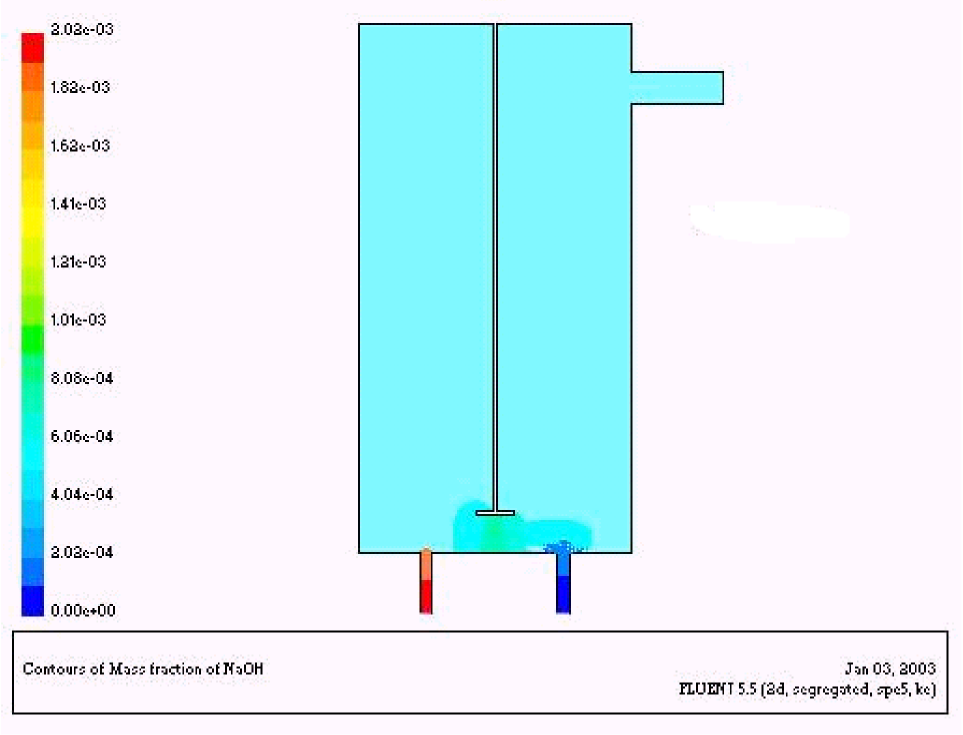

Fig. 4 MASS FRACTION OF NaOH FOR 750 rpm IMPELLER SPEED FOR IMPELLER AT 2 cm FROM BOTTOM

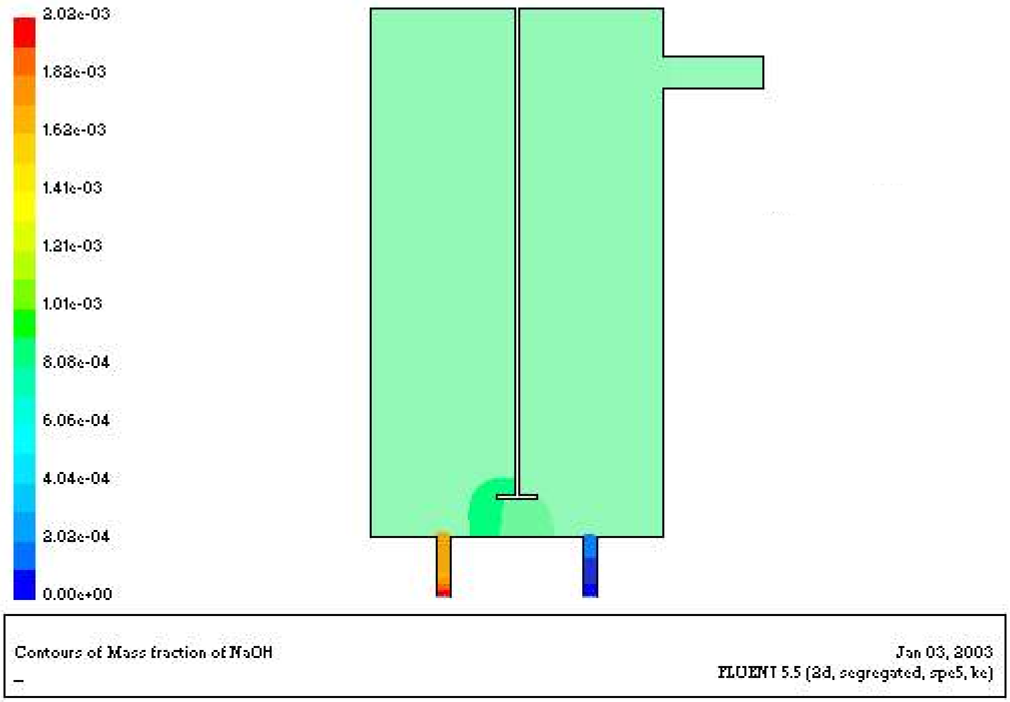

Fig.5 MASS FRACTION OF NaOH FOR 1000 rpm IMPELLER SPEED FOR IMPELLER AT 2 cm FROM BOTTOM

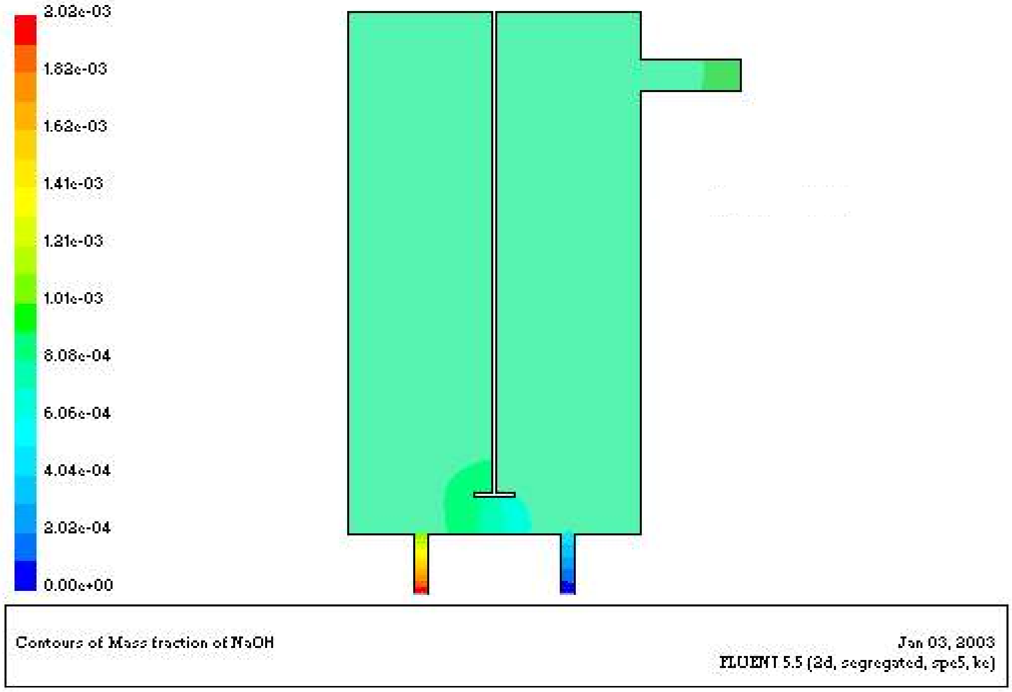

Fig. 6 MASS FRACTION OF NaOH FOR 2000 rpm IMPELLER SPEED FOR IMPELLER AT 2 cm FROM BOTTOM

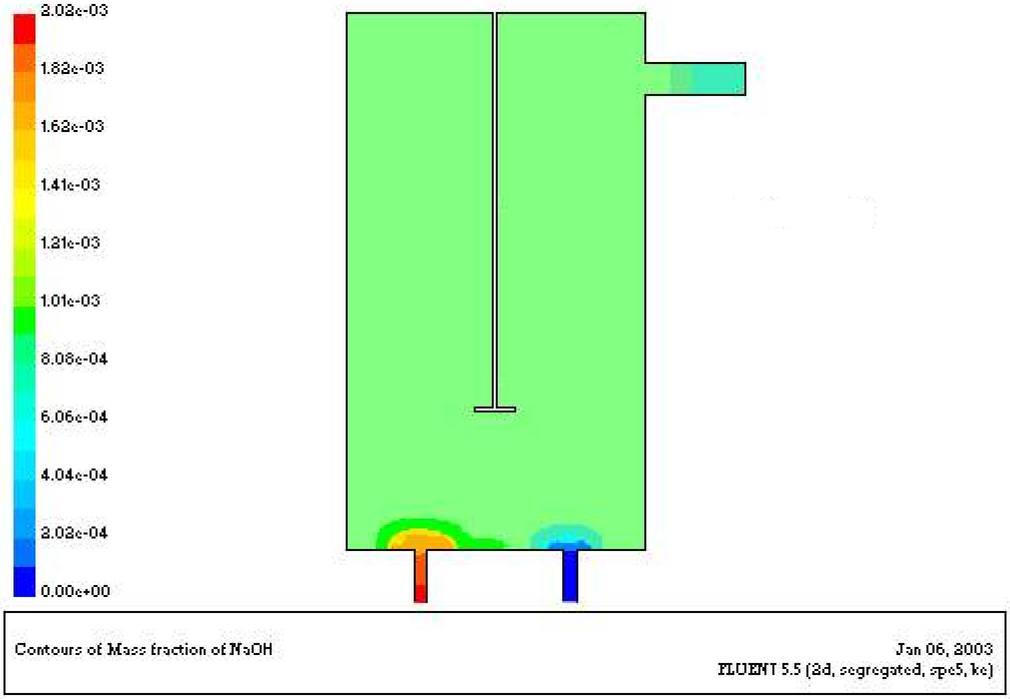

Fig. 7 MASS FRACTION OF NaOH FOR 500 rpm IMPELLER SPEED FOR IMPELLER AT 7 cm FROM BOTTOM

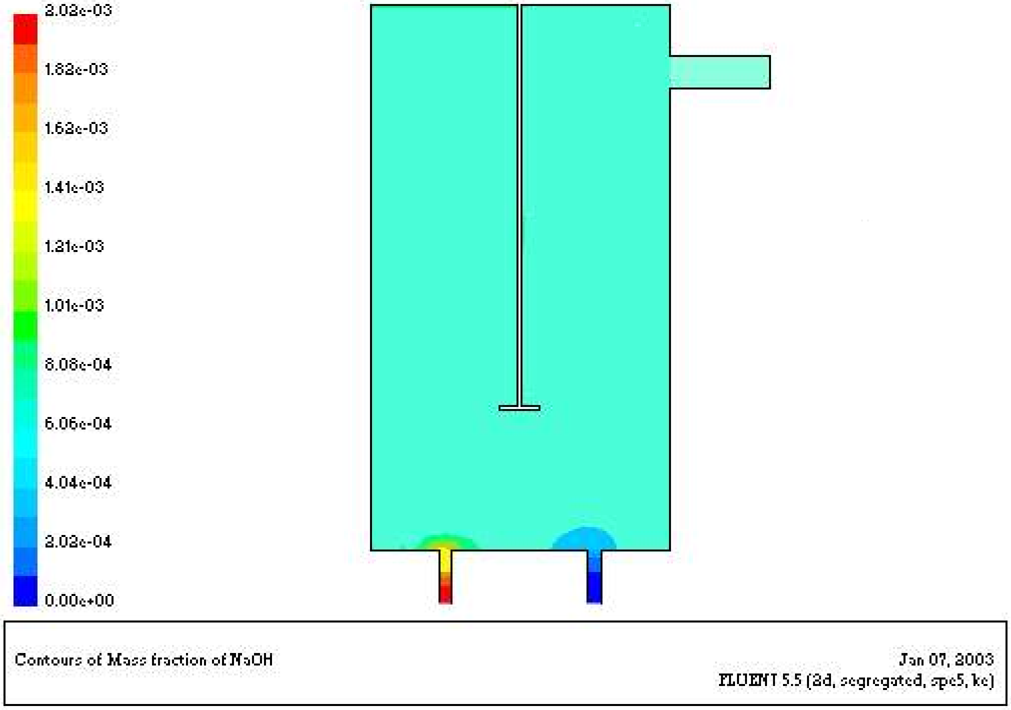

Fig. 8 MASS FRACTION OF NaOH FOR 750 rpm IMPELLER SPEED FOR IMPELLER AT 7 cm FROM BOTTOM

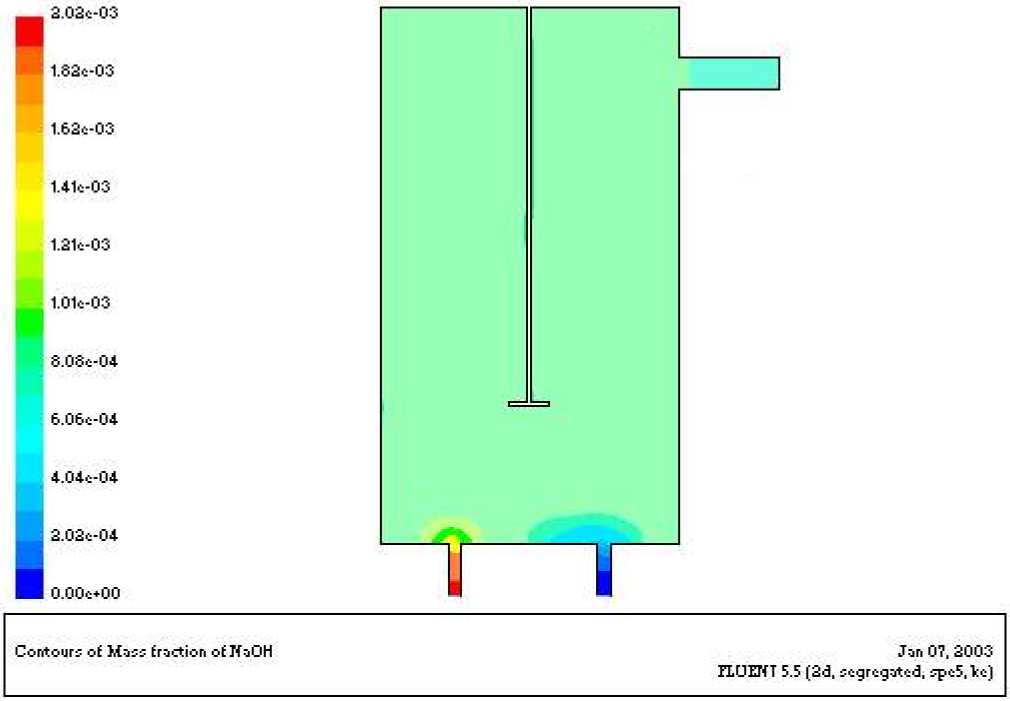

Fig. 9 MASS FRACTION OF NaOH FOR 1000 rpm IMPELLER SPEED FOR IMPELLER AT 7 cm FROM BOTTOM

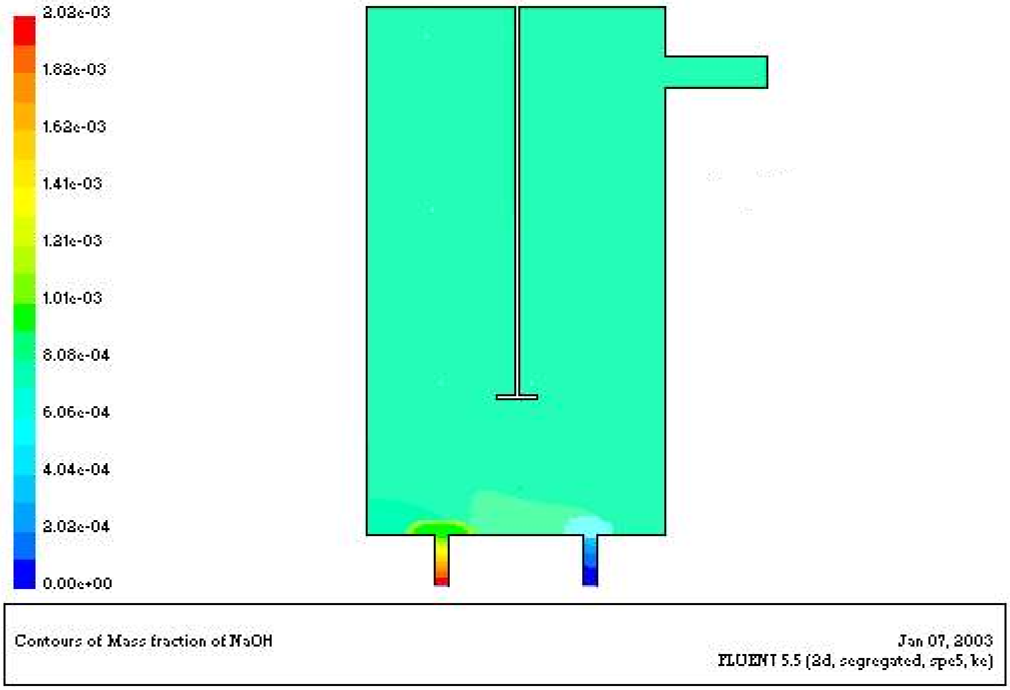

Fig. 10 MASS FRACTION OF NaOH FOR 2000 rpm IMPELLER SPEED FOR IMPELLER AT 7 cm FROM BOTTOM

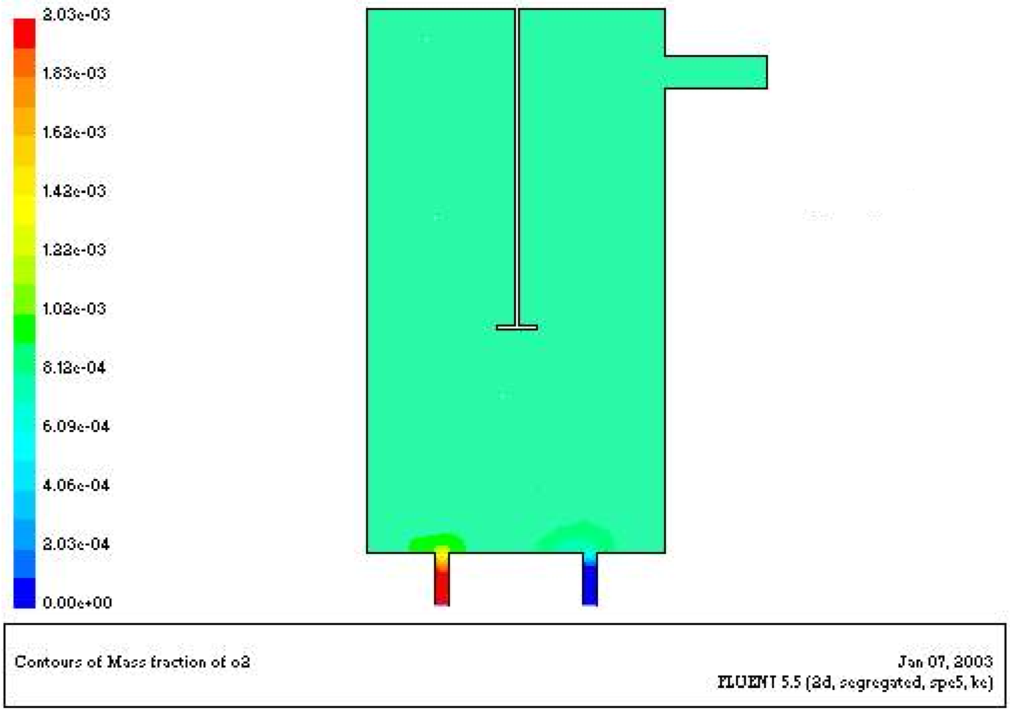

Fig. 11 MASS FRACTION OF NaOH FOR 500 rpm IMPELLER SPEED FOR IMPELLER AT 11 cm FROM BOTTOM

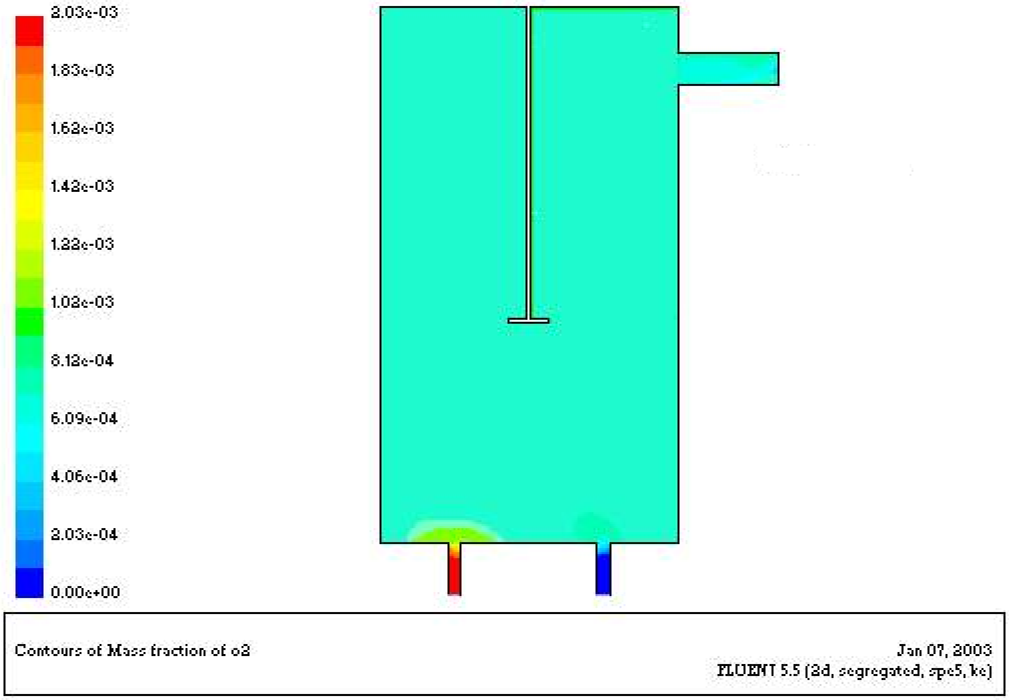

Fig. 12 MASS FRACTION OF NaOH FOR 750 rpm IMPELLER SPEED FOR IMPELLER AT 11 cm FROM BOTTOM

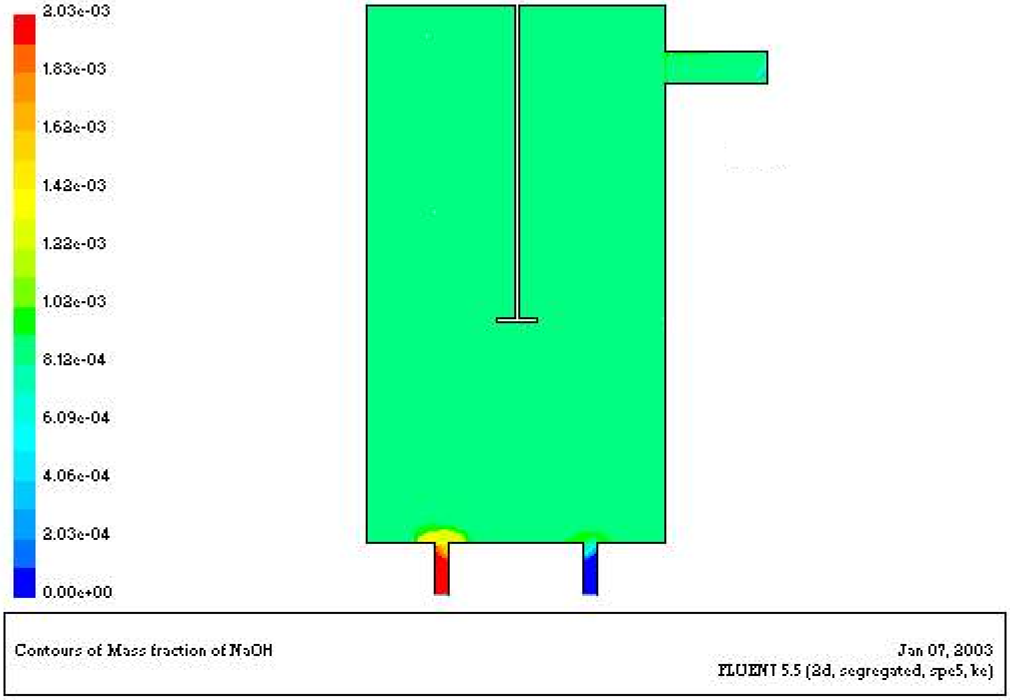

Fig. 13 MASS FRACTION OF NaOH FOR 1000 rpm IMPELLER SPEED FOR IMPELLER AT 11 cm FROM BOTTOM

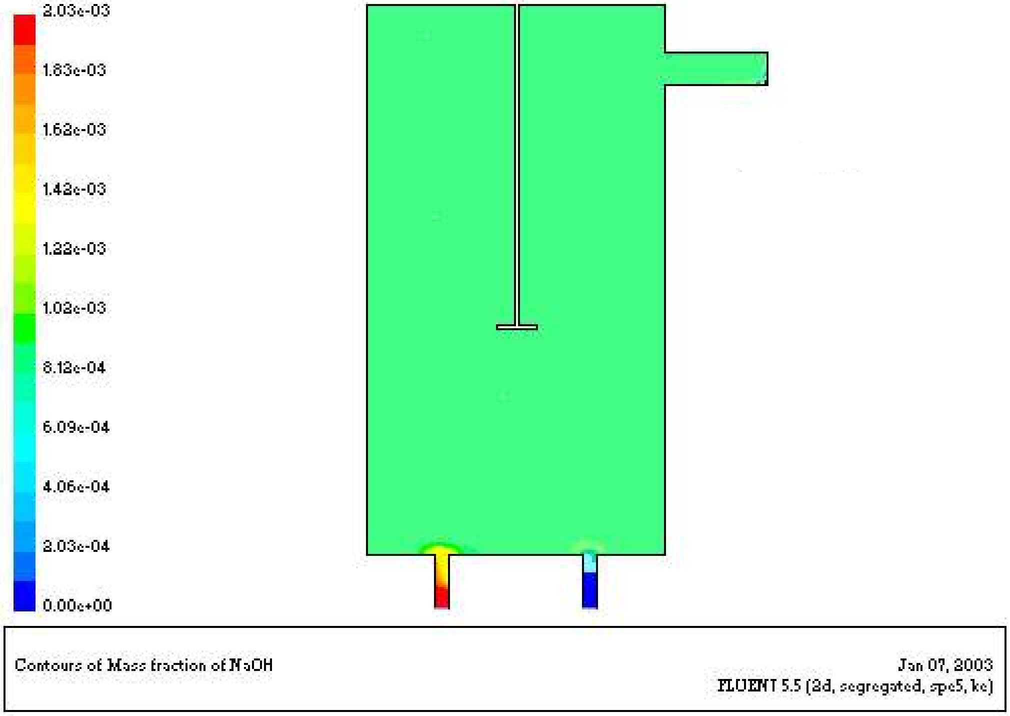

Fig. 14 MASS FRACTION OF NaOH FOR 2000 rpm IMPELLER SPEED FOR IMPELLER AT 11 cm FROM BOTTOM

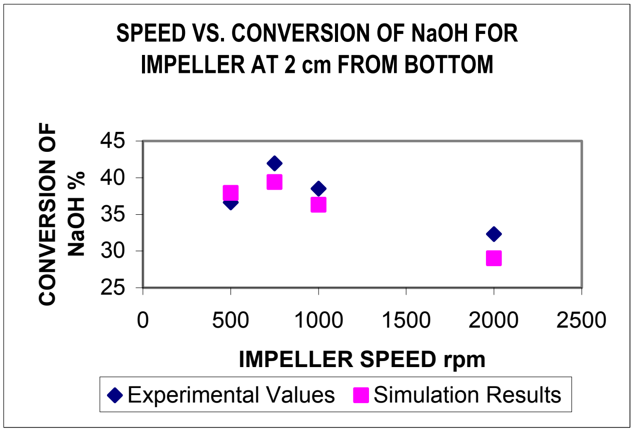

Fig.15 EFFECT OF IMPELLER SPEED ON CONVERSION OF NaOH FOR MPELLER AT 2 cm FROM BOTTOM

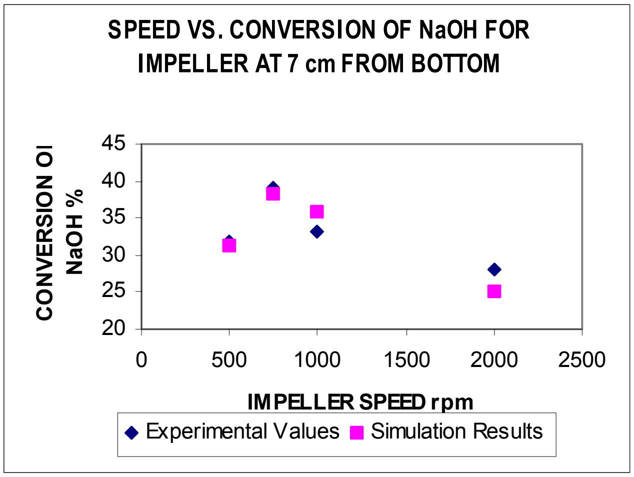

Fig.16 EFFECT OF IMPELLER SPEED ON CONVERSION OF NaOH FOR IMPELLER AT 7 cm FROM BOTTOM

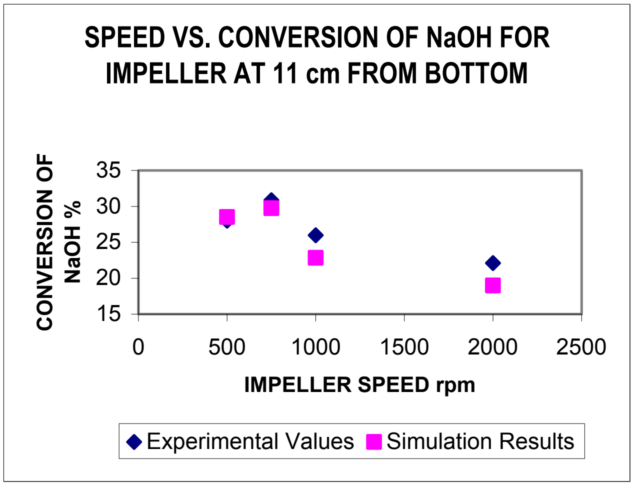

Fig.17 EFFECT OF IMPELLER SPEED ON CONVERSION OF NaOH FOR IMPELLER AT 11 cm FROM BOTTOM