ISSN XXXX XXXX © 2017 IJESC

IJESC

Research Article Volume 7 Issue No.5

Modelling of an Airlift Bioreactor using CFD and PBE for Production of PHB from Molasses

Lavanya.D.K[1], Dr. Vidya Niranjan[2]
PG student[1], Professor& Associate Dean[2]
Department of Biotechnology
R.V College of Engineering, Bengaluru, India

Abstract:
In present work, a 3D simulation of airlift bioreactor using computational fluid dynamics (CFD), FLUENT package. The population balance model (PBM) and Eulerian model were used to investigate the production of polyhydroxybutarate (PHB) in airlift bioreactor performed by Tavares et al. Biosynthesis of PHB in modelled airlift bioreactor was examined and the results were validated against the experimental PHB production rate by Tavares et al suitably. Also, the case study was conducted to get improved yield of PHB from the cheap source and the results thus obtained are compared with validated results within the bioreactor.

Keywords: Computational fluid dynamics (CFD); Polyhydroxybutarate (PHB); airlift bioreactor.

I. INTRODUCTION

Industriousness of plastics has brought about ecological issues. Use of biodegradable biopolymer is answer for the issues. Polyhydroxybutarate (PHB) is biopolymer which can be biodegradable and have comparative properties of thermoplastics. PHB is accumulated in microorganisms with deficient supply of supplement, for example, nitrogen and mineral salts. PHB is accumulated for storage of carbon and energy materials. Because of high cost, the use of PHB and its copolymer is constrained and a few works have been completed to defeat this issue utilizing distinctive methodologies. The works with utilization of mathematical model, neural and metabolic networks helped in enhanced production of PHB. Today a capable technology Computational Fluid Dynamics (CFD) is utilized for considering simulation of flow conduct and nearby hydrodynamics in bubble columns, membrane bioreactors, airlift and stirred tank reactors. This is first way to deal with comprehend utilizing governing equations of continuity, momentum and energy for each phase. The benefit of CFD package is that the column geometry and scale impacts are consequently accounted. As CFD is commercially available apparatus it can be utilized rather than high cost of experiments, with in availability to all areas in the system and turbulent multiphase flow, which should be possible utilizing CFD. Thus CFD can be utilized for examination and forecast of various characteristics. The best possible displaying of energy trade or drag co-productive amongst gas and fluid stages are vital for the achievement of CFD re-enactment methodology. In the course of the most recent decade there is momentous advance in CFD demonstrating of ward gas-fluid two phase streams. The Euler – Euler (E-E) model and Euler-Lagrange (E-L) model are utilized to study hydrodynamics of airlift bioreactor and bubble column reactors. Airlift reactor is an air pocket segment with draft tube to course the liquid in the reactor. Due to the useful profitable, for example, mechanical straightforwardness, great blending, low shear rateand lower operation cost. Thus airlift bioreactors are appropriate decision for large scale manufacturing of PHB.
CFD is an effective device which dissect both air pocket section and PHB creating carrier bioreactors. CFD is likewise used to investigate distinctive attributes, for example, gas burglary, shear push, mass exchange and stream elements in airlift reactors. Past deals with ferrous biooxidation in a two stage framework with airlift bioreactor was finished by CFD simulation in Eulerian outline work to depict the hydrodynamics of the bioreactor (Mousavi et al.). Phenol biodegradation by immobilized *Candida tropicali*s in three-stage bubble section was explored utilizing CFD displaying to create 3-D transient CFD show for recreating the dynamic conduct of group phenol biodegradation (Jia et al.). The review on three-stage transport bioreactor for bio-treatment of toluene waste gas by immobilized *Pseudomonas putida* utilizing a transient CFD displaying (Wang et al.). The CFD display with two-measurement axisymmetric to enhance the inward structure of a tube shaped carrier bioreactor (Xu et al.). The work was to improve the structure plan of a carrier sonobioreactor for furry root culture utilizing two dimensional CFD show. Another outline of airlift bioreactor was mimicked utilizing CFD. They got result was having a huge change in the execution the bioreactor by the expansion of mass exchange and the abatement of shear stress (Bannri et al.). The present review expects to design airlift bioreactor producing PHB with hydrodynamics attributes (gas holdup, volumetric oxygen exchange co-productive and shear push) and furthermore PHB biosynthesis response utilizing CFD in the Eulerian outline work. The PHB biosynthesis response was analyzed utilizing metabolic model of PHB biosynthesis and was utilized as a part of the recreation. Advance enhancement of active parameters for forecast of trial information in the bioreactor was done.

II. METHODOLOGY

(A). KINETIC EQUATIONS

The PHB pathway of the bacterium *Ralstoniaeutropha* comprises three noteworthy strides including thiolase, reductase and synthase. For examination of the PHB creation in the bioreactor, a model proposed by Leaf and Srienc was utilized. The numerical model conditions introduced by Leaf and Srienc are

$$\frac{d[AACOA]}{dt} = R_{\text{thiolase}} - R_{\text{reductase}} - \mu_s[AACOA] \quad (1)$$

$$\frac{d[3HBCOA]}{dt} = R_{\text{reductase}} - R_{\text{synthase}} - \mu_s[3HBCOA] \quad (2)$$

$$\frac{d[PHB]}{dt} = R_{\text{synthase}} - \mu_s[PHB] \quad (3)$$

The three response rates of PHB production and their relating constants, and furthermore metabolites values as indicated by Leaf and Srienc, have been used. It ought to be noticed that for execution of response in the recreation, the accompanying rearranged response was got from metabolic responses to use in the production

$$C_6H_{12}O_6 \rightarrow \text{PHB monomer}(C_4H_6O_2) + 6H^+ + 2CO_2 \quad (4)$$

(B). GOVERNING EQUATIONS

Eulerian model with two-phase flow (air dispersed in liquid phase) was applied in this study.
The continuity equation is written as

$$\frac{\partial}{\partial t}\left(\alpha_j \rho_j\right) + \nabla.\left(\alpha_j \rho_j \overrightarrow{u_j}\right) = 0 \quad (5)$$

Where αj is volume fraction, ρj is density, and →u j is the average velocity for the jth phase.
The momentum equation is written as

$$\frac{\partial}{\partial t}\left(\alpha_j \rho_j \rightarrow u_j\right) + \nabla.\left(\alpha_i \rho_i \overrightarrow{u_j}\,\overrightarrow{u_j}\right) = -\alpha_j \nabla p + \nabla.\bar{\bar{\tau}}_j + \alpha_j \rho_j \bar{g} + \sum_{i=1}^{n} \overrightarrow{R_{ij}} + \alpha_j \rho_j \left(\overrightarrow{F_j}\right) \quad (6)$$

The right term of Eqn depicts all forces acting on the phase j including pressure gradient, viscous stress, gravity, and interfacial force between two phases such as drag, lift, and virtual mass forces.
The conservation equation for transport species has the following form,

$$\rho\left(\frac{\partial Y_i}{\partial t}\right) + \rho \nabla.\left(\overrightarrow{u} Y_i\right) = -\nabla.J_i + S_i \quad (7)$$

Where Yi represents the local mass fraction of ith species, Ji the diffusion flux of species i, and Si is the source term for ith species due to the reaction.
Diffusion flux can be shown as

$$J_i = -\rho D_{i,m} \nabla Y_i \quad (8)$$

Di, m is the ith species diffusion coefficient in the mixture.

III. MODEL VALIDATION

(a).Creation of geometry

Cylindrical shaped airlift bioreactor was displayed by utilizing CATIA V5 demonstrating device. The distance across of the draft tube to bioreactor breadth 0.8mm and the edge of the cone shaped base is 250°. Inlet and outlet of the bioreactor and its symmetry were picked as boundary limits of reactor. Inlet limit is of velocity and outlet limit is pressure outlet. Discretizing is done for the produced computer aided design model of bioreactor by utilizing ABAQUS/CAE. The figure beneath demonstrates the meshed model of bioreactor. For modelling, hexahedral components are utilized for the geometric unpredictability. Next stride is to make a discretized model to acquire exceedingly exact outcomes, the organized framework discretization plan is utilized. This procedure basically includes separating the model into hexahedral mapped volumes. This split volumes are coincided utilizing consistent hexahedral modelled components.

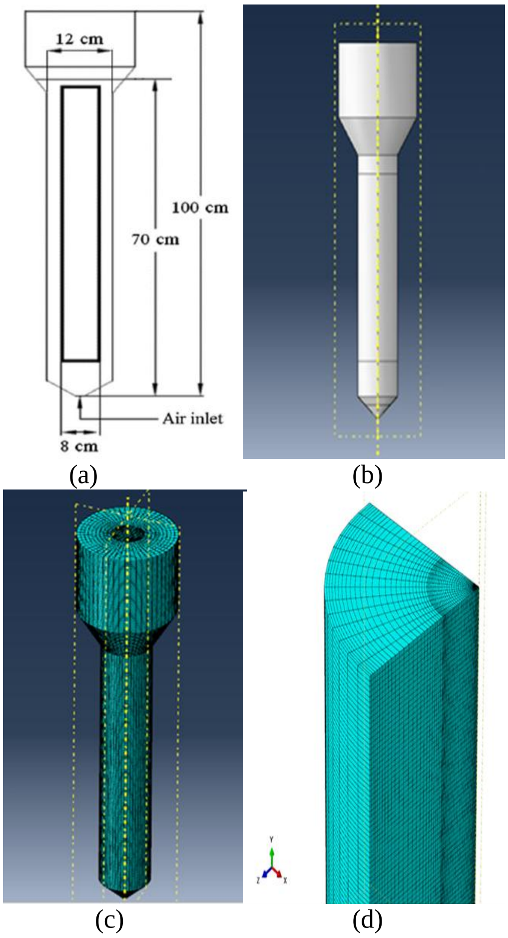

Figure.1. (a) Shows schematic diagram of airlift bioreactor (b) pre-processor model (c) hexahedral mapped model (d) symmetric view of hexahedral model

(b). Initialization and boundary conditions

The population balance equations, the Sauter mean bubble diameter was used in calculations. The boundary conditions for the walls were defined as no-slip for the liquid phase and free-slip for the gas phase. The reactor was symmetrical from both sides. The aeration rate was set to 30 L/min. The number of the orifices was 16 with a diameter of 0.8mm. Multiphase reaction model is chosen to characterize the connection between the fluid and air stages. The first order upwind technique was utilized for discretization of basic conditions. Air was utilized as the gas phase and liquid phase was assumed as blend of glucose, water, H+, CO2, and PHB monomers, as per the simplified reaction. Liquid and air phases are set up and physical properties were characterized under Eulerian Multiphase model. K-Epsilon show with two stages is chosen for continuous phase. The Turbulence Reaction model is characterized for the velocity fluctuations that are experienced in the dispersed bubbly stream. Discrete phase model utilized for analysing the 16 orifice air infusions at the inlet boundary condition. Population Balance model with quadrature methodology is defined to calculate a reactive balance momentum accuracy in each cells. The bubble diameter with maximum and minimum sizes and moments are defined for proper dispersion in the reactor.

Table.1. Material properties

Components	Density (kg/m3)	Molecular Weight (Kg/kgmol)	Enthalpy (Kj/kgmol)	Entropy (j/kgmol-k)
Carbon –dioxide	1.79	44.00995	-393532	213720.2
Glucose	1540	180	-1271	209200
Water	998.20	18.02	-285841	69902
Atomic hydrogen	898.80	1.00742	-153624	108827
PHB monomer	1250	86.09	-	-

PHB- Polyhydroxybutarate.

IV. CASE STUDY SIMULATION

Investigation was carried out by defining the alternative carbon source from sugar industry as cheap source for the generation of PHB monomer. Simulations were performed to analyse the PHB concentration profile from molasses as substrate. The kinetic equations considered for the simulation are presented below**:**

$$C_{12}H_{22}O_{11} + H_2O \rightarrow 2C_6H_{12}O_6 \quad (9)$$

$$C_6H_{12}O_6 \rightarrow PHB\ monomer(C_4H_6O_2) + 6H^+ + 2CO_2 \quad (4)$$

The conversion of molasses to glucose is carried out by enzyme invertase and the glucose thus produced is broke down to PHB monomer. The addition invertase as catalyst improves production rate of PHB. Population Balance model with quadrature methodology is defined to calculate a reactive balance momentum. Liquid and air phases are set up and defining Eulerian Multiphase model, K-Epsilon realization model with two phases is chosen for continuous operation. The velocity contour of the bubble column bio-reactor which has the inlet boundary condition of 16 orifices air injections which has the mass flow inlet of 30LPM with a diameter of bubble 0.8mm.

Table.2. Material property for Molasses

Components	Density (kg/m3)	Molecular Weight (Kg/kgmol)	Enthalpy (Kj/kgmol)	Entropy (j/ kgmol-k)
Molasses	1400	46.06	-	-

V. RESULTS AND DSCUSSION

(a).Validation results

To investigate the production of PHB in the bioreactor the accumulation phase, the Eqns (1)–(3) were solved and their results were compared with the experimental results of Tavares et al.,. Required parameters for calculating KLa like gas holdup were called from simulation data. The results close to experimental data are shown in figure 2.The experimental data of Poorya Mavaddat et al, are related to aeration rate of 30 L/min, which was obtained as a nearly optimized value and at higher aeration rates, no significant difference in performance of production reported and this indicates that the oxygen transfer was not a limiting factor at higher aeration rates than 30 L/min is shown in figure 3.Thevelocity profile of liquid and volumetric oxygen transfer co efficient are obtained and compared with experimental data of Poorya Mavaddat et al. shown in figure 4 (a) and (b).

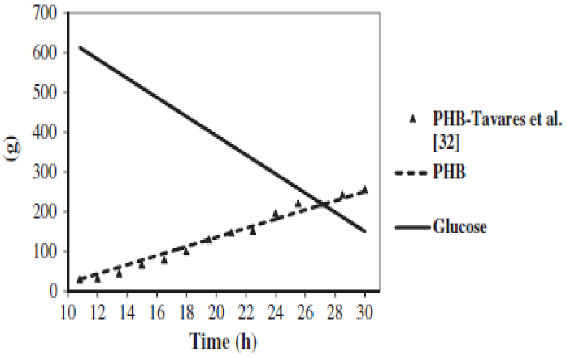

Figure.2. Variation of the modeled polyhydroxybutyrate and glucose and experimental data by Tavares et al.

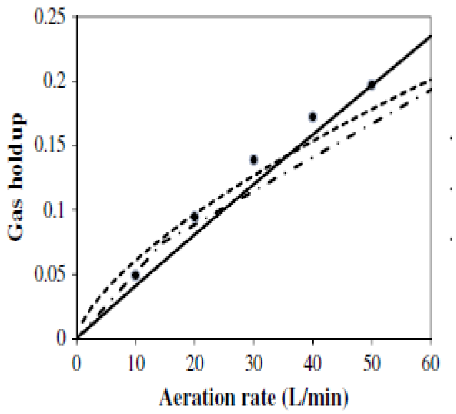

Figure.3. Gas holdup obtained by simulation andvarious correlations vs aeration rate data by Poorya Mavaddat et al.

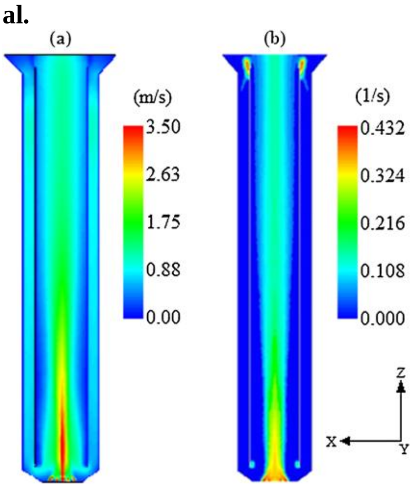

Figure.4. Profile of (a) liquid velocity in the bioreactor(b) volumetric oxygen transfer coefficient calculated by Eqn 42 at aeration rate of 30 L/min data by Poorya Mavaddat et al.

The correlation of velocity at various regions of bioreactor is shown in the figure5 (a). The velocity form of the airlift bioreactor which has the channel orifice 16 holes for air infusions which has the mass flow rate of 2.0417e-5 kg/s (30LPM) .Maximum velocity obtained is of 4.28 m/s. The pressure at various regions of reactor is shown in figure 5 (b). The pressure distinction inside the airlift bioreactor, which has the maximum pressure of 21.5 Pa. Simulations were carried out to analyse the molar concentration of glucose and PHB in bioreactor. The glucose concentration with aeration rate of 30 L/Min obtained is 0.77 mol /L and the PHB molar concentration with aeration rate of 30 L/Min is 0.55 mol / L. The results are shown in figure5 (c) and (d).The figure 6 shows the graphical representation of residual plots and convergence parameters for transient simulation performed.

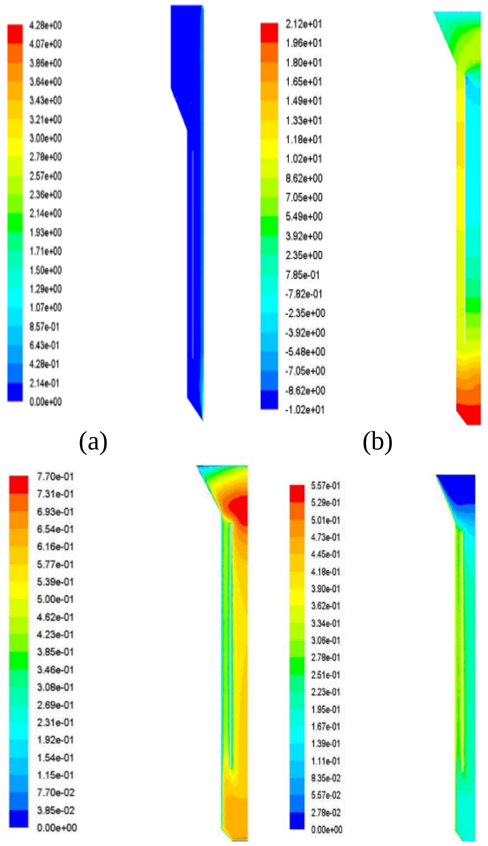

Figure.5.(a) air velocity contour (b) pressure contour (c) glucose mass fraction (d) PHB mass fraction, of validated model

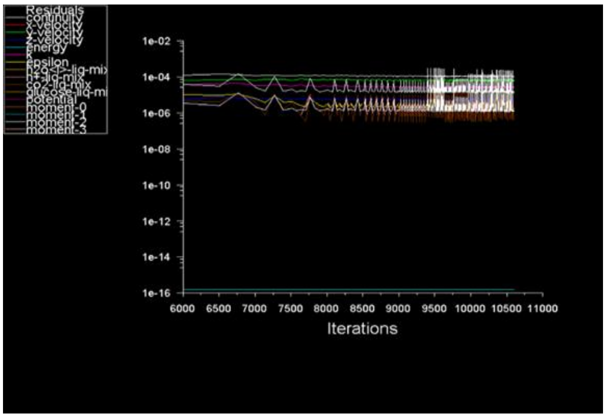

Figure.6. Simulated graph of convergence under transient condition

(b). Case study simulation results

The use of cheap source of substrate i.e. molasses from sugar industry and alongside extra kinetic reaction responses the transformation from molasses to glucose and after that glucose to PHB has given enhanced yield of PHB monomer in above approved model of airlift bioreactor which can be easily visualized after outcomes. The velocity contour of air phase of bubble column bioreactor which has the inlet boundary condition of 16 orifices air injections which has the mass flow inlet of 2.0417e-5 kg/s. Maximum velocity observed is of 3.19m /s and maximum pressure of 15.4 Pa are shown figure7 (a) and (b).The molar concentration of glucose and PHB obtained is more compared to with approved validated model. Simulations were carried out to investigate the molar concentration of glucose and PHB in bioreactor, the glucose concentration with aeration rate of 30 L/Min obtained is 1.72 mol/L and the transformation of glucose to PHB monomer concentration is 0.77 mol/L are shown in figure 7 (c) and (d).

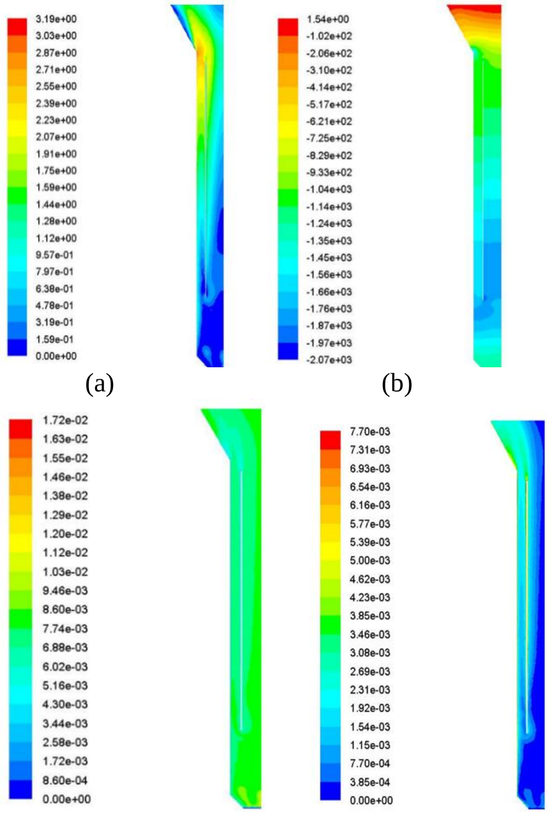

Figure.7. (a) air velocity contour (b) pressure contour (c) glucose mass fraction (d) PHB mass fraction, of the case study.

VI. CONCLUSION

In this paper we have proposed the model of airlift bioreactor using CFD with FLUENT software package. As the usage of airlift bioreactor consumes less power and understanding the mechanical operation is easy compared to other reactors. We analysed the airlift bioreactor model with validation of proposed model against the experimental data. The case study conducted showed improved yield of glucose and PHB monomer concentration by usage of molasses as cheap source of carbon from sugar industry and the improved results obtained are verified by comparing to the values of validated model successfully.

NOMENCLATURE

Symbols

ACOA - Acetyl_CoA

AACOA - Acetoacetyl_CoA

ADP - Adenosine diphosphate

ATP - Adenosine triphosphate
DL - Oxygen diffusivity in liquid, m2/s
Di,m - Diffusion coefficient of ith species in the mixture, m2/s
d - Diameter, m
d_{32} - Sauter mean diameter, m
→F - External body force, N
f - Drag function
Fr - Froude number, dimensionless
g - Gravitation acceleration, m/s^2
HSCOA - Coenzyme A
I- Unit tensor
J - Diffusion flux, $mol/(m^2s)$
K - Turbulent kinetic energy, m^2/s^2
PHB – Polyhydroxybutyrate
→R - Interaction force, N
T - Temperature, K
U - Superficial gas velocity, m/s
u - Velocity, m/s
ubt - Terminal velocity of an isolated bubble, m/s →u - Average velocity, m/s
v - Bubble volume, m^3
Y- Local mass fraction, dimensionless

Greek letters
α - Volume fraction, dimensionless
ε - Turbulent dissipation rate, m^2/s^3
λ - Bulk viscosity, Pa s
μ - Viscosity, Pa s
μs - Specific growth rate, 1/s
μt,m - Turbulent viscosity, Pa s
ρ - Density, kg/m3
σk - Constant, dimensionless
σε - Constant, dimensionless
τ - Particulate relaxation time, s
τ - Shear stress, Pa
τ - Stress–strain tensor, Pa

Subscrpit
i - ith phase, class index
j - jth phase
L - Liquid phase
m – Mixture
r - Riser
t - Whole column

VII. REFERENCES

[1]. J. L. Ienczak, L. K. Quines, A. A. de Melo, M. Brandellero, C. R. Mendes,W. Schmidell and G. M. F. Aragao High cell density strategy for poly(3-hydroxybutyrate) production by cupriavidus necator. Brazilian Journal of Chemical Engineering Vol. 28, No. 04, pp. 585 – 596, 2011.

[2]. Lana Zanetti Tavares, Elda Sabino da Silva, José Geraldo da Cruz Pradella. Production of poly(3-hydroxybutyrate) in an airlift bioreactor by Ralstonia eutropha. Biochemical Engineering Journal vol 18-21–31, 2004.

[3]. M. Schmidt, J. L. Ienczak, L. K. Quines, K. Zanfonato,W. Schmidell and G. M. F. Aragao. Poly(3-hydroxybutyrate) production by cupriavidus necator supplemented with miniemulsified soybean oil. Brazilian Journal of Chemical Engineering. Vol. 33, No. 01, pp. 13 – 20, 2016.

[4]. Poorya Mavaddat, Seyyed Mohammad Mousavi, Ershad Amini and Hamidreza Azargoshasb. Modeling and CFD-PBE simulation of an airlift bioreactor for PHB production. Asia-Pac. J. Chem. Eng, 2014.

[5]. R.A.J. Verlinden, D.J. Hill, M.A. Kenward, C.D. Williams and I. Radecka .Bacterial synthesis of biodegradable polyhydroxyalkanoates. Journal of Applied Microbiology ISSN 1364-5072, 2007.

[6]. Valkirea Matos Nascimento, Luiziana Ferreira Silva, Jose Gregorio Cabrera Gomez and Gustavo Graciano Fonseca. Growth of Burkholderia sacchari LFM 101 cultivated in glucose, sucrose and glycerol. Sci. Agric. v.73, n.5, p.429-433, 2015.

[7]. A.K.H NorAslan, M.D Mohd Ali, N.A Morad and P. Tamunaidu .Polyhydroxyalkanoates production from waste biomass. International Conference on Chemical Engineering and Bioprocess Engineering. Vol 36-012040, 2016.

[8]. M. Novak, M. Koller, G. Braunegg, and P. Horvat.Mathematical modelling as a Tool for Optimized PHA Production. Chem. Biochem. Eng. Q., 29 (2) 183–220, 2015.

[9]. Samuel Talvy, Arnaud Cockx and Alain Line. Modeling Hydrodynamics of Gas–Liquid Airlift Reactor. AIChE Journal Vol. 53, No. 2, 2007.

[10]. Pratap R. Patnaik. Dispersion optimization to enhance PHB production in fed-batch cultures of Ralstonia eutropha. Bioresource Technology 97.1994–2001, 2006.

VIII. AUTHORS

Ms. Lavanya.D.K received the B.E. Degree in Biotechnology from VTU Belagavi in 2015. She is currently Second year M Tech student of Biotechnology in RVCE, Bengaluru. Her research area of interest are genetics, enzyme technology, microbiology, drug discovery and bioinformatics. Now work focusing on implementation of CFD based real time distributed automotive systems for bioreactor designing and analysis.

Dr. Vidya Niranjan is presently Professor& Associate Dean in Department of Biotechnology in R.V college of Engineering, Bengaluru. She has teaching experience of 10 years. She has submitted many papers in international journals and conferences. Her area of expertise isNGS Data Analysis, Structural Bioinformatics and Drug Discovery.