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Simulation of Preparation of Silver Hydrogen Peroxide using Computational Fluid Dynamics (CFD)

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Abstract
This work deals with the production of silver hydrogen peroxide (AgH2O2) from silver nitrate and hydrogen peroxide. In this procedure, the unstable hydrogen peroxide is balanced by introducing silver, where the antimicrobial silver nitrate activator can be observed. Silver hydrogen peroxide is not harmful for environment and human beings. Silver hydrogen peroxide is mostly used as disinfectant in the industries as it is antifungal and antibacterial in nature. Pathogen removal and sterilization is key requirement. As an activated H2O2, all forms of active oxygen compounds are formed (radicals, anions etc.), however the interactive forces among Ag and H2O2 in silver hydrogen peroxide causes the active compounds to attain higher kinetic energy. Higher kinetic energy facilitates the active compounds to penetrate cell wall more easily and more rapidly and oxidize microbial cell walls more efficiently. In this work lab scale production of silver hydrogen peroxide is performed using CFD simulations. The results obtained from simulations were compared with the ideal batch reactor.

Keywords – *Antimicrobial, silver nitrate, disinfecting, oxidize, sterilization.*

I. INTRODUCTION

Silver hydrogen peroxide is a disinfectant dependent on hydrogen peroxide. Silver hydrogen peroxides are a mixture of hydrogen peroxide, silver nitrate and various different segments which are all kept extremely unknown by the different manufactures. Different substances are important to keep detailing stable. The actual variation among AgH_2O_2 and H_2O_2 lies within the sight of the $AgNO_3$ which has its very own antibacterial activity. The silver nitrate likewise goes about as an activator. The peculiarity of the silver nitrate is that it possibly activates the AgH_2O_2 when it is exposed to contamination. Under the power of silver, H_2O_2 turns out to be emphatically activated in contact with organic material [1]. Just similarly as with typically activated hydrogen peroxide a wide range of active oxygen compounds are produced. Although since interaction forces between the silver activator and the hydrogen peroxide particles, the shaped radicals and anions have a high kinetic energy.

This facilitates them to go through the cell divider easily, so that the inside oxidation of the microbial cell takes place more proficiently. Here after AgH_2O_2 sanitizes far superior than usual H_2O_2.Depot action a better sanitization can be guaranteed throughout a long time, whenever dosed accurately. Hydrogen peroxide activation ceases once all the organic material is oxidized. Toward the finish of the oxidative reaction the non-reacted hydrogen peroxide remains balanced out (H_2O_2). Then again, the reacted hydrogen peroxide which is changed over in active oxygen breaks down in water (H_2O) and oxygen (O_2) after the oxidation of the organic material. $AgNO_3$

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doesn't separate and in this way stays in the environment. Conversely with typically activated hydrogen peroxide the reaction is reversible so just the hydrogen peroxide, essential for the total oxidation of the present organic substance, is separated. Residual non-reacted hydrogen peroxide stays steady and preserved in relationship with the silver nitrate.

Due to long term efficiency silver hydrogen peroxide is used as an effective disinfectant in industries. It is viable even in low compositions utilized. It is used in broad range of temperatures up to the boiling point. Delicate to the skin, Silver nitrate is one of the most dangerous types of heavy metal. Silver precipitates out in contact with chlorites hence can't be utilized with ground water [2].

II. COMPUTATIONAL FLUID DYNAMICS

Chemical reactors are categorized by batch, fed-batch, continuous operations or kind of impeller type. The mixed vessel tank is one of the most regularly utilized gadgets in the creation business. For the reasonable homogeneity, sufficient blending is necessary which relies upon the design and size of the moving parts. Static parts connected to a mixing tank in certain circumstances may significantly affect mixing phenomena. A thorough simulation of the fluid dynamics can support to determine the operating regimes. Depending upon the specific parameters the amount of products can be increased in the process. Many readings of process are to be taken for detailed study using several criteria and the device must be tested for all environmental adversities to remedy any skewness of values. It takes lot of time to gather adequate data to construct a model [11].

At times, it is hard to acquire experimental data too. Pilot plant tests can be deliberated as a choice; yet the appearance of computational fluid dynamics (CFD) has left this ordinary technique far apart. Due to its principal benefit, the CFD models examine the actual process in 3-Dimensions beside with the scaling option. This work uses OpenFOAM 6.0in which a lab reactor with impeller was simulated at various rotational speeds, for example, 20, 30, 40 and 50 rpm. Velocity, pressure and concentration profiles at different planes were obtained and studied. The accomplished outcomes are shown in three dimensional animations employing Paraview.

The flow is expressed by the Navier-Stokes equations given as follows:

$$\rho\frac{\partial u}{\partial t}+\rho\ (u.\nabla)= \nabla.\left[-pI+ \eta(\nabla u+(\nabla u)^{T})\right]+ F \quad (1)$$

$$\nabla.u=0 \qquad (2)$$

The continuity equation is as follows:

$$\frac{\partial \rho}{\partial t}+ \nabla.(\rho u)= 0 \qquad (3)$$

Two models are used for deciding turbulence modeling variable k-ε models, Reynolds number and Navier-Stokes equation. The stresses are determined as mean stresses to reduce the computation requirement. Equation indicates the stress tensor (P_K). Here u signifies for velocity (m/sec), ρ for density (kg/m^3), **η** for dynamic viscosity (Pas), and P the pressure (Pa) [3].

III. BATCH REACTOR

Reactants are initially fed into the batch reactor and are well mixed, and are left to react for a specific period of time. The resultant mixture is then discharged. This is an unsteady state operation where composition changes with respect to time and the composition of reactor is uniform at any instant. A typical batch reactor comprises of tank with an agitator and integral heating/cooling system. Such vessels can vary in size from less than 1 liter to 15,000 liters. They are normally assembling in stainless steel, glass-lined steel or exotic alloy. Liquids and solids are normally charged via means of connections in the top front of the reactor. Vapors and gases likewise release through connections in the top. Liquids are generally released from the bottom.

a) IDEAL BATCH REACTOR

In a batch reactor, as the composition is uniform at all times, it can be accounted for the entire reactor. Taking note of that no liquid enters or leaves the reaction mixture during reaction, which is written for component A, becomes

Input = Output + Disappearance +Accumulation

Input = Output = 0

(Rate of loss of reactant A within reactor due to chemical reaction) = - (Rate of accumulation of reactant A within the reactor)

Disappearance of A by reaction =

$$(-r_A)V = \frac{\text{moles of A reacting}}{(\text{time})(\text{volume of fluid})}\ (\text{volume of fluid}) \quad (4)$$

$$\text{Accumulation of A} = \frac{dN_A}{dt}$$

By replacing these two terms, we get

$$(-r_A)V = N_{A0}\frac{dX_A}{dt} \quad (5)$$

Rearranging and then integration gives,

$$t = N_{A0}\int_0^{X_A}\frac{dX_A}{(-r_A)V} \quad (6)$$

Equation (6) gives the correlation between time and desired conversion X_A for isothermal or non-isothermal system. The volume of reacting fluid and the reaction rate remain under the integral sign; generally both vary as reaction proceeds [4]. This equation might be interpreted for various circumstances. Considering the density of fluid to be constant, we acquire performance equation of batch reactor written as follows:

$$t = C_{A0}\int_0^{X_A}\frac{dX_A}{(-r_A)} \quad (7)$$

IV. DIFFICULTIES IN REACTOR SCALE UP

Industrial Expansion of reactors is a major challenge and is a profound stage towards the developmental and streaming of industrial processes. The scale up operation reflects the integration of the information that has been acquired in different process. Typically, the word "scale up" was described as how to build a "pilot plant or industrial reactor capable of replicating the results obtained in the laboratory". Regarding chemical reactor as a first procedure, there is no broad guideline and no direct method to accomplish these goals. Causes are given as:

1. The reactive system is characterized by kinetic data

2. Industrial scale expertise is not often correlated to lab scale equipments even if industry fully comprises of lab equipments.

3.
For the same reaction, completely different appara tus is possible and the reactions may take place in various phases

Other issues like catalyst aging, impurity, fouling, corrosion, safety and environmental assets are also important to process [5].

a) OBJECTIVES OF THE WORK

- Lab scale method development for production of Silver hydrogen peroxide.
- Scaling up the lab batch reactor to industrial reactor and performing the CFD analysis using OpenFOAM for batch reactor with rotating impeller.
- To obtain pressure, velocity and concentration profile at the various sections in reactor and effect of shaft rpm on these profiles using Paraview.
- Comparing the results with ideal reactors in order to find the deviation from ideal batch

reactor and applications of Silver hydrogen peroxide as disinfectant.

V. QUENCHING OF CHLORINATION DISINFECTION

Since the detection of trihalomethanes (THMs) during water chlorination, extensive research has been conducted into disinfection by-products (DBPs). Presently it has been seen that THMs are the major type of DBPs that can be obtained from water chlorination [6]. In research facility tests, some DBPs are carcinogenic and promote mental results, while in people; epidemiological examinations propose powerless relationship between specific cancers, regenerative and formative impacts and chlorinated surface water. The sanitizer, $Ag+/H_2O_2$ formulation, can be intended after an essential disinfectant e.g., UV, ozone, or chlorine. Research of inactivation with E. coli shows strong microbicide potential of Ag^+ and H_2O_2. For instance, 1-h exposure to 30 ppb of silver ion and 30 ppm of H_2O_2 yields five logs of inactivation of E. Coli B [9].

a) SILVER HYDROGEN PEROXIDE SPRAY FOR SOFT SURFACE FUMIGATION

Most of the cleaning and sterilization efforts concentrate on hard surfaces; there is considerable evidence that soft surface contamination is frequent in health care facilities. For example, clinic security draperies are often infected with pathogenic microorganisms that can be transmitted to hands of healthcare workers or patients. Due to the fact that delicate surfaces cannot be washed and disinfected with a considerable number of products used on hard surfaces, new strategies are required to disinfect delicate surfaces. The IHP (Improved Hydrogen Peroxide) solution applied as a spray without manual washing has proven effective in disinfecting safe isolation curtains [7].

BLEACHING POWDER

Silver hydrogen peroxide is odorless and produces no unpleasant odor like chlorine. Chlorine is profoundly corrosive to metallurgy whereas silver hydrogen peroxide is non-corrosive. Silver hydrogen peroxide does not change the taste of water, unlike chlorine. Silver hydrogen peroxide does not cause irritation to eye or skin. Silver hydrogen peroxide is non-allergenic as chlorine is allergenic in nature. Table 1 shows the specifications of silver hydrogen peroxide [8].

TABLE 1: SPECIFICATIONS OF SILVER HYDROGEN PEROXIDE

Particulars	Value
Hydrogen Peroxide(H_2O_2) IP Grade	49.5% to 50%
Nano Silver IP Grade	490 to 510 ppm
Value of pH	1.5 - 2.0
Shelf life	24 months

VI. METHODOLOGY OF EXPERIMENTS

Here a lab scale reactor is used. Such vessels are about around 50 to 1000 milliliters in size. They are used in production systems for the preparation of small amounts of medicinal substances. The trouble in modeling this sort of reactors is modeling of rotation. It comprises of a reactor vessel of radius 50 mm and height 90 mm. Impeller is connected to a turning shaft. Stationary little pivoting shaft is attached to a long shaft. Impellers are surrounded by a multiple reference frame approach (MRF) zone.

a) MATERIALS AND APPARATUS

In this work the chemicals used are as follows: Silver nitrite ($AgNO_3$), Sodium borohydride ($NaBH_4$), Hydrogen peroxide (H_2O_2), Sodium dodecyl sulphate (SDS), Distilled water. Glass beakers, 500 ml Batch Reactor, conical flask, measuring cylinder and magnetic stirrer with needle.

VII. SYNTHESIS OF SILVER NANOPARTICLE

a) Optimizing the mole ratio

In order to obtain the desired particle size, different mole ratio of silver nitrite and sodium borohydride were taken and the solution obtained from each batch was used to calculate the maximum wavelength using UV visible spectroscopy [10]. Optimization of mole ratio is shown in Table 2.

TABLE 2: OPTIMIZATION OF MOLE RATIO

Sr. No.	Mole ratio $AgNO_3 : NaBH_4$	λ_{max}	Particle Size Range nm
1	1 : 1	550	150 and above
2	1 : 2	380	8-12
3	3 : 1	425	40-55

Reaction:

$$AgNO_3 + NaBH_4 \rightarrow Ag + 1/2H_2 + 1/2B_2H_6 + NaNO_3 \quad (8)$$

Stepwise route:

1. Solution 1- 16.9 mg of silver nitrite ($AgNO_3$) is mixed with 100ml distilled water.

2. Solution 2- 22.8 mg of $NaBH_4$ is mixed with 300ml of distilled water.

3. Solution 1 is placed at room temperature in a reactor of volume 500ml.

4. Surfactant (SDS) is added in terms of percentage of the total volume of the solutions in the reactor containing solution of silver nitrite.

5. Surfactant is added 1%, 1.25%, 1.5% of total volume of the solution taken.

6. Solution 2 is taken in burette and released dropwise in the reactor containing solution of silver nitrite and SDS.

7. Constant stirring of 35-45 rpm is provided with the help of magnetic stirrer.

VIII. SIMULATION USING OPENFOAM

a) FreeCAD

FreeCAD is a 3-D modeler made to design real objects of desired size. Parametric modeling enables us to effortlessly modify the design by returning into model history and changing its parameters. FreeCAD is configured to utilize other open-source resources from thescientific computing sector. Among them are Open CASCADE, coin 3D, the Qt GUI system and Python, a well-known scripting language. FreeCAD itself can be used as a library by different projects.

Initially lab scale batch reactor of radius 50 mm and height 90 mm was designed using FreeCAD. The designed reactor also has a 4-bladed impeller of height 60 mm and radius 10mm. Fig. 1 shows the solid geometry of batch system.

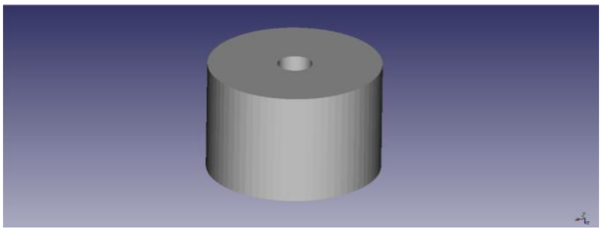

Fig.1. Solid geometry of batch reactor

b) OpenFOAM

OpenFOAM is a platform for creating program executables in a range of around 100C+ libraries utilizing bundled features. With about 250 pre-incorporated applications, OpenFOAM comes with two sections: solvers, designed to solve fluid mechanics issue and utilities, designed to perform data control activities. OpenFOAM is supplied with pre-processing and post-processing situations. The interface to the pre and post-processing are themselves OpenFOAM utilities, consequently guaranteeing consistent data

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handling across all situations which have been shown in Fig. 2.

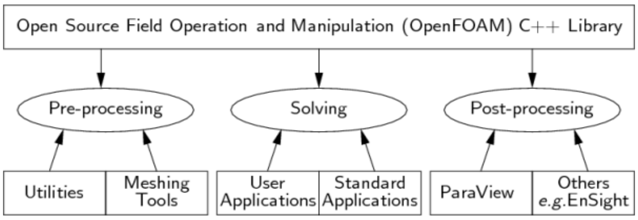

Fig.2. Overview of OpenFOAM structure

c) SnappyHexMesh

OpenFOAM ensures that the mesh fulfills a truly rigid arrangement of validity constraints and will fail to operate if the constraints are not met. Of course, OpenFOAM describes a mesh of arbitrary polyhedral cells in 3-D, bounded by arbitrary polygonal faces, e.g. the cells can have an infinite number of faces where there are no limitations on the quantity of edges or constraints on their orientation of each face. In OpenFOAM a mesh with this general form is called a Polymesh.

The SnappyHexMesh utility produces 3-dimensional meshes that contain hexahedra (hex) and split-hexahedra (split-hex) automatically from triangulated surface geometries in Stereolitho-graphy (STL). Through iteratively improving a starting mesh and transforming the resulting split-hex mesh to the surface, the mesh around it conforms to the surface.

d) ParaView

ParaView is a multi-stage data examination and representation application (see Fig.3). ParaView users can develop perceptions to break down their data using qualitative and quantitative techniques. The data analysis can be done interactively in 3D or programmatically using the batch processing capabilities ParaView. ParaView runs on distributed and shared memory parallel and single processor frameworks. ParaView uses Visualization Toolkit (VTK) as the data processing and rendering engine and has a UI composed using Qt [11].

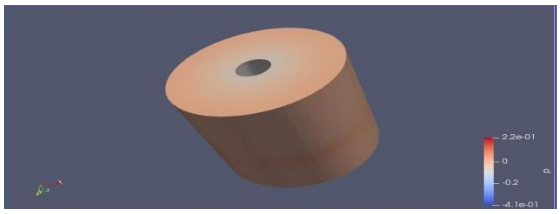

Fig.3. Solid geometry of batch reactor in ParaView

IX. RESULTS AND DISCUSSION

a) Characterization

Reactors are major asset of the any industry. Adaptive reactor parameters are needed for more economically effective industry. Here we have considered a stirred batch reactor having radius R=50 mm and height H = 90mm. The impeller dimensions are, for shaft r = 10 mm and h = 60 mm, for blade l×w×h = 25×12.5×10. The total volume that can be occupied by the fluid = 0.684 L. Fig 4 indicates the comparison in Theoretical and simulated concentration for reaction without flow.

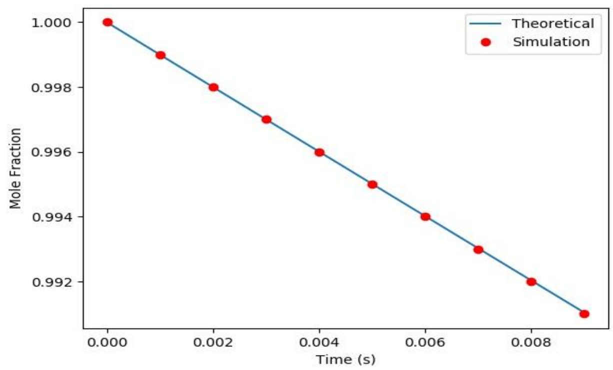

Fig.4. Comparison between Theoretical and simulated concentration for reaction without flow

The blue line in the above graph shows the theoretical concentration and red points show the simulated concentration. Since the two values are very close to each other it means the designed reactor is almost ideal. Table 3 shows the Maximum Velocity Magnitude for different rpm of impeller.

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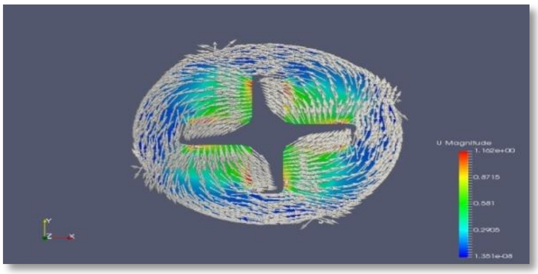

Fig.5. Distribution of the velocity magnitude in the impeller plane (20 rpm)

TABLE 3: MAXIMUM VELOCITY MAGNITUDE FOR DIFFERENT RPM OF IMPELLER

Sr. No.	Impeller Speed (rpm)	Maximum velocity (m/s)
1	20	1.162
2	30	1.161
3	40	1.245
4	50	1.246

The primary Paraview filter used for creating Fig. 5 is glyph filter. In these figure oriented, scaled and coloured lines for each of the velocity vectors is seen. Velocity vectors for different rpm are shown in figures. Maximum velocity profile is almost flat i.e., it is same for different rpm of impeller which implies that mixing is uniform in the reactor and hence the designed reactor is almost ideal.

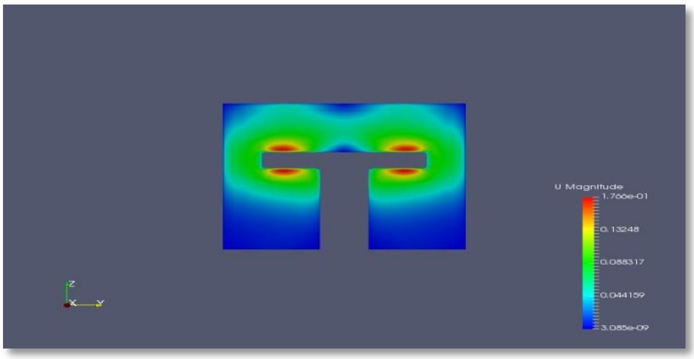

Fig.6. Axial flow velocity distribution in the plane perpendicular to the propeller plane (20 rpm)

Fig. 6 shows the velocity profile in the plane perpendicular to propeller. It basically shows the axial mixing in the reactor for different rotational speed of impeller. It can be seen from the figures that velocity is maximum just above and below the propeller and velocity decreases as distance from propeller increases. Blue coloured zones near wall of the reactor are called dead zone.

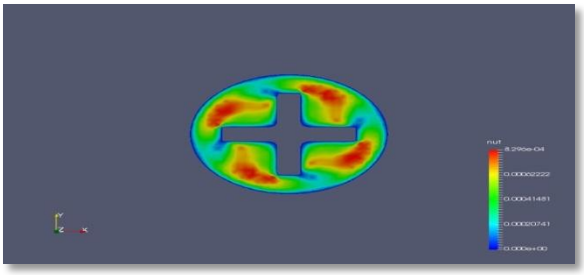

Fig.7. Turbulent viscosity (nuT) for 20 rpm

Fig. 7 represents turbulent viscosity of fluid. Eddy viscosity is the proportionality factor that defines the turbulent energy transfer arising from moving eddies, resulting in tangential stresses. Greater turbulent viscosity implies fluid is highly viscous and more power is required by the impeller.

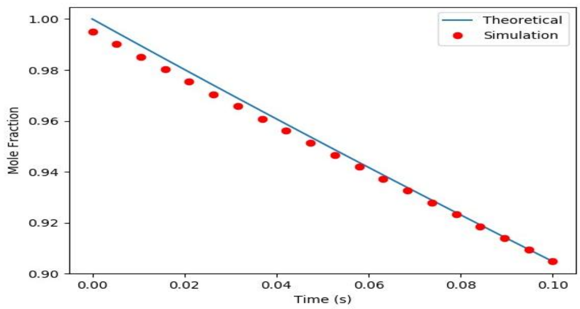

Fig.8. Comparison between theoretical concentration and simulated concentration for flow and reaction

Fig. 8 shows the comparison between theoretical concentration and simulated concentration for 1 mol/lit of initial concentration. The blue line in the above graph shows the theoretical concentration and red points show the simulated concentration. Since the two values are very close to each other it means the designed reactor is almost ideal.

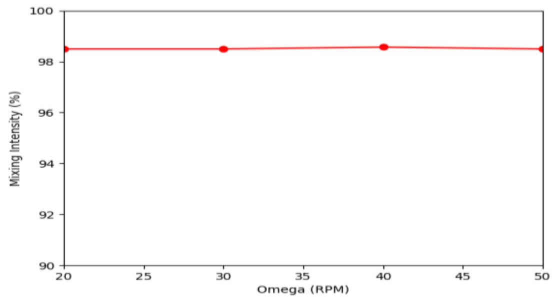

Fig.9. Mixing Intensity vs different rpm

b) Mixing Indices

Mixing indices are calculated by pixel intensities over a cross-section of a grayscale picture. Simplest index is determined by equation given below:

$$\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(I_i - \langle I \rangle)^2} \quad (9)$$

where I_i - local pixel intensity, $\langle I \rangle$- average of the pixel intensities in the cross-section, and N- No. of pixels.

The scale of RMI extends from 0 to 1. Fig. 9 represents the mixing index variation with omega. Value of mixing index (RMI) is 98.5%, which shows the reactor is almost ideal [12].

Fig. 10 and Fig. 11 show the comparison of theoretical and simulated concentration analysis for 20 rpm and 50 rpm respectively.

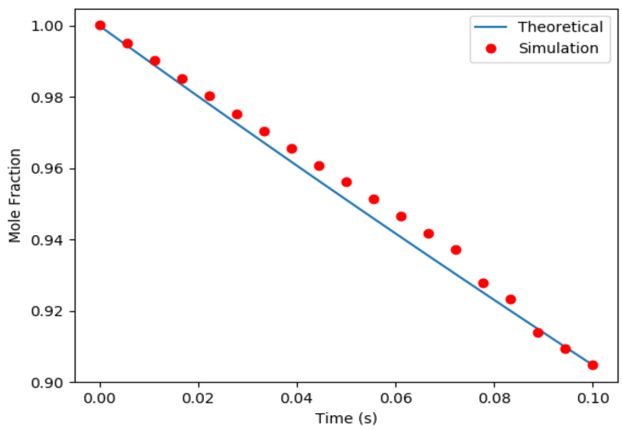

Fig.10.Comparison of theoretical and simulated concentration analysis for 20 rpm

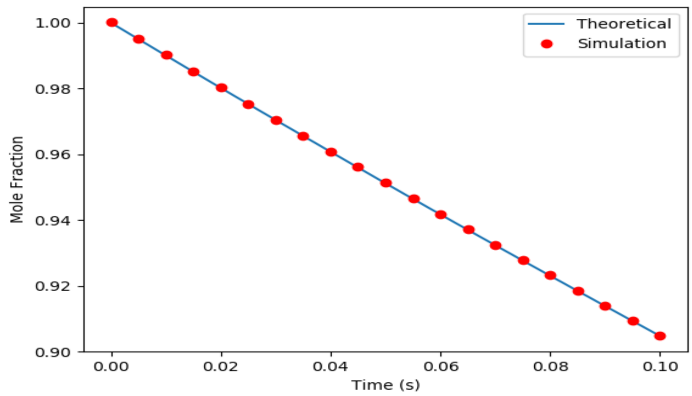

Fig.11. Theoretical and simulated concentration analysis for 50 rpm

X. CONCLUSION

Silver hydrogen peroxide from hydrogen peroxide and silver nitrate is environmentally safe and not harmful to humans. Due to its excellent antiviral, antifungal and antibacterial qualities, silver activated hydrogen peroxide has a higher position in the variety of disinfectants. Pathogen reduction and sterilization has become a key requirement. The computational fluid dynamics (CFD) is being used to investigate velocity profile and mixing in stirred vessels.

In order to understand the various effects like reactor geometry, speed, baffles, and properties of fluids on mixing process, an impeller configuration is the most important factor. Same simulation can be done in future for, multi-impeller systems, continuous systems and higher revolution speed. The results obtained from these lab scale reactor simulations are similar to an ideal batch reactor. The various shape of reactors (viz, ellipsoidal) with different type of impellers like T-Shaped, rotating disc, three-bladed impeller of the ideal batch reactor can be used for further advancement of production of silver hydrogen peroxide.

XI. REFERENCES

1. B. M. Andersena, M. Rasch, K. Hochlin, K. Jensen, F-H Wismar, P. and Fredriksen, "Decontamination of rooms, medical equipment and ambulances using an aerosol of hydrogen

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peroxide disinfectant", J. Hospital Infection, 62 (5), pp 149-155, 2005.

2. A. Filippi, "The Disinfecting Action of Ozonated Water and of Hydrogen Peroxide/Silver Ions in Vitro", Ozone: Science & Engineering, 22 (4), pp 441-445, 2000.
3. Praveen Patel, Pranay Vaidya, Gurmeet Singh "An Overview of Impellers, Velocity Profile and Reactor Design", proceedings of COMSOL conference in Bangalore, 2014.
4. Octave Levenspiel, "Chemical Reaction Engineering", John Wiley & Sons. 3rd Ed., 1998.
5. Gianni Donati, Renato Paludetto "Scale up of chemical reactors", Catalysis: Today, 34(3-4), pp 483-533, 1997.
6. Mohammad Hosein, Kalantar Motamedi, FinaNavi, AshkanBadkoobeh, Maryam Rezaei &Javad Zardrang "Hydrogen Peroxide-Silver 6%: an Effective Eco-Friendly Disinfectant for Contaminated Instruments" Global journal of medical research: C Microbiology and Pathology , 15 (2) , pp 249-279 , 2015.
7. Cadnum, J. L., Mana, T. S. C., Jencson, A., Thota, P., Kundrapu, S., & Donskey, "Effectiveness of a hydrogen peroxide spray for decontamination of soft surfaces in hospitals". American Journal of Infection Control, 43(12), pp 1357–1359, 2015.
8. Web ref: https://www.chemtexlimited.com/hydrogen-peroxide-with-silver.html
9. Rami Pedahzur, Ovadia Lev, Badri Fattal, Hillel I. Shuval, "The interaction of silver ions and hydrogen peroxide in the inactivation of E. coli: A preliminary evaluation of a new long acting residual drinking water disinfectant", Water science and technology, 31 (5-6), pp 123-129, 1995.
10. Kandarp Mavani, Mihir Shah, "Synthesis of Silver nanoparticles by using Sodium Borohydride as a reducing agent", International Journal of Research and Technology, 2 (3), pp 57-62, 2013.
11. Lomax, H., Pulliam, T., Zingg, D., & Kowalewski, T., "Fundamentals of Computational Fluid Dynamics", Applied Mechanics Reviews, 55(4), pp B61- B82, 2002.
12. Hashmi, A., Xu, J., "On the Quantification of Mixing in Microfluidics", Journal of Laboratory Automation, 19(5), pp 488–491, 2014.