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Design, Modeling and Simulation of Electrochemical Sensor for Zn Detection

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***Abstract*— Electrochemical sensors are becoming vital and an integral part in our everyday life. Many of the application are biomedical and biochemical. Most popular, and the most expressive, electrochemical sensor is the self-regulation blood glucose meter assist in controlling Diabetes. The other application of electrochemical sensor includes gas sensor which is used in homes to detect CO, metal sensor for water quality Analysis. The electrochemical sensors have also been used in Medical Diagnostic, Food monitoring. This Project confers design and modelling of electrochemical sensor for determining Zn ion in Potassium Hydroxide solution. This model consists of three electrodes reference electrode working electrode counter electrode. In this model electrolyte is taken as Potassium Hydroxide (KOH) which is liquid binary electrolyte and analyte is taken as the zinc [Liquid, tested at 450C (723K)] and carbon material is taken as electrode. The Zinc substance is taken 50mmol/m^3 in the Potassium Hydroxide solution. The main reaction takes place at the working electrode applying potential 0.5V at the working electrode will get the peak current which is proportional to the Zn substance Concentration. Electroanalysis physics is used in COMSOL for the simulation of this project.**

Keywords: Electrochemical sensor, amperometry Analysis, concentration, metal ion

I. INTRODUCTION

A sensor can be defined as a device that takes input and gives sensed output. All sensors convert the output into a detected signal on present day instrumentation. They have major position out of the presently available sensor that have extend the commercial stage and which have found have a vast range of important application in the field of environmental, agricultural analysis, industrial clinical field. There are three types of electrochemical sensor, potentiometric sensor in which voltage is detected amperometry sensor in which current is detected conductometric sensor in which conductivity is detected [1-3]. With the increase of present -day industry the result of chemical pollution, and the heavy metal pollution chemical ion pollution which become serious condition for humans. Hence, it is very important to correctly detect, compute and control the chemical pollutants. The measuring techniques used are, electrochemical analysis, mass, spectrometry, spectroscopic analysis. These methods have complex pretreatment, long detection cycle, other side electrochemical sensor have acting as a fast detection chemical ion, electrochemical sensor which measure the solution concentration by electrochemical analysis. Presently electrochemical sensors are extensively used in Pharmaceutical and other fields due to their quality low-cost fast detection [3-6]. Environmental contaminants such as mercury, copper, cobalt is very harmful for human body. Which require the design and development of analytical methods to detect such species. Electro analytical method is considered systematic, high accuracy, rapid responses and they are inexpensive method. Collection of these metals leads to serious harm to human body such as the kidney, liver and transforms into serious diseases lung damage, cancer, digestive issues. This condition has driven us to develop sensors that are inexpensive, portable, sensitive [7-10]. The increased concentration of several metals exceeding guidelines recommendation in water samples. This encourages research on the development of electrochemical sensors. Undoubtedly, the global economic expansion and industrial developments necessary to meet demand and the continued sustainability of human lives have been appreciated worldwide. At the same time, the discharges from the increased chemical processes, agricultural processes, and energy conversions, amongst other applications, have elevated water pollution. The statistics published by the World Health Organization (WHO), based on the 2017 figures, pronounce that 785 million people lack basic drinking-water services, including 144 million people who are dependent on surface water. Globally, at least 2 billion people use a drinking water source contaminated with faces, leading to the transmission of diseases such as; diarrhea, cholera, dysentery, typhoid, and polio, amongst others. It is well known that a class of essential trace elements, such as; zinc (Zn), copper (Cu), molybdenum (Mo), selenium (Se), chromium III (Cr), cobalt (Co), manganese (Mn), amongst others, play significant roles in nutrition balance and other biological aspects 17,81. However, their excessive ingestion above the maximum permitted guidelines provided by the World Health Organization (WHO) may lead to various adverse effects ranging from acute to chronic impacts, de-pending on the type, species and level of exposure[4]. Pollution from heavy metals challenges environmentally friendly structures and poses a great global sustainability challenge. Heavy metals are the major contributors to water contamination, resulting in a severe human tragedy in this paper the procedure have mentioned all the three electrodes were manufactured on the basis of carbon nanotubes thread in the electrochemical cell [11-13]. Electrochemical sensors are essential part of our daily life. It has Many applications such as biomedical and biochemical. The other Applications of electrochemical sensors include, detection of CO as a gas sensor, metals sensor for water quality analysis. The electrochemical sensors are also used in Environmental monitoring, Medical Diagnostic, Manufacturing Automotive, in this technique, the current and potential is measured. Based on this there are major techniques. In Voltammetry a varying potential is applied to working electrode and current is being measured and fix potential is applied and thereby current is measured [14, 15].

SOFTWARE USED: COMSOL Multiphysics is used by engineers and scientists to simulation purpose in all fields of scientific research, engineering and manufacturing. Finite element Analysis software Packages such as ANSYS, COMSOL, Covent ware used to design of electrochemical sensor. In this work COMSOL result gives simulation of electrochemical sensor. The purpose of this work to measure total current proportional to the ion concentration

II.PROPOSED SYSTEM

The Proposed system consists of three carbon electrodes which are made up of carbon materials namely as working electrode, reference electrode, counter electrode. In this system electrolyte is taken as Potassium Hydroxide (KOH) which is liquid binary electrolyte and analyte is taken as the zinc [Liquid, tested at 450C (723K)] carbon material is taken as electrode. In this model the transport of analyte can be done by three modes which are: Diffusion, Migration, convection. Diffusion: Movement of analyte from higher concentration to the lower concentration. Migration: The Movement of ions from working electrode to the counter electrode. Convection: The Movement of material in response to a mechanical force such as strain solution. As we have taken substance 50mmol/L in electrolyte concentration as this substance increases from 10mmol/L to 50mmol/L the current is also increases.

III.MODELLING AND SIMULATION OF SENSOR

The sensing structure in figure consist of typical electrochemical sensor which has three electrode working electrode, counter electrode, reference electrode, the main reaction takes place at the working electrode. The electrochemistry module of 5.6 Multiphysics simulation tool is used for modeling and simulation of sensor. Fig. 1, 2, 3, describe the geometry of working electrode, counter electrode and reference electrode in a rectangular shape.

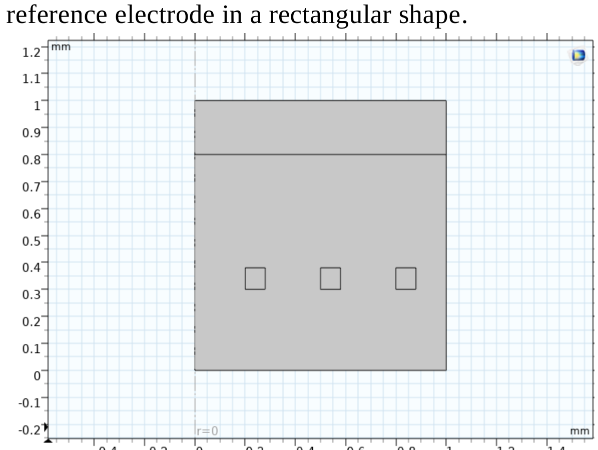

Fig 1. Arrangement of electrochemical cell

Fig. 1. Shows the proposed electrochemical cell. Fig. 2, presents the arrangement of electrochemical cell

with three carbon electrodes. Fig. 3, presents the arrangement of electrochemical cell with electrolyte. In fig. 4, shows the arrangement of electrochemical cell with analyte.

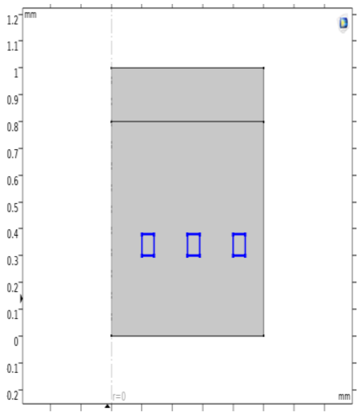

Fig 2. Arrangement of electrochemical cell with three carbon electrodes

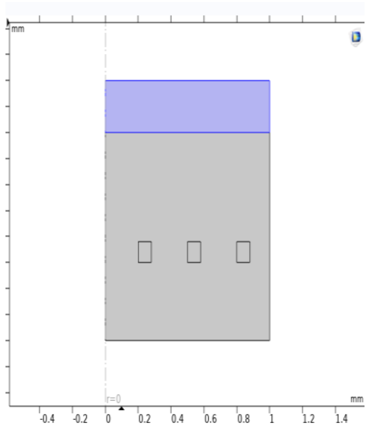

Fig 3. Arrangement of electrochemical cell with electrolyte

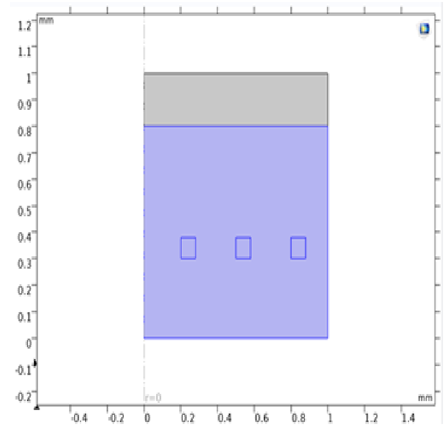

Fig 4. Arrangement of electrochemical cell with analyte

Table.1, 2, 3 describe the properties of the electrodes viz., carbon material, electrolyte and analyte respectively.

Property	Variable	Value	Unit	Property group
Electrical conductivity	sigma_...	25000[m...	S/m	Basic
Diffusion coefficient	D_iso ;...	1.6e-9	m^2/s	Basic
Density	rho	1.34	kg/m^3	Basic
Equilibrium potential	Eeq	Eeq_int1...	V	Equilibrium potential
Temperature derivative of equil...	dEeqdT	dEeqdT_...	V/K	Equilibrium potential
Reference concentration	cEeqref	56250[m...	mol/m^3	Equilibrium potential
Maximum electrode state-of-c...	socmax	1	1	Operational electrode st...
Minimum electrode state-of-ch...	socmin	0.43	1	Operational electrode st...

Table 1. Properties of carbon material

Property	Variable	Value	Unit	Property group
Diffusion coefficient	D_iso ;...	0.75e-9[...	m^2/s	Basic
Density	rho	(A_rho(T...	kg/m^3	Basic
Electrolyte conductivity	sigmal...	(A*M+B...	S/m	Electrolyte conductivity
Transport number	transp...	0.22	1	Species properties
Activity dependence	fcl	2	1	Species properties

Table 2. Properties of electrolyte

Property	Variable	Value	Unit	Property group
Thermal conductivity	k_iso ;...	k_liquid_...	W/(m·K)	Basic
Resistivity	res_iso...	res_liqui...	Ω·m	Basic
Coefficient of thermal expansion	alpha_...	(alpha_li...	1/K	Basic
Heat capacity at constant press...	Cp	C_liquid...	J/(kg·K)	Basic
Electrical conductivity	sigma_...	sigma_li...	S/m	Basic
Density	rho	rho_liqui...	kg/m^3	Basic
Dynamic viscosity	mu	eta_liqui...	Pa·s	Basic
Tangent coefficient of thermal...	alphat...	CTE(T[1/...	1/K	Thermal expansion
Thermal strain	dL_iso...	(dL_liqui...	1	Thermal expansion

Table 3. Properties of Analyte

IV.SIMULATION RESULTS

Simulation results of the electrochemical sensor are described in this section. Fig. 5 & 6 presents the concentration of analyte and electrolyte. Amperometric and potentiometric analyses of the sensor are carried out. Fig. 7 presents the oxidation concentration of the analyte and electrolyte. The details of the simulation parameters used for the simulation of the proposed electrochemical sensors is shown in Table. 4. The model is simulated and the results obtained are described in Fig. 8 & 9 respectively.

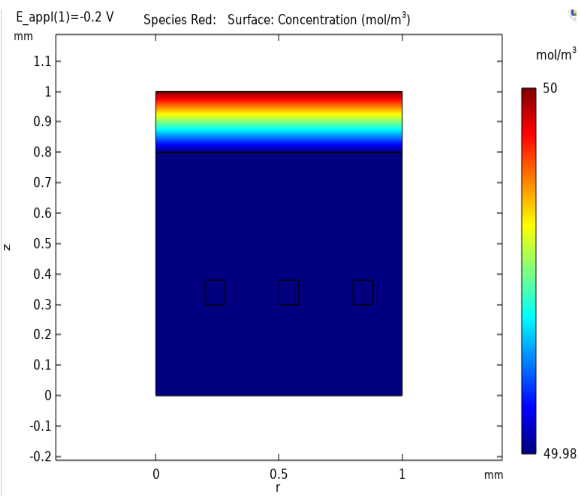

Fig 5. Surface: concentration (mol/m^3)

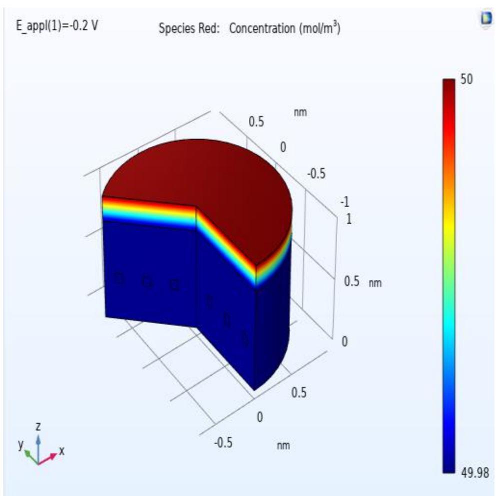

Fig 6. Concentration (mol/m^3) in 3D

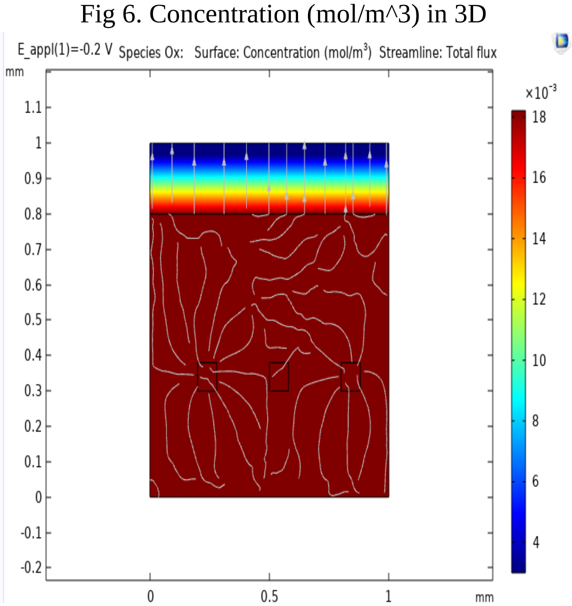

Fig 7. Oxidation surface concentration (mol/m^3)

Parameters

Label: Parameters 1

Parameters

Name	Expression	Value	Description
E_appl	0.5[V]	0.5 V	Applied potential
Ef	0[V]	0 V	Formal potential
c_bulk	1[mmol/L]	1 mol/m^3	Reactant concentration
re	10[um]	1E-5 m	Electrode radius
r_max	25*re	2.5E-4 m	Size of simulation space
D1	1e-9[m^2/s]	1E-9 m^2/s	Reactant diffusion coeffi...
D2	1e-9[m^2/s]	1E-9 m^2/s	Product diffusion coeffici...
i0ref	1000[mol/(m^2*s)]*F_const	9.6485E7 A/m^2	Reference exchange curr...
E_start	-0.2[V]	-0.2 V	Start potential
E_vertex	0.2[V]	0.2 V	Vertex potential
E_step	10[mV]	0.01 V	Potential step (output)
c_bulk_2	50[mmol/L]	50 mol/m^3	Mixed Substance concent...
VCell	2[V]	2 V	RE Volt

Table 4. List of Parameter used

The plot of Total Current vs applied potential is shown in Fig. 8. Fig. 9 presents plot of total current vs Mixed substance concentration.

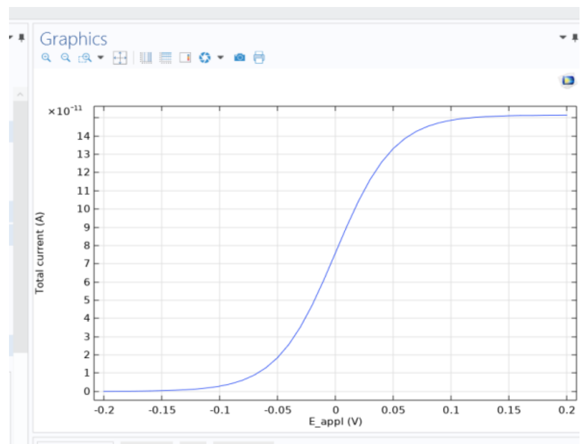

Fig 8. Plot of Total current vs E applied

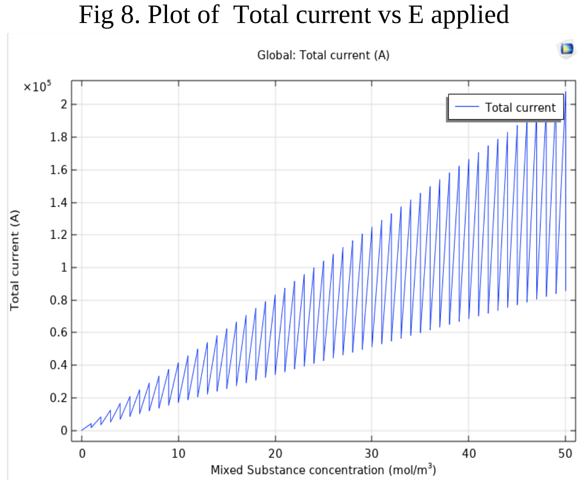

Fig 9. Plot between Total current vs Mixed Substance Concentration

V.CONCLUSION

The paper present electrochemical sensor for detection of Zn in KOH solution. The model is simulated in COMSOL Multiphysics. 0.5V potential is applied for the model. Zn substance concentration of 50 mmol/L in the KOH electrolyte concentration is considered. In the plots it can be observed that as this substance quantity is increases the current also increases. The results obtained for increase in Zn concentration in the electrolyte is shown in Table. 5.

Table. 5. Current vs Zn concentration

Mixed Substance Concentration (mol/m^3)	Current Observed (A)
10	0.4
20	0.8
30	1.2
40	1.6
50	2

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