Nano World Journal

https://doi.org/10.17756/nwj.2023-s1-051

Research Article

Open Access

Simulation Model for the Corrosion Behavior of Additively Manufactured Iron in Electrolytic Environment Using COMSOL Multi-physics

Pawan Sharma[1], Dayanidhi Krishana Pathak[2*] and Anusha Gowerneni[3]

[1]*Indian Institute of Technology, Banaras Hindu University, Varanasi, Uttar Pradesh, India*
[2]*G. B. Pant Govt. Engineering College, New Delhi, India*
[3]*Veljan Hydrair Private Limited, Hyderabad, Telangana, India*

***Correspondence to:**
Dayanidhi Krishana Pathak
G. B. Pant Govt. Engineering College,
New Delhi, India.
E-mail: dk.pathak50@gov.in

Received: November 24, 2022
Accepted: April 12, 2023
Published: April 14, 2023

Citation: Sharma P, Pathak DK, Gowerneni A. 2023. Simulation Model for the Corrosion Behavior of Additively Manufactured Iron in Electrolytic Environment Using COMSOL Multi-physics. *Nano World J* 9(S1): S260-S265.

Published by United Scientific Group

Abstract

The modelling of the corrosion behavior of additively manufactured iron (Fe) as biomaterials is the subject of this research work. The electrochemical interaction of metal in the electrolytic environment, such as screw plate couplings, initiates the biocorrosion process. The body tissues have an electrolytic characteristic due to the discharged ions, enzymes, and hormones, making the environment extremely active in terms of corrosion potential. As a result, it becomes very important to assess biometals' toxicity and corrosion behavior by simulating the corrosion degradation process, which will focus on substitute biomaterial designs that might decrease or avoid corrosion degradation behavior's effects. The corrosion potentials of the biometal couples of additively manufactured Fe material are compared in this work utilizing the finite element based COMSOL electrochemical analysis technique for a two-dimensional (2D) model in the electrolyte solution and a three-dimensional (3D) model in two distinct electrolytes of bone and muscle. The simulated Fe corrosion behavior findings are then compared to those of the experimental corrosion. The higher corrosion current density resulted in many active implants exhibiting a faster degradation of biodegradable porous Fe.

Keywords

Biodegradable, Corrosion, Iron, Model, Simulation

Introduction

Metal corrosion is a complicated phenomenon that is influenced by geometric, mechanical, and chemical solution factors. Radiological analysis of degraded metal products in body tissues is required to be studied. The quantity of oxidizing agents produced by these chemical processes provides an unfavorable environment for metals and alloys [1]. Initially, every metal used in human implantation corrodes, creating a slim barrier layer. These metals would react aggressively with the neighboring chemical environment if this barrier was not present, eventually disintegrating. This layer can be broken down by mechanical forces, exposing reactive metal atoms to corrosion [2]. The surrounding tissues are affected by the corrosion process, which is influenced by cells' behavior. Mild corrosion can cause various symptoms, ranging from local discomfort in the degraded region to severe pain, reddening, and swelling across the device's surrounding vicinity [2]. Elevated concentrations of certain alloying elements of implants might result from organ-specific accumulations of specific metal ions combined with simultaneous ion-specific excretion rates from the body. This might throw off the general balance created by toxin tolerance in the body.

In contrast to effective biomaterials for biological aspects, implant and prosthetic failures are growing due to galvanic corrosion processes in the electrolytic environment, such as the human body. The implants' integrity depends on the corrosion rate of materials as materials tend to degrade from the surface and form corrosion products/debris [3]. Debris can move via the circulatory system to different body regions, affecting numerous bodily systems [4]. Corrosion debris can lead to aseptic weakening, rupture, tissue infection, and vascular snag, leading to implant failure.

A paired oxidation-reduction reaction occurs during the corrosion process by electron transfer from one species to another [5]. Because electrochemical corrosion processes include electron transfer, which results in an electric current, corrosion rate and velocity may also be described relating to the quantity of freed electrons or the current density of the degrading material [6].

So, the present work aims to model a corrosion process utilizing Fe-based software, i.e., COMSOL, that uses an electric current distribution in an electrolytic environment method. Different studies for 2D and 3D spaces are simulated and compared with experimental potentiodynamic polarization findings of additively manufactured Fe. The 2D models of different porosities are also simulated and compared with experimental results [7]. Change in thickness of electrode material with time; more specifically, the tiny screws that are supposed to hold the implant for a longer duration of time should be studied, which is complicated and resource consuming. To overcome this significant limitation, numerical modeling of corrosion behavior is required, which takes the Tafel data of experimental corrosion tests along with material-specific properties [7] to compute the corrosion behavior and change in thickness of the model for any number of days. The simulation becomes important for assessing degradation behavior and reducing the subsequent detrimental effects of corrosion.

Materials and Methods

Material

In orthopedics, dentistry, and vascular surgery, several biomaterials are required for healing the tissue and or organ fractures. The connection of metallic couples in an electrolytic environment may cause implant corrosion. As a result, engineering approaches must be used to quantify and understand the corrosion potentials of particular metals [8]. Fe has been suggested as the material sustaining high mechanical loads for bone replacement and fixation owing to its medium corrosion and excellent mechanical properties. Table 1 presents the mechanical properties of pure Fe [7].

Geometry, modelling, and study factors

Figure 1 shows the schematic of the used 2D computation domain. In order to achieve the corrosion rate simulations of bimetallic in a physiological environment, geometries of electrodes, as shown in figure 2 in 2D and 3D models similar to bone fixation plate and screw, have been modelled in COMSOL. The modelling has been done for simulating the electrochemical corrosion behavior utilizing the corrosion current density and distribution methods. The entire simulations are performed with the help of COMSOL's electrochemical analysis module. The electrodes in the 2D model are in contact with the electrolyte of conductivity 1.75 S/m. The electrodes in the 3D model are arranged for two distinct electrolytic conditions in orthopedic applications, such as muscle and bone. Table 2 and table 3 present the electrode reaction factors, the additively manufactured dense iron environment, and different porosity samples (S1, S2, S3) for 2D and 3D spaces, respectively [6, 9].

Table 1: Mechanical properties of pure Fe [7].

Young's Modulus (GPa)	Ultimate Tensile Strength (MPa)	Yield strength (MPa)	Density (g/cm^3)	Molar mass (kg/mol)
200	180 - 210	120 - 150	7.81	0.055

In orthopedic applications, the simulation factors are electrode potentials, exchange current density, and electrolytic conductivity of the materials. Due to the diverse aged population and area, implants and bimetallic couples undergo different body loads. As a result of the stress corrosion process, altering loading on bimetallic couplings for various locations in the human body would affect the corrosion potential and current density. In addition, the mechanical load increases the electrolytic current density and localized corrosion growth potential close to the bimetallic intersection [9].

The boundary conditions at the anodic and cathodic surfaces are critical for predicting the true corrosion rates. Experimental polarization data for Fe are utilized as the boundary

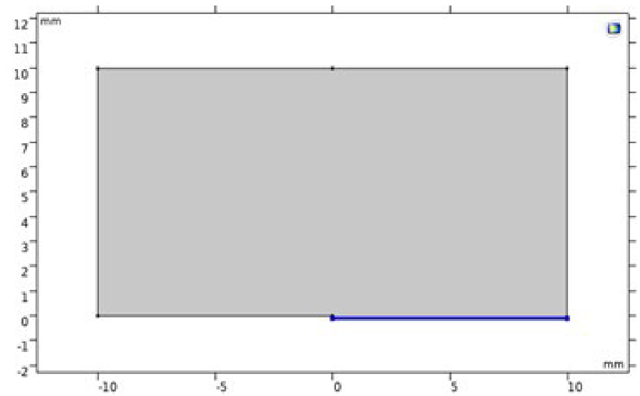

Figure 1: The schematic of a computational 2D domain (blueline represents anode).

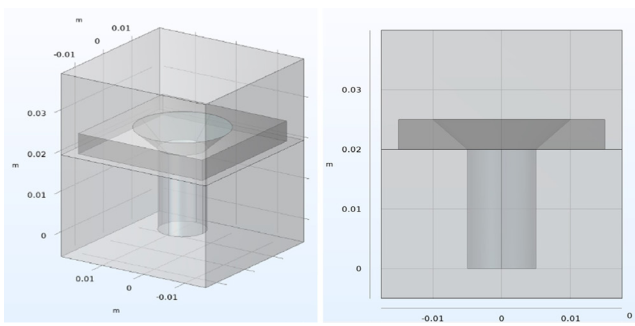

Figure 2: The schematic of a computational 3D domain similar to screw in bone model.

Table 2: Electrode reaction parameters in the 2D simulation [6, 9].

Sample	Porosity	Electrolyte conductivity	Equilibrium potential	Exchange current density	Anodic Tafel slope	Cathodic Tafel slope
	(%)	(S/m)	(V)	(A/m²)	(mV)	(mV)
Dense Fe	2.25	1.75	0.5734	0.12638	423	185
S1	16.83	1.75	0.631	0.463	314.5	253.91
S2	29.80	1.75	0.712	0.6671	151.42	276.41
S3	39.60	1.75	0.7737	0.8458	374.54	300.4

Table 3: Electrode reaction parameters in the 3D simulation [6, 9].

Sample	Electrolyte conductivity of bone	Electrolyte conductivity of muscle	Equilibrium potential	Exchange current density	Anodic Tafel slope	Cathodic Tafel slope
	(S/m)	(S/m)	(V)	(A/m²)	(mV)	(mV)
Dense Fe	0.2	0.62	0.5734	0.12638	423	185

condition for anodic and cathodic surfaces [6]. Simulation is performed using different porosity sample data on a 2D model, and results are compared with the experimental study.

For 3D simulation, the geometry is a simplified version of a screw holding a plate on a bone and muscle. There were different electrolytic mediums. One was a bone (bottom box) with an electrolyte conductivity of 0.2 S/m, and another one was a muscle (top box) with an electrolyte conductivity of 0.6 S/m [9]. The geometry of the 3D model is shown in figure 2, where the screw threads were omitted, and the model is simplified to decrease computation time and geometrical errors while solving the study.

Corrosion growth rate analysis

Using the experimental Tafel data of additively manufactured iron, as shown in table 2 and table 3 [6, 9], corrosion behavior was computed for 365 days for the 3D model and 300 hours for the 2D model. Using the corrosion module of COMSOL, total thickness change along with electrode potential and electrolyte current densities were calculated for both models. In COMSOL, the Corrosion rate (CR) is calculated using the equation of Faraday's law [10].

$$CR = \frac{M}{zdF} j$$

Where, M represents for material's molar mass, j denotes the current density of the electrolyte, z signifies the electron number, d represents the material density, and F denotes Faraday's constant = 96,485.34 C/mol. With the flow of current through the cathode from the anode, particles dissolve, resulting in a decrease in thickness of the material over a period measured in millimeters per year (mmpy).

Results and Discussion

In the 2D simulation study, the difference in electrode potential led the materials to behave as anode and cathode. Figure 3 shows the flow of electrolytic current density for the 2D simulation of additively manufactured dense Fe. It is

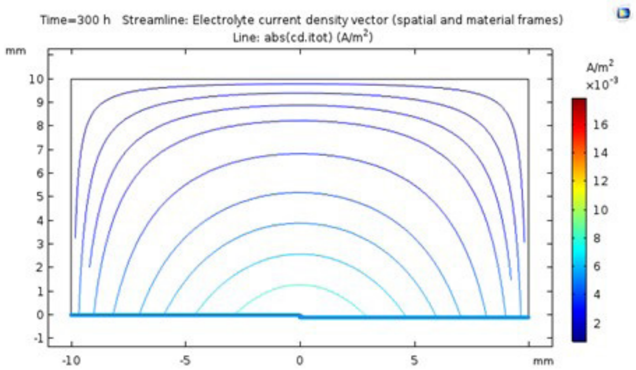

Figure 3: Electrolytic current density vector of dense Fe (2D simulation).

observed that the current is flowing from the anode towards the cathode with maximum electrolytic current density at the contacting surface. After calculating the corrosion rate from current density using CR equation and comparing it with the experimental results [6], it is found to be within the permissible range, and it can be seen that the corrosion growth is maximum at the point of contact. These results are obtained using the secondary current distribution module of multiphysics solver COMSOL. It is also observed from the plots that current density is dependent on the distance between cathodic and anodic regions. The electrolyte potential and electrode thickness change plot can be seen in figure 4 and figure 5.

Similarly, the simulations are obtained for different porosities (16.83%, 29.8%, and 39.6%) of additively manufactured Fe by using experimental data from Sharma et al. [6], and corrosion rates are calculated using current densities from the plots in figure 6, figure 7, and figure 8. When comparing these values with the experimental results, it is found to be within the permissible range. Further, it is inferred that the corrosion growth enhanced with rising porosity values. Simulation results described that porous Fe possessed an increased degradation rate in comparison to dense Fe sample, thereby supporting the experimental findings where the corrosion rate increases with increasing porosity values of additive manufactured Fe as more surface when exposed to the electrolyte.

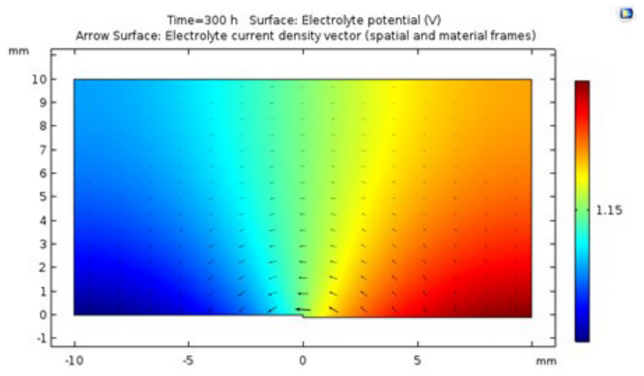

Figure 4: Electrolyte potential of dense Fe (2D simulation).

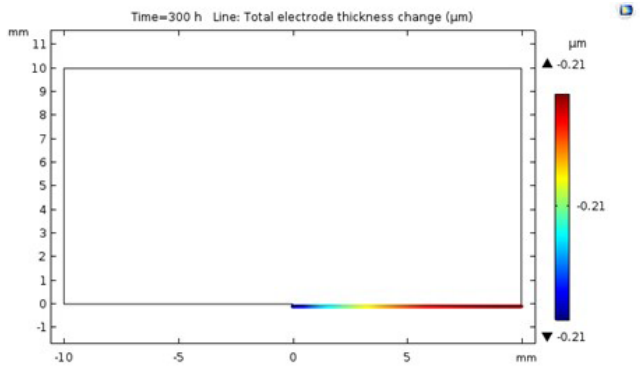

Figure 5: Total change in electrode thickness after 300 hrs of dense Fe (2D simulation).

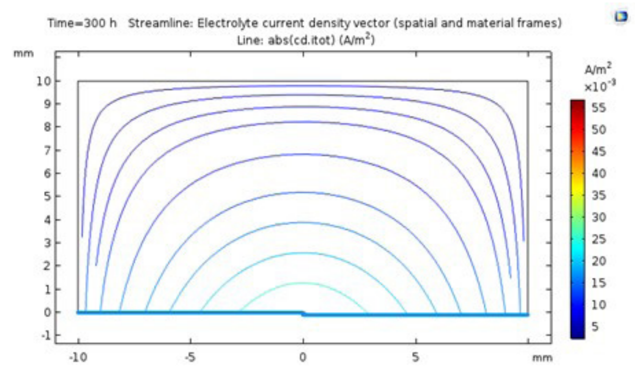

Figure 6: Electrolytic current density vector of Fe with 16.83% porosity (2D simulation).

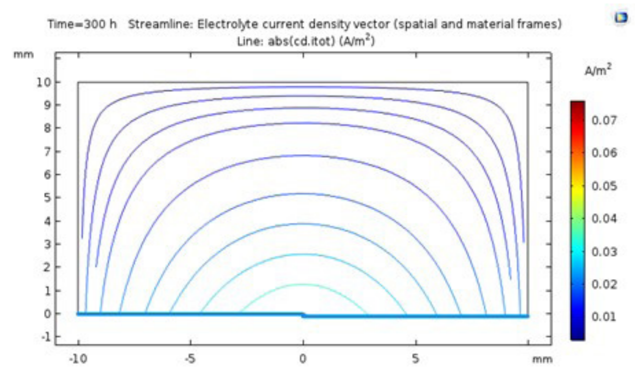

Figure 7: Electrolytic current density vector of Fe with 29.8% porosity (2D simulation).

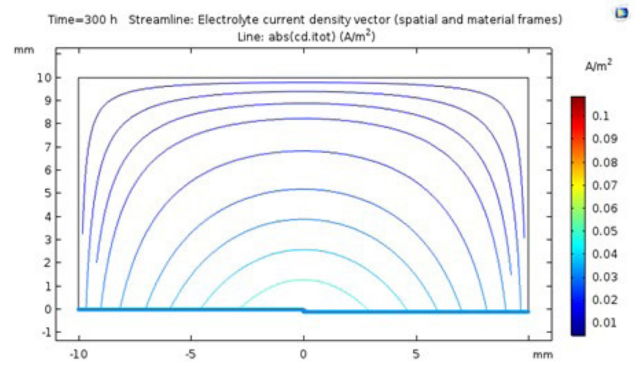

Figure 8: Electrolytic current density vector of Fe with 39.6% porosity (2D simulation).

From figure 9, variation of electrode potential or Ecorr can be seen. It was observed that the maximum corrosion growth occurred in muscle region as compared to bone region. The reason behind this is the higher electrolytic conductivity of muscle with a value of 0.62 S/m compared to 0.2 S/m of bone. The maximum electrolytic current density was found to be at the contacting surface inside the muscle region. As shown in figure 10, from 3D simulation, the electrolytic current density vector can be observed to move from anodic region of screw towards the cathodic region inside bone and muscle, where arrows show the direction of current flow. From figure 11, it can be observed that the maximum amount of reduction in electrode thickness takes place around the periphery of head within the contact of plate.

Experimental results from the study and results of 2D and

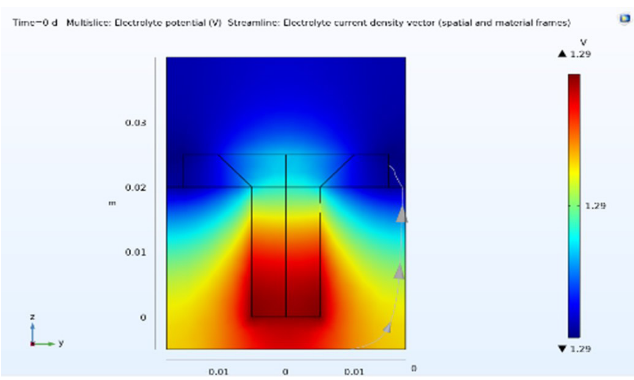

Figure 9: Electrolyte potential (3D simulation).

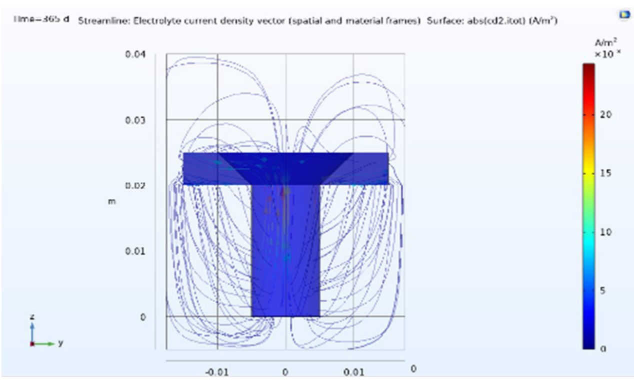

Figure 10: Electrolytic current density vectors of dense Fe (3D simulation).

Table 4: Comparison of previously reported experimental results and 2D simulated results.

Sample	Porosity (%)	Corrosion properties			Fabrication technique	Reference
		Experimental results	Simulation results			
		Corrosion rate (mmpy)	Current density (A/m²)	Corrosion rate (mmpy)		
Dense Fe	2.25	0.13 ± 0.01	0.016	0.1856	Additive Manufacturing	[6]
S1	16.83	0.50 ± 0.04	0.055	0.638		
S2	29.80	0.76 ± 0.03	0.07	0.812		
S3	39.60	0.98 ± 0.10	0.1	1.16		

Table 5: Comparison of previously reported experimental results and 3D simulated results.

Sample	Porosity (%)	Corrosion properties			Fabrication technique	Reference
		Experimental results	Simulation results			
		Corrosion rate (mmpy)	Current density (A/m²)	Corrosion rate (mmpy)		
Dense Fe	2.25	0.13 ± 0.01	0.02	0.232	Additive Manufacturing	[6]

3D simulations are tabulated, and corrosion rates are compared, which can be observed in table 4 and table 5. Additively manufactured samples had lower exchange current densities resulting in lower corrosion rates. The cumulative distribution causes a maximum electric current in the cathodic area. As a result, cathodic protection techniques are used in the majority of corrosion prevention applications and research. By manufacturing parts of the implants using additive manufacturing, the customized parts can be manufactured easily, and better corrosion-resisting properties can also be found in AM fabricated parts.

Conclusion

The bimetallic couple in the presence of electrolyte causes corrosion. The corrosion behavior of additive manufactured Fe has been studied from the simulation results obtained when Fe electrodes are in contact with virtual body environment using secondary distribution module of multi-physics software COMSOL. From the simulation results, the corrosion rate of porous iron is greater than dense Fe, and the corrosion rate increases with increasing porosity values, supporting the experimental findings of previous studies. As the current density value increases, the corrosion rate increases. A very low corrosion rate i.e., 0.1856 mmpy was obtained for dense Fe, making it more corrosion resistant material compared to porous Fe samples fabricated using AM. Furthermore, it could be inferred that the developed simulated model could be applied for the evaluating the degradation behaviour of complex geometry in any electrolytic environment, making it an effective method for biodegradable implant applications.

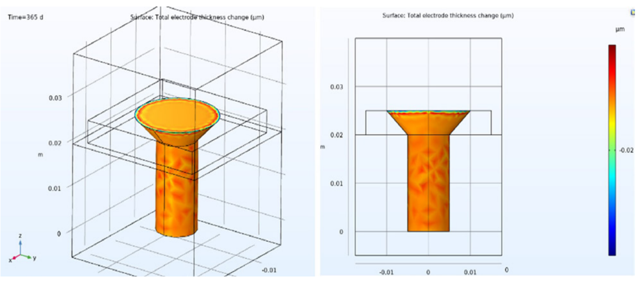

Figure 11: Total change in thickness electrode after 365 days.

Acknowledgements

None.

Conflict of Interest

The authors declare no conflict of interests that are relevant to the content of this article.

Credit Author Statement

Pawan Sharma: Resources, Investigation, Formal analysis, Writing - original draft preparation, Writing - review and editing, Supervision; Dayanidhi Krishana Pathak: Writing - original draft preparation, Writing - review and editing; Anusha Gowerneni: Conceptualization, Methodology, Investigation, Formal analysis. All the authors read and approved the manuscript.

References

1. Wegener B, Sichler A, Milz S, Sprecher C, Pieper K, et al. 2020. Development of a novel biodegradable porous iron-based implant for bone replacement. *Sci Rep* 10(1): 9141. https://doi.org/10.1038/s41598-020-66289-y
2. Villapún VM, Carter LN, Gao N, Addison O, Webber MA, et al. 2020. A design approach to facilitate selective attachment of bacteria and mammalian cells to additively manufactured implants. *Addit Manuf* 36: 101528. https://doi.org/10.1016/j.addma.2020.101528
3. Manthe M, Blasser K, Beauchamp C, O'Connor MI. 2016. Trunnion corrosion causing failure in metal-on-polyethylene total hip arthroplasty with monolithic femoral components. *Reconstructive Rev* 6(1): 13-22. https://doi.org/10.15438/rr.6.1.131
4. Matharu GS, Berryman F, Dunlop DJ, Judge A, Murray DW, et al. 2019. Has the threshold for revision surgery for adverse reactions to metal debris changed in metal-on-metal hip arthroplasty patients? a cohort study of 239 patients using an adapted risk-stratification algorithm. *Acta Orthop* 90(6): 530-536. https://doi.org/10.1080/17453674.2019.1659661

5. Mohanakrishna G, Abu-Reesh IM, Al-Raoush RI. 2018. Biological anodic oxidation and cathodic reduction reactions for improved bioelectrochemical treatment of petroleum refinery wastewater. *J Clean Prod* 190: 44-52. https://doi.org/10.1016/j.jclepro.2018.04.141
6. Sharma P, Pandey PM. 2019. Corrosion behaviour of the porous iron scaffold in simulated body fluid for biodegradable implant application. *Mater Sci Eng C* 99: 838-852. https://doi.org/10.1016/j.msec.2019.01.114
7. Sharma P, Pandey PM. 2019. Corrosion rate modelling of biodegradable porous iron scaffold considering the effect of porosity and pore morphology. *Mater Sci Eng C* 103: 109776. https://doi.org/10.1016/j.msec.2019.109776
8. Olanipekun AT, Faola AE, Oluwabunmi KE, Oladosu TL. 2014. Galvanic corrosion of a mild steel bolt in a magnesium alloy (AZ91D) plate simulation using COMSOL multiphysics. *Int J Sci Eng* Res 5: 1329-1332.
9. Istanbullu OB, Akdogan G. 2021. A simulation study of galvanic corrosion potential on the surface of implantable biometallic couples. *J Bio Tribo Corros* 7(1): 25. https://doi.org/10.1007/s40735-020-00462-8
10. Deshpande KB. 2010. Validated numerical modelling of galvanic corrosion for couples: magnesium alloy (AE44)–mild steel and AE44–aluminium alloy (AA6063) in brine solution. *Corros Sci* 52(10): 3514-3522. https://doi.org/10.1016/j.corsci.2010.06.031