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CORROSION SIMULATION OF AUTOMOTIVE MATERIALS UNDER EXPOSURE IN BIODIESEL

S Y CETIN[1,2]*; M A MALEQUE[3]; H H MASJUKI[2]; A HAMDANI[2] and M M RAHMAN[4]

ABSTRACT

Biodiesel being an eco-friendly and renewable alternative fuel has gained attention due to its clean nature. However, the corrosion behaviour of automotive component materials in the presence of biodiesel is well known. Therefore, a computational fluid dynamics simulation on corrosion phenomena of automotive component materials has been done under exposure of biodiesel over varying time intervals. Two different types of steel materials (carbon steel and stainless steel) were chosen for the simulation of corrosion under biodiesel exposure. However, the corrosion was predominantly observed in both carbon steel and stainless steel materials. A notable finding emerged as stainless steel demonstrated significantly superior corrosion resistance compared to carbon steel when subjected to biodiesel-induced corrosion. Furthermore, the corrosion resistance of both stainless steel and carbon steel was found to be within the acceptable range for utilising biodiesel in automotive engines. This finding underscores the viability of biodiesel as a sustainable and viable alternative fuel for the automotive industry.

Keywords: automotive materials, biodiesel, CFD simulation, corrosion.

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INTRODUCTION

Corrosion is an undesirable phenomenon that affects the durability of materials and is caused by an electrochemical interaction between metals with their environment. This process arises from prolonged exposure to hostile environmental conditions, impacting the reliability and safety of various alloys (Mitrović *et al*., 2018). In everyday life, corrosion represents a common form of surface degradation that affects metallic structures negatively and employs a considerable economic impact. Industrial and personal assets such as automotive engine components, underground piping systems, bridges, storage tanks, furniture with metal accessories and household items such as kettles and white goods can all succumb to corrosion. From automotive engine components to underground piping systems, bridges, storage tanks, and household utilities, such as kettles and white goods are subjected to corrosion. In the sphere of design, the importance of considering corrosion when incorporating metallic materials is considerable. Consequently, considering corrosion during material design becomes imperative. While its effects may not be immediately evident, the damage it inflicts gradually surfaces over time (The Electrochemical Society, 2016). Corrosion occurs in the presence of corrosive media, typically acidic or basic solutions, where metals react according to their composition and electrochemical properties. This phenomenon manifests in various types, as depicted in *Figure 1* (Oxyplast UK Limited, 2018).

Biodiesel presents a promising cleaner energy source, derived from renewable resources, holding significant potential as a future alternative fuel.

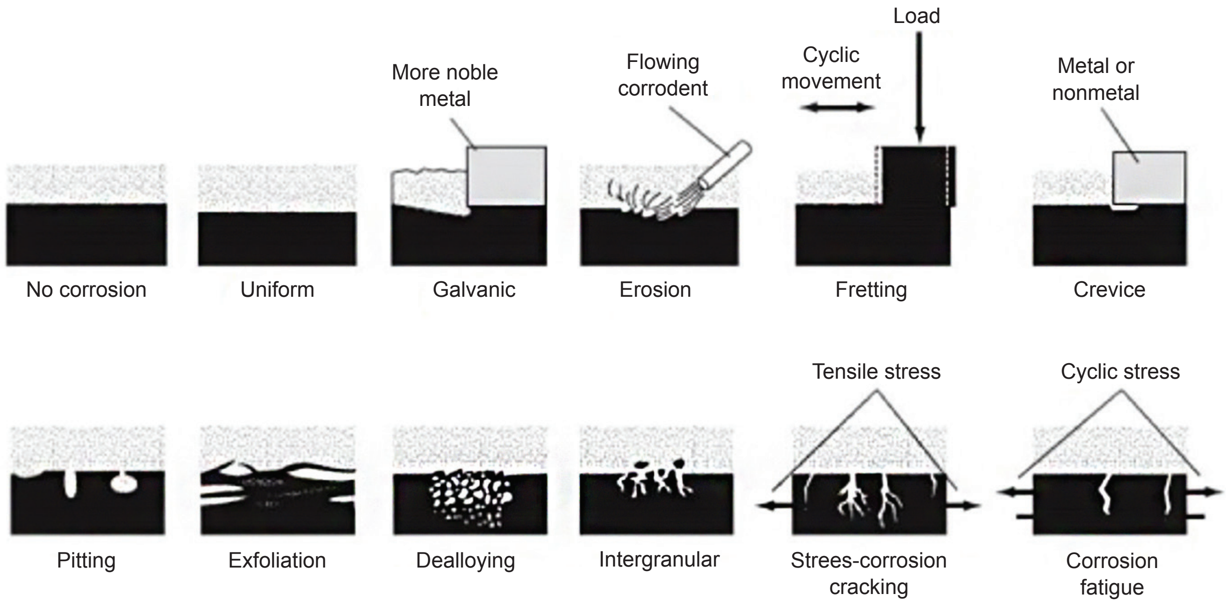
[1] Institute of Structural Durability and Railway Technology, Graz University of Technology, 8010 Graz, Austria.

[2] Department of Mechanical Engineering, International Islamic University Malaysia, 53100 Kuala Lumpur, Malaysia.

[3] Department of Manufacturing and Materials Engineering, International Islamic University Malaysia, 53100 Kuala Lumpur, Malaysia.

[4] College of Engineering, Universiti Malaysia Pahang Al-Sultan Abdullah, 26300 Pahang, Malaysia.

* *Corresponding author e-mail: s.y.cetin@tugraz.at*



Source: Oxyplast UK Limited (2018).

Figure 1. Various types of corrosion.

Countries with agricultural economies can reduce their dependence on oil by using biodiesel. It's superior lubricating properties can reduce wear on engine components and extend the engine life (Maleque *et al*., 2015). Moreover, biodiesel is an environmentally friendly fuel which makes it promising for the future, such as reduced toxic exhaust emissions and minimised visible smoke during ignition, highlight its appeal (Maleque *et al.,* 2015). Nonetheless, biodiesel does possess some disadvantages, including aggressive corrosive tendencies that limit its industrial utilisation (Jakeria *et al.,* 2015). The presence of dissolved water, emulsified water, oxygen and free fatty acids in biodiesel adversely affects automobile engine components, leading to corrosion (Maleque & Abdulmumin 2014). Researchers have identified the hygroscopic nature and oxidation of biodiesel as potential threats to the integrity of metallic components in automotive engines (Sazzad *et al*., 2016). Consequently, it is evident that biodiesel has a detrimental impact on automotive engine components, particularly regarding the interaction with metallic materials which is subjected to corrosion.

Technological developments in automobile industry are advancing with each passing day, hence, manufacturers continually pursue materials with superior resistance, strength, usability, and affordability. After paying attention on the interaction and corrosive effects between metals and biodiesel, research has been undertaken on this subject in the recent times. Baena and Calderón (2020), studied corrosive dynamics of carbon steel and stainless steel under biodiesel exposure for 3, 6 and 12 months periods. As a result of the study, the corrosion rates observed 0.001000, 0.000500 and 0.000240 mm/yr, respectively. Complementing these findings, referring to Ahmmad *et al.* (2018), stainless steel showed approximately 0.000500 mm/yr corrosion rate in presence of biodiesel for 2 months. Sterpu *et al.* (2012) found that the corrosion rate of carbon steel was 0.000855 mm/yr after 49 days of immersion period by sunflower oil biodiesel. These divergent results across different investigations can be attributed to a variety of variables such as temperature variations, movement of metal components, the specific type of biodiesel used, the velocity of the biodiesel fluid and other unique experimental conditions. This underlines the multifaceted and complex nature of the corrosive process involved in this context. The tribological behaviour of the metal components with several factors such as temperature, sliding time, biodiesel conditions and non-aqueous phase are investigated by Maleque *et al.* (2000). The complex nature of this corrosive process necessitates the use of different models to predict corrosion rates under varying parameters, ultimately reducing the need for numerous experiments (Anderko & Young, 1999).

Very minimum information on the computational fluid dynamics (CFD) simulation study that realistically addresses possible damage on metal surfaces, allowing the identification of potential failures in presence of biodiesel are available in literature. Such simulations can prove biodiesel's corrosive behaviour on metals and help to identify suitable material for automotive engine components. It is believed that simulation studies yield results close to real-life conditions, however, experimental studies under similar conditions are necessary for comparison and verification. Therefore, the main aim of this work is to simulate corrosion phenomena of automotive component materials under exposure of biodiesel over varying time intervals.

MATERIALS AND METHODS

Materials

In this study, stainless steel and carbon steel were used as representative materials. Renowned for their robust strength, both stainless steel and carbon steel are commonly used in the automotive industry. Stainless steel is an iron-based alloy that contains 10.5% or more of chromium and a maximum of 1.2% carbon thus resulting a self-regenerative surface layer that provides remarkable corrosion resistance. The nomenclature `stainless steel` derives from the fact that these steels do not stain, corrode and rust unlike many other types of steel. Owing to its alloy characteristics and type, this material is frequently referred to as corrosion-resistant steel.

Therefore, stainless steel has a high resistance to corrosion and oxidation in many natural and artificial environment. Conversely, carbon steels are iron-carbon alloys, which contain manganese, silicon, sulphur and phosphorus. All the properties of carbon steels are directly related to their respective structures, depending on the amount of carbon content. Thereby, hardness, yield and tensile strength increase with the increase in the amount of carbon content. Following the thread of investigation previously established by (Maleque *et al.*, 2022), the present study maintains the focus on the same chemical composition for both stainless steel and carbon steel. This strategy allows for a consistent examination and correlation of results, ensuring that the results remain robust and meaningful within the overarching context of the original research.

3D Modelling

In the modelling phase of this simulation, two identical sketches were meticulously designed and the biodiesel liquid environment was created in ANSYS Fluent and ANSYS Mechanical. Subsequent to the completion of the sketching process, the contact relation has been created between materials and the liquid. Following these initial steps, all bodies within the simulation were meshed. *Figure 2* presents the meshed geometry of the corrosion simulation specimens and palm biodiesel environment.

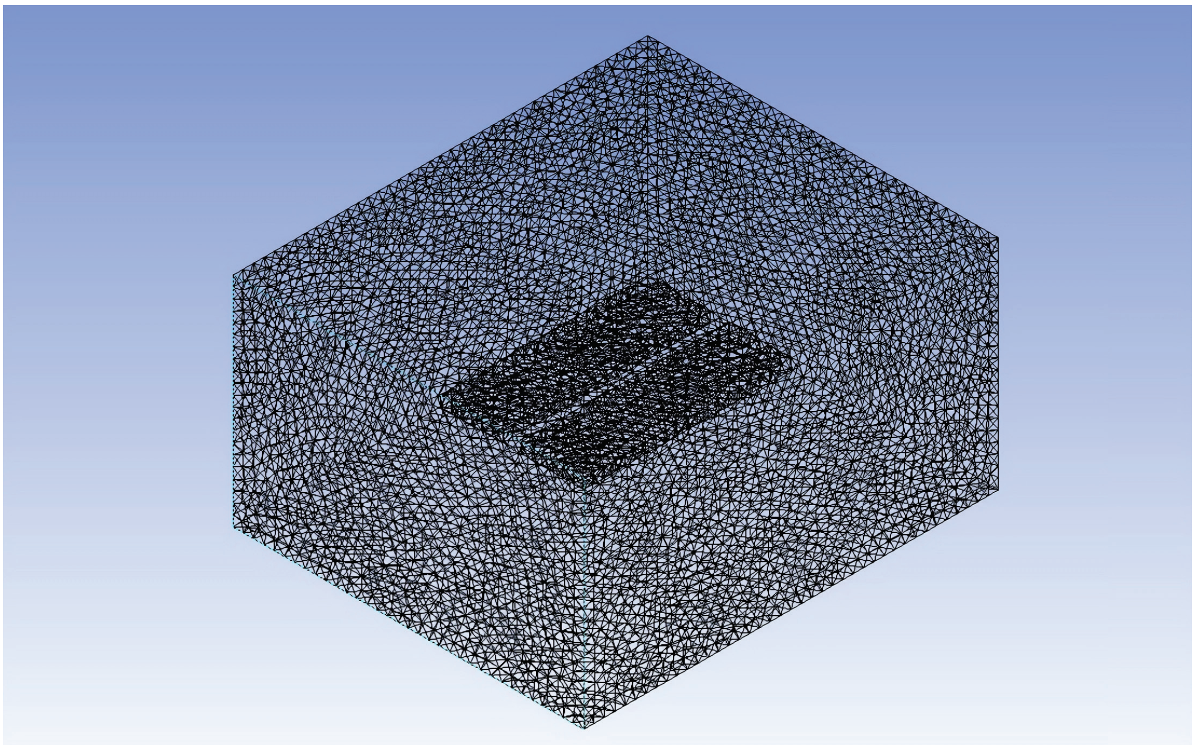


Figure 2. Meshed geometry of corrosion analysis.

Simulation Procedure

Numerous simulation methods are available, such as numerical simulation, computational simulation and computer aided simulation *etc.* A crucial aspect of simulation is the definition of the simulation procedure before the process is initiated. Real-life conditions, including simulation time, temperature, pressure and the characteristics of the liquid to be used, should be replicated as accurately as possible in the simulation. The corrosive impact of biodiesel on automotive engine components is widely recognised. Therefore, predicting the severity, type and exposure time of biodiesel corrosion is of great importance. Proactive measures can be taken based on early detection of corrosion. Consequently, material surfaces can either be reinforced or alternative materials can be considered for the engine components. In addition, a realistic simulation can help to minimise the factors that potentiate the corrosion, thereby ensuring enhanced durability and life of the components.

At the beginning of the simulation study, boundary box was created. As can be seen in *Figure 3*, biodiesel entered through the inlet section of the boundary box and, left the system by the outlet section after contact with specimens of stainless steel and carbon steel.

The reference temperature was regulated at 25°C as the room temperature. The pressure-velocity method was preferred as "coupled" to keep high accuracy of the results. Furthermore, standard wall functions were used together with the realisable k-epsilon model. The simulation performed for 100 iterations. The entry of biodiesel liquid was provided from the inlet section of the boundary box at a constant speed of 1 m/s.

Finally, the calculation method of the test determined and adjusted. The type of transport model was selected and the reaction set as "volumetric". Turbulence-chemistry interaction was determined as "Eddy-Dissipation". Palm biodiesel was given 1 m/s velocity for ease of calculation. "Inlet diffusion" and "Diffusion Energy Source" was activated as options of the model. In consequence, the "mass fraction of O_2" was taken as a reference for the corrosion rate.

Corrosion Rate Measurement

Recognising the extensive toolbox available for the investigation of corrosion phenomena, it is worthwhile to acknowledge the contribution of established electrochemical techniques, although their application is outside the boundary of this particular study, which used computational fluid dynamics simulation as its primary investigative tool. Among these acknowledged electrochemical methodologies, polarisation curves represent a fundamental analytical resource providing a graphical correlation between the electrode potential and the corresponding current. Through this relationship, a comprehensive assessment of corrosion rates can be made, thereby delineating the degree of corrosion resistance inherent in the materials under investigations. Similarly, Electrochemical Impedance Spectroscopy (EIS) which uses modest voltage or current perturbations to provoke a system response, is another laudable technique. The resultant impedance characteristics grant us to assess the performance of materials under different environmental conditions, providing valuable insight into the dynamics of the corrosion process. Furthermore, potentiometric polarisation, a technique characterised by gradual change in electrode potential to establish a comprehensive current versus potential profile, provides a significant depth of understanding

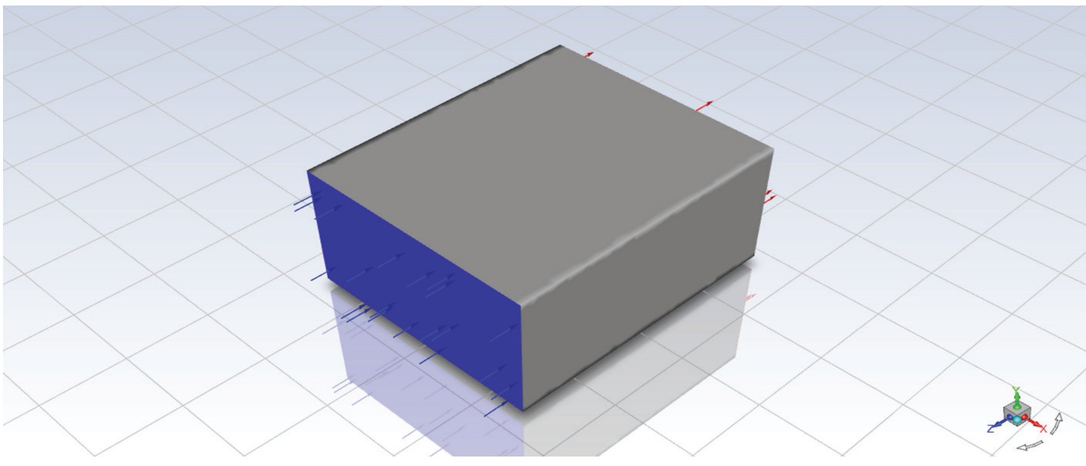


Figure 3. Boundary box.

of the kinetics of corrosion reactions. The value of this technique lies in its ability to clarify the mechanisms and rates of electrochemical process.

This study pursued an alternative but equally rigorous route, using computational simulations to elucidate the behaviour of materials under biodiesel exposure. The unit of measures is defined as the metal mass that moves away from unit surface in unit time. In general, the unit used to express corrosion rate is g/dm^2 per year.

$$\frac{g}{dm^2 \times yr} \tag{1}$$

As another unit, metal thickness reduction over a certain period of time can also be used.

$$\frac{mm}{yr} \tag{2}$$

The corrosion rate can be found by the help of the formula that is shown in Equation (3):

$$Corrosion\ rate\left(\frac{mm}{yr}\right) = \frac{K \times W}{DAT} \tag{3}$$

where, K is a constant, W is the weight loss in milligrams, D is the metal density in g/cm^3, A is the area of the test specimen in m^2 and T is the exposure time in hours. Besides, the mass fraction is one of the preferred parameters in corrosion studies to analyse the interaction between metal and chemical substances. Equation (4) shows the general equation for mass fraction.

$$W_i = \frac{m_i}{m_t} \tag{4}$$

where mass fraction of specimen is W_i, component mass m_i and m_t is the total mass of the mixture.

RESULTS AND DISCUSSION

Corrosion rates for materials predicted are based on the data obtained from the simulation software. Since the ANSYS software is not suitable for real-time long interaction tests, weight loss was considered for the corrosion rate calculations. In general, "mm/yr" is used as the corrosion rate which means the metal thickness in mm that was removed from the surface of the material by corrosion in one year. Equation (3) presents the formula of corrosion rate. Moreover, the mass fraction formula is presented in Equation (4). Herein, the simulation was performed for the mass fraction of O_2 of both materials. Based on the simulation results, maximum mass fraction of carbon steel monitored was 1.04×10^{-1}. Besides, stainless steel showed 1.68×10^{-1} mass fraction of O_2. *Table 1* presents the mass fraction of O_2 in different regions of both carbon steel and stainless steel specimens.

According to the simulation results, after three months of exposure to biodiesel, the corrosion rate of carbon steel was recorded as 0.000213 mm/yr. Meanwhile, stainless steel exhibited a corrosion rate of 0.000193 mm/yr over the same exposure time. Besides, carbon steel displayed 0.000106 mm/yr and stainless steel displayed 0.000096 mm/yr for 6 months of contact with palm biodiesel. After 1 yr of exposure, it was observed that corrosion rate of carbon steel decreased to 0.000053 mm/yr. Furthermore, stainless steel displayed 0.0000482 mm/yr of corrosion rate. *Figure 4* presents corrosion rates of stainless steel and carbon steel under exposure of palm biodiesel at different time periods. Moreover, *Figure 5* shows corroded surfaces of the materials after exposure of palm biodiesel. From a metallurgical point of view, the corrosion behaviour of both carbon steel and stainless steel when exposed to biodiesel can be interpreted in terms of their respective material compositions and the way they interact with the

TABLE 1. MASS FRACTION OF O_2 OF THE MATERIALS

Reference position of carbon steel (m)	Mass fraction of O_2 for carbon steel	Mass fraction of O_2 for stainless steel	Reference position of stainless steel (m)
0.012	1.16×10^{-2}	9.41×10^{-2}	0.027
-0.008	2.16×10^{-2}	9.38×10^{-2}	0.032
0.000	5.08×10^{-2}	1.01×10^{-1}	0.043
0.002	7.25×10^{-2}	1.68×10^{-1}	0.049
0.009	9.07×10^{-2}	1.29×10^{-1}	0.052
0.018	1.04×10^{-1}	4.90×10^{-2}	0.057

Note: Reference coordinate is (-0.012 m, 0.058 m), carbon steel placed (-0.012 m, 0.018 m) and stainless steel placed (0.027 m, 0.057 m).

corrosive environment. Carbon steel, which has mainly higher mass fraction of oxygen, indicates more extensive oxidation, resulting in a slightly higher corrosion rate. This phenomenon mainly due to the absence of a protective oxide layer that could resist corrosive agents. On the other hand, stainless steel, an alloy with a significant chromium content, exhibits a lower corrosion rate. The chromium in the alloy reacts with oxygen in the environments to form a thin, adherent, invisible surface layer of chromium-rich oxide. This layer is self-repairing and provides a barrier to prevent oxygen diffusion to the underlying steel surface. Thus, slowing the corrosion process. The slightly lower mass fraction of oxygen found in stainless steel compared to carbon steel in the simulation study is evidence of this inherent corrosion resistance property. The results of this study also demonstrate that the corrosion rate for both types of steel decreases over time when exposed to biodiesel, suggesting a possible adaptation or saturation effect of the corrosive biodiesel environment. These findings provide valuable insights for material selection in industries where equipment is exposed to similar corrosive conditions.

Although there is no common corrosion rate as standards for palm biodiesel, carbon steel and stainless steel, it is important to note that these rates are inherently variable. Furthermore, they depend on the number of factors such as material composition, environmental conditions and the specific operating parameters under which they are utilised. Particularly in the industrial applications, the specific requirements of the materials may vary due to the dynamic nature of their role, requiring an adaptable approach to corrosion management. The adaptability of materials and the diversity of their applications underline the importance of a sophisticated understanding and management of material corrosion in different industrial contents. The way metallic materials degrade or corrode in biodiesel blends is influenced by several factors. These include the chemical composition of the fuel, how long the material is immersed in the fuel and the environmental conditions. According to the Dharma *et al.* (2023) the rate at which mild steel corrodes decreases as the amount of biodiesel in the fuel increases. The reason behind this finding is that biodiesel contains less sulphur and aromatic compounds than regular diesel fuel. These compounds are known to contribute to metal corrosion. Biodiesel also contains more oxygen and fatty acid methyl esters which can form a protective layer on the metal, slowing down corrosion. However, the impact of biodiesel on the rate which metal corrodes is not simple. It can be influenced by other factors such as the type of metal, impurities in the fuel and environmental conditions. Therefore, more research is needed to fully understand how metallic materials corrode in biodiesel blends and to find the effective ways to handle these corrosion problems in engines running on biodiesel.

The results of the current investigation are broadly consistent with previous research, although the existence of the minor variations due to different experimental conditions is acknowledged (*Table 2*). The study by Fazal *et al.* (2011) reported a corrosion

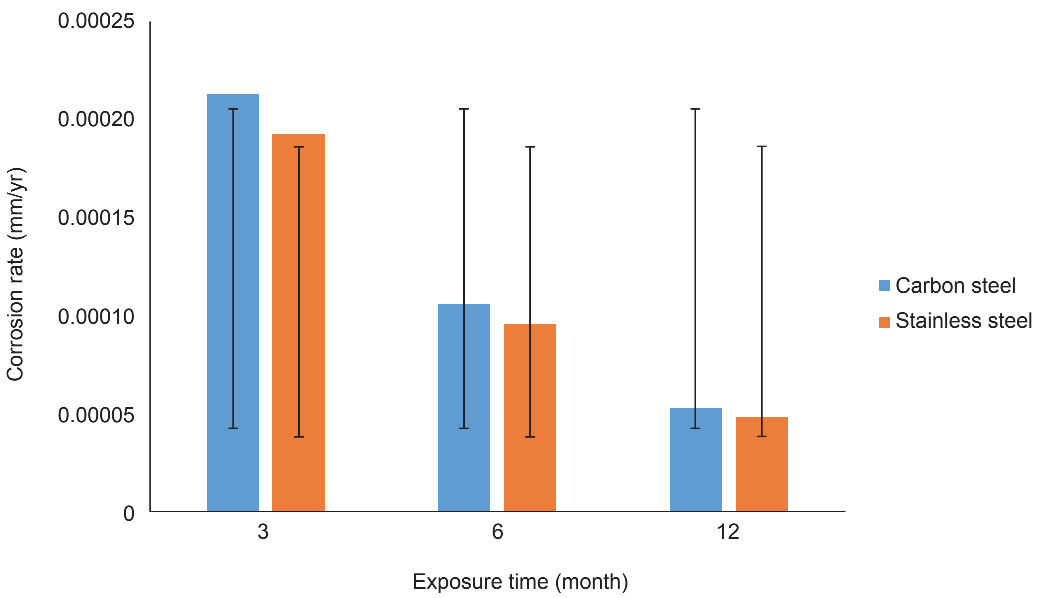


Figure 4. Corrosion rates of the materials.

rate for mild carbon steel in biodiesel approximately 0.001320 mm/yr after 1,200 hr of immersion test. Although, the results show slightly higher values than those obtained in this study, considering the difference between the immersion times in both studies, the results provide evidence that these two studies can support each other. Similarly, Fazal *et al.* (2010) investigated the corrosion rate of stainless steel in palm biodiesel and diesel at 80°C for 1,200 hr. The authors reported the corrosion rate of stainless steel immersed in diesel and biodiesel as 0.000586 and 0.000879 mm/yr respectively. Therefore, these results explicitly demonstrate the effect of temperature on the results. Likewise, Alves *et al.* (2019) investigated the influence of stainless steel corrosion on the oxidative stability of biodiesel during storage. The study explored the relationship between biodiesel degradation and corrosion of stainless steel used for storage. The authors measured lower corrosion rates for stainless steel in biodiesel conditions ranging from approximately 0.00000381 to 0.00001905 mm/yr than those found in this study. Thangavelu *et al.* (2015) analysed the effect of biodiesel blends on corrosion rate, fuel properties and fuel composition changes. The carbon steel specimens were exposed to static immersion test for 800 hr at 25°C-30°C and 400 hr at 60°C respectively. The corrosion rate of carbon steel in biodiesel was found to be 0.1817 and 0.2612 mpy which are approximately equals to 0.004615 mm/yr and 0.006634 mm/yr at room temperature and 60°C, respectively. As highlighted earlier, the differences may be due to the immersion time, the use of different fuel blends and test conditions, emphasising the role of certain fuel properties influencing the corrosion rates. In addition, some chronic differences can be observed between simulation-based studies and experimental analyses performed in laboratory environments. These differences may be due to the limitations of the simulation software, the use of incorrect parameter inputs, incomplete or incorrect implementation of the simulation process, and inadequate conditions for the experiments. Therefore, it is very important to determine the most appropriate conditions to use as input in simulation studies. In the current simulation study, the most suitable conditions evaluated and attempts were made to emphasise the importance of simulation studies in predicting the corrosive properties of materials in advance. However, it should be noted that an experimental study that fully meets the same conditions is required for a complete and accurate comparison.

TABLE 2. CORROSION RATES OF PREVIOUS EXPERIMENTAL STUDIES ON STAINLESS STEEL AND CARBON STEEL WITH DIFFERENT KIND OF BIODIESEL

Biodiesel type	Temperature (°C)	Duration (hr)	Corrosion rate		References
			Stainless steel	Carbon steel	
Palm oil	80	600	0.015 mpy	-	Fazal *et al.* (2010)
	60	-	-	0.1497 mm/yr	Prasojo *et al.* (2019)
Palm biodiesel	25	2,190	0.000213 mm/yr	0.0001930 mm/yr	Present work
		4,382	0.000107 mm/yr	0.0000965 mm/yr	
		8,765	0.000530 mm/yr	0.0000482 mm/yr	
Fatty acid methyl esters (FAME)	At room temperature	720	0.00055 mpy	-	Alves *et al.* (2019)
			0.00045 mpy		
		1,440	0.00020 mpy		
Fatty acid ethyl esters (FAEE)		2,160	0.00015 mpy		
			0.00015 mpy		
			0.00015 mpy		
Sunflower oil	25-30	1,176	-	0.000855 mm/yr	Sterpu *et al.* (2012)
Rapeseed oil				0.000760 mm/yr	
Corn oil				0.001164 mm/yr	

Note: mpy - mils per year.

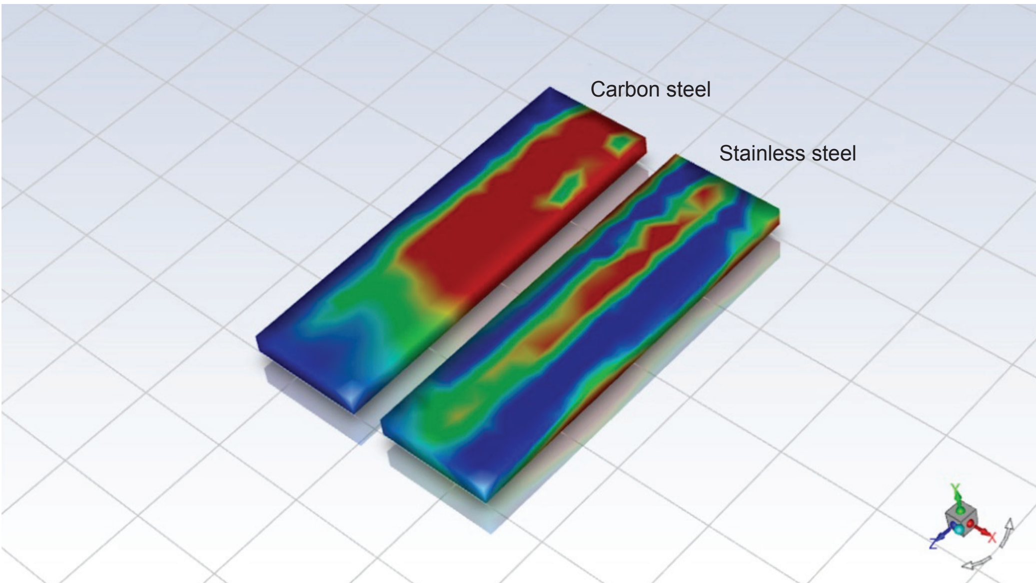


Figure 5. Corroded surfaces of carbon steel and stainless steel after biodiesel exposure.

CONCLUSION

Corrosion, with its potential to cause product loss and contamination, it is highly demanded to consider its effect and pre-determine the behaviour with materials. In this pursuit, the utilisation of simulation tools, incorporating basic material properties, emerges as a highly effective and scientifically sound approach to predict corrosion behaviour when exposed to biodiesel. The simulation employed palm biodiesel as the operating liquid at 25°C. This study shows that it was feasible to simulate corrosion behaviour of automotive component materials under biodiesel for the prediction of such phenomenon in real life. It is possible to achieve the process parameters for the corrosion rate providing accurate predictions for stainless steel and carbon steel specimens under biodiesel exposure with the ANSYS simulation software. The findings showcased a corrosion rate of 0.000213 mm/yr for carbon steel specimens after three months of biodiesel exposure, while stainless steel specimens exhibited a slightly lower corrosion rate of 0.000193 mm/yr over the same duration. After one year of exposure, corrosion rates were recorded at 0.000053 mm/yr for carbon steel and 0.0000482 mm/yr for stainless steel, respectively. As a conclusion, this study illustrates the efficiency of simulation studies to predict the behaviour of materials, saving valuable time and resources in the process. Nonetheless, to validate these results under real-time operations, it remains crucial to conduct future experimental studies, ensuring the exact conditions are met.

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