Enhancing the thermo-mechanical properties of the interface in composite materials based on the polysulfone polymer matrix

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doi https://doi.org/10.5937/vojtehg73-53376

FIELD: materials sciences
ARTICLE TYPE:original scientific paper

Abstract

Introduction/purpose: Extensively engaged nanocomposite and biocomposite polymers reinforced with natural fibers as fillers possess the capability to not only augment material properties but also actively tackle challenges within green ecosystems. This versatile application underscored the dual benefits of improved material performance and a proactive commitment to environmental sustainability. The purpose of the present study was to investigate the temperature-induced damage to the fiber-matrix interface in various composite materials.

Methods: The study examined carbon/polysulfone, glass/polysulfone, and alfa/polysulfone biocomposite materials. A genetic approach based on the probabilistic formalism of Weibull was employed to model and analyze the interface damage caused by temperature variations.

Results: Notably, the alfa/polysulfone biocomposite emerged as a compelling alternative, showcasing cost-effectiveness and minimal environmental impact. Its fiber-matrix interface behavior closely paralleled that of carbon/polysulfone. The results revealed the remarkable resilience of the carbon/polysulfone composite's fiber-matrix interface to temperature impacts, distinguishing it from its counterparts.

Conclusions: This nuanced understanding provided valuable insights into the distinct responses of composite materials to temperature variations. It also underscored the advantageous characteristics of the alfa/polysulfone biocomposite, positioning it as a sustainable and efficient option in the field of reinforced polymers for modern applications.

Keywords: polysulfone, carbon, alfa, glass, interface, temperature

Introduction

The remarkable attributes of composite and biocomposite polymers have spurred researchers and manufacturers to delve deeper into this field (Manu et al., 2022; Agustiany et al., 2022; Chichane et al., 2023). The pursuit is centred on not only augmenting their existing properties but also innovating to introduce new materials suitable for a diverse array of contemporary applications. This exploration reflects a dynamic quest for advancements, aiming to continually broaden the scope of materials available for various present-day uses (Akhil et al., 2023; Mann et al., 2023). Composite materials are designed and produced through the arrangement of diverse components, including fibers (whether synthetic or natural), matrices (either thermoset or thermoplastic), fillers, and more (Sharma et al., 2023; Akter et al., 2024; Elfalehet al., 2023; Seydibeyoğlu et al., 2023). These constituents, initially immiscible, undergo a transformative process, resulting in the creation of new materials endowed with superior mechanical, thermal, and physicochemical properties (Rajeshkumar et al., 2023). These composites often exhibit superior strength (Syduzzaman et al., 2023), durability (Zuccarello et al., 2023), and resistance to environmental factors compared to their individual constituents (Nagalakshmaiah et al., 2019; Das Lala et al., 2018). Moreover, the advent of biocomposite polymers, where natural fibers or fillers are incorporated into a polymer matrix, reflects a conscious effort toward sustainability and eco-friendliness in material design (Lee & Jai, 2009; AL-Oqla & Omari, 2017). The applications of these advanced materials are far-reaching, from aerospace to automotive industries (Asyraf et al., 2022; Al Maadeed & Ponnamma, 2023), in construction to offer novel solutions for durable and sustainable building materials (Alam et al., 2021). Additionally, the medical field benefits from biocomposite polymers, where their biodegradability and compatibility with biological systems open avenues for innovative biomedical devices and implants (Sivaraman et al., 2012; Teoh et al., 2016). In this study, we focus on a detailed examination of the influence of three specific fiber types: carbon fiber, glass fiber, and alfa fibers on the properties and performance of polysulfone (UPS). PSU is an amorphous matrix with an amber-colored transparency that resembles in its properties. This type of plastic with very good performance has a balanced ratio between high thermal stability, rigidity, toughness and high creep resistance. Due to its long-term strength and limited tendency to creep, PSU is predestined for long-term exposures. The primary objective is to gain a comprehensive understanding of how these reinforcing materials impact the polymer matrix. In the literature, numerous recent research studies have delved into the multifaceted impact of polysulfone across an array of practical and innovative applications. In (Nica et al., 2023), Nica et al. have characterized high-performance nanocomposite materials based on modified polysulfone using various amounts of modified carbon nanotube fillers for electronic applications. The study's findings unveiled a substantial improvement in the electrical conductivity of composite materials. This enhancement was particularly pronounced at higher filler loadings, suggesting promising prospects for the development of advanced electronic applications using these modified polysulfone nanocomposites. In another study (Stepashkin et al., 2023), Stepashkin et al. have investigated the impact of carbon fiber type, polymer mass fraction, and loading rate on tensile strength of polysulfone polymer using a polymer solution method. Scanning Electron Microscopy (SEM) analysis provided further insights, revealing that at low loading rates, elementary filaments within the impregnated fiber could align themselves along the applied load axis. This alignment, facilitated by the flow of the thermoplastic matrix under tensile stresses, led to more effective realization of the fiber's strength properties in thermoplastic-based composites compared to analogous composites with an epoxy matrix. In (Li et al., 2022), Li et al. studied the repercussions of hydrothermal aging on the long-term durability, specifically focusing on stress relaxation and creep properties, for both virgin and recycled PSU, where specimens of virgin and recycled polysulfone PSU were subjected to exposure to pure hot water at temperatures of 98 °C for varying durations ranging from 1 to

12 months. The findings of the study reveal that virgin PSU demonstrates exceptional resistance to hydrothermal aging across various mechanical parameters, including tensile, flexural, impact, and fracture toughness properties, as well as stress relaxation and creep resistance, even after a year of aging in 98 °C hot water. Additionally, the investigation establishes that the activation energy required for stress relaxation in PSU is consistent with that needed for creep. In another recent study (Lim et al., 2022), the authors have investigated the separation characteristics of polysulfone hollow fiber membranes for the removal of carbon dioxide and sulfur compounds from biogas. The research offers valuable insights into the impact of various operating conditions on the membrane's separation performance. Their findings revealed that the polysulfone membrane exhibited robust removal efficiency for sulfur compounds, ranging between 70% and 80%, within a feed pressure range of 2.3-2.6 bar. Importantly, the presence of sulfur compounds was observed to have a negligible effect on the separation performance of the polysulfone membrane. Building upon recent studies, this investigation focuses on probing the temperature-induced damage to the fiber-matrix interface in carbon/polysulfone and glass/polysulfone composite materials, as well as in alfa/polysulfone biocomposite material. The interesting mechanical properties of alfa fibers show that they can present an interesting alternative for the reinforcement of different polymer matrices.The study of morphological, physical and mechanical properties showed that alfa fibers present promising properties for use as reinforcement in composite materials. Its potential as reinforcement in composites requires the understanding of its microstructure, its mechanical properties, adequate control of fiber extraction as well as the transformation process (Brahim & Cheikh, 2007 ; Paiva et al., 2007; Bessadok et al., 2007; Bessadok et al., 2009; Arrakhiz et al., 2012; Marrakchi et al., 2012; Hamza et al., 2013; Mounir et al., 2014; Helaili & Chafra, 2014 ; Ghali et al., 2006).Traditional material characterization methods are efficient, but to characterize the behavior of a new material requires numerous physical tests (fracture, shear, bending, buckling, torsion, relaxation, etc.). These problems can be solved by adopting a more powerful AI-based strategy. This offers speed and precision in the development of new materials.

Artificial Intelligence (AI) tools, in our case, the approach employed is a genetic one, grounded in the probabilistic formalism of Weibull, can exploit and analyze large quantities of data to predict the properties of these materials, reducing the need for expensive and time-consuming physical testing. The obtained results revealed that the fiber-matrix interface of the carbon/polysulfone composite remained relatively unaffected by temperature variations when contrasted with the interfaces of the alfa/polysulfone and glass/polysulfone composite and biocomposite materials. This insight contributes to a nuanced understanding of the diverse responses of different composite materials to temperature-induced stress, emphasizing the unique advantages and characteristics of the alfa/polysulfone biocomposite in this context.

Materials, models and methods

Polysulfone matrix (PSU)

Polysulfone (PSU) has one of the highest service temperatures of all high-performance melt-processable polymers. The high temperature nature of PSUs allows them to be used in demanding applications that other polymer materials cannot satisfy. PSU is highly resistant to acids, alkalis and electrolytes, oxidizing agents, surfactants and hydrocarbon oils. PSU is one of the so-called thermostable technical thermoplastic polymers. Indeed, the systematic presence, on the main chain, of aromatic nuclei, explains in particular the high thermal resistance of this polymer. Mechanical properties are retained by PSU over a wide range of temperatures. In addition, PSU is resistant to temperature, UV, gamma and X-ray radiation (De Leon et al., 2016; Mujika et al., 2002; Chukov et al., 2019; Solodilov et al., 2015; Yao et al., 2018; Anne, 2019).

Fibres

Carbon fiber (CF)

A number of carbon fiber reinforced composites based on thermoplastic have been developed and studied. Among thermoplastics, high-performance polymers are of particular interest due to their thermal stability and high mechanical properties. Carbon fiber composite materials are very popular for their lightness and strength, especially compared to steel, aluminum and even titanium. Aeronautics, for example, uses them extensively: in fact, the main cost of operating an aircraft is fuel and we reduce fuel consumption by reducing the weight of the plane. Carbon fiber is obtained by spinning a precursor prepolymer, generally polyacrylonitrile (or PAN). It is an unhardened plastic material that is made into a very fine wire. The latter is treated at high temperature in order to eliminate anything that is not pure carbon. This is carbonization: a process close to pyrolysis and similar to that which transforms wood into charcoal. The use of carbon rather than metals reduces weight without compromising the mechanical strength of the device. Motor racing, luxury cars, or manual devices also use it, mainly for its lightness coupled with its resistance. Carbon is also used in luxury areas, for its beautiful appearance despite its high cost (Chukov et al., 2018). Figure 1 presents the structure of the composites reinforced with carbon fibers (a) initial and (b) oxidized at 500 °C (Chukov et al., 2018).

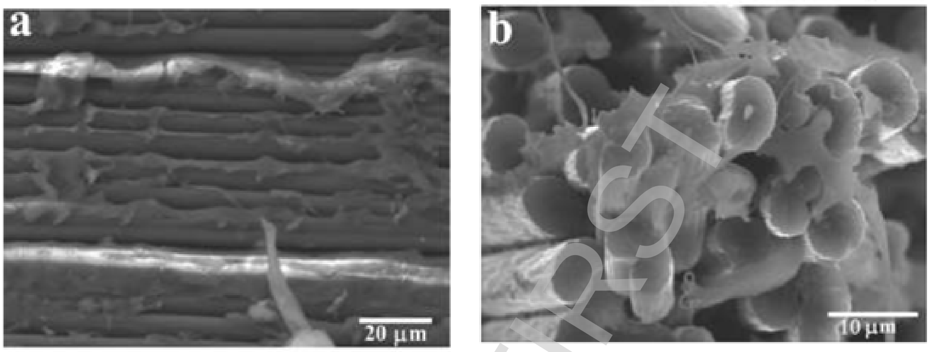

Figure 1– Structure of the composites reinforced with carbon fibers: (a) initial and (b) oxidized at 500 °C (Chukov et al., 2018).

Alfa fiber

Alfa plant fibers, also called lignocellulosic fibers, are rigid micro-fibrillar structures mainly composed of cellulose, hemicelluloses and lignin and in relatively small proportions of extractables and mineral materials. These natural fibers are low cost and low density fibers; they have specific properties, biodegradable and non-abrasive fibers (Saad, 2013). It has been studied from the point of view of chemical composition, evolution of the structure with the biological cycle, possibility of developing composites, surface modification by physico-chemical treatments, grafting, bleaching and production of paper with a study of the impact of various actions undergone by this fiber.

Glass fiber

As opposed to glass in massive forms, fiber glass with a diameter not exceeding a few microns loses its fragility and its sensitivity to cracking. Glass fibers show good mechanical characteristics. Depending on their composition, there are five types of glass fibers: E glasses which are for general use and which have good electrical properties, D glasses which have high dielectric properties, A glasses which have a high alkali content, C glasses which have good chemical resistance, and R and S glasses which have good mechanical resistance. Glass fibers are made up of silica, alumina, lime, magnesia, boron oxide, fluorine, iron oxide, titanium oxide, sodium oxide, and oxide of potassium. The composition in percentage by mass of each chemical component varies from one type of fiber glass to another. (Hamlaoui, 2022).

Different physical properties of the constituents of the composite and biocomposite materials used in the genetic program have been mentioned in Table 1.

Table 1 – Physical properties of the constituents of the composite and biocomposite materials used in the genetic program.(Anne, 2019 ; Hamlaoui, 2022 ; Bourahli & Osmani, 2013 ; Biagiotti et al., 2004 ; Rowell, 2008; Moghaddam et al., 2016 ; Rao et al., 2007 ; Monteiro, 2011 ; Berthelot, 2005

Materials	Young's modulus (GPa)	Deformation at break (%)	Density (g/cm3)	Stress to break (MPa)
Carbon	230	4	1.7	4000
Alfa	21.5	2.4	1.4	247
Glass	73	4.4	2.6	3400
Polysulfone	3.1	4	1.24	80

Analytical models and genetic simulation

Thermal stress

Equation (1) is used to represent the thermal stresses that arise from the differential expansion of fibers and matrices. This occurs during the cooling process after the composite has been prepared at elevated temperatures (Weibull, 1939).

$$\sigma_f^T = E_f \frac{a}{a+1}(M_2 - M_0) \tag{1}$$

with:

$$M_0(T) = \int_{T_0}^{T_e} (\alpha_m - \alpha_f) dT$$

$$M_2(T) = \int_{T_e}^{T} (\alpha_m - \alpha_f) dT$$

- T_0: room temperature;
- T_e: temperature during the development process;
- T : test temperature; and

- α_f and α_m :expansion coefficients of the fiber and matrix, respectively. ($\alpha_{f\text{-}Carbon}$=1.2*10^{-6}/°C, $\alpha_{f\text{-}Glass}$= 1.2*10^{-6}/°C, and α_m=82*10^{-6} /°C)

Weibull approach

Weibull's statistical method has been utilized in the analysis of composite materials, assuming a uniform distribution of applied stress. The expressions for matrix and fiber damage are denoted by equations (2) and (3), respectively, and are elaborated upon in detail in reference (Lebrun, 1996). This approach involves using Weibull statistics to model stress distribution in composite materials, with equations (2) and (3) offering a quantitative representation of the damage to the matrix and fibers, guided by this statistical framework.

$$D_m = 1 - exp\left\{-\frac{V_{eff}}{V_0}\left(\frac{\sigma_f}{\sigma_0}\right)^m\right\} \quad (2)$$

with :

- σ_f: applied stress;
- V_{eff}: matrix volume;
- $mand\sigma_0$: Weibull parameters; and
- V_0: initial volume of the matrix.

$$\mathbf{D_f = 1 - exp\left\{-A_f * L_{equi} * \left(\frac{\sigma^f_{max}}{\sigma_{of}}\right)^{m_f}\right\}} \quad (1)$$

with:

- σ^f_{max}: maximum stress applied to the fiber;
- σ_{0f}: initial stress applied to the fiber;
- m_f: Weibull parameters;
- A_f =π*a²; and
- L_{equi} : length of the fiber at equilibrium.

Genetic model

In this study, we will investigate the effect of temperature on the resistance and behavior of the fiber-matrix interface of composite materials (carbon/polysulfone and glass/polysulfone) and Alfa-polysulfone biocomposite material. The final performance of a composite material strongly depends on the quality of the fiber-matrix interface. This interfacial bond is quite difficult to model using deterministic models; in our case, we

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chose genetic modeling based on the two Weibull equations (2 and 3) determining the damage of the fiber and that of the matrix. Our objective is to calculate the damage of the interface using the two aforementioned damage cases by the crossing operator (see the flowchart presented in Figure 2) (Lebrun, 1996; Belhadj et al., 2022; Belkheir et al., 2023; Mokaddem et al., 2012; Mokaddem et al., 2014; Benyamina et al., 2021).

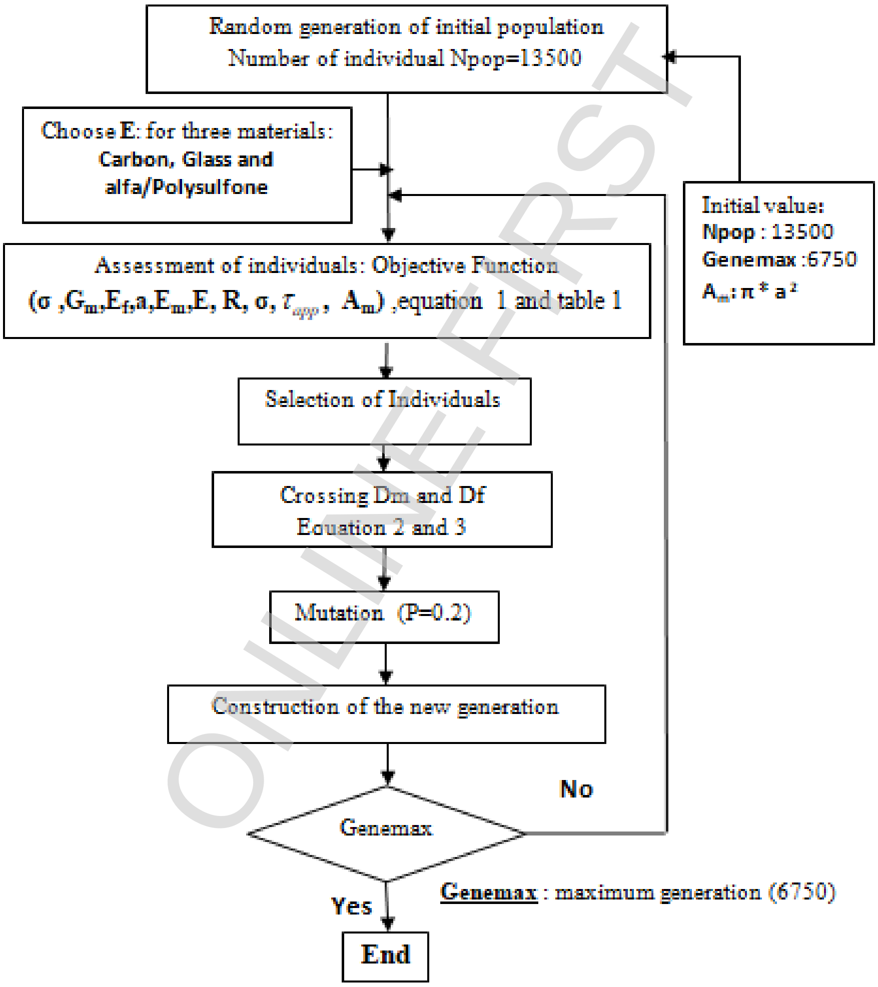

Figure 2– Genetic program flowchart

Results and discussion

In this work, the effect of temperature on damage to the fiber-matrix interface of carbon/polysulfone and glass/polysulfone composite materials, and alfa/polysulfone biocomposite material was investigated using a genetic approach based on the probabilistic formalism of Weibull (equations 2 and 3) (Belkheir et al., 2022; Belkheir et al., 2023). The damage at the interface was calculated by the genetic operator (crossover) using the two damage cases, one of the matrix and the other of the fiber given by equations (2) and (3), respectively. The random variables of the population consist of chromosomal genes representing the following variables: tensile stress (σ=600, 750, 900, 1050 and 1200MPa), Young's modulus, shear modulus of the matrix, fiber diameter, length of each fiber, and the half-distance R. This initial generated population is composed of 13500 individuals, which will be improved each time by the genetic operator mutation with a mutation probability of 0.2 (Mokaddem et al., 2020; Mokaddem et al., 2014). In each case, we used different values of the Young's modulus of each fiber and the Polysulfone matrix (Table1).The temperature variation for the five values of the mechanical stress and its influence on the damage of the interface was calculated and verified by equation (1). The results presented in Figures 3 to 5 refer to the level of interfacial damage as a function of temperature to the three composite and biocomposite materials studied (see the program flowchart in Figure 2).

Figures (3-5) show that the interface damage is strongly linked to the damage of the matrix which has the weakest constituent compared to the reinforcements (fibers), and show that the different temperature values applied to the three composite and biocomposite materials caused fiber-matrix interface damage which was lower for carbon/PSU, medium for Alfa/PSU and higher for glass/PSU. The fiber-matrix interface of the carbon/PSU composite was not influenced by temperature compared to the other interfaces of Alfa/PSU biocomposite material and glass/PSU composite material. The effect of temperature on the interface damage of the three studied composite and biocomposite materials shows almost the same results as those found by Dilyus Chukov et al.(Chukov et al., 2019). It should be noted that the alfa/polysulfone biocomposite material remains an interesting alternative given its very low environmental impact, a very low cost compared to other composite materials and that its fiber-matrix interface has a value that is close to the carbon/polysulfone interface. In this theoretical study, the fiber-matrix interface of the carbon/PSU composite was not influenced by the temperature compared to other interfaces of the Alfa/PSU and glass/PSU composite and biocomposite materials. The results found, in particular those relating to the carbon/polysulfone interface, are in good agreement with the results found by Dilyus Chukov et al.(Chukov et al., 2019).

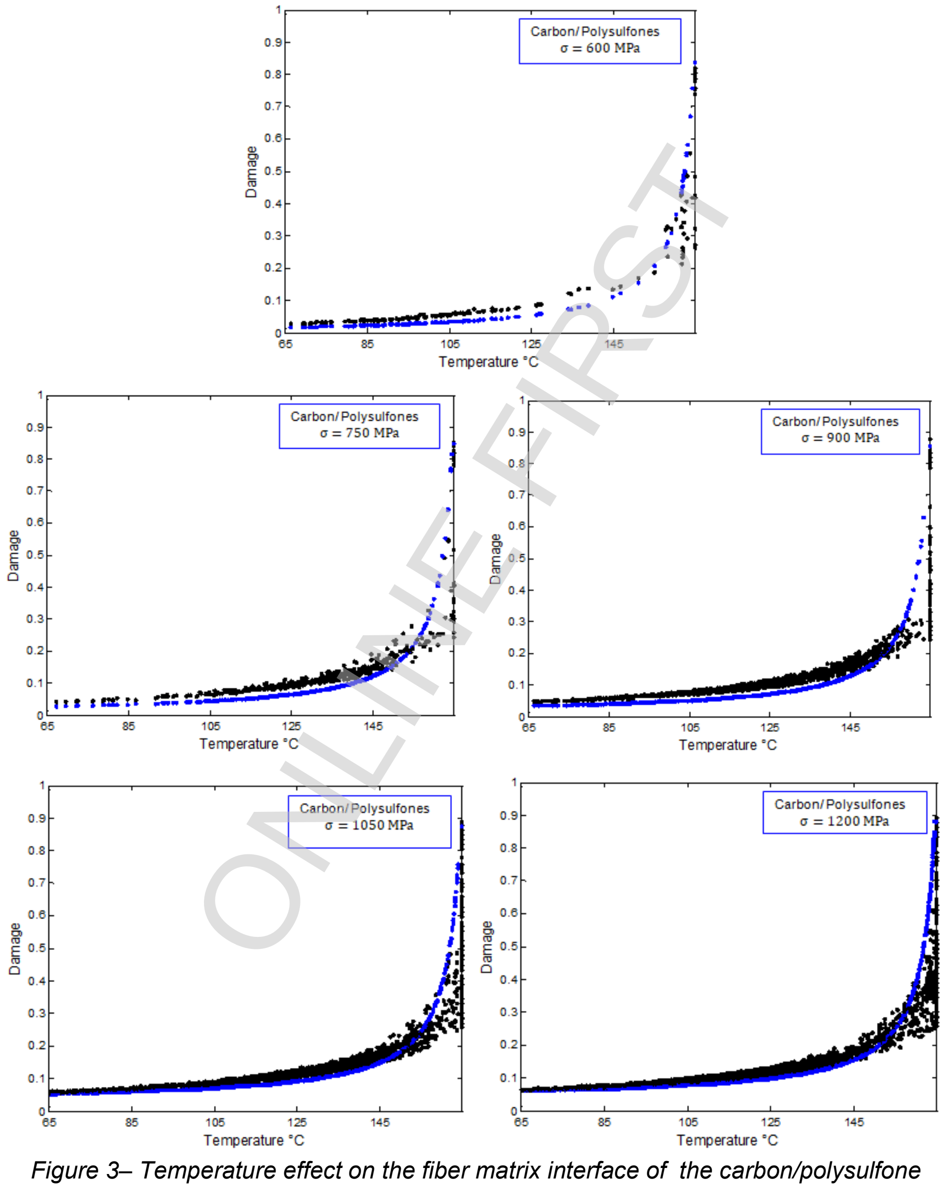

Figure 3– Temperature effect on the fiber matrix interface of the carbon/polysulfone composite

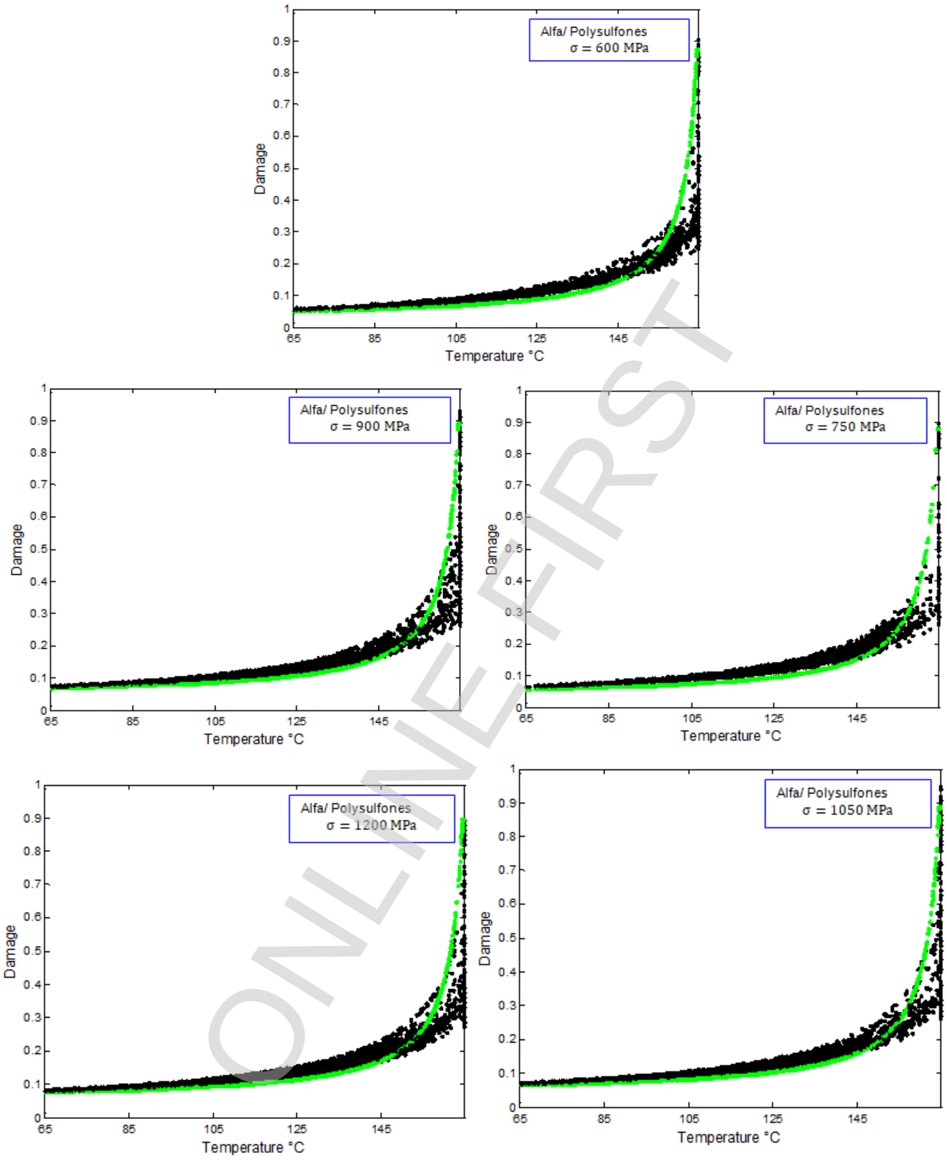

Figure 4– Temperature effect on the fiber matrix interface of the alfa/polysulfone biocomposite

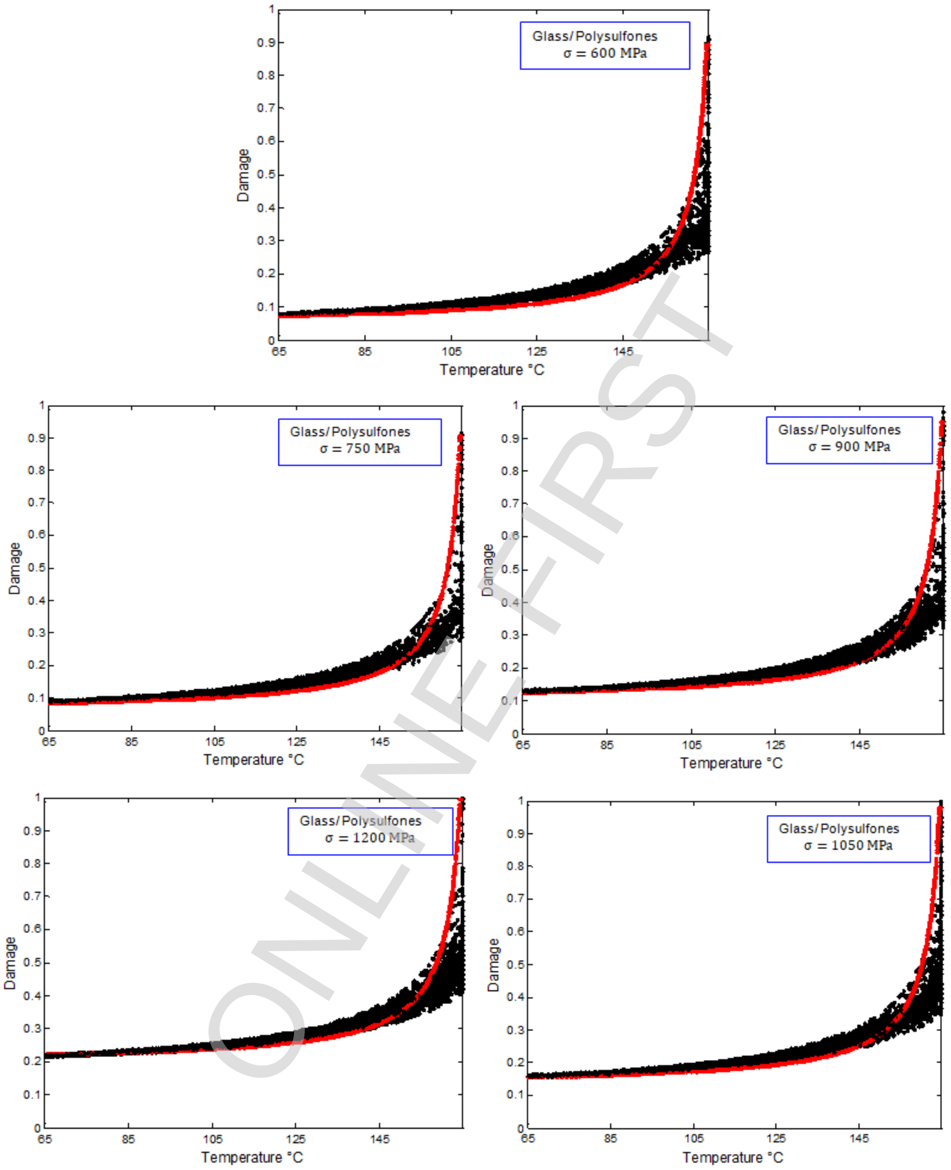

Figure 5– Temperature effect on the fiber matrix interface of the glass/polysulfone composite

In various studies carried out on composite materials, the fiber has a direct influence on the behavior of the fiber-matrix interface in relation to the matrix because fibers transmit their mechanical properties to the matrix and this in terms of rigidity, resistance to breakage, hardness, etc. The reinforcements also confer their physical properties to the resin. Among these properties, we can cite Young's modulus, mechanical behavior, fire resistance, and abrasion resistance (Prakash et al., 2021; Pan, 2022; Ramesh et al., 2021).

Conclusions

The present study focuses on the influence wielded by three distinct fiber types (carbon fiber, glass fiber, and alfa fibers) on the properties and performance of polysulfone. The overarching objective is to attain a comprehensive understanding of how these reinforcing materials exert their influence on the polymer matrix, based on a genetic approach. In the theoretical exploration conducted, it was observed that the fiber-matrix interface of the carbon/PSU composite exhibited a notable resistance to temperature effects in contrast to the interfaces of the Alfa/PSU and glass/PSU composite and biocomposite materials. This finding emphasizes the distinct thermal behavior exhibited by these composite interfaces, highlighting the relative stability of the carbon/PSU composite's fiber-matrix interface under varying temperature conditions. This insight contributes to refining the understanding of how different composite materials respond to temperature-induced stress on their fiber-matrix interfaces.

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Побољшавање термомеханичких својстава интерфејса код композитних материјала на бази полисулфонске полимерне матрице

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Сажетак:

Увод/циљ: Универзално употребљавани нанокомпозитни и биокомпозитни полимери ојачани природним влакнима као пунилима имају способност не само да побољшавају својства материјала него и активно решавају изазове у зеленим екосистемима. Овом разноврсношћу употребе наглашава се двострука корист – побољшане перформансе материјала, као и проактивна посвећеност еколошкој одрживости. Циљ ове студије био је испитивање оштећења проузрокованог температуром на интерфејсу влакно-матрица у различитим композитним материјалима.

Методе: Испитивани су карбон-полисулфонски, стакло-полисулфонски и алфа-полисулфонски биокомпозитни материјали. Генетички приступ заснован на пробабилистичком формализму Вејбула примењен је за моделовање и анализу оштећења интерфејса услед температурних варијација.

Резултати: Алфа-полисулфон биокомпозит показао се као одлична алтернатива захваљујући исплативости и минималном утицају на животну средину. Понашање његовог интерфејса влакно-матрица веома је слично понашању интерфејса карбон-полисулфон. Резултати су показали изузетну отпорност интерфејса влакно-матрица код карбон-полисулфонског композита на утицај температуре, што га издваја од осталих.

Закључак: Представљени су драгоцени увиди у различите одговоре композитних материјала на температурне варијације. Такође, наглашене су карактеристике алфа-полисулфонског биокомпозита које му, као одрживом и ефикасном решењу, дају предност у области ојачаних полимера за модерне примене.

Кључне речи: полисулфон, карбон, алфа, стакло, интерфејс, температура

Paper received on: 11.09.2024.
Manuscript corrections submitted on:10.12.2024.
Paper accepted for publishing on: 22.01.2025.