Chapter 3

New Advances in Thermoplastic Commingled Composites: Processing and Molecular Dynamics

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New Advances in Thermoplastic Commingled Composites: Processing and Molecular Dynamics

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Abstract

This chapter addresses a current and innovative topic related to thermoplastic commingled composites. Computational molecular dynamics simulations represent a very sophisticated technique for characterizing microstructures, but it is still not widely explored in the area of high-performance thermoplastic polymers. The molecular dynamics technique evaluates the movements of atoms as a function of time and temperature, according to external demands and boundary conditions of the molecular system. Based on thermodynamics, atomistic and classical mechanics theories, molecular dynamics simulations with empirical potentials aim at (i) the development of new polymeric materials, (ii) the optimization of polymer properties, and (iii) the characterization of these materials. The molecular dynamics technique provides a prediction of mechanical and thermal behavior of high-performance polymeric microstructures, reducing the number of tests and experimental practices, which increases the operational cost of engineering projects and the characterization of structural composite materials. Furthermore, this chapter also includes a scientific and technological literature background to demonstrate and highlight the conjuncture between thermal processing parameters, thermal degradation kinetics, processing optimization, thermal and mechanical characterization techniques. It also includes literature and experimental background based on previous studies.

Keywords: Molecular dynamics; thermoplastic commingled composites; thermal consolidation.

1 Introduction

Interatomic potentials are mathematical functions that describe the interaction between pair of atoms or the interaction between groups of atoms, considering the condensed phase or systems with very large number of atoms. From this perspective, computational simulations using molecular dynamics (MD) with empirical potentials have been used to explain and predict the thermal and mechanical behavior of polymeric materials. The atomic microstructure is investigated according to the movements of the atoms in three-dimensional space.

Typically, polymeric materials display amorphous or semi-crystalline structures, which makes it difficult to realistically simulate interatomic movements. The molecular structure of thermoplastic polymers is composed of high entropy thermodynamic systems. This condition limits the precise determination of the positions of atoms in three-dimensional space. The validation of the technique for characterizing high-performance thermoplastic polymers using MD simulations depends on the level of representativeness of the models and the reliability of the theoretical and experimental data.

MD method is based on mathematical calculations of potential energies. The calculations measure the displacement of atoms as a function of time and temperature. Scientific studies with an emphasis on MD of polymeric microstructures are promising and have attracted the attention of researchers and companies, favoring partnerships and technological advances. The use of computer simulations in engineering projects creates opportunities for new scientific work in a continuous and integrated way. Computational analyzes work together with experimental practices, offering support to companies and research centers. In addition to reducing project time and costs, the use of computer simulation provides a competitive advantage in the development of new materials and products.

MD simulations that describe the behavior of thermoplastic materials have been an active research area with great potential for impact in basic and applied research. These simulations can be used to conduct mathematical tests to predict and simulate the material behavior.

2 Theorical Background

2.1 Thermal Processing and Degradation

Commingled yarns are hybrid structures in which two different materials are mixed to form continuous filament tow. This technology provides easier storage and drapability [1], due to the ability of textile preforms to conform to the surface of molds. Thus, thermoplastic commingled materials allow the preform conformation to make a rigid structure [2] under applied temperature and pressure. Thermoplastic commingled composites are versatile materials, recyclable, with high performance and significant manufacturing costs reduction [2]. Focusing on the overall reduction of production costs, the use of thermoplastic commingled composites reduces the weight of components and establishes the best characteristics of geometry, materials, and processing parameters [3].

The processing of thermoplastic composites, however, involves thermo-oxidative degradation of the matrix during consolidation. The thermal degradation directly affects the mechanical properties of the composite structures. Degradation kinetics methodologies determine the limits of temperature and time in which the material can be processed. Friedman's isoconversional kinetic model is an example of how to investigate the matrix thermo-oxidative degradation. Any variation in processing parameters can cause significant changes in the mechanical behavior of these materials [4,5].

Friedman's model [6] calculates the activation energy (E_a), defined as the minimum energy required for chemical reaction. The pre-exponential factor (A_α) is determined by the linearization of the degradation degree rate $\left(\frac{d\alpha}{dt}\right)$, as a function of the temperature inverse ($1/T$) for each degree of degradation (α). Equation 1 allows for calculating the variation of the rate constant of a chemical reaction with temperature, in which $-\frac{E_a}{RT}$ and lnA_α are equivalent to the line's equation slope and intersection, respectively:

$$ln\left(\frac{d\alpha}{dt}\right) = lnA_\alpha - \frac{E_a}{RT}; \tag{1}$$

Friedman's method correlates the degradation degree as a function of time for a given temperature, according to:

$$\alpha = A_\alpha \exp\left(-\frac{E}{RT}\right)t, \tag{2}$$

resulting in a time/temperature graph, considering the time and temperature required to provide the softening range of the thermoplastic matrix without reaching its degrees of temperature onset damage degradation [7]. Thermal degradation must be considered when processing thermoplastic composites. To estimate the degree of degradation using Friedman's kinetic model, thermogravimetry (TGA) must be performed with at least three different heating rates.

Darcy's law [8] is a constructive equation used to predict how a viscous fluid is able to impregnate the reinforcing fibers of the composite material [8]. This period can be estimated by the impregnation time t_{imp}. Darcy's law has been used to precisely define the soak time (isothermal), defined in Equations 3 and 4, considering the pressure rate $\frac{dP}{dx}$ constant:

$$u_p = \frac{dx}{dt} = \frac{K}{\eta}\frac{dP}{dx}, \tag{3}$$

$$t_{imp} = \frac{\eta D_p^2}{2KP}, \tag{4}$$

where u_p is the impregnation velocity of the viscous polymer, K is the reinforcing fibers coefficient of permeability, η is the polymer viscosity, $\frac{dP}{dx}$ is the pressure gradient, and D_p is the impregnation distance related to the thickness of the laminate. Figure 1 represents a viscous flow impregnating the reinforcement fibers by external pressure.

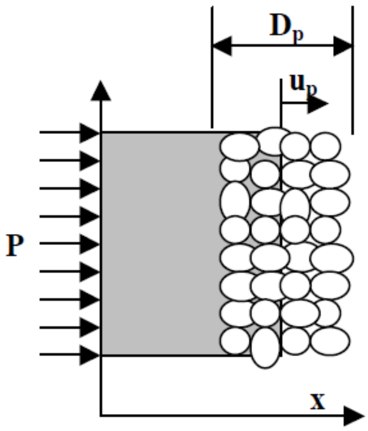

Figure 1: Schematic of impregnation under pressure of the reinforcing fibers by a viscous flow (adapted from [8]).

The determination of the processing pressure is usually obtained empirically. Total consolidation is considered until there are no more detectable defects and voids within the laminate. The consolidation pressure P should be enough to reach these conditions, but not allow the polymer matrix to leak beyond the reinforcement fibers out of the metal matrix. Finally, the viscosity η of the polymeric matrix can be obtained by rheology analysis.

2.2 Statistic Modeling and Soft Computing Techniques

Multiple regression models (MRM) can be used to describe a studied process or a material behavior as a three-dimensional (3D) plane, or response surface. The 3D plane refers to independent explanatory variables such as processing time, temperature, and the target property. Optimizing the thermal processing of thermoplastic commingled composites reduces production costs and optimizes the composite properties.

MRM was developed to predict a mechanical property as a function of (i) thermal and viscoelastic properties of the matrix; (ii) kinetic parameters of degradation, and (iii) consolidation parameters. The regression coefficients β_1 and β_2, (Equations 5 and 6) indicate the variation in the mean response to each unit of the independent variable x_1, when the other variables are kept fixed. Y is the response-dependent variable [9],[10]:

$$\beta_1 = \frac{(\sum x_2^2)(\sum x_1 Y) - (\sum x_1 x_2)(\sum x_2 Y)}{(\sum x_1^2)(\sum x_2^2) - (\sum x_1 x_2)^2}; \tag{5}$$

the parameter β_2 indicates the variation in the mean response to each unit of x_2, when x_1 is kept constant [9],

$$\beta_2 = \frac{(\sum x_1^2)(\sum x_2 y) - (\sum x_1 x_2)(\sum x_1 y)}{(\sum x_1^2)(\sum x_2^2) - (\sum x_1 x_2)^2}. \tag{6}$$

The least-squares method (LSM) is a statistical technique used to find the best fit for a set of data points, precisely predicting the behavior of dependent variables or responses. Based on the MRM and LSM, the maximum likelihood function L (Equation 7) must be minimized. L represents a function to measure the probability of observing a set of dependent variable values [9–12]:

$$L = \sum_{i=1}^{n} \left(Y_i - \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}\right)^2. \tag{7}$$

Another important step of the optimization process refers to variable selection, specifically the stepwise method. This statistical tool automatically chooses the best predictive variables to fit regression models. Akaike Information Criterion (AIC) is based on this fit to estimate the likelihood of the MRM to predict or estimate future values. The minimum AIC (Equation 8) defines the variables which were included or removed from the model [13],[14], i.e.,

$$AIC = -2log\left(L_p\right) + 2[(p+1)+1], \tag{8}$$

where, L_p is the maximum likelihood function and p the number of explanatory variables.

Soft computing techniques including artificial neural networks (ANN) and machine learning offer new prospects to predict the mechanical behavior of thermoplastic commingled composites. Recent studies [15–22] have been used to predict the mechanical behavior of structural composite materials by computational modeling [23]. ANN technique has been applied to improve the behavior of structural composite materials [24], including the design optimization of composite components [25], structural behavior of natural fibers reinforced composite [26], recyclability of thermoplastics composites [27], and to improve mechanical properties of these materials [28],[29]. Systematic and interactive approaches involving composite materials allow to achieve the ideal characteristics of the material.

ANN has been used to (i) investigate mechanical properties of composite materials, (ii) properties optimization, (iii) understand the effects of manufacturing parameters, and (iv) develop new computational methods for materials characterization. Basically, ANN is a computational system arranged of processing elements operating in parallel, whose function is obtained according to the network structure, the connection strengths, and the processing performed at computing elements or nodes.

In general, a neural network is a processor with a natural tendency for storing experiential knowledge and making it available for practical use. ANN resembles the human brain in two respects: (i) knowledge is acquired through a learning process, and (ii) interneuron connection forces are used to store knowledge [30].

2.3 Initiating molecular dynamics in thermoplastic composites

MD-based on empirical potentials established a new generation of characterization of thermoplastic structures. Essentially, MD is a computer simulation method to analyzes atomic movements and, thus, predict thermal and mechanical behavior of polymeric molecules. The benefits associated with advances in MD for thermoplastic composites are promising and attractive for the science and technology of high-performance composite materials, potentially reducing the material's development time. The main scientific challenge is to establish the atomic and molecular positioning criteria that can contribute to a more realistic result of computer simulations.

MD simulations that describe the behavior of polymeric materials have been an active research area with great potential for impact in basic and applied research. Computational practice is a procedure that uses advanced software to conduct mathematical tests to predict and simulate material behavior.

The innovation proposed consists of the development of analytical models, experimental analyzes, and MD simulations to investigate the thermal and mechanical behavior of polymers. MD simulations will be conducted to evaluate intermolecular movements and investigate the thermal and mechanical behavior of thermoplastic matrices. The literature presents modeling and simulation gaps when thermoplastic composites are involved. This topic has raised great scientific interest because of the practical results: (i) assist decision-making in the selection of polymeric materials, (ii) determine optimal processing parameters, (iii) predict the thermal and mechanical behavior of polymers, and (iv) optimize the performance of thermoplastic commingled structures.

3 Experimental Practices

This topic involves the experimental results consisting of raw material characterization, processing procedures, thermal degradation kinetics, optimization of the material properties, and an initial approach to MD simulations applied to thermoplastic composites.

3.1 Commingled technology

The CF/PA commingled tow combines 37 µm PA yarns into 12k 7 µm carbon fibers, as shown in the SEM micrography in Figure 2.

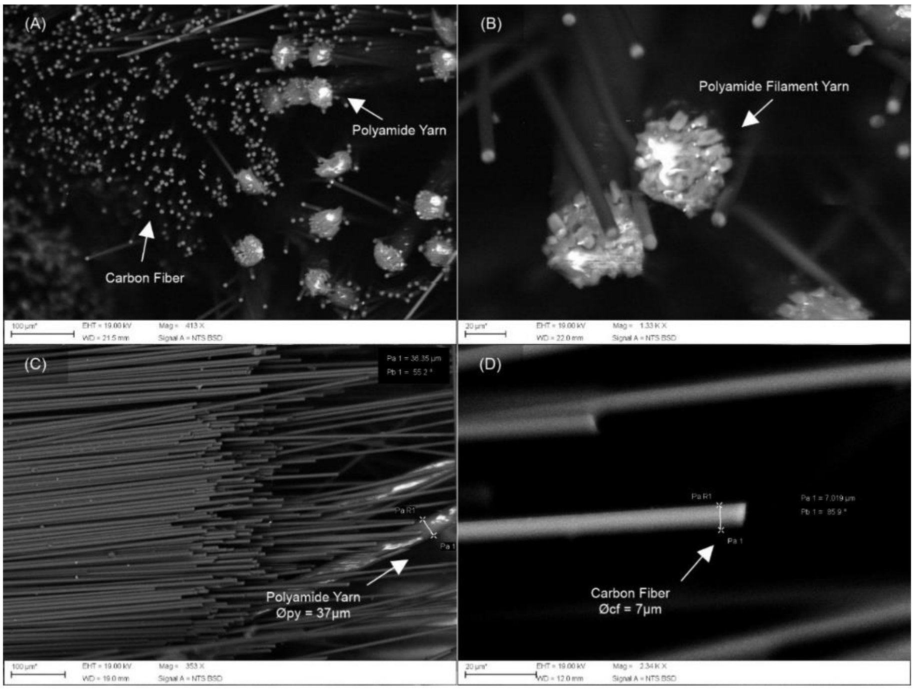

Figure 2: SEM micrography of CF/PA6 commingled tow to measure fibers and yarn diameters (adapted from [7]).

The constituents of CF/PEEK commingled tow are shown in Figure 3. According to the SEM micrography, the material is composed by 12k 7 µm carbon fibers and 26 µm PEEK yarns.

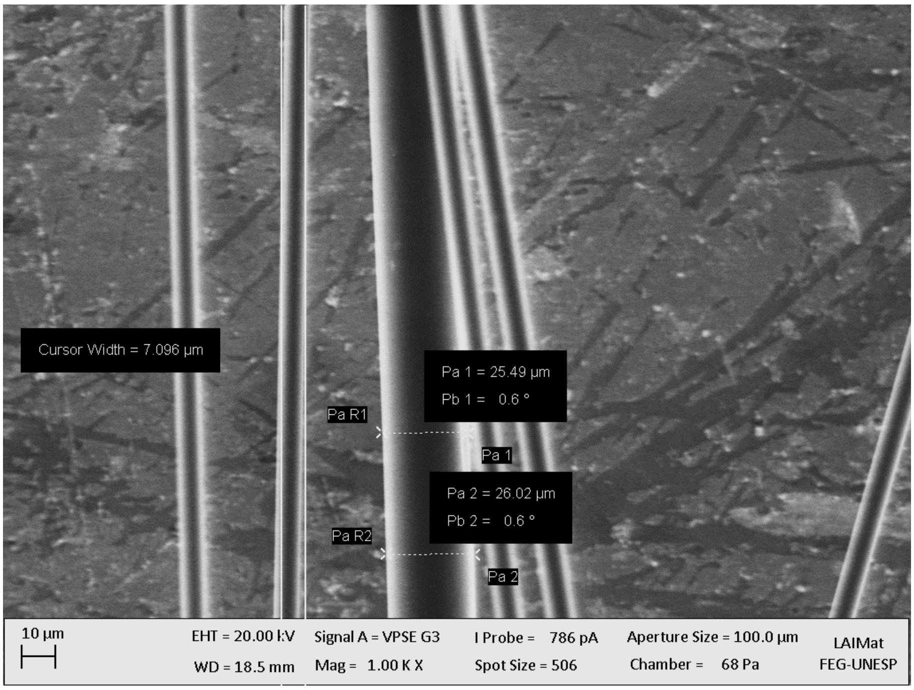

Figure 3: SEM micrography of CF/PEEK commingled tow to measure fibers and yarn diameters (adapted from [31]).

3.2 Thermal analysis

Differential scanning calorimeter (DSC) analysis reveals the phenomena that occur during thermal cycles, and it guides the selection temperatures to process CF/PA commingled composite. The result of DSC analysis is shown in Figure 4.

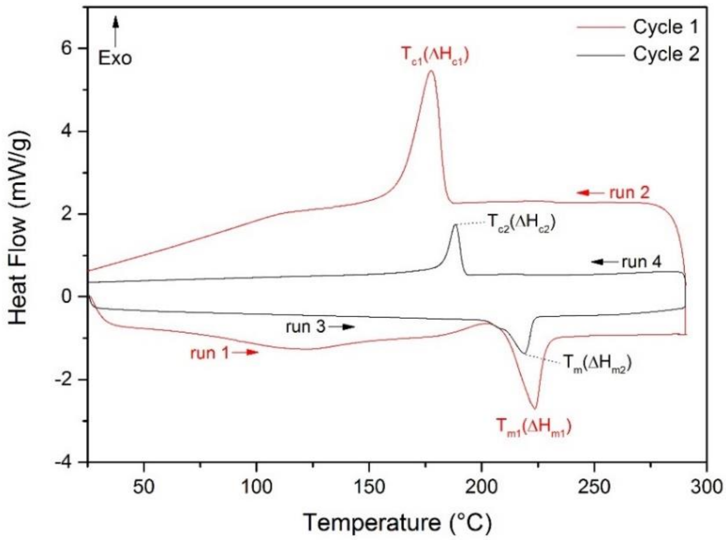

Figure 4: DSC thermal cycles of thermoplastic polymer to reveal endothermic and exothermic peaks associated to melting point and crystallization (adapted from [7]).

The DSC was conducted in two steps. The first cycle erases the thermal history of the sample associated with its previous processing [32]. The second cycle allows the calculation of more accurate values for melting point (Tm) and crystallization temperature (Tc) disregarding the thermal history influence. The melting and crystallization enthalpies, ΔHm and ΔHc, were also identified. To process a thermoplastic commingled composite efficiently the processing cycle should consider the temperatures Tm and Tc and the cooling rate.

The crystallization degree of semicrystalline polymers should be as high as possible to enhance the mechanical and thermomechanical properties of composite structures. Therefore, a low cooling rate favors crystalline structure formation, and it can be calculated by relating ΔHm and ΔHc.

3.3 Degradation Limits

Friedman's isoconversional method allows for the prediction, as a function of time and temperature, of the degree of degradation and establishes the processing window. Graphically, the result of the degradation kinetics study shows the limits of temperature and time in which the composite material should be processed (see Table 1).

Table 1: Thermal degradation kinetics parameters obtained by Friedmann`s isoconversional method.

Material	Temperature, T (°C)		Time, t (min)		Ea (α=0.05) kJ/mol	Molecular Mass (g/mol)
	melt	*onset*	*melt*	*onset*		
PA	220	320	112	4.5	93.70	113
PEEK	338	550	142	12.3	73.26	228

Figure 5 shows the results of the degradation kinetics analysis for the CF/PA6 commingled composite. It reveals the relation between the activation energy E_a and α in (a) and the limits of degradation according to T_p in (b). Figure 6 shows the degradation kinetics analysis of the CF/PEEK commingled composite.

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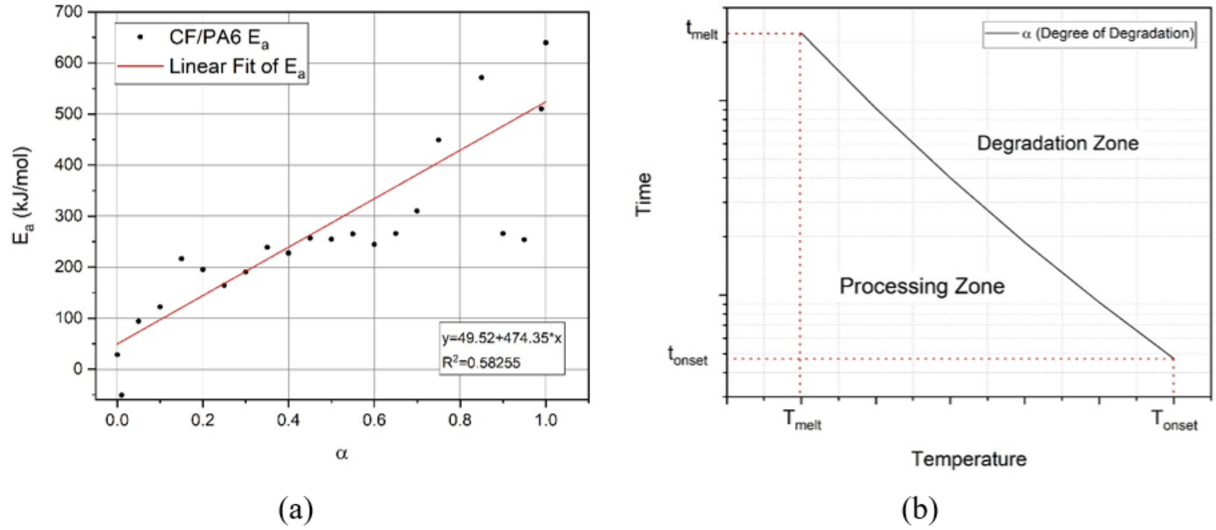


Figure 5: Thermal degradation kinetics analysis for CF/PA6. (a) E_a *versus* α. (b) Thermal degradation limits plot (Adapted from [31]**)**

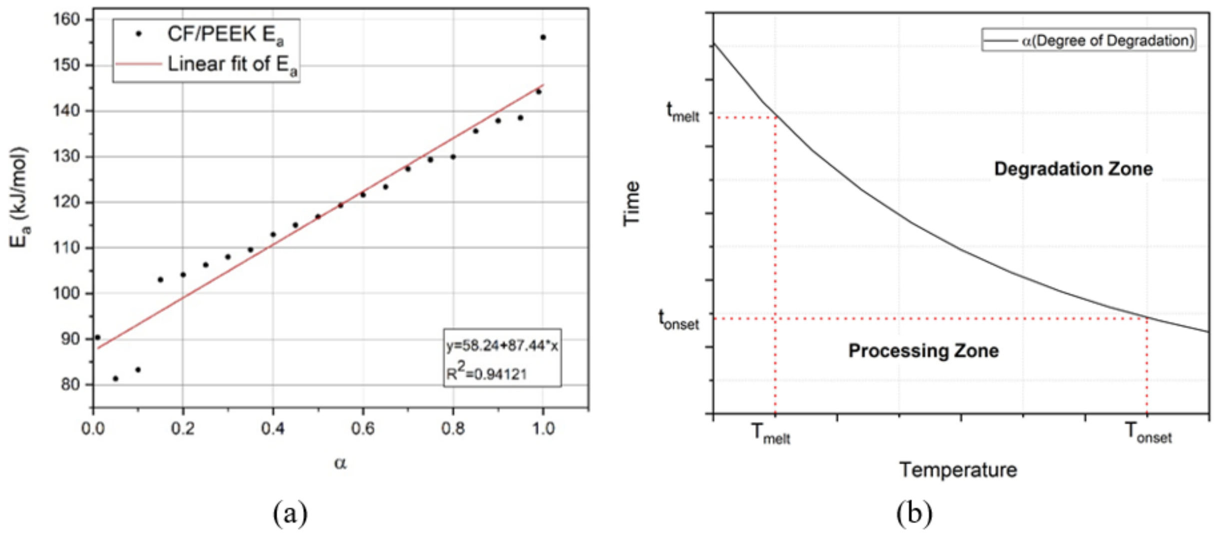


Figure 6: Thermal degradation kinetics analysis for CF/PEEK. (a) E_a *versus* α. (b) Thermal degradation limits plot (adapted from [31]**).**

3.4 Composite Layup and Processing

The consolidation of thermoplastic commingled composites requires high temperature and pressure. A metallic mold with an integrated heating system can be used to fabricate the composite material as shown in Figures 7 and 8.

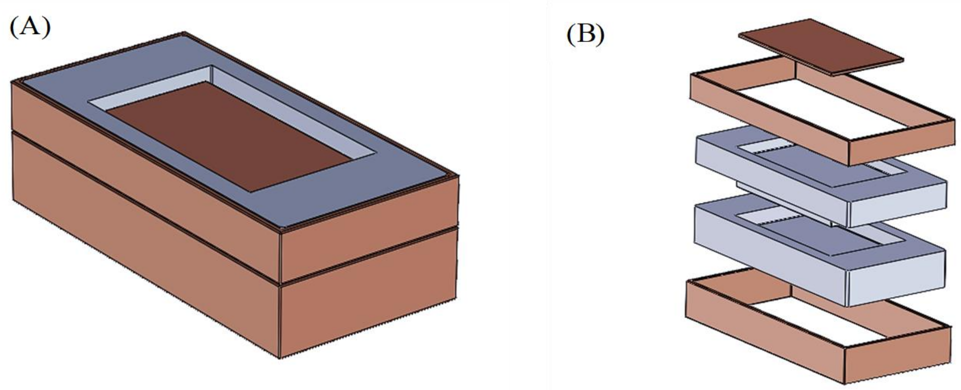


Figure 7: Heating system and metallic mold assembly developed to manufacture the thermoplastic commingled composites. (A) Metallic mold with heating system used to consolidate the materials. (B) Exploded view to show the assembly (adapted from [33]**).**

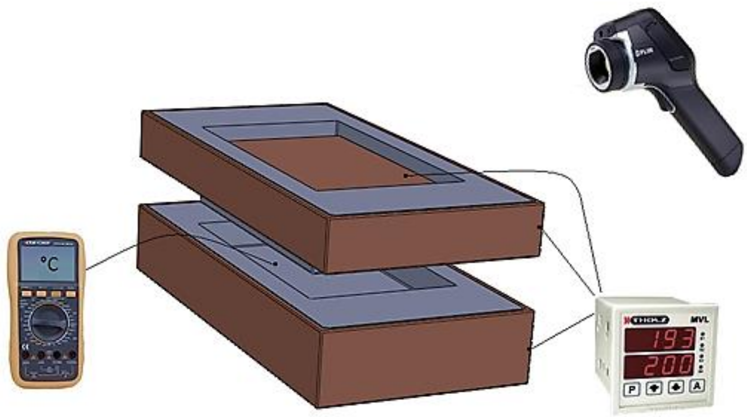


Figure 8: Integrated temperature control and monitoring systems during the thermoplastic composite consolidation.

Next, the thermal processing of the commingled composites was performed. Figure 9 shows the filament winding process and thermal consolidation using the metallic mold with the integrated heating system.

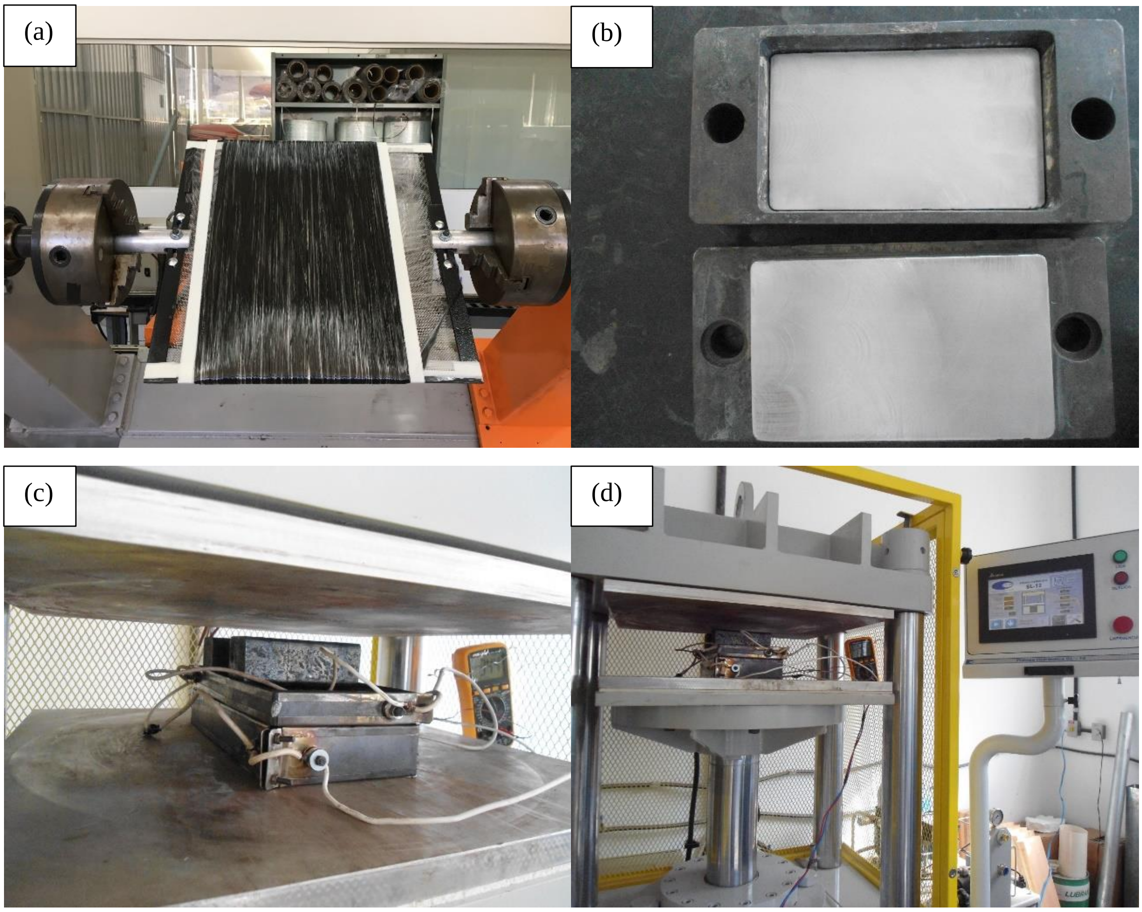
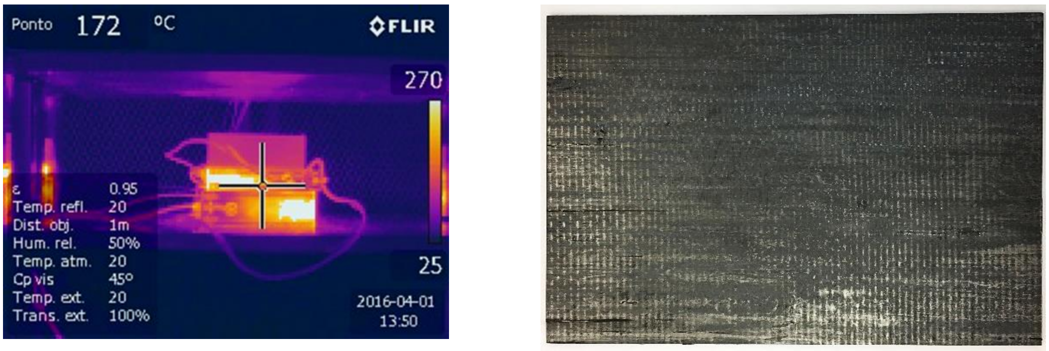


Figure 9: Thermal processing of thermoplastic commingled composites. (a) Filament winding to construct the laminate layers. (b) Metallic mold used to consolidate the composite. (c) Heating system assembly. (d) Hydraulic press used on the commingled composite consolidation (Adapted from [33]**).**

The manufacturing of thermoplastic materials requires a high level of heating control. Thus, the thermal inspection was conducted simultaneously with the consolidation as demonstrated in Figure 10 (a). A specimen of commingled composite with 10 layers (3mm thickness laminate) is shown in Figure 10 (b).

The optimization of the mechanical and thermomechanical properties of commingled thermoplastic composites depends on the appropriate processing cycle that reduces process time and cost, but also guarantees a high degree of crystallinity, mainly because it is associated with the cooling rate.



(a) (b)

Figure 10: Thermal monitoring during processing of thermoplastic commingled composites. (a) Thermal inspection. (b) 10 layers laminate manufactured.

3.5 Ultrasound Inspection

The ultrasound inspection assessed the quality of the composite by performing a surface scan. This technique ensures a precise quality inspection in which defects, voids, and delamination can be identified. Ultrasonography is also used to determine the minimum consolidation pressure, capable of eliminating all voids and air from the interior of the material, until the total consolidation of the composite has been concluded.

As an example, Figures 11 and 12 present an ultrasound scan using insufficient processing pressure. The presence of voids can be seen, indicating that the pressure used to fabricate the thermoplastic material was insufficient.

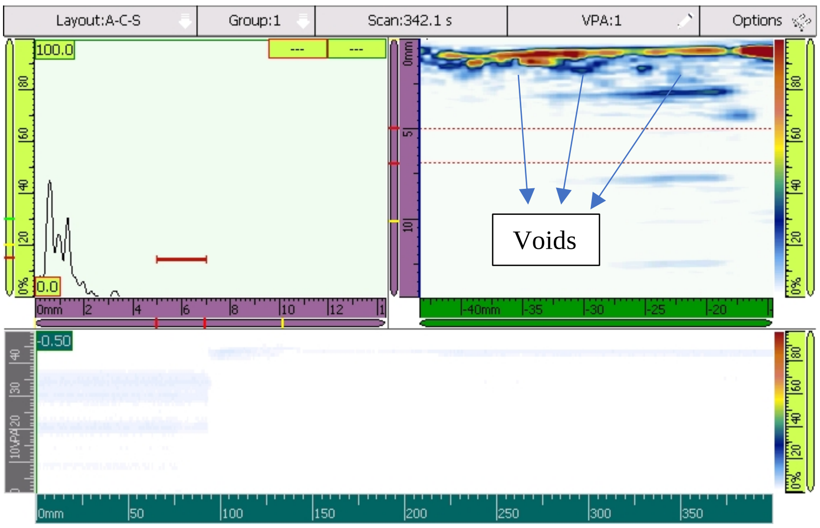


Figure 11: CF/PA ultrasound scan indicating voids in the laminate when insufficient pressure was used.

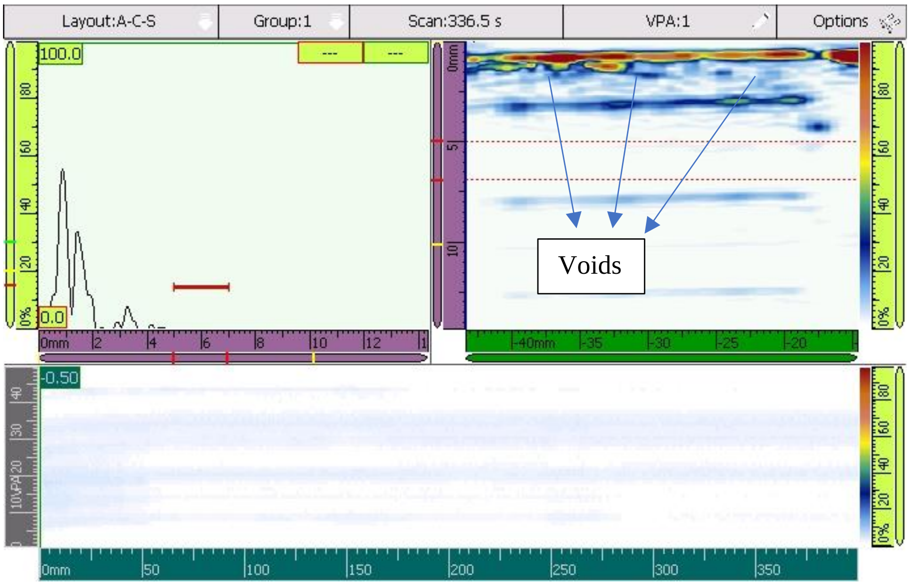


Figure 12: CF/PEEK ultrasound scan indicating voids when insufficient pressure was used.

The presence of voids inside the material represents a high risk of premature failure. This defect is therefore associated with insufficient pressure during consolidation. When the pressure is correctly adjusted to the material, the ultrasound inspection does not show the presence of voids. Figures 13 and 14 are ultrasound inspections with no defects detected in the laminate. It served to determine the pressure P=0.30 MPa that is needed to impregnate the reinforcing fibers by the molten polymer.

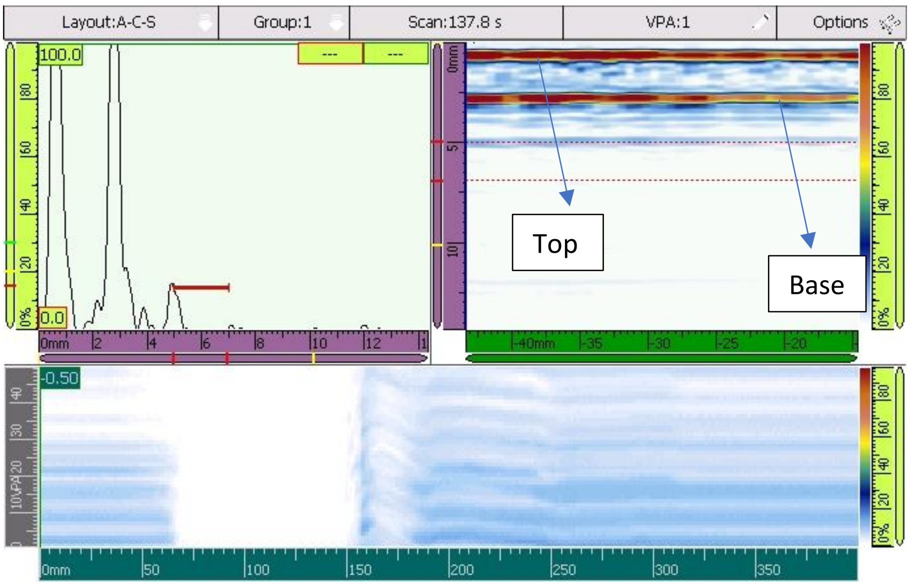


Figure 13: CF/PA ultrasound scan with no presence of defects when an appropriate pressure was used on fabrication.

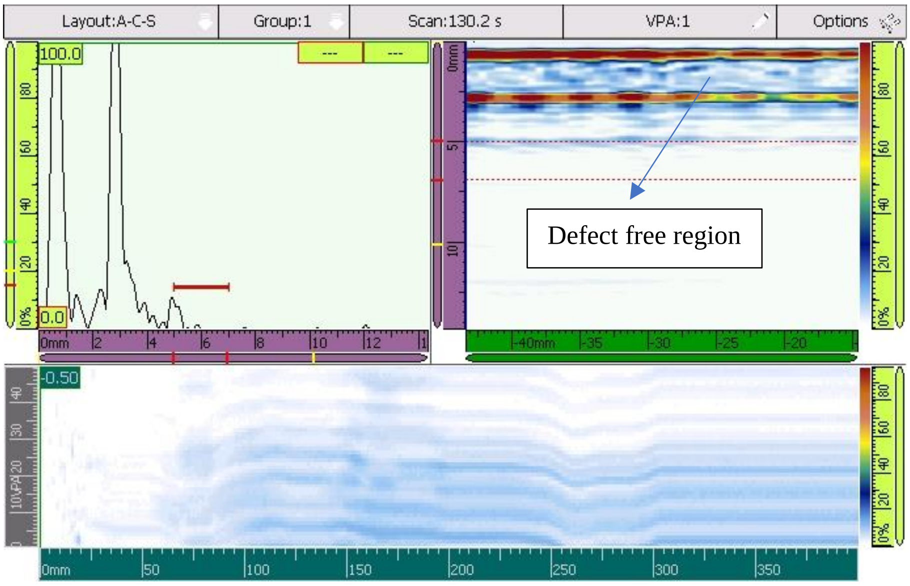


Figure 14: CF/PEEK ultrasound scan with no presence of defects when an appropriate pressure was used on fabrication.

3.6 Statistics and Modeling

3.6.1 Multiple regression and artificial neural network

A multiple regression model was developed to predict a specific property. The impact energy absorption (IEA) capability of thermoplastic commingled composites is an extremely important parameter to guarantee high-performance components. The regression model was obtained in a previous work of Di Benedetto et al. (2019) [34], and can be written as follows (Equation 9):

$$IEA = \beta_0 + \beta_1 \left(\frac{-E_a}{ln\left(\frac{\alpha}{A_\alpha} t\right)} \right) + \beta_2 \left(\frac{\nu D_p^2}{2KP} \right); \quad (9)$$

where β_0, β_1, and β_2 are the regression coefficients.

The regression model established a relationship between the degradation limits with the consolidation parameters. As a result, it predicts the IEA capability of commingled composites based on the matrix degradation, the matrix properties, thermal degradation kinetics, and the processing parameters.

Design of experiments (DOE) is a quality tool used to analyze the effect of the processing parameters, polymeric matrix properties, and the thermal degradation kinetics, on the IEA. The data acquisition obtained according to Equation 9 was used as input for the DOE analysis. A Pareto chart is used to evaluate the effect of each variable. The absolute values of the standardized effects are shown as a bar graph. Figure 15 is a Pareto chart of the IEA of thermoplastic commingled composite.

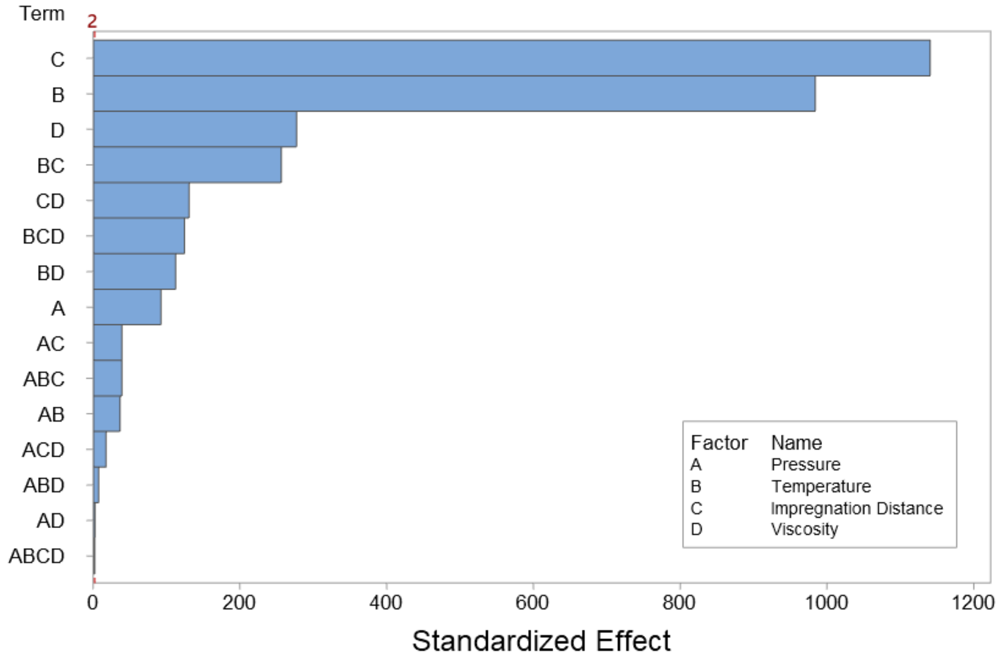


Figure 15: Pareto chart of the standardized effects on *IEA* revealing the level of the effects and its interaction (adapted from [31]).

The Pareto chart exhibits a reference line (t_{calc}=2) to indicate which effects are statistically significant. According to the results in Figure 15, the impregnation distance D_p and temperature T are the independent variables that have stronger effects over IEA. The matrix viscosity ν and the interaction between processing temperature T_p and impregnation distance D_p have similar effects on IEA. Lastly, the consolidation pressure P was the variable with less effect compared to the others. No significant effect on IEA was observed in the interaction between all these four parameters.

Another resource of DOE analysis is the surface response plot. This surface indicates how the behavior of the material changes as a function of temperature T_p, pressure P and impregnation distance D_p. The regression model was applied considering a reduction of the impregnation distance as demonstrated by the response surface in the Figure 16.

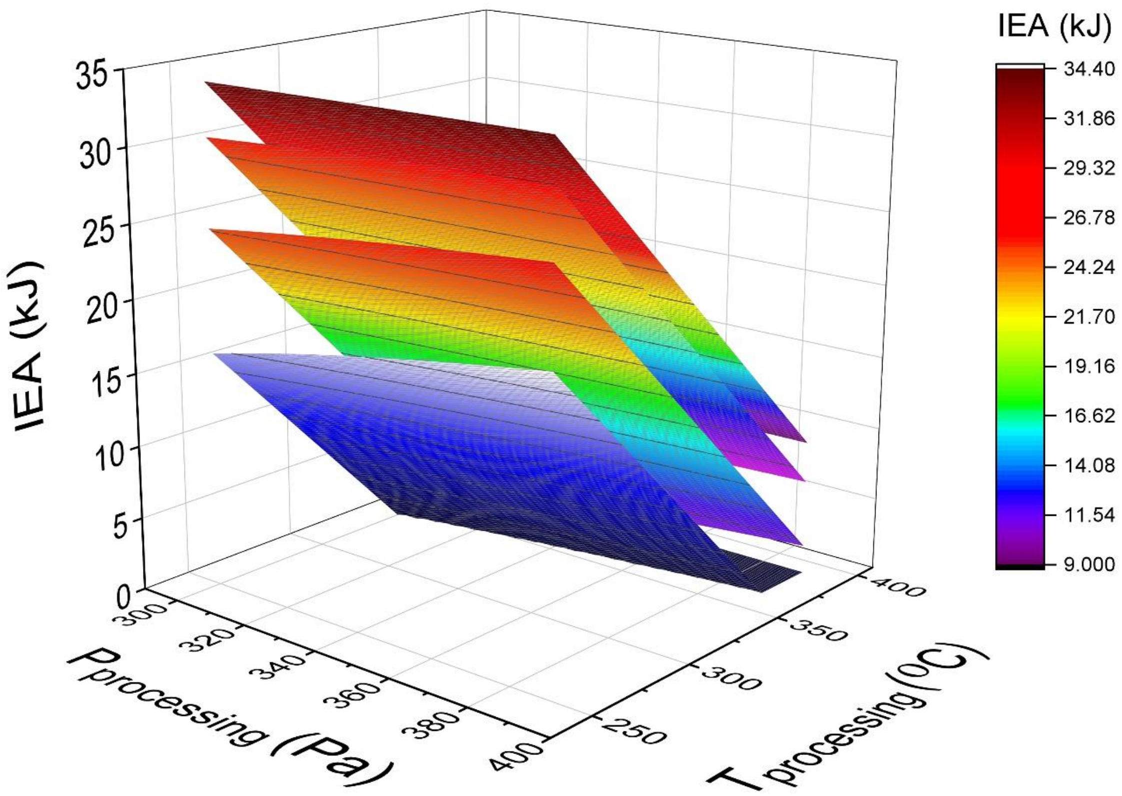
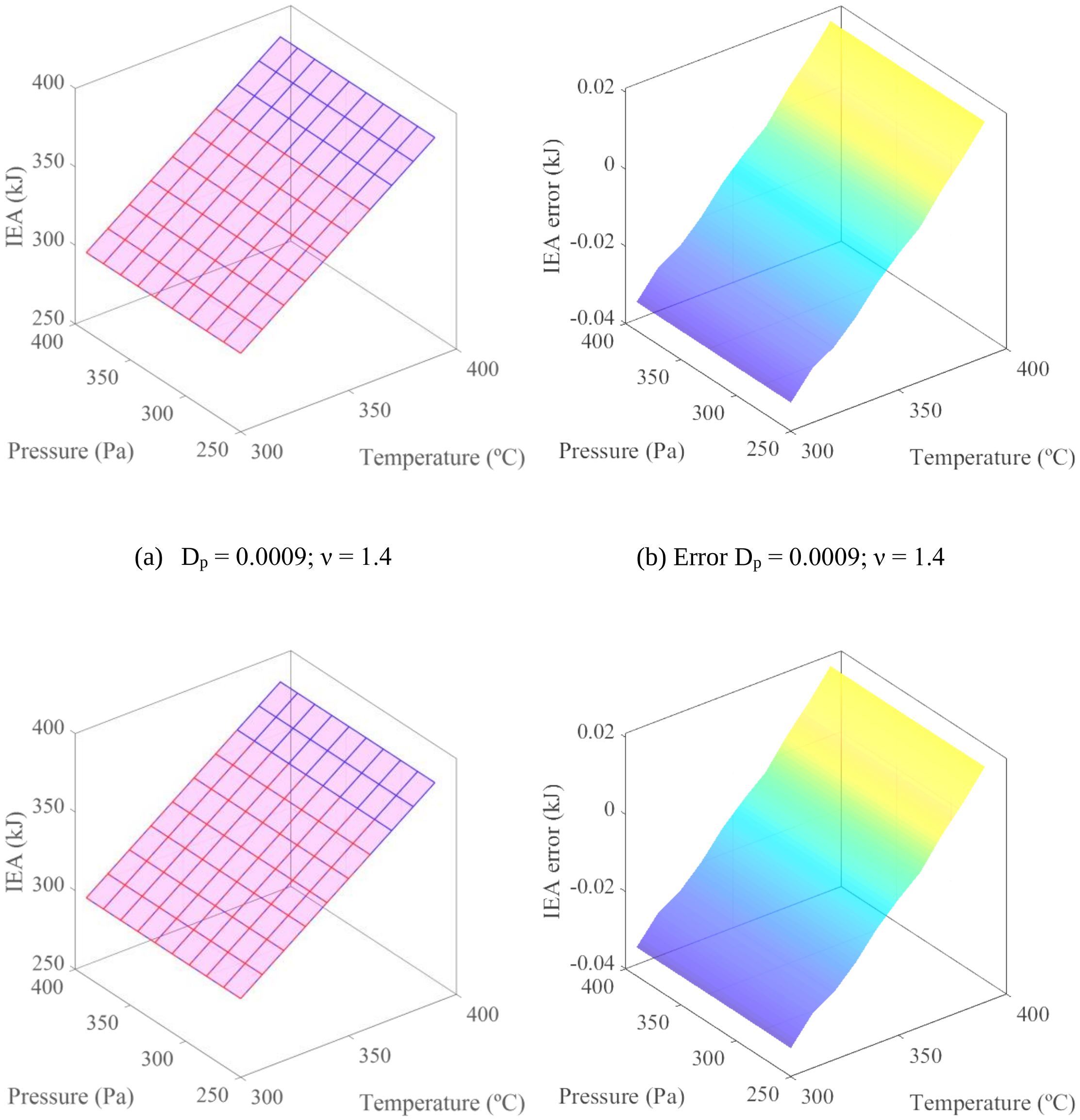


Figure 16: Representative 3D response surface considering the increase of impregnation distance D_p (adapted from [31]).

Technically, the surface response identifies the combination of input variable settings that optimize the IEA response. The optimization corresponds to the combination of P=390Pa, T_p=250°C, D_p=0.3mm, and ν=2000Pa.s, which provides the maximum IEA value (36.09 kJ), for example.

The artificial neural network developed by Di Benedetto, et. al (2021) [35] was applied to Carbon Fiber/PA6 and Carbon Fiber/PEEK specimens subjected to a low-velocity impact test (LVI). The goal was to collect data from Equation 9 for the training phase of a neural network. Temperature, pressure, impregnation distance, and viscosity were selected as input variables. The output of the neural network is then targeted focusing on the dynamic impact energy absorption property.

Figure 17 shows the graphical results of the IEA standard as a function of pressure and temperature for fixed values of impregnation and viscosity. Figures 17(a) and (c) show the overlapping experimental results and those obtained by ANN. It turns out that the planes are practically overlapping. Figures 17(b) and 17(d) show the error obtained, that is, the difference between trained (IEATR) and experimental (IEAEXP) data, i.e., IEAE-IEATR. The global difference for the known data from the neural network is of the order of 0.02 kJ (< 1%).



(a) $D_p = 0.0009$; $\nu = 1.4$ (b) Error $D_p = 0.0009$; $\nu = 1.4$

(c) $D_p = 0.0012$; $\nu = 1.4$ (d) Error $D_p = 0.0012$; $\nu = 1.4$

Figure 17: Graphical results of the IEA standard for trained data known (legend: — Experimental — ANN) (Adapted from [35]).

Figure 17 reveals an excellent agreement between the modeled and experimental data. Accurate results have been obtained in the testing and validation stages. Therefore, ANN has exceptional predictive abilities that can be used in the development of new thermoplastic composites with desired mechanical impact properties.

3.7 Initiating Molecular Dynamics to Thermoplastic Materials

The application of atomistic molecular dynamics techniques to high-performance polymers depends directly on knowing the conformation of the microstructure. The steric hindrance defines free axes of rotation of thermoplastic molecules. The challenge of realistically defining the position of atoms imposes specific boundary conditions that during the geometry optimization. Figure 18 is an example of a generic polymeric chain (n=16) and Figure 19 shows the result of the MD simulation.

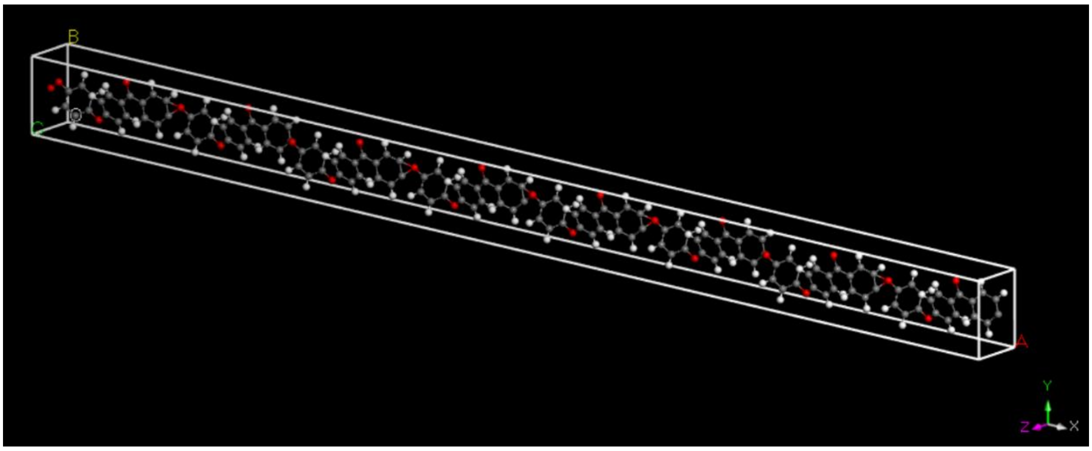


Figure 18: Molecule geometry optimized by MD simulation considering the effect of steric hindrance and distance between atoms.

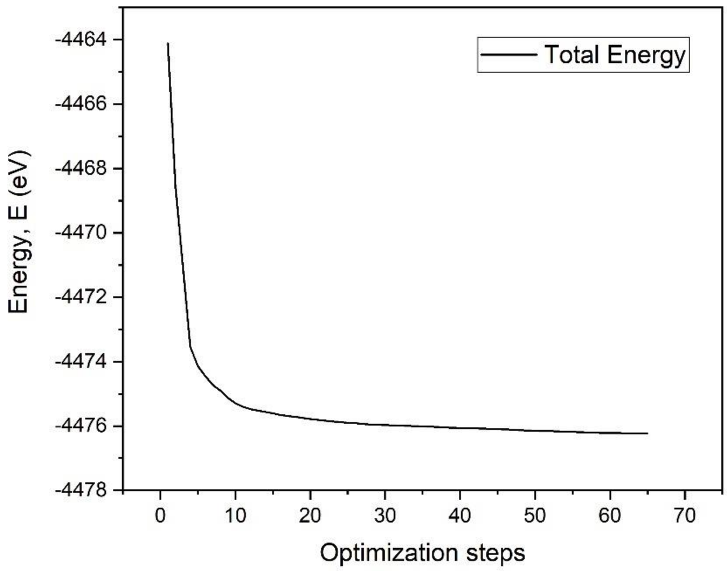


Figure 19: Number of optimization steps in the geometry simulation showing the minimum energy state.

From these results, calculation parameters are established to assemble polymeric macrostructures with better-defined positions in a 3D space. The combination of MD simulation and experimental practices is an innovative approach to high-performance structural composites. However, for the molecular dynamics technique to work as a sophisticated technique for characterizing thermoplastic polymers, more precise information on the atomistic structure of the composites is a necessary first step.

For this reason, new studies are being carried out to create parameters of molecular positioning in semi-crystalline structures. Therefore, studies are being carried out to create new parameters of molecular positioning in semi-crystalline structures. The goal is to (i) establish a conformation criterion for macromolecular polymers, (ii) identify, in each case, the most stable position of atoms in a polymeric structure through energy and force minimization, and (iii) compare potential energy results for each type of conformation.

4 Conclusion

This chapter addressed a design for characterizing composites. The research stages were described pointing out the most important scientific findings, including a recent review of thermoplastic commingled composites processing and properties.

The combination of Darcy's law and Friedman's isoconversional method proved to be a powerful tool to optimize the performance of thermoplastic composites and, thus, define specific parameters to perform thermal consolidation.

It was concluded that the ANN is an alternative to traditional methods to determine the processing parameters for the manufacturing of commingled composite. The use of an analytical multiple regression model as a new approach of ANN architecture was a promising approach which caused an increase of ANN's reliability to predict composite properties.

Developing a technique for characterizing high-performance polymeric materials by simulating molecular dynamics with empirical potentials is the main objective of our near-future research. New advances in the molecular dynamics of thermoplastic polymers have the potential to contribute to new techniques for characterizing composites, reducing operating costs, optimizing structures and materials, and determining their properties.

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