Experimental analysis and numerical optimization of a thermoplastic composite in crashworthiness

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Abstract. In this work, we present an experimental analysis and a numerical optimization study for the material parameter identification of an impact attenuator made of a brand new All-PP thermoplastic composite material subjected to an axial impact load. After an experimental characterization of the material, a Finite Element (FE) numerical model of the impact attenuator is created and simulated using the LS-DYNA explicit software. Subsequently, in order to capture the force-displacement trend of the crush experimental test, a fine-tuning of some relevant material parameters through surrogate-based optimization techniques is performed. The optimization process mainly consists of (1) defining a set of target points on the load-displacement curve where to evaluate the Mean Squared Error (MSE) between the numerical and the experimental values; (2) using a Design of Experiments technique to provide a sample set on which expensive deterministic simulations are performed; (3) constructing as many surrogate approximations as the number of target points in order to predict how the load values change over the parameters’ domain; (4) predicting an overall MSE surface that is optimized by means of a genetic algorithm in a sequential domain reduction iterative procedure. Results show a good agreement between the numerical and the experimental impact load and energy curves, and hence confirm that surrogate-based optimization is a valuable technique to refine the material parameters in the numerical simulation of composite structures.

1. Introduction

Over recent decades, passive safety is gaining more and more interest among scientists and engineers due to its high contribution to reducing the risk of serious injury and allowing drivers and passengers to ride out a crash. On the one hand, the increasing importance of vehicle safety has led to more strict legislative regulations requiring the introduction of more sophisticated protective systems. On the other hand, the environment and sustainability are becoming topics of major concern, leading to the necessity of vehicles getting more ecological by using less fuel. To couple both these requirements, the automotive industry has put much emphasis on the production of car body components in composite materials. Composite materials have received always more attention over conventional ones such as steel, because their light weight, high strength, corrosion resistance, and long life offer significant advantages [1]. In particular, composites have a greater capacity to absorb energy than metals, due to the different modes of failure that influence energy absorption. However, standard composite materials - mostly glass
and carbon fiber reinforced with thermosetting plastics - require expensive production processes and are not easy to dispose of at the end of their life cycle due to their thermosetting matrix. To overcome these shortcomings, thermoplastic composites represent a good solution. Indeed, they show many advantages like melt and fast processing, easy recycling and reuse in different applications contexts, greater toughness than thermosets, and resistance at high temperatures [2,3]. Despite the many advantages, one significant drawback is that thermoplastic resins (such as polyether ether ketone-PEEK and Polyetherimide-PEI) turn out to be significantly expensive. Besides the production itself, this represents a bottleneck in the experimental campaigns aimed to test the mechanical properties of structural components in thermoplastic material, which are gaining more and more interest in many end markets that are quite price sensitive, the automotive among the others. As a consequence, substantial effort has to be put into the project and design phase of the new products. This can be efficiently addressed thanks to the development of Computer-Aided Design (CAD) methods and the progress in numerical simulations with the Finite Element Method (FEM). Moreover, to identify the best trade-off between lightweight and good crash performance, numerical optimization is particularly useful [4–7]. Recent studies [8, 9] demonstrate that surrogate modeling techniques represent a valuable tool when dealing with structural optimization in crashworthiness. In fact, crash applications are characterized by severe numerical noise, discontinuities in the objective function to be optimized, and physical bifurcation in crash response, leading to a lack of gradient and sensitivity information. Therefore, gradient-based optimization algorithms are not useful in such applications. In crash optimization problems, an objective function evaluation requires to simulate a numerical model, which needs, in turn, significant computational time. Based on a certain number of finite element analyses, surrogate models allow for the construction of a computationally cheap-to-evaluate approximation of the considered expensive objective function [10]. In this way, the direct optimization of the real objective is replaced with the optimization of the approximating model. As a result, many more evaluations can be performed to capture the crash response and reach an optimal parameters configuration.

In this work, we present an experimental investigation and a numerical optimization study to identify relevant material parameters in the numerical model of an impact attenuator made of a brand new All-PP thermoplastic composite material [11] subjected to an axial crush load. In particular, the optimization study is conducted using the external software LS-OPT [12] and aims to calibrate some numerical and non-physical model’s material parameters in order to capture the global crush behavior of the impact attenuator during the experimental crush test. Firstly, the physical material parameters are identified through mechanical tests on standard specimens and the component itself [11,13,14]. Secondly, the FE numerical model of the impact attenuator is created and simulated through the LS-DYNA explicit software. Finally, some relevant parameters of the material card are tuned through surrogate-based optimization techniques to capture the force-displacement trend of the crush experimental test. Once the optimization strategy is performed, the numerical and experimental load and energy curves are compared, highlighting a good agreement and a visible improvement over the curve resulting from numerical simulations where the considered parameters are tuned by trial-and-error. Therefore, it can be stated that surrogate-based optimization represents a powerful tool for the identification of material parameters in the numerical modeling of mechanical components made of thermoplastic composite material. Moreover, due to their novelty, thermoplastic composite materials are still undergoing intense analysis studies. Thus, the outcome of this work represents a significant step in the numerical characterization of the investigated material, from which future research studies can also benefit.
2. Material

The impact attenuator under investigation is a crash absorber device, placed in the frontal part of a Formula SAE vehicle. As shown in Figure 1a, it has a truncated-cone shape, with a rectangular cross-section. The section width changes along the axis of the attenuator. The bottom section has a width of 265 mm and is supposed to be anchored with the vehicle frame. The upper section comes instead into contact with the crushing object and has a width of 225 mm. The thickness of the impact attenuator is not constant along the axis: the first part of the attenuator (red in Figure 1a) has a thickness of 1.68 mm, the central part (green) has a thickness of 2.16 mm, and the bottom part (blue) has a thickness of 2.4 mm. The increase in thickness along the axis of the component is a specific design criterion, since this characteristic guarantees a progressive energy absorption trend while the component is crushing. The impact attenuator is manufactured with an innovative thermoplastic composite material. This material, shown in Figure 1b, is fully made of polypropylene (PP) and it is known with the commercial name of PURE©. The PURE© sheets are made up of several stacked laminas. Each lamina is composed of balanced woven tapes. The tape has an A:B:A structure: the core (B) is PP homopolymer and the skins (A) are the PP copolymer. While the core presents highly oriented chains to enhance strength, the skins shape the matrix of the whole material and have a lower melting temperature than the core. This condition is necessary to process the tapes with co-extrusion. The tapes are then woven into balanced fabrics. The final composite sheets are obtained with a hot-compacting process. This thermoplastic composite material presents several advantages in terms of production process, sustainability, and impact response when compared to conventional thermosetting composite materials. Indeed, the PURE© material is fabricated with a large sealing window (130 – 180°) and requires a short cycle time at pressure. This makes the production process suitable for a mass market. Both the matrix and the reinforcement of the PURE© are composed of PP, making this composite material fully recyclable. Furthermore, unlike the common thermosetting composites, it shows a ductile and progressive crush response.

![Figure 1](image)

Figure 1: Characteristics of the analyzed impact attenuator: (a) geometry and (b) PURE© thermoplastic composite material.

3. Method

In this section, the material parameter identification methodology is presented. The LS-DYNA material library provides several material models that can reproduce the composite behavior, and, in the literature, many researchers used these models to simulate common thermosetting composite materials (e.g., [15, 16]). However, the failure mode of the PURE© thermoplastic is mainly dominated by plastic deformation and delamination. To globally capture this peculiar crush behavior, an optimization study for material parameter identification was performed. In
the first step, the material was characterized by standard experimental test. In a second stage, a crush test on the full component was executed. The experimental crush response was then compared with a numerical simulation, where the material model parameters were set according to the results from the standard tests. However, the statistical uncertainties and the necessity to tune non-physical parameters of the material card make a trial-and-error approach not accurate and time-demanding. Accordingly, a surrogate-based optimization was performed to fine-tune the most influencing material parameters, taking as reference the load-displacement trend of the experimental crush test.

3.1. Experimental tests

Standard tests on PURE c⃝ specimens were performed to evaluate the mechanical properties of the material. The standard tests consist of tension, compression, shear, and a three-point bending test, according to the ASTM standards D3039, D3410, D5379, D790. Afterward, the PURE c⃝ impact attenuator was experimentally tested. In this test, the component is crushed in a quasi-static condition using a Zwick Z100 electro-mechanical machine for a universal tension-compression test, where the crush load is applied along the axis of the attenuator. The bottom section of the component is placed on a planar plate, and a moving plate made of steel gets in contact with the upper face of the impact attenuator with a fixed motion rate of 0.5 mm/sec. Figure 2a shows the test configuration. From the image, some imperfections and undulations can be noted on the upper and bottom edges. In addition, the cutting process leads to the formation of splinters and debris, due to the detachment of the tapes from the woven fabrics.

3.2. Numerical model

A numerical model of the impact attenuator was created and simulated through the commercial finite element code LS-DYNA. As illustrated in Figure 2b, the component is modeled with square fully integrated shell elements of 2.5 mm of size. In order to define the thickness of the component, the keyword PART_COMPOSITE is used. This card allows for setting the correct orientation and ply-thickness of each stacked layer. A moving rigid-wall that gets in contact with the upper section is defined through the keyword RIGID_WALL_MOVING_FORCES. On the opposite edge of the model, a fixed rigid wall in contact with the bottom surface constrains the X-translation of the component. The AUTOMATIC_SINGLE_SURFACE keyword guarantees self contacts and correct interaction between the rigid-wall and the component. The material card MAT_54/55 is chosen to reproduce the mechanical characteristics of the PURE c⃝ material. The Chang Chang criterion is set as failure law. The characteristic loading curve of the element has an elastoplastic stress-strain relationship, and maximum strains can be set to define the failure of the integration point. Considering the compression case, the behavior of the element is dominated mainly by three parameters: the Young modulus in the fiber direction, the strain to failure, and the strength. The linear loading phase is defined according to the Young modulus in fiber direction Eaa and the longitudinal compressive strength Xc. This is the strength in the fiber direction. Once this value is reached, the linear hardening is followed by a plastic stage in which the load is constant, until the maximum compressive strain (DFAILC) is reached. At this point, the element fails. In crashworthiness simulation, a crush front reduction factor called SOFT can be set. This factor strongly influences the crush simulation result. It is a non-physical parameter that reduces the strength of the element row ahead of the crush front. When the rigid wall gets in contact with the first row of elements, there is a load increase followed by a sharp load drop due to the deletion of the element row. The SOFT parameter can be used to reduce these mathematical instabilities. The numerical model also presents a trigger in the upper section of the impact attenuator. The trigger is modeled with a row of reduced thickness elements (0.5mm), in order to simulate the imperfections and undulations of the impact attenuator edges.
3.3. Optimization strategy
In this work, an optimization strategy composed of several building blocks has been adopted. The external optimizer LS-OPT was used to carry out all the phases of the optimization procedure. First of all, as shown in Figure 3b, a set of 36 target points $F_i$, for $i = 1, \ldots, 36$, is chosen on the load-displacement curve resulting from the experimental tests in order to evaluate the Mean Squared Error (MSE), defined in Equation (1), between the numerical and the experimental values of the force at different displacements. Afterward, the Design of Experiments methodology [10] is used to sample the design space in order to describe the variation of the objective function based on the values of the design variables affecting the process. In particular, a Latin Hypercube sampling is chosen to locate a set of evenly distributed points over the prescribed domain and evaluate the objective function value corresponding to such configurations of parameters. Based on that, as many surrogate-approximations as the number of target points are constructed to predict the force value for every target displacement on the unsampled areas of the search domain. Here, the Kriging surrogate model is adopted due to its ability to estimate the potential error committed in the approximation. At each iteration of the optimization algorithm, the Kriging surrogate surfaces are refitted and the parameters characterizing the approximation are estimated. Subsequently, the MSE between the numerical and the experimental curve values computed on the 36 target points is evaluated at each point of the domain, leading to an overall MSE surface. At the end of each iteration, the minimum of such a surface is found through a Genetic Algorithm (GA). To reach the optimum, a sequential domain reduction procedure of four iterations is followed, as shown in Figure 3a. The optimization terminates with a verification simulation on the computed optimum.

3.3.1. Optimization problem When defining a numerical model, many material card parameters can be identified through preliminary experimental tests. However, the model is also characterized by non-physical parameters that are commonly chosen based on the engineer’s expertise. This trial-and-error methodology is usually very time-expensive, and an optimization study can help to define the most critical values of the numerical model. In particular, the optimization problem consists of minimizing the mean squared residual force, i.e., the difference in y-values between the experimental and numerical load-displacement curves, with the material...
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Figure 3: Optimization settings: (a) LS-OPT Graphical User Interface and (b) choice of the target points on the experimental curve.

parameters DFAILC and SOFT as the unknown optimization variables. It is stated as follows:

$$\min_x \quad \text{MSE} = \sum_{k=1}^{P} \left( \frac{f_k(df_{c1}, s1) - F_k}{M_k} \right)^2$$

subject to

$$-0.35 \leq df_{c1} \leq -0.15,$$

$$0 \leq s1 \leq 1.$$

(1)

where $P=36$ is the number of target points, $F_k$, $k = 1, \ldots, P$, are the values on the target curve $F$, and $f_k(df_{c1}, s1)$ the corresponding components on the computed curve $f$. $M_k$ is defined as the maximum targeted absolute value of the experimental load-displacement curve, i.e., $M_k = \max |F_k|$. The design variables are $df_{c1}$ and $s1$, which refer to the DFAILC and SOFT parameters, respectively.

3.3.2. Kriging model  Kriging is named after D. G. Krige, who first developed the method in 1951 [17]. The main idea is based on the concept that the DoE observed responses are viewed as a result of a stochastic process, even if they result from deterministic numerical simulations. This can be visualized through the following formula:

$$y(x) = f(x) + Z(x),$$

(2)

where $y(x)$ is the unknown function value at location $x$, $f(x)$ is the value of the approximating polynomial function, and $Z(x)$ is the stochastic component with mean 0 and covariance:

$$\text{Cov}[Z(x^i), Z(x^j)] = \sigma^2 R([R(x^i, x^j)]).$$

(3)

In Equation (3), $\sigma^2$ represents the variance of the samples and $R$ is the $n \times n$ correlation matrix between the random variables, where $n$ is the number of sample points. At position $(i, j)$, the matrix $R$ contains the correlation function between the data points $x^i$ and $x^j$. After an extensive analysis, Gaussian correlation functions were chosen in this work to construct the surrogate surface. These are defined as:

$$R(x^i, x^j) = \exp \left( -\sum_{k=1}^{L} \theta_k \left( x^i_k - x^j_k \right)^2 \right).$$

(4)
The Kriging response surface strongly depends on the choice of the appropriate correlation function, which characterizes the level of regression of the surrogate approximation. Gaussian correlation functions lead to a more regressive fitting of the data, which is a valuable feature when dealing with crash optimization problems, strongly characterized by noise. Moreover, such a choice allowed for avoiding a phenomenon that is typical of interpolating approximations, i.e., overfitting [18]. In Equation (4), the $\theta_k$, for $k = 1, \ldots, L$, represent the unknown parameters to be estimated. Such an aim is fulfilled by maximizing the likelihood function of the predicted data $y(x)$ [10]. The trend model has also a significant role since it represents the polynomial component of the surrogate approximation. Here, a quadratic trend model was chosen to have an accurate polynomial approximation even if requiring more DoE points than a constant or linear trend for the model construction. It needs $(n + 1)(n + 2)/2 + 1$ points, where $n$ is the number of variables of the optimization problem.

3.3.3. Genetic Algorithms At each iteration, the optimization of the surrogate approximation is solved by using a real-coded GA. A GA is a nature-inspired global population-based search algorithm that was first introduced by John Holland in 1960 [19]. Needing no gradient information to drive the search towards the optimum, it starts from a randomly initialized population of individuals - the parent population - and, after evaluating the population, it relies on the operators of mutation, crossover, and selection, which lead to the generation of the offspring population. After that, elitism is applied, i.e., the worst individuals in the child population are replaced by the best individuals from the parent population and a new population is available for the next generation of the algorithm. Such a scheme continues until a prescribed termination condition is met. In this study, the population consists of 100 individuals and the number of generations is limited to 250. The Tournament method is used as selection operator, where only 2 elite members pass to the next generation. For real crossover, the Simulated Binary Crossover (SBX) operator is used with a distribution index of 10 and crossover probability of 1.0. The mutation probability is instead 100, with a mutation probability set to 0.5.

4. Results and discussion

4.1. Experimental and numerical results

From the crush test on the impact attenuator, it can be observed that the failure mode is dominated by plastic deformation and the attenuator walls fold while crushing (Figure 4a). Due to its ductile behavior, the edges of the attenuator slid inward, causing the faces to bend and fold. The load-displacement curve of the experimental crush test on the impact attenuator is shown in Figure 5, denoted by a black-dashed line. Four peaks of force can be distinguished in the curve. These peaks are due to thickness discontinuity, as illustrated in Figure 2b, and layer compaction. The material did not splitter: the faces folded and compacted, causing a progressive increase of the load.

The numerical material model was set-up according to the outcome of the standard test.

![Figure 4: Crush behavior: (a) experimental test and (b)-(c) numerical simulation.](image)
experimental tests: the Young modulus, the ultimate strain, and the stress in tension and compression were computed experimentally and then used as input parameters. However, these parameters are affected by statistical uncertainties, and the SOFT non-physical factor cannot be experimentally evaluated. Accordingly, a trial-and-error process was necessary to fine-tune the material parameters. The red curve in Figure 5 shows the force-displacement trend of the numerical simulation. The curve represents quite accurately the experimental trend up to the peak corresponding to a displacement of about 30 mm, when the first thickness discontinuity occurs. After 30 mm, the global trend is well captured, even if some discrepancy can be observed in terms of force peaks and oscillations. Indeed, the faces of the experimental attenuator undergo to buckling and layer compaction (Figure 4a). Instead, the faces of the numerical model do not compact due to element failure and deletion (Figure 4b-4c).

4.2. Optimization results

The optimization strategy has been set according to a sequential domain reduction iterative procedure. It is composed of four iterations, each of which starting from a DoE sample set of 8 points that are located on the domain according to suitable schemes. In the first iteration, a D-optimal scheme, which favours the exploration of the boundaries of the domain, is adopted (Figure 6a). Afterward, a Latin Hypercube scheme allows for generating samples that are evenly distributed allover the search domain, as shown in Figures 6b-6d. The MSE response surface is fitted on the 8 points of the current iteration in order to obtain a locally accurate approximation by avoiding the phenomenon of overfitting. The parameters configurations defining the computed
optima found in the four iterations are in the order: \((dfc1, s1) = (-0.16, 0.18), (-0.17, 0.56), (-0.18, 0.38), \) and \((-0.18, 0.67)\). It can be noted that the DFAILC parameter, which can be roughly estimated based on the experimental tests, is only slightly modified throughout the optimization procedure and with respect to the value characterizing the baseline model: \((dfc1, s1) = (-0.18, 0.17)\). In contrast, the SOFT parameter undergoes deep changes and ends up reaching a much higher value than originally assumed.

In Figure 7, we compare the load-displacement (Figure 7a) and the absorbed energy (Figure 7b) curves extracted from the experimental tests to the ones resulting from the simulations that are set according to the results of the optimization procedure. Here, Computed Optimum refers to the combination of parameters that is found at the end of the sequential optimization strategy as the point that optimizes the MSE objective function, while the Best Computed is the parameters configuration that shows the lowest MSE among all the points that have been evaluated during the optimization procedure. It can be assessed that both the Computed Optimum and the Best Computed curves are able to capture the experimental behavior, except for the load-displacement curves on the \([0,10]\) displacement range, due to initial contact instabilities between the impacting rigid wall and the component in the numerical simulations. Therefore, a focused optimization study for improving the triggering phase is planned.

In order to assess the accuracy of the load-displacement numerical curves compared to the experimental one, three error measures have been evaluated: the Root Mean Squared Error (RMSE), the coefficient of determination \((R^2)\), and the maximal residual error \((\epsilon_{\text{max}})\). Good agreement is stated when the RMSE and the \(\epsilon_{\text{max}}\) measures present a small value, whereas the \(R^2\) should have a value close to the unit [12]. From Table 1, it can be observed that the baseline curve is less accurate of either the best computed or the computed optimum curves according to each error measure, proving an improvement due to the optimization methodology.

**Table 1:** Accuracy estimation of the load-displacement numerical curves. Bold style highlights the best results.

|             | RMSE  | \(R^2\) | \(\epsilon_{\text{max}}\) |
|-------------|-------|---------|---------------------------|
| Baseline    | 0.6385| 0.8910  | 1.704                     |
| Best Computed | **0.5335** | 0.6999 | **1.253**                     |
| Computed Optimum | 0.6072 | **0.9112** | 1.343                     |

Figure 7: Experimental and FEM optimized curves: (a) shows the load-displacement curves (b) illustrates the absorbed energy trends.
5. Conclusions
An experimental investigation and a numerical optimization study of an All-PP thermoplastic composite impact attenuator subjected to an axial impact load were carried out. The material parameters were identified through standard mechanical and full component crush tests. A FE crush simulation was then performed, and two material parameters have been detected to highly influence the simulation results. In the first stage, they were calibrated with a trial-and-error approach. Afterward, to increase the accuracy of the results, a surrogate-based optimization with sequential domain reduction was set-up to identify the suitable values of this couple of material parameters. The simulations on the optimized models are in a better agreement with the experimental results if compared to the one performed on the model defined using the trial-and-error approach. The improvement of the matching between the load-displacement curves was assessed by evaluating different well-known accuracy estimation indexes, which confirmed that surrogate-based optimization is a valuable methodology for material parameter identification. Most of all, the final estimates of the parameters allowed for obtaining a proper numerical characterization of the thermoplastic composite under investigation and, as such, they can be useful for future analyses involving this novel composite material.

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