Finite Element Thermal Modeling of Paperboard Formability Using Abaqus

Lappeenranta–Lahti University of Technology LUT

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ABSTRACT

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Keywords: Thermoforming, PETG-coated paperboard, finite element simulation, temperature-dependent deformation, thermal softening

Thermoformed polymer-coated paperboards are a promising solution for sustainable packaging applications. This study examines the influence of temperature on the thermoforming behavior of Polyethylene Terephthalate Glycol (PETG) coated paperboard sheets using finite element simulations in Abaqus/Standard. The composite shell model consisted of two layers: a paperboard substrate of 0.475 mm thickness and a PETG coating of 0.05 mm, modelled using composite shell elements. Composite shell models representing a substrate paperboard with PETG coating at 80 °C, 100 °C, 120 °C, and 140 °C were analyzed, while maintaining constant geometry, contact friction, and an applied pressure of 0.2 MPa. The results show that with the temperature increasing, the material stiffness and peak von Mises stress decrease gradually, and the formability increases. Within the studied ranges, a temperature of 120 °C was found to be optimal for forming, having the highest values of in-plane principal strain, highest plastic strain values, and maximum forming depth of 16.5 mm. In the comparison of the two material layers, the PETG coating exhibited consistently higher stress and plastic strain levels than the paperboard substrate. Increasing the temperature from 120 °C to 140 °C did not lead to further improvement in formability, indicating that the thermal softening effect saturates in this temperature range. The results across 80–140 °C reveal a clear trend of reducing stiffness and increasing formability, peaking at 120 °C, offering quantitative benchmarks for industrial process parameter selection and future coupled thermo-mechanical modelling.

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Robiul Hasan

Lappeenranta

SYMBOLS AND ABBREVIATIONS

Roman characters

E	Young's modulus	MPa
G	Shear modulus	MPa
P	Pressure	MPa
T	Temperature	ºC, K
t	Time	s
v	Poisson's ratio	
μ	Friction coefficient	

Abbreviations

MD	Machine Direction
CD	Cross Direction
ZD	Thickness Direction
LE	Logarithmic Strain (Max. In-Plane Principal)
PEEQ	Equivalent Plastic Strain
U2	Vertical displacement
ALLAE	Artificial Strain Energy
PETG	Polyethylene Terephthalate Glycol
ABAQUS	Finite element analysis software
FEM	Finite Element Method
SNEG	Negative surface (Abaqus)

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DECLARATIONS

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AI tool, ChatGPT was used to assist some minor language editing and clarity. All conceptualization, result interpretation, and writing were conducted solely by the author.

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1 Introduction

Thermoforming of polymer sheets is a deformation-based manufacturing process where the final shape is obtained through an interaction between various properties, geometries, and process parameters (Patil et al., 2019). Temperature is one of the most important parameters for such processes since it directly affects the stiffness and formability of the sheet being formed. Even small variations in temperature have a direct effect on stress distribution, deformation, and plasticity of thermoformed parts during the forming process of PETG-coated paperboard composite (Afshariantorghabeh, Kärki and Leminen, 2022). Such temperature differences can affect both the quality and depth of the part that is produced during the thermoforming process. Moreover, differences in temperature might cause defects like wrinkling, thinning, incomplete or irregular forming during the forming process of PETG-coated paperboard. The structure makes things more complicated since the paperboard and the PETG coating have different mechanical responses to temperature (Afshariantorghabeh et al., 2023). Therefore, a clear comprehension of how the mechanical properties change with respect to temperature is the main target of this research. This study aims to provide detailed information about the deformation behavior of thermoformed parts through controlled numerical studies within an exact temperature interval. Unlike general statements about temperature-dependent mechanical responses, a concrete answer to how temperature affects the forming process is the purpose of this work.

1.1 Background and Context

The thermoforming process refers to the manufacture of parts through heating, followed by deforming a sheet into a certain shape through pressure application onto a mold. During the thermoforming process, there are substantial amounts of deformation on the sheet, including stretch and bend deformation. This results in an extremely non-uniform mechanical response that is characterized by stress and strain localization within the deformed sheet. Temperature plays a critical role in the mechanical behavior of thermoplastics such as PETG during thermoforming (Ragoubi et al., 2024). The material gets less stiff as the temperature goes

up. At the same time, the material's resistance to stress is lowered, which changes how stresses are spread and how strains form during the forming process. In this sense, there is a link between deformation, outside forces, and the properties of materials that change with temperature. In industrial forming processes, this interaction is particularly important in areas where the shape of the material changes, like its edges and cavity (Ciganas et al., 2022). These zones handle the deformation pattern because they experience the most bending and tensile deformations. Therefore, it is essential to consider how temperature affects the movement of stresses and the growth of strains in these key areas. (Ragoubi et al., 2024)

1.2 Research Problem

It is clear how changes in temperature affect the process of thermoforming, but it is not clear how the mechanical behaviour changes under a certain set of conditions. In numerous experiments, various alterations in temperature were implemented to enhance the material's deformability; however, variations in stress, strain, and plastic deformations were not systematically examined across a controlled temperature range. Failure to systematically study this relationship limits the understanding of deformation mechanisms. In other words, lower stresses may indicate reduced resistance to deformation; however, excessively low stresses may also reflect insufficient structural integrity. Also, higher strains or plastic deformations could mean more flexibility, but they could also mean too much localization, which could cause some defects in the material. This is especially important for cases where the material behaves in ways that are not expected and are not linear. Hence, to ensure that the trends are valid and properly analyzed, it is necessary to conduct systematic comparisons under controlled settings.

1.3 Objective of the Study

The purpose of the present study is to examine the impact of temperature on the mechanical behaviour of PETG-coated paperboard when formed under thermoforming with similar forming conditions. The current study involves direct comparisons regarding various temperatures ranging from 80 °C to 140 °C so that the evolution of the deformation behaviour could be properly observed.

The research examines four important areas in relation to the mechanical behaviour of PETG-coated paperboard. Displacement behaviour is first analysed to evaluate the resulting shape and forming depth across different temperatures. Secondly, stress behaviour is examined in terms of variations in the load-bearing capacity and stress concentration regions. In addition, in-plane strain behaviour is also included to examine the development of deformation and local strain. Finally, the level of plastic deformation is considered as well.

It is not just about identifying the trends in mechanical behaviour but also about explaining why the deformation mechanisms shift from stiffness to plasticity.

1.4 Methodological Approach

The simulation is conducted using the finite element method utilizing Abaqus/Standard. In this case, the process of thermoforming will be modeled, keeping its parameters under controlled conditions. Shell elements are used for the composite sheet, which will be deformed by applying the necessary pressure load until acquiring the geometry of the predefined mold. Also, the interaction between the sheet and mold will be considered using a frictional contact.

To analyze the effect of temperature independently, all other parameters in the simulation should be kept the same. Geometry, constraints, loading conditions, and contact type will be set consistently throughout all the simulations. However, the material property will be changed according to different temperatures, applied through predefined fields.

The deformation of the sheet will be simulated using the static general step, depicting its behavior at the end of the process. After obtaining the result, several plots will be analyzed, including displacements, stresses, strains, and plastic deformations. For consistent analysis, scales on all the plots will be uniform among the different temperatures.

1.5 Scope and Limitations

The scope of this research is restricted to the purely mechanical properties of the PETG-coated paperboard undergoing thermoforming under certain temperatures. The temperature

change during the deformation process will be ignored to perform uncoupled modeling and to analyze deformation behavior under certain predefined temperature conditions only.

Furthermore, the material's response is not investigated, considering such factors as rate dependency or viscoelastic properties, which may significantly affect the deformation of material characteristics during processing. Also, thickness changes are not considered, as the main concern of the work is the material's response under certain temperatures in terms of stress and strain behaviour. Despite certain limitations, however, the proposed approach allows obtaining clear results regarding the influence of certain temperature conditions on deformation behaviour.

The study also does not account for moisture effects, which are known to influence the mechanical response of paperboard significantly. Since both temperature and moisture affect fibre bonding simultaneously in real processing conditions, isolating temperature as the sole variable provides a controlled basis for comparison but does not fully represent industrial thermoforming environments. Additionally, the contact model used assumes a constant friction coefficient throughout the simulation, whereas in practice, friction may vary with temperature and contact pressure. Finally, the results are based on a single geometry and a fixed pressure of 0.2 MPa, meaning that the findings cannot be directly generalized to other mold geometries or loading conditions without further investigation.

2 Literature Review

Thermoforming consists of highly complicated interactions of material behavior depending on temperature, deformation mechanics, and contact conditions. Material mechanical behavior at the stage of sheet forming depends on the development of stress, strain, and plastic deformation states, significantly affected by temperature.

The chapter highlights the important issues concerning material behavior and modeling of this process that should be considered in connection with thermoforming technologies. Temperature effects on deformation behavior, heat transfer analysis, and finite element modeling of forming processes are discussed. Despite the large number of research papers related to the forming process with paperboard and other fiber-based materials, principles of thermo-mechanics are applicable also to plastic sheet forming.

The main purpose of the present review is the establishment of the theoretical background required to develop thermo-mechanically based modeling of the process studied in this thesis.

2.1 Paperboard Material Properties

Paperboard is a composite material of fibrous origin having a complicated structure and behaviour, which depends on the hierarchical structure of the material, its anisotropic fibre arrangement, and multi-layered structure. Unlike traditional materials, the mechanical properties of paperboard are very sensitive to the environment; therefore, its proper characterization is crucial for forming and modelling. Anisotropy and nonlinearity of paperboard have been extensively discussed in the literature both experimentally and computationally; however, there exists no consensus about its behaviour under various conditions in machine direction (MD), cross direction (CD), and thickness direction (ZD). (Alajami, Li and Simon, 2018)

2.1.1 Composition and Structure

Paperboard consists of cellulose fibres, hemicellulose, and lignin to form a fibre matrix with a porous structure. It is manufactured through fibre suspension, fibre deposition, compression, and drying processes. In this case, hydrogen bonds form between the fibres, such that no adhesion is required to hold them together. This process forms a heterogeneous microstructure, in which fibres align in the machine direction. (Hirn and Schennach, 2015; Parsa Sadr, Bosco and Suiker, 2022)

In terms of the microscopic scale, a single fibre has a structure of layers in its cell walls and achieves its rigidity from cellulose microfibrils. These fibres can interact using means of mechanical interlocking and hydrogen bonding. Such a structure acts like a network, and the behaviour of such a system depends upon the orientation of fibres, density of fibres, and their bonding. Such complexity could not be modelled using all scales at the same time. (Simon, 2021)

However, in the actual world, paperboard will usually be made up of more than one layer with varying degrees of fibres and density. For instance, there may be some dense outer surfaces compared to inner ones, which are thick but soft. Moreover, the areas where layers meet are always mechanically weak, hence can easily peel off due to delamination under load. Also, materials such as polyethylene and PET are used on the paperboard to increase its barriers. (Nygårds, 2022)

2.1.2 Anisotropy and Directional Behaviour

The anisotropic behaviour of paperboard is one of the key features of the material. Because of fibre orientation, there will be great differences between the mechanical properties along MD, CD, and ZD directions. Studies have demonstrated that stiffness of paperboard along the MD axis may be much larger compared to the stiffness in the CD, while stiffness along ZD is relatively low because of poor fibre interaction (Alajami, Li and Simon, 2018). Such an anisotropic behaviour impacts deformation. Along MD, stretching occurs, thus leading to relatively high stiffness, whereas deformations along CD are related to the fibre rotation and bond deformation, which causes extensibility but limits the strength of the material (Labossikre and Neale, 1991). The paperboard displays strong anisotropy, with high

nonlinearity even at low deformation levels. The stress-strain behavior is not only orientation-dependent but also depends on structural heterogeneity and fiber orientation heterogeneity (Hagman, 2016). This makes it essential to incorporate orthotropic material models in numerical simulations to accurately represent directional behaviour.

To capture the plastic response associated with this directionality, an appropriate anisotropic yield criterion must be used. The Hill yield criterion (introduced by Rodney Hill (1948)) is one of the most established yield criteria to describe anisotropic plastic deformations and is formulated as a direct extension of the von Mises yield criterion in quadratic form. The criterion introduces six independent material constants (F, G, H, L, M, N), which must be calibrated experimentally, each of which is representative of the directional yield stress characteristics of the material, thus making it particularly well-suited to orthotropic fibrous materials such as paperboard for which the principal material axes (MD, CD, ZD) are clearly defined. The Hill (1948) criterion has been one of the most used models to describe the plastic behavior of sheet-like materials in analytical and numerical simulations of forming processes. (Chen, Wen and Cui, 2013)

The Hill criterion has been demonstrated to match well with bi-axial tension experiments on fibre network materials in the context of paperboard modelling, where the asymmetric tension-compression response is not of primary interest, indicating its usefulness in capturing in-plane anisotropic plastic behaviour. However, the Hill criterion has major limitations for paperboard applications. The main limitation of the Hill plasticity model is that it considers only the symmetric behaviour in tension and compression, which is not suitable to describe the through-thickness response of paperboard, where the compressive strength is much greater than the tensile strength. Furthermore, the significant disparity between the out-of-plane and in-plane strength could result in a severely distorted form of the yield surface, leading to computational difficulties. These limitations motivate the development of more sophisticated constitutive frameworks specifically for fibrous materials. Therefore, a three-dimensional anisotropic constitutive model directly constructed from the measured yield strengths in different loading directions, capable of describing the highly anisotropic elastic-plastic behavior of paper and paperboard. Further developments and extensions have improved the model by reducing the required number of material parameters and including out-of-plane plastic response, extending the applicability of the model to packaging forming operations (Eberle and Moll, 2021). In the thickness direction,

the fibre network will densify under compressive loads by pore collapse and compaction of fibres. This will induce nonlinear stiffening and non-recoverable strains. This is particularly important in forming operations where out-of-plane deformation is critical.

2.1.3 Elastic–Plastic Response

Paperboard material behaves non-linearly as it possesses elastic-plastic properties due to the interactions of fibres and bonding mechanisms in the material. The initial behaviour of paperboard is elastic and depends on the stretching of bonds and the flexural behaviour of fibres. Beyond the elastic limit, the material deforms plastically depending on fibre sliding, breaking of bonds, and reorientation.

The plasticity of paperboard is dictated by the fibre structure. Research work has proved that elastic behaviour may be modelled by means of anisotropic constitutive models (Qiu and Lin, 1999). Additionally, continuum models separating in-plane and out-of-plane behaviour have been developed to capture different deformation mechanisms in different directions.

2.1.4 Through-Thickness Characteristics

The thickness (ZD) behavior of paperboard is considerably lower compared to its in-plane response, due to the characteristics of inter-fiber bonding. Under mechanical loading, especially bending and shear, the material is prone to delamination, where layers separate along weak interfaces. Delamination is one of the key modes of failure in formability processes and has been widely investigated from a modelling perspective for composites. Delamination has been simulated through continuum approaches coupled with interface models, which permit delamination between layers when subjected to various loads. The multi-layered nature of paperboard further assists in this behavior as stresses are concentrated at interfaces between layers due to different densities and rigidities of each layer. The importance of this concept comes into play particularly during thermoforming, as both stretching and bending take place.

Thermal conduction in ZD ($\approx 0.1–0.2$ W m^{-1} K^{-1}) is also far lower than in-plane ($\approx 0.3–0.4$ W m^{-1} K^{-1}) (Marin and Nygårds, 2020). The delay in internal heating causes steep gradients

during thermoforming, which makes it even more important to accurately characterize the thickness of the material.

2.1.5 Influence of Environmental Conditions

Paperboard's mechanical behaviour depends on the environment, specifically humidity and temperature. Increased moisture absorption results in a weakening of hydrogen bonds between fibres, which causes a great loss in rigidity and strength. The effect of humidity has been demonstrated by experimental research that showed elastic modulus reduction by 20% to 53% (Fadiji et al., 2017) . Temperature also influences the ability of the network to move around. With higher temperatures, there is a weakening of the bonds between fibres; hence, there is increased flexibility of the material. It is important to note that when both moisture and temperature act on materials, the result may be more complicated. (Linvill and Östlund, 2014)

The impact of the environment adds another layer of variation in the characteristics of materials, thereby making it difficult to formulate reliable parameters for modelling purposes. In most cases, a controlled approach is used to examine specific impacts, like temperature, as in this case. (Robertsson et al., 2018)

2.1.6 Structural Inhomogeneity and Local Deformation Behaviour

The paperboard material is heterogeneous by nature owing to varying fibre arrangement, bonding, and density. In turn, such heterogeneity creates the possibility of deformation behavior at specific locations within the material, where both strain and stresses are unevenly distributed. Strain localization may occur owing to microstructural heterogeneity (Baum, 1993). Localized effects are especially relevant in forming processes, as they result in the formation of wrinkles or other types of failures.

Structural heterogeneity adds complexity to numerical modelling, which would necessitate an explicit microstructure-based model or efficient continuum models. Continuum models have been widely used in macroscopic problems, and inhomogeneity is considered through material properties. (Hagman, 2016)

2.2 Thermal behaviour of Paperboard

Paperboard is highly affected by the effect of temperature on its mechanical behaviour as well as the process of heat conduction. Paperboard does not have the ability to melt like the thermoplastics but rather exhibits behaviour of gradual softening because of fibre rearrangement and fibre bonding. It thus displays a gradual transformation of its mechanical properties without exhibiting a distinct change of state.

2.2.1 Mechanisms of Thermal Softening

When hydrogen bonds between cellulose fibres break down, paperboard becomes soft. When the temperature rises, the molecules stimulate, which weakens the bonds between them. This lets the fibres move against each other. This makes paperboard less stiff and more flexible when it is under less stress. Thermal and moisture effects are typically analyzed concurrently, as both affect the bonding characteristics of cellulose fibres. When both thermal and moisture effects are considered, paperboard becomes much less stiff and much more flexible. (Linvill and Östlund, 2014)

According to experiments, increasing the temperature reduces the stresses involved during the formation process while increasing the strain capability of the material. Peak stresses are found to decrease by more than 50% as temperatures rise (Tanninen et al., 2018). The behavior is important for the process of formation because it affects how well it can change shape without breaking.

At higher temperatures, the behavior also changes from being controlled by bonds to being controlled by the network. It lets the fiber network change when it is loading, which makes it easier to shape, but it also makes it more likely to become unstable.

2.2.2 Influence of Temperature on Mechanical Response

Temperature significantly affects the mechanical properties of paperboard concerning stress and strain. Paperboard is very stiff at low temperatures and does not stretch much, which makes it brittle. As the temperature rises, stiffness decreases and strain ability increases,

which is what paperboard shows. Moreover, the strength of bonds between fibres diminishes and movement within them increases; such trends become pronounced. (Afshariantorghabeh, Kärki and Leminen, 2022)

Research indicates that at temperatures exceeding 90 °C, fiber networks start to deform more readily without fracturing, signifying a shift from bond-controlled behavior to network-controlled deformation (Under and Lofqvist, 2012). Still, better formability comes at the cost of lower strength. This is a compromise between the two properties, which limits the range of temperatures in which formability can be achieved. The material should be sufficiently softened to allow deformation but not so hot that it loses structural stability or is excessively thinned or damaged.

2.2.3 Through-Thickness Temperature Gradients

These kinds of gradients cause stress to build up and change the way they deform, which can lead to problems like wrinkles, delamination, and inconsistent deformations. When one side is heated, the temperature difference in the thickness can be more than 40 °C (Tanninen et al., 2014). These gradients cause the softening to happen unevenly, with the surface layers becoming more flexible and the core staying stiff, which causes internal stresses even before deformation begins.

2.2.4 Heat-Transfer Mechanisms and Anisotropy

The main way that heat moves through paperboard is through conduction in the fiber matrix. Along with conduction at high temperatures, convection and radiation can also happen. Because it is an anisotropic material, the paperboard has anisotropic thermal conductivity. The thermal conductivity in the plane is higher than the thermal conductivity in the thickness. The plane of the sheet has a thermal conductivity of 0.3 to 0.4 W m^{-1} K^{-1}, and the thickness direction has about half of this value (Marin and Nygårds, 2020). This anisotropy helps the material heat up by creating temperature differences. The surface layer also affects how heat moves. Using a polymer coating makes the surface layer better at conducting heat, but it can also trap air between the two surfaces (Franke et al., 2021). Thus, both material and surface effects control how heat moves overall. For computational analysis, such phenomena are

typically represented using effective thermal material properties. This study employed temperature dependent material properties to model the influence of thermal behavior on mechanical performance.

2.2.5 Contact Conditions and Pressure Effects

The way the sheet and forming tool interact has a big effect on how heat moves during the forming operation. High pressure makes it easier for heat to move from the tool to the part by closing the air gap. Too much pressure will make the fiber denser, which will change how well it conducts heat. Because of this, the paperboard will not soften evenly, which will cause it to change shape and break, changing its properties. The Abaqus analysis in this case makes the interactions between the paperboard and the forming tool by having them interact with each other through friction. But this modeling process does not include the transfer of heat. Instead, the properties of contact have a big effect on deformation and stresses that happen at certain temperatures. (Mergel, Scheibert and Sauer, 2020)

2.2.6 Coupled Thermal–Mechanical Effects

The thermoforming process demonstrates a significant interconnection between thermal and mechanical components. This indicates that temperature influences material stiffness and deformation behaviour, while deformation in turn affects contact conditions and local density, which govern heat transfer. A full coupled thermo-mechanical analysis solves both heat transfer and deformation at the same time. This gives very accurate predictions; however, such models are computationally expensive and complex to implement. (Kartovaara et al., 1985)

Another way is to use the temperature's effect on how materials behave by making it a predefined field in the mechanical model. This way, the effects of temperature can be considered without implementing a complete thermal analysis. (Safwa, Yeddu and Leminen, 2024)

For this thesis, temperature will be analyzed by a specified temperature field within Abaqus. By changing the temperature while keeping the other variables the same, different

temperatures can be simulated. This makes it possible to study thermo-mechanical behavior effectively in a controlled simulation setting.

2.2.7 Residual Stresses and Recovery

After the paperboard is formed, it cools down, which changes the temperature and makes the paperboard shrink in an uneven way. The outer layers cool and harden faster than the inner layers, which puts stress on the material. These kinds of stress are known to change the shape of the paperboard. This is especially true when the process is done at high temperatures. (Wallmeier, Hauptmann and Majschak, 2016)

However, keeping the pressure on even during the cooling stage could help reduce these effects by making sure the shape stays the same. This, on the other hand, takes a lot of time and may not be possible in most manufacturing settings. (Crespo, Juan and Amigo, 2012)

For this thesis, the simulations do not consider either cooling or residual stresses. Still, it can be seen how they affect things indirectly by looking at the changes that happen because of the simulation results. Residual stresses are not considered because the deformation processes being examined are contingent upon the material's temperature.

2.2.8 Thermal Degradation Limits

At sufficiently high temperatures, paperboard undergoes thermal degradation, which leads to irreversible changes in material properties. Cellulose fibres begin to degrade through oxidation and thermal decomposition, resulting in reduced mechanical strength, embrittlement, and visible discoloration. (Tanninen et al., 2018)

Studies on thermal ageing have shown that prolonged exposure to elevated temperatures significantly weakens the material and reduces its mechanical performance (Lessard et al., 1996). This imposes an upper limit on the temperature range used in forming processes.

However, the effects of thermal degradation are not studied explicitly in the present study. The simulations are carried out in the temperature range of application (80-140 °C), where temperature-dependent material properties are used to model the softening behaviour of the

material. In this range the temperature effect is mainly visible as a reduced stiffness, lower stresses and increased deformation.

2.3 Simulation Approaches Using Finite Element Modelling (FEM)

Thermoforming paperboard requires a lot of different things to happen at the same time, including thermal, mechanical, and contact effects. Thermoforming paperboard is different from thermoplastics because it doesn't melt and flow. Instead, it involves reorienting fibres and mechanics between layers. Because of this, the process of thermoforming paperboard is much more difficult than the process of forming thermoplastic sheets, and more research is needed. Thermoforming studies can be hard to do in the lab, but finite element method analysis can help us understand what's going on better. Finite element modelling enables the integration of anisotropy and temperature dependence of materials within their constitutive laws to forecast forming behaviour.

2.3.1 Development of Paperboard Forming Models

In early studies of paperboard formation using FEM, relatively simple isotropic elasticity-plasticity formulations were adopted. Although these formulations sufficed for small deformation analysis, their inadequacies included ignoring behaviors like anisotropy, wrinkling, and thermality. (Nygårds, Just and Tryding, 2009; Wallmeier et al., 2015)

More advanced models used orthotropic material descriptions to show how paperboard behaves in different directions. An example is an orthotropic elastic-plastic model in Abaqus, showing that temperature reduces stress concentrations and improves drawability. This marked a shift toward more realistic modeling of forming processes. (Hauptmann and Majschak, 2011)

Further developments included multilayer modeling approaches. Models with multiple plies and cohesive interfaces to simulate delamination between layers. These approaches improved the representation of the layered structure of paperboard and enabled better prediction of failure mechanisms. (Huang and Nygårds, 2012)

These studies demonstrate that accurate modeling of paperboard requires consideration of anisotropy, multilayer structure, and temperature-dependent behaviour.

2.3.2 Coupled Thermal–Mechanical Simulations

Since paperboard properties change significantly with temperature, accurate simulation requires consideration of both thermal and mechanical effects. Fully coupled thermo-mechanical simulations solve heat transfer and deformation simultaneously, providing detailed predictions of forming behaviour.

A coupled modelling approach that incorporates anisotropic thermal conductivity together with temperature-dependent mechanical properties has been shown to significantly improve the representation of thermoforming behaviour. The findings indicate that neglecting thermal coupling can result in an overestimation of material stiffness and an underprediction of deformation. (Marin and Nygårds, 2020)

Further improvements in simulation accuracy have been achieved through the implementation of user-defined subroutines that dynamically update material properties and heat-transfer behaviour during deformation. These approaches highlight that coupling between heat transfer and mechanical response is essential for realistic prediction of forming behaviour (Domaneschi et al., 2017). However, fully coupled simulations are computationally expensive and require extensive material data, which limits their practical use.

2.3.3 Role of Process Parameters

Temperature, pressure, and forming rate can all influence thermoforming behavior. However, in this study, pressure and other process conditions are kept constant, allowing the effect of temperature on material stiffness, stress distribution, and plastic deformation to be investigated separately. The force pushes the material against the mold and makes sure it sticks to the surface properly. High pressure makes things flexible and makes materials denser (Awais et al., 2018). The thermoforming process also depends on the friction between the paperboard and the die. It changes how materials flow, how stresses are spread out, and how heat moves. Experiments and simulations have demonstrated that an accurate

characterization of friction is essential (Huang and Nygårds, 2012). Moreover, variations in the process itself, like heat sealing and tray forming, make things even more complicated. This is because heat sealing and tray forming both put stress on the material in both thermal and mechanical ways. (Niini et al., 2021)

2.3.4 Modelling of Contact and Friction

Contact interaction between the paperboard and the forming tool is a critical aspect of thermoforming simulations. Accurate representation of contact conditions is essential for predicting deformation behaviour, stress distribution, and heat transfer.

Friction plays a significant role in controlling material flow during forming. High friction may limit material movement, causing stress concentrations and problems, whereas low friction may result in improper deformation control. Simulations have revealed the importance of precisely setting friction coefficients to accurately simulate real processes. (Huang and Nygårds, 2012)

In contact modelling, surface-to-surface interactions are used to simulate sliding, adhering, and detaching by applying normal contact stress and friction. This kind of behaviour is needed to show how the sheet and mold work together.(Afshariantorghabeh, Kärki and Leminen, 2022).

2.3.5 Challenges in Modelling Paperboard Forming

Even though numerical modelling has come a long way, it's still hard to model paperboard thermoforming accurately. The problem arises from the complex interplay of material behavior, heat transfer, and contact mechanics. The first challenge is modeling the anisotropic and nonlinear behavior of materials. Simulating paperboard is challenging because it behaves differently in different directions, and its uneven structure makes accurate modelling more challenging.(Safwa, 2024)

Another problem is the interactions between heat and mechanics. Fully coupled analyses yield more accurate results; however, they are computationally intensive and require

substantial experimental data. Consequently, most researchers employ simplified methodologies that regard temperature as established domain of inquiry.

Furthermore, turning experimental data into quantitative models isn't easy. The values derived from experiments conducted in highly controlled settings cannot be directly applied to models for the manufacturing process, which is characterized by numerous complexities. (Domaneschi et al., 2017).

2.3.6 Relevance to the Present Study

The literature indicates that temperature significantly affects the formability of sheet materials during the forming process. There have been many studies on paperboards, but the same mechanical principles that cause temperature-related softening and stress redistribution also apply to polymer sheet forming. (Franke et al., 2021).

In this research work, a simplistic model is used where the temperature is introduced as a predefined field in Abaqus. Several models are studied at different temperatures but with constant geometry and boundary conditions, and contacts. This enables comparison between deformation characteristics and stresses at various temperatures.

The model includes:

- Anisotropic material behaviour through layered composite definitions
- Surface-to-surface contact with friction between the tool and paperboard
- Pressure-driven forming conditions
- Temperature-dependent material properties

This method makes it easy to accurately measure how temperature affects formability while still showing how the forming process works in real life.

2.4 Damage and Failure Mechanisms in Paperboard Forming

Paperboard’s thermoforming process is constrained by a few failure modes that emerge because of its anisotropic and laminar nature. In contrast to isotropic materials, the

occurrence of failure in paperboard can be attributed to a series of interfacial interactions and cannot be easily explained through a simple criterion.

2.4.1 Tensile Failure and Fracture Behaviour

Tensile failure is one of the primary failure modes of paperboard that must be considered during forming processes. Tensile stresses acting on fibers and fiber bonds during the deformation process cause tensile failure. When the tensile strain is greater than the material's strain capacity, it will fail. Tensile strain at failure is an important factor in figuring out how formable something is (Afshariantorghabeh, Kärki and Leminen, 2022). The factor is greatly affected by temperature and humidity because both factors influence fibre bonding and network formation. At low temperatures, the ductility of the material is less, resulting in fragile failure, while at high temperatures, more ductility is achieved, but strength is reduced.

2.4.2 Compressive Instability and Wrinkling

When compressive stresses are applied to a material, particularly in regions where material flow is restricted, wrinkling occurs. Wrinkling happens when the sheet buckles in a certain way, which depends on the structure's anisotropy, the boundary conditions, and the friction. The anisotropy of paperboard causes MD and CD to behave differently when they are compressed.

Numerical and experimental findings validate the existence of a correlation between the compressive behaviour of the material and its inhomogeneous structure (Hagman, 2016). These effects are difficult to predict and require advanced modelling approaches.

2.4.3 Thermal Effects on Failure Mechanisms

Temperature is important when it comes to failures because it changes the strength and ductility of materials.

With increasing temperature, the substance becomes more flexible and loses bonding ability, making it easier to manipulate but unstable. As the temperature rises, the substances become

more ductile, making them less likely to break and easier to shape. However, high temperatures can cause some defects, such as wrinkles and delamination. Furthermore, when a substance is exposed to high temperatures, it degrades (Lessard et al., 1996) . These opposing effects set the limits of thermoforming and show how important it is to choose the right temperature conditions.

2.5 Research Gap and Motivation

Even though there has been a lot of study on how paperboard behaves when it is mechanically, thermally, and formed, there are still some problems that make it hard to accurately predict and improve thermoforming processes.

2.5.1 Limitations in Existing Studies

Previous research has primarily focused on specific properties of paperboard material behaviour, such as mechanical, thermal, or formation-related phenomena. This approach gives some insight into the issues, but it can also be overly specific. (Simon, 2021)

Experimental studies are widely used, but they are insufficient to simulate the complex interaction of temperature, deformations, and contact. However, highly sophisticated numerical models that attempt to simulate these parameters necessitate massive computational resources and a thorough understanding of materials. (Lindberg and Kulachenko, 2022). Furthermore, many modelling approaches rely on assumptions, such as the uniformity of temperatures or the specific reactions of certain materials. Such assumptions may lead to discrepancies between the simulation results and actual formation processes. (Nygårds, Just and Tryding, 2009)

2.5.2 Gaps in Thermoforming Modelling

One of the major research gaps is the study of the effect of temperature on formability using experimental methods. Despite the influence of temperature on formability, relatively few studies have isolated its effect under controlled conditions, making it difficult to determine the temperature's role in the formability process. Furthermore, coupled thermomechanical

models are extremely precise, but their use in industrial settings can be challenging due to the requirement of high computational costs. (Crespo, Juan and Amigo, 2012; Vishtal et al., 2014)

Inconsistency is also observed in the modeling approaches used by different researchers. Variations in geometry, dimensions, and material composition have an impact on the comparability and generalization of thermoforming processes.

2.5.3 Motivation of the Present Study

Given all these limitations, computationally efficient modelling approaches are required. This can be seen by taking simpler approaches, such as using the temperature as a predefined field rather than coupling. (Kibirkštis et al., 2007)

Such procedures enable opportunities to investigate the effect of temperature on material behavior without incurring a significant computational burden. However, such an approach necessitates distinguishing the effect of temperature from other variables. The purpose of this study is to investigate the effect of temperature on the thermoforming of paperboard using a uniform finite element modeling approach.

The main contribution of this work is:

- analyzing deformation behaviour across a defined temperature range
- maintaining constant geometry, boundary conditions, and loading
- isolating the effect of temperature on stress, strain, and plastic deformation

By adopting a simplified yet systematic approach, the study provides a clear understanding of how temperature influences formability, while avoiding the complexity of fully coupled simulations.(Wallmeier et al., 2015)

In effect, this method helps to fill the important gap between the very complicated process of theoretical modelling and the real-world engineering applications that are used. By using this method, it is possible to get important scientific information that is useful and relevant to industrial applications.

3 Methodology

This chapter describes the numerical method used to investigate the thermoforming behaviour of a coated paperboard sheet under various temperature conditions. The analysis was carried out using the finite element method implemented in Abaqus/Standard. The modelling framework was constructed so that the influence of temperature could be isolated, while geometry, boundary conditions, contact interaction, and loading remained unchanged across all cases.

The thermoforming system consists of a layered sheet material and a rigid female mold. The sheet represents a composite structure composed of a paperboard substrate and a PETG coating, while the die defines the final geometry of the formed part. Four temperature conditions were examined: 80 °C (353.15 K), 100 °C (373.15 K), 120 °C (393.15 K), and 140 °C (413.15 K). For each case, the same model was used, and only the temperature-dependent material properties were modified. This ensured that any differences observed in the results arose directly from the variation in material behaviour with temperature.

3.1 Thermoforming Model Development

The thermoforming model was developed to represent the deformation of a coated paperboard sheet into a rigid female die under quasi-static loading conditions. The analysis was performed in a three-dimensional modelling space, where the sheet was defined as a deformable body and the forming tool as a discrete rigid body. This approach ensured that all deformation occurred within the sheet, while the die remained geometrically unchanged during the simulation.

The sheet was represented using conventional shell elements, which are well-suited for modelling thin structures undergoing large deformation. The use of shell elements allowed efficient computation while still capturing both bending and in-plane behaviour.

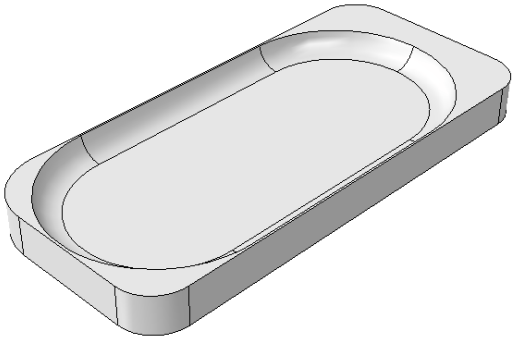

Figure 1. Rigid Female Mold

As shown in (Figure 1) the rigid female mold has an outer dimension of 242.5 mm (length) × 111.2 mm (width) and a total height of 40.0 mm. The inner cavity measures 241.5 mm × 109.2 mm at the top opening, with a cavity depth of 30.0 mm and a base thickness of 10.0 mm. The cavity walls feature a draft angle of 61.1° and a corner radius of 11.8 mm (Afshariantorghabeh et al., 2023). The paperboard is modelled as a flat rectangular sheet measuring 350 mm × 200 mm, with a thickness of 0.475 mm. The sheet is positioned centrally above the female die before forming. The layered structure of the material was incorporated using a composite shell layup, where two plies were defined to represent the paperboard substrate and the PETG coating. The paperboard layer had a thickness of 0.475

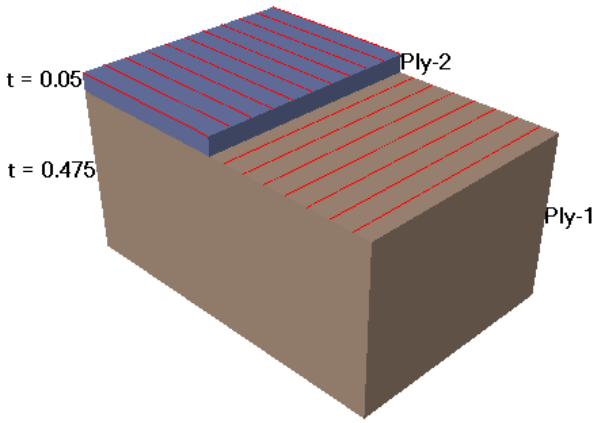

Figure 2. Composite shell layup (paperboard substrate + PETG coating)

(Figure 2), showing the composite shell layup definition of the coated paperboard sheet. The first ply is made of paperboard and is 0.475 mm thick. The second ply is made of PETG coating and is 0.05 mm thick. The part global coordinate system was used to set the layup orientation, with the thickness direction lined up with the normal axis. The paperboard layer was given an angle for the fibre orientation of 90°, showing its anisotropic structure, while the PETG coating was given a rotation angle of 0°. Using Simpson's rule and three integration points per layer, through-thickness integration was done. This made it possible to accurately show how stress and strain change across the thickness. (Lindberg and Kulachenko, 2022)

3.2 Geometry, Boundary Conditions and Loading

The geometric configuration of the model used for testing remained consistent across all temperature conditions. The paperboard sheet was placed above the female die and positioned over the shape of the cavity.

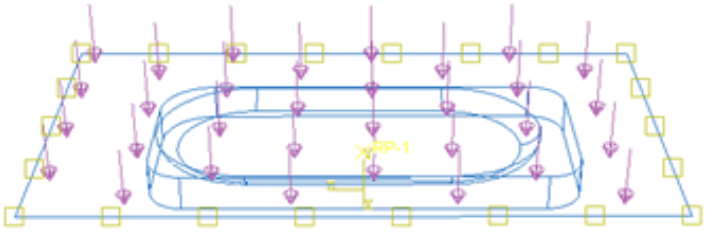

Figure 3. Boundary conditions and loading

A displacement boundary condition is used to limit the edges of the sheet to simulate clamping conditions. These constraints prevent rigid body motion and ensure that deformation is concentrated within the forming region.

(Figure 3) Geometry, boundary conditions, and loading of the thermoforming model. The forming tool (mold) is modelled as a rigid body and fixed in space using an ENCASTRE boundary condition (all translational and rotational degrees of freedom constrained). A uniform pressure load of 0.2 MPa is applied to the sheet during the forming step. These

conditions are kept constant for all temperature cases (Safwa, 2024). Since this value remained unchanged for all temperature cases, it did not influence the comparative analysis.

As a result, any variation in deformation behaviour could be directly attributed to the temperature-dependent material properties.

3.3 Contact Interaction

The interaction between the sheet and the die was modelled using a surface-to-surface contact formulation in Abaqus/Standard. The inner surface of the die cavity was defined as the main surface, while the bottom surface of the sheet was defined as the secondary surface. The proposed configuration aided in the deformation and relative motion of the sheet and die during the process. The contact law was created using the mechanical interaction model. To prevent penetration along the normal direction, hard contact was used. Along the tangential direction, a penalty approach based on the Coulomb friction law was used. The coefficient of friction ($\mu = 0.3$) was assumed to be isotropic. It was kept constant across all temperature conditions to avoid friction-induced variability.

The contact interaction was activated during the forming step, allowing progressive contact between the sheet and the die as deformation occurred.

3.4 Step Definition and Numerical Control

The simulation was performed using two static general steps with geometric nonlinearity enabled. The first step, referred to as the preheating step, was used to establish a stable interaction between the sheet and the die. This step was defined with a period of 2 s, using automatic incrementation with a maximum of 10000 increments, an initial increment size of 0.01, a minimum increment of 1×10^{-8}, and a maximum increment of 0.1. No stabilization was applied in this step.

The second step, referred to as the forming step, represented the main deformation stage. A period of 3 s was defined, and automatic stabilization was introduced with a dissipated energy fraction of 0.002. Adaptive stabilization was used with a maximum ratio of stabilization to strain energy of 0.05. Automatic incrementation was applied with a

maximum of 100 000 increments, an initial increment size of 0.01, a minimum increment of 1×10^{-6}, and a maximum increment of 0.05. This two-step approach ensured numerical stability by separating the contact establishment and forming processes.

3.5 Material Definition and Temperature Cases

The material system consisted of a paperboard substrate and a PETG coating layer. The paperboard was modelled as an anisotropic elastic–plastic material using engineering constants, while the PETG coating was defined as an isotropic elastic–plastic material.

For the paperboard, the elastic behaviour was defined using directional moduli E_1, E_2, and E_3, along with shear moduli G_{12}, G_{13}, and G_{23}, all expressed in MPa. The plastic behaviour was defined using stress–strain data, and a damage model based on a potential criterion was included to represent material degradation. The PETG coating was defined with isotropic elastic properties, where Young's modulus E is expressed in MPa, and Poisson's ratio is dimensionless. Its plastic behaviour was also defined using stress–strain data (Robertsson et al., 2018; Lindberg and Kulachenko, 2022). Four temperature conditions were considered: 80 °C (353.15 K), 100 °C (373.15 K), 120 °C (393.15 K), and 140 °C (413.15 K).

The material properties used in the finite element model are summarised in (Table 1) for both the paperboard substrate and the PETG coating layer. The paperboard is modelled as a fully orthotropic elastic-plastic material, with nine independent engineering constants capturing the directional stiffness differences between the machine direction (MD, direction 1), cross direction (CD, direction 2), and thickness direction (ZD, direction 3). The significant reduction in stiffness from MD to ZD reflects the preferential alignment of cellulose fibres along the machine direction during manufacture.

Table 1. Paperboard and PETG material properties used in the FE model (Safwa, 2024)

Paperboard Material Properties		PETG Material Properties	
Density, kg/m³	816	Density, kg/m³	1290
Expansion Coefficient, °C⁻¹	1E-05	Expansion Coefficient, °C⁻¹	7E-05
Specific Heat, J/(kg °C)	1400	Specific Heat, J/(kg °C)	1200
Thermal Conductivity, W/(m·K)	0.095	Thermal Conductivity, W/(m·K)	0.285
E_1, MPa	5857	Young's Modulus, MPa	2200
E_2, *MPa*	2437	Yield Stress, MPa	50
E_3, *MPa*	800	Poisson's Ratio	0.33
G_{12}, *MPa*	2201		
G_{13}, *MPa*	916		
G_{23}, *MPa*	400		
v_{12}	0.33		
v_{13}	0.32		
v_{23}	0.32		

Table 2. Anisotropic yield stress ratios for Paperboard (Xia, Boyce and Parks, 2002; Jessen and Groche, 2025)

Anisotropic parameters					
R_{11}	R_{22}	R_{33}	R_{12}	R_{13}	R_{23}
1	0.403	0.406	1.105	1	1

The Hill yield criterion is applied to the paperboard because its cellulose fibres align preferentially along the machine direction (MD) during manufacture, making the isotropic von Mises criterion physically inappropriate. In Abaqus, anisotropy is introduced via the Potential keyword. MD uniaxial yield stress taken from the first point of the plastic hardening curve $R_{11} = 1.0$ by definition, while $R_{22} = 0.403$ and $R_{33} = 0.406$ encode the CD and ZD yield stresses at approximately 40% of the MD value, consistent with the MD/CD strength ratio of factor (Xia, Boyce and Parks, 2002). For packaging paperboard and reflecting the dominant fibre alignment along MD, the slight deviation of R_{33} from its physically expected lower value is a deliberate modelling choice to maintain a positive-definite yield surface, as the Hill criterion imposes mathematical constraints on how far the through-thickness ratio can deviate from the in-plane values. $R_{12} = 1.105$ reflects the marginally elevated in-plane shear yield stress typical of fibrous networks, where shear activates fibre bonds across multiple directions. $R_{13} = R_{23} = 1.0$ are set to the isotropic default due to the absence of experimental out-of-plane shear data, consistent with standard practice in paperboard finite element modelling.

3.6 Meshing

The meshing method used was designed to accurately and efficiently model the deformation phenomenon. Traditional shell elements were used to model the paperboard material. The deformable coated paperboard sheet was meshed with S4RT shell elements, which are four-node reduced integration shell elements designed for thin sheet structures. This element type was chosen for its ability to efficiently capture both membrane and bending deformation during thermoforming while also representing temperature-dependent material behaviour. The rigid female die was meshed with R3D4 and R3D3 rigid shell elements, which defined the forming tool's contact surface while preventing die deformation.

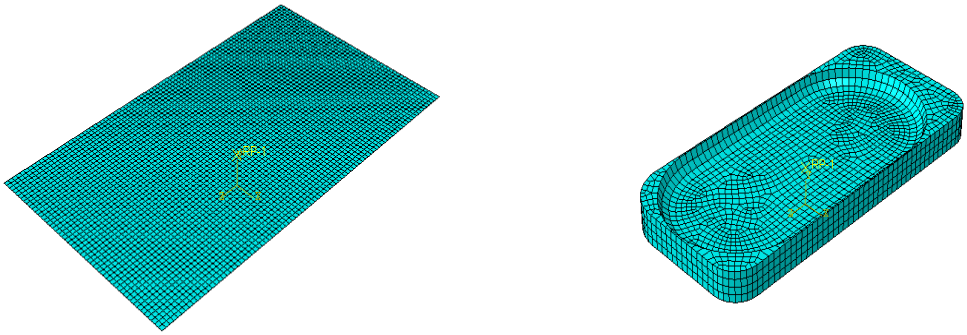

Figure 4. Finite element mesh of the paperboard sheet and rigid die

A refined mesh was used to reduce element distortion and ensure accurate representation of deformation into the die cavity. The mesh density was selected according to the optimal combination of accuracy and efficiency. The same mesh was employed in all simulations, regardless of the paperboard temperatures. A uniform meshing strategy was used for the whole paperboard, which guaranteed an even distribution of elements in all parts of the geometry. This was done to ensure that no bias in the results would appear because of selective refinement, as well as to keep the same numerical accuracy in all parts of the geometry, namely in the flat bottom, side walls, and their intersections. The rigid die was also separately meshed, although keeping the same approach of uniformity for accurate contact detection.

4 Results and Discussion

The thermoforming behaviour of the Polyethylene terephthalate glycol (PETG) coating layer paperboard sheet was examined through a series of finite-element simulations conducted at four different temperatures, namely 80 °C, 100 °C, 120 °C, and 140 °C, while keeping the applied pressure load constant at 0.2 MPa. The temperature-dependent elastic–plastic properties of both the paperboard substrate and the PETG coating layer were updated for each case according to the material model described in Chapter 3. The results are presented through detailed contour plots of the deformed configuration at the end of the forming step, followed by quantitative comparisons of the key response variables. The results are presented on the negative surface (SNEG, fraction = -1.0, Layer = 1), which is the inner surface of the sheet in contact with the forming tool. This ensures that the presented values accurately reflect the material response at the tool-sheet interface, which typically experiences the highest stresses, strains, and deformation effects during the thermoforming process. In the layer-wise plots, 1st ply refers to the paperboard layer and 2nd ply to the PETG coating layer.

4.1 Contour Plots of Thermoforming Response at Each Temperature

To better understand the effect of temperature on the thermoforming behaviour, the deformation response is analysed individually at each temperature level, starting from the lowest temperature, where the material remains relatively stiff.

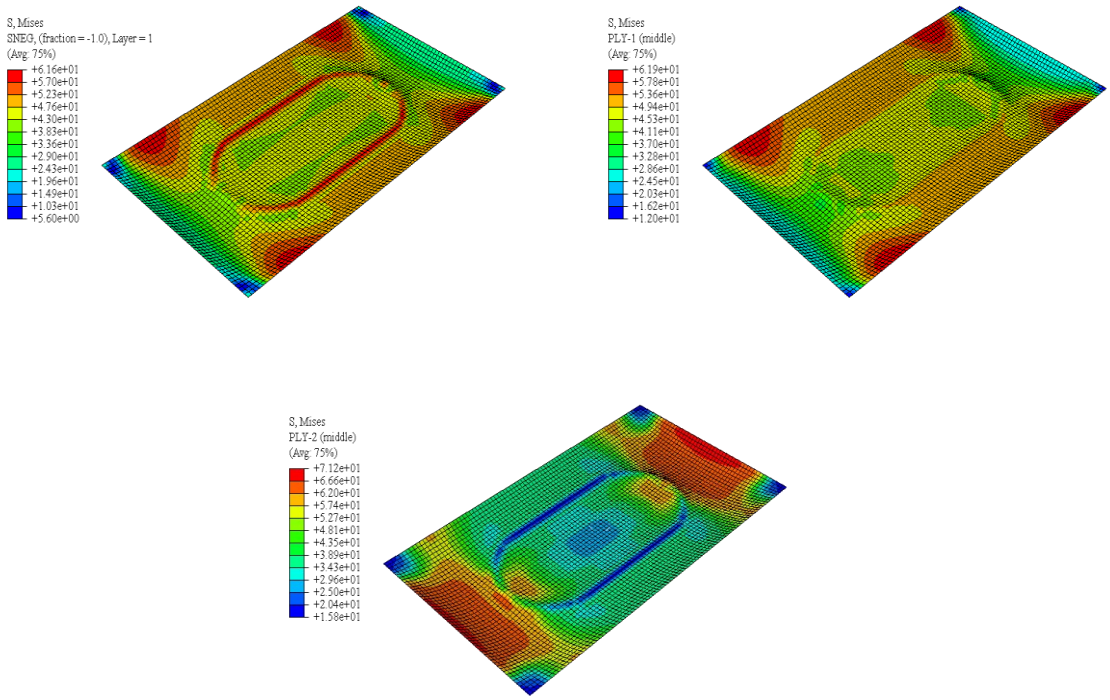

Figure 5. Von Mises stress contours at 80 °C

(Figure 5) shows at 80 °C, the material exhibits a relatively stiff response. The von Mises stress reaches its highest values in this study, with approximately 61.6 MPa on the overall surface, 62.7 MPa in 1st ply, and 71.4 MPa in 2nd ply. The stress contours clearly show concentration in the side walls and transition regions, indicating resistance to deformation. The observed behaviour is consistent with what is expected from bond-controlled mechanics at this temperature. The fiber network and the PETG coating work together to resist the applied load. At this temperature, the material properties indicate a high-stiffness regime, so the applied pressure of 0.2 MPa will not cause any plastic deformation. Analyzing each layer individually shows that the stress levels in both the first and second plies are nearly identical. However, the stress in the PETG coating is slightly higher than that in the fiber substrate because the latter is stiffer. This difference in stress between the layers indicates how they respond and behave at elevated temperatures.

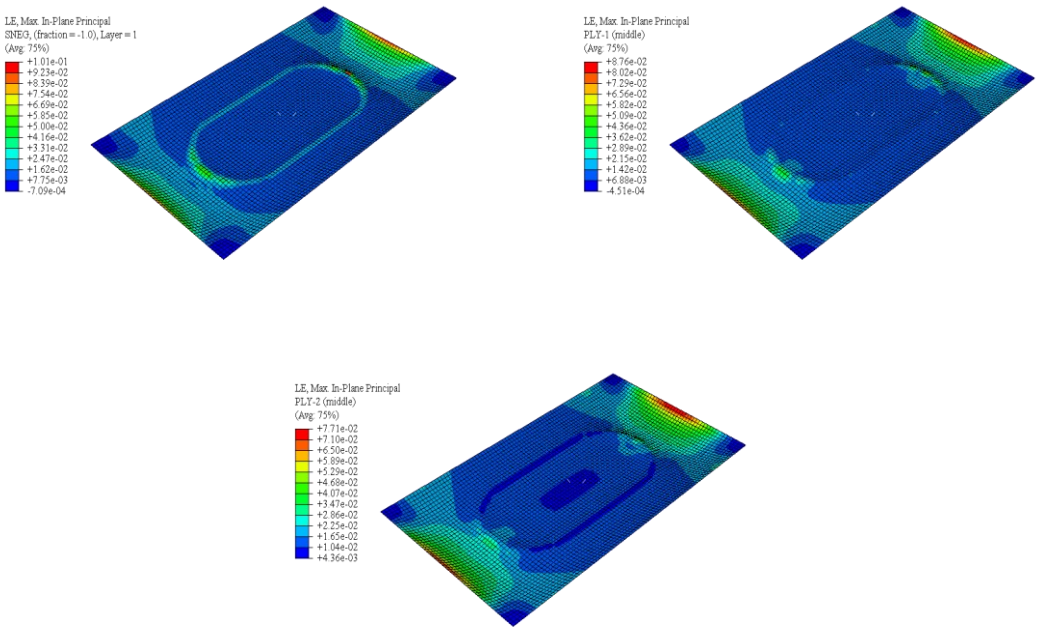

Figure 6. Maximum in-plane principal strain contours at 80 °C

For both the surface and the first ply, the maximum value of the in-plane principal strain is very small, at 0.101 (Figure 6). The second ply has an even smaller value. This means that the extension didn't spread evenly across the sheet; instead, it only happened in a few important places, since most of the sheet was under less stress. The strain contours indicate that high strain regions are limited to the rounded corners and transition zones of the stamp, where bending occurs under load. The center and flange area remain unstrained, reflecting uniform blue contours, which suggests the sheet material cannot conform to the mold's geometry at this temperature. Additionally, the 2nd ply shows lower strain than the 1st, indicating that while PETG is more deformable, it hasn't reached a state to accommodate strain independently. At 80 °C, the thermal softening of the PETG is insufficient to induce strain, causing it to deform similarly to the substrate. Overall, at 80 °C, the material still exhibits elastic properties.

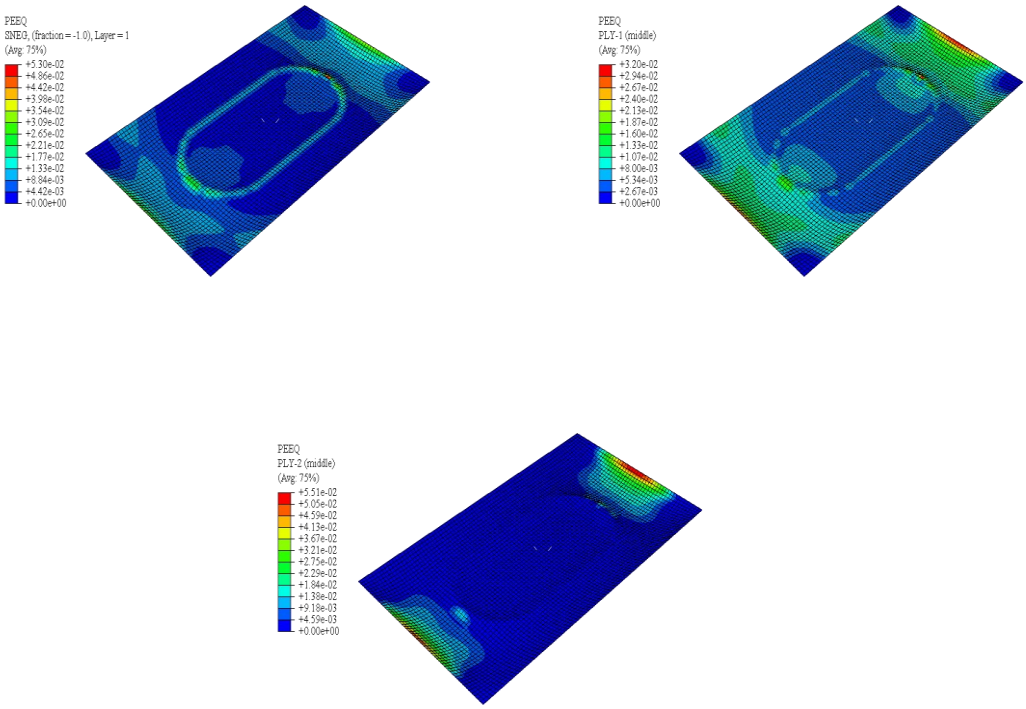

Figure 7. Equivalent plastic strain (PEEQ) contours at 80 °C

(Figure 7) shows that the equivalent plastic strain (PEEQ) is also bounded, having a value only around 0.053 on the inner surface for the 1st Ply and about 0.056 for the 2nd Ply. This indicates that plastic deformations are minimal even at this temperature, meaning that the behavior of the material is mostly elastic.

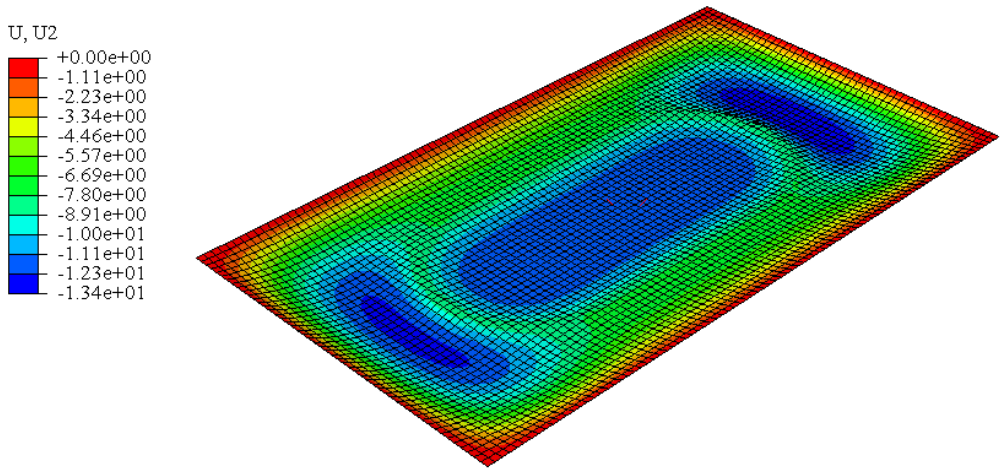

Figure 8. Vertical displacement (U2) contour at 80 °C

Looking at the center of the cavity, the U2 displacement contour has a maximum forming depth of -13.37 mm. In this case, the displacement field is shallow and smooth, indicating that the sheet is unable to conform to the shape of the die. (Figure 8)

As a result, the low values of the LE and PEEQ parameters, combined with the shallow U2 displacement, show that a temperature of 80°C is insufficient for a successful thermoforming process because the sheet retains its rigidity.

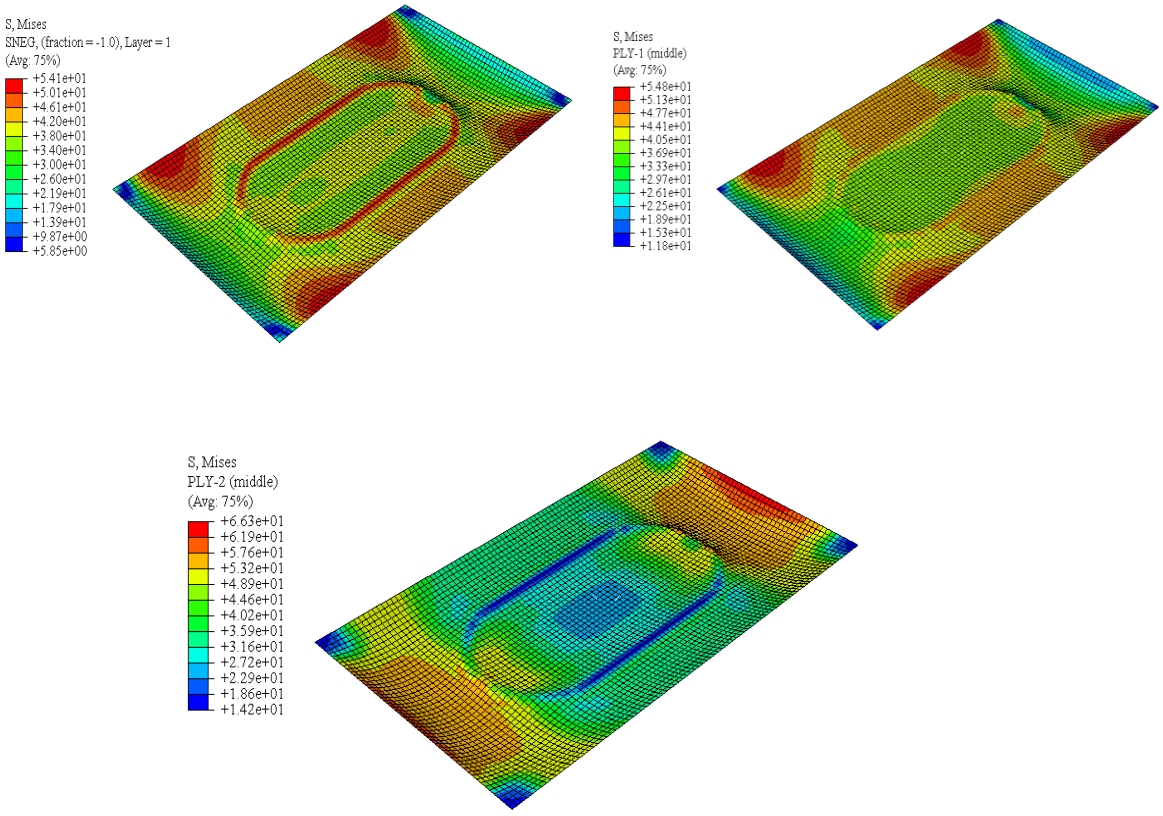

Figure 9. Von Mises stress contours at 100 °C

(Figure 9) shows a clear change in the way the material behaves, with a softening effect. The von Mises stress drops to about 54.0 MPa over the whole surface area, including the first ply. Though the stress level in the second ply is high compared to other plies, it is less than

that at 80°C. The distribution seems to be more even, particularly on the side walls and bottom surface.

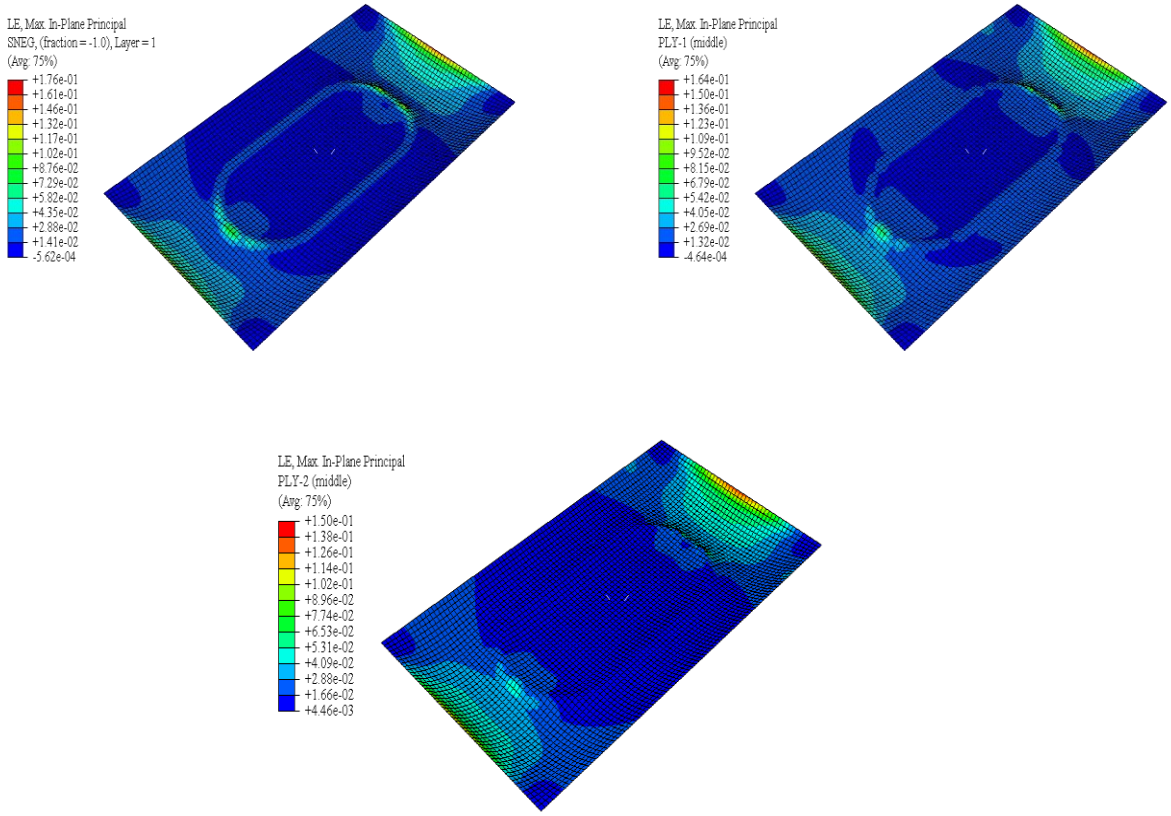

Figure 10. Maximum in-plane principal strain contours at 100 °C

The largest in-plane principal strain LE value rises to around 0.176 both on the entire surface and the 1st ply. However, the 2nd ply also exhibits quite close values of strains. It can be concluded that both layers have become involved in the process. Strain distribution on the geometry reveals a greater spread of deformations across the entire geometry compared to the previous cases. Shown in (Figure 10).

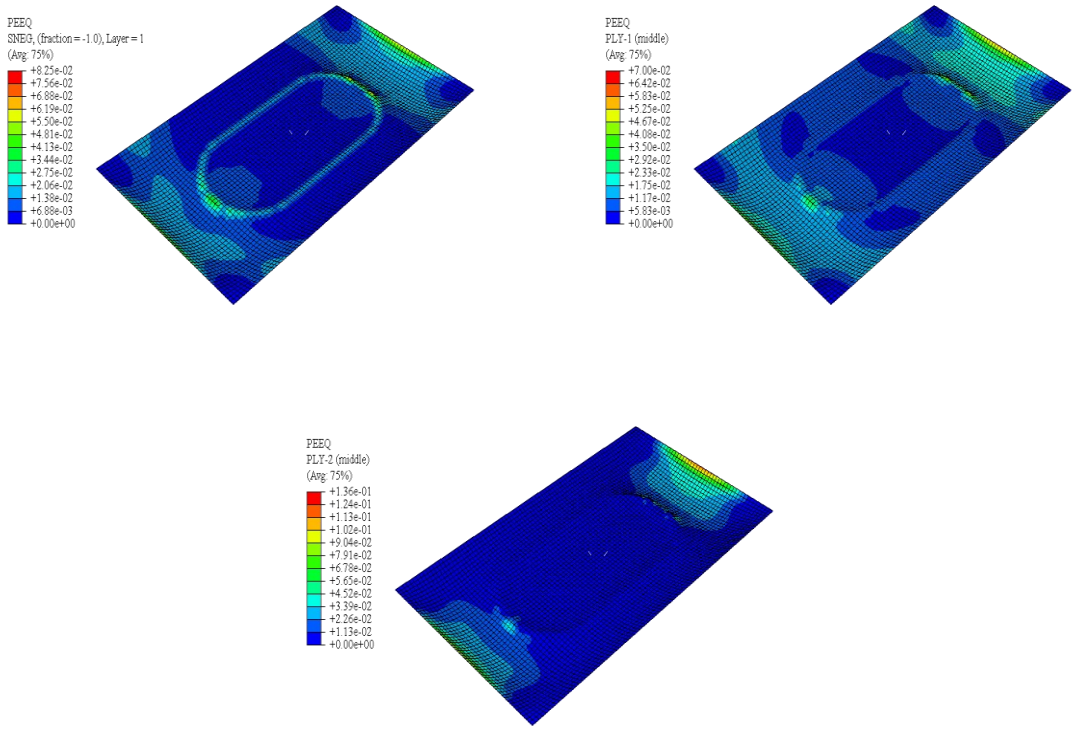

Figure 11. Equivalent plastic strain (PEEQ) contours at 100 °C

The equivalent plastic strain (PEEQ) rises significantly, attaining around 0.082 in the 1st ply and up to 0.138 in the 2nd ply, signifying that plastic deformation becomes more evident, especially in the PETG coating layer. The areas of the corners and the side walls have the highest plastic strain in both plies since they deform by both bending and stretching simultaneously. The 2nd ply shows significantly higher values of PEEQ than the 1st ply at this temperature due to the fact that the yield point of the PETG coating is lower than that of the paperboard substrate. The substrate has become more plastic in comparison with 80 °C, but its fibre structure restricts its ability to undergo irreversible deformation.

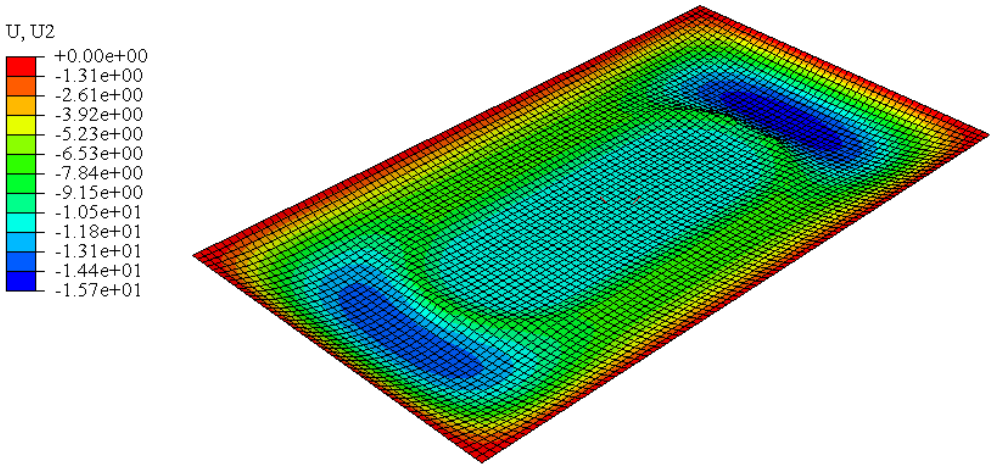

Figure 12. Vertical displacement (U2) contour at 100 °C

The displacement value of U2 is increased to -15.7 mm, resulting in a more pronounced cavity shape at the sheet's center. The smoothness of the displacement pattern indicates a better fit between the sheet and the mold. Overall, the increased values of LE, PEEQ, and U2 at 100°C demonstrate that this temperature level improves formability. As the temperature increases from 80 °C to 100 °C, the distribution of displacement becomes noticeably more uniform. At 80 °C, the material had difficulty conforming to the mold's shape, but at 100 °C, there is a more significant gradient of displacement observed on the side walls. This suggests that the material is beginning to follow the mold's contours more effectively while maintaining a pressure of 0.2 MPa. However, the flange area hasn't deformed much, and the forming depth of -15.7 mm indicates that the entire cavity has yet to be filled.

With further increase in temperature, the deformation becomes more uniformly distributed, and plastic flow becomes dominant in both layers, as shown in (Figure 13). At 120 °C, the forming response reaches its most effective condition within the investigated temperature range.

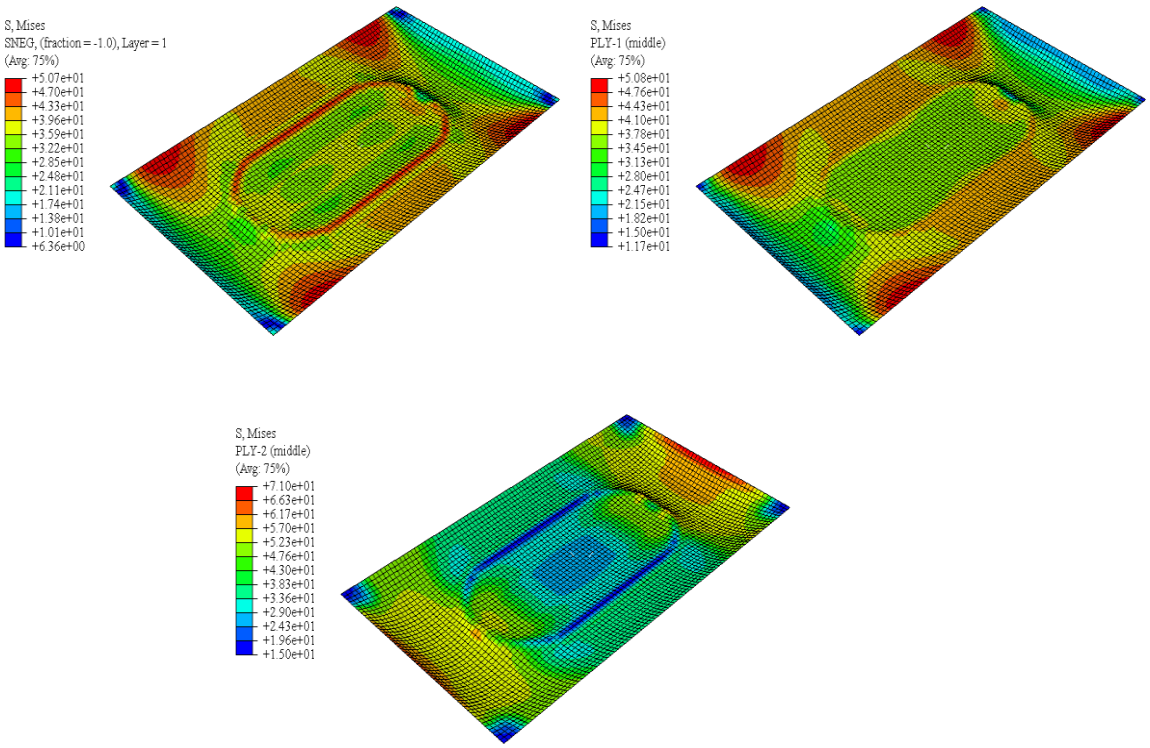

Figure 13. Von Mises stress contours at 120 °C

The von Mises stress decreases further, with a peak value of approximately 50.8 MPa in 1st ply, while 2nd ply continues to show slightly higher localized stress concentrations, particularly near the sidewall transitions and corner regions, although the stress within the PETG film coating layer remains relatively high locally, the stress distribution throughout the entire film is much more uniform than at lower temperatures, implying that film deformation occurs under more stable conditions. The decrease in the magnitude of maximum stress, combined with the smoother contour of the film surface, indicates that its formability has been significantly improved.

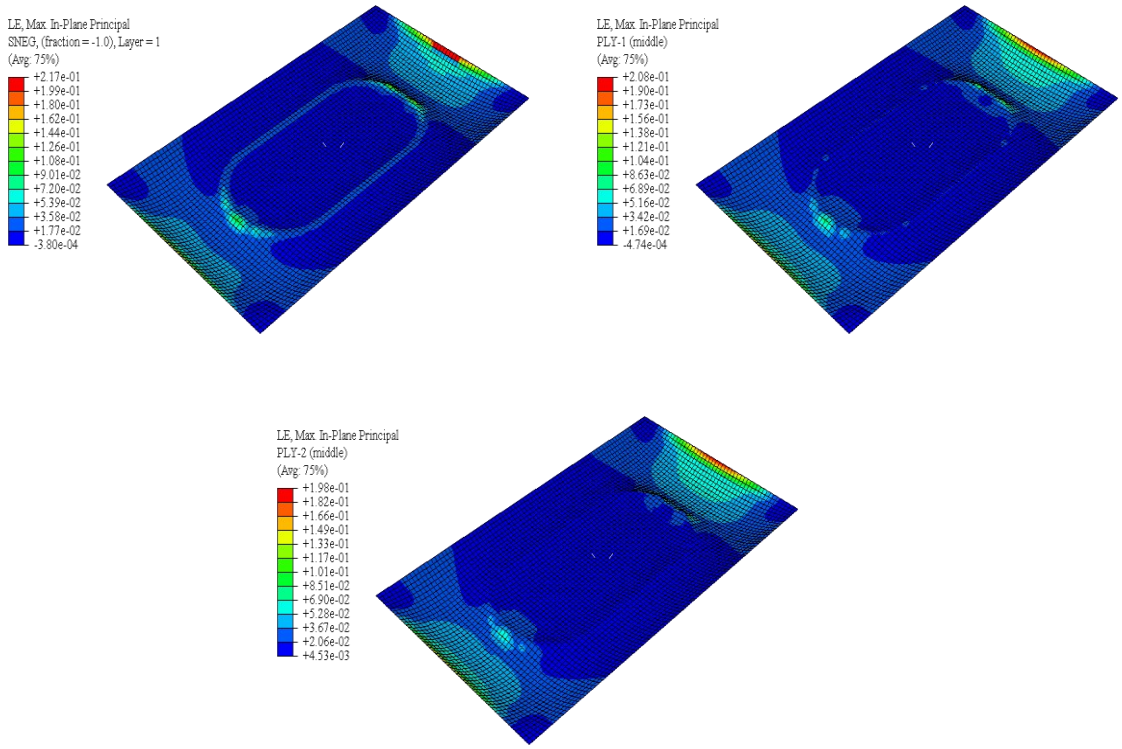

Figure 14. Maximum in-plane principal strain contours at 120 °C

The maximum in-plane principal strain (LE) increases to approximately 0.217 in the 1st ply, with the inner surface showing nearly identical values, while the 2nd ply reaches slightly lower peak strain values of around 0.200. The substrate board clearly exhibits greater elongation than the coating layer, even though the two layers now participate equally in the deformation process. The strain contour pattern has also changed, with deformation occurring much more widely around the formed part rather than just in pockets. This is especially noticeable in the bottom cavity and the transition from it to the side walls. At 120 °C, the stress distribution in both layers becomes more even, spreading out from narrow bands along the side walls to the entire forming region. This allows a larger area of the sheet to participate in stress transfer due to the lower stiffness at this temperature.

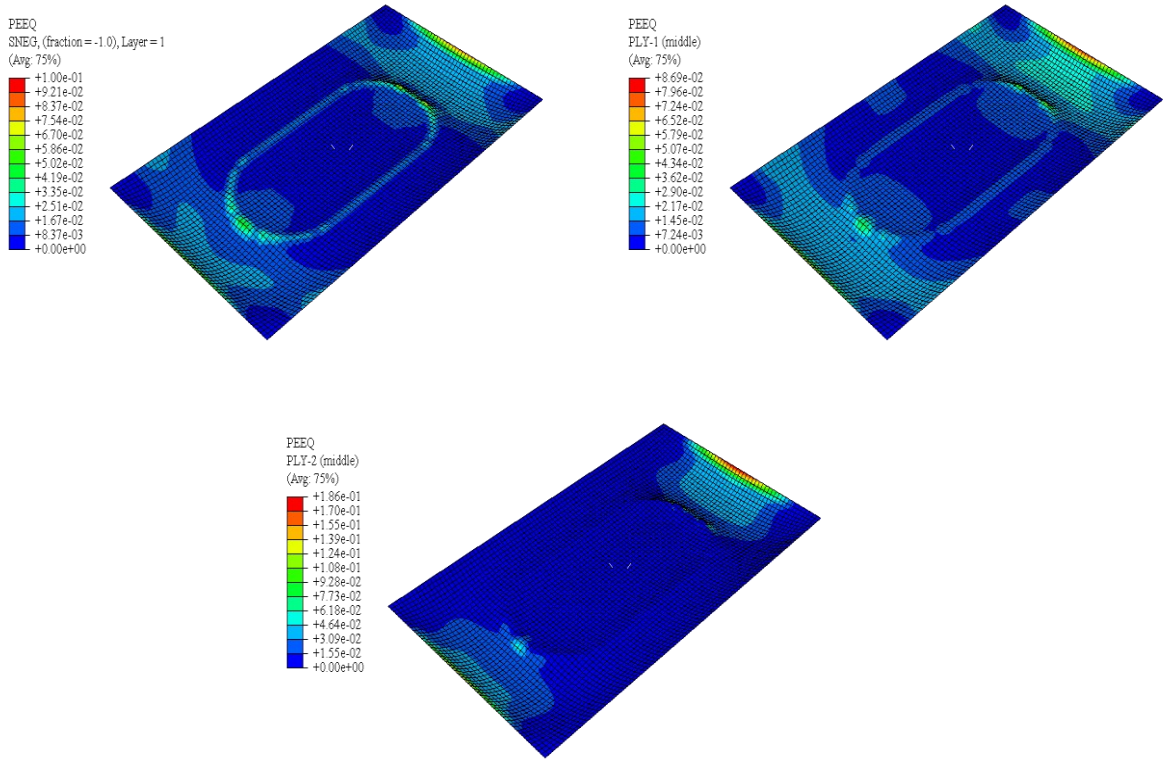

Figure 15. Equivalent plastic strain (PEEQ) contours at 120 °C

The equivalent plastic strain (PEEQ) reaches its highest level in the entire study at this temperature. The current temperature point is the highest value of the PEEQ parameter for the whole experiment. The value of the parameter is about 0.100 for the 1st ply, but it jumps up to 0.187 for the 2nd ply. The PETG film layer changes shape the most permanently. The higher PEEQ level in the 2nd ply indicates that the coating layer plays a major role in accommodating irreversible deformation once the temperature becomes sufficiently high. At the same time, the fact that 1st ply also shows increased plasticity means that the substrate is no longer only resisting deformation but is actively contributing to the forming process. The vertical displacement (U2) reaches its maximum value of approximately –16.5 mm, which is the deepest forming depth obtained among all four temperature cases.

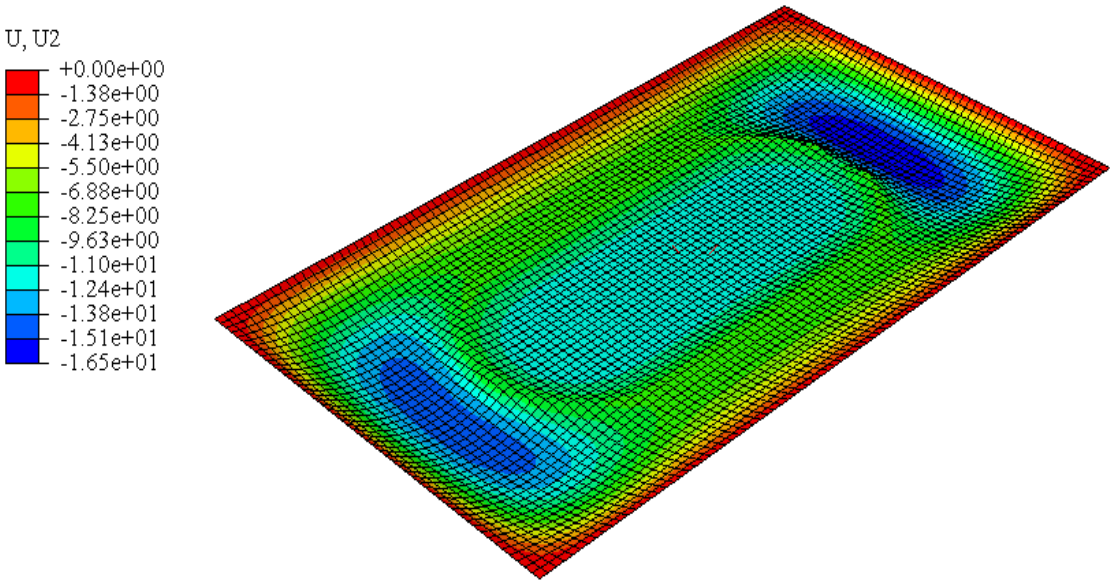

Figure 16. Vertical displacement (U2) contour at 120 °C

The displacement contour shows a well-developed cavity shape with smooth transitions from the flat flange region to the side walls and bottom surface. Compared with 80 °C and 100 °C, the sheet follows the mold geometry more completely, which indicates that the material has reached a highly favourable balance between stiffness reduction and deformation capability. Taken together, the stress, strain, plastic strain, and displacement results show that 120 °C appears to provide the most favourable thermoforming condition within the investigated parameter range, where the sheet achieves maximum deformation with controlled stress levels and extensive but stable plastic flow across both layers. The maximum forming depth of -16.5 mm was reached at the highest temperature, indicating that a pressure of 0.2 MPa works most efficiently here. At this temperature, the material bends and shapes into the mold more easily. Moreover, the transition between the flange and cavity base is noticeably smoother compared to the lower temperatures of 80 °C and 100 °C.

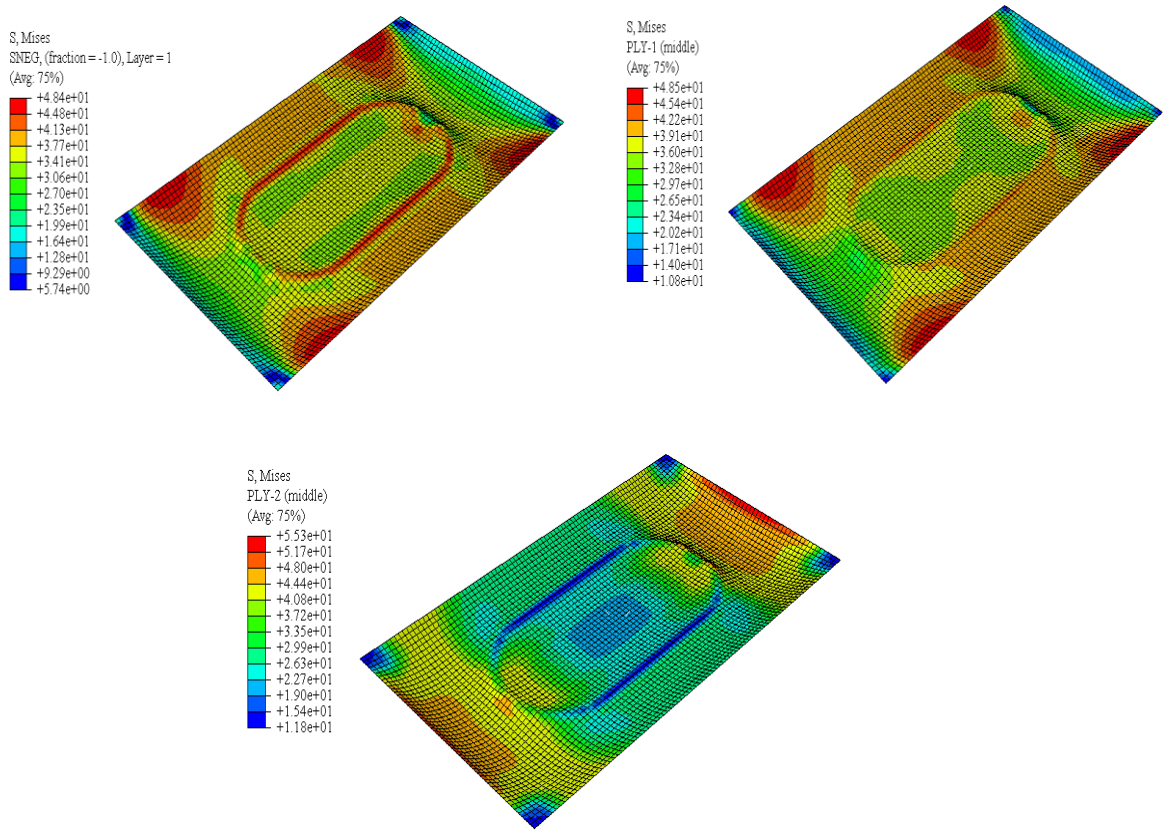

Figure 17. Von Mises stress contours at 140 °C

The material gets even softer at 140 °C, but the change in how it deforms is only small compared to the 120 °C case. Von Mises stress goes down a little, with a maximum value of about 48.4 MPa in the 1st ply. The 2nd ply, on the other hand, has even higher localized stress areas, especially around edges, side wall transitions, and corners. Even though this is the smallest value compared to other temperature conditions, the contour pattern above shows that lowering stress does not help the shape formation process. The reduction in stress levels indicates that thermal softening has lowered the material's resistance to deformation. In contrast to the behaviour observed between 80 °C and 120 °C, the reduction in stress at 140 °C does not appear to be linked to any meaningful enhancement in deformability. This observation suggests that the material has likely reached its softening saturation point. Furthermore, the observed stress concentrations in the second ply, particularly at the corners and transition zones, highlight that the PETG layer is still taking on a disproportionate amount of the stress.

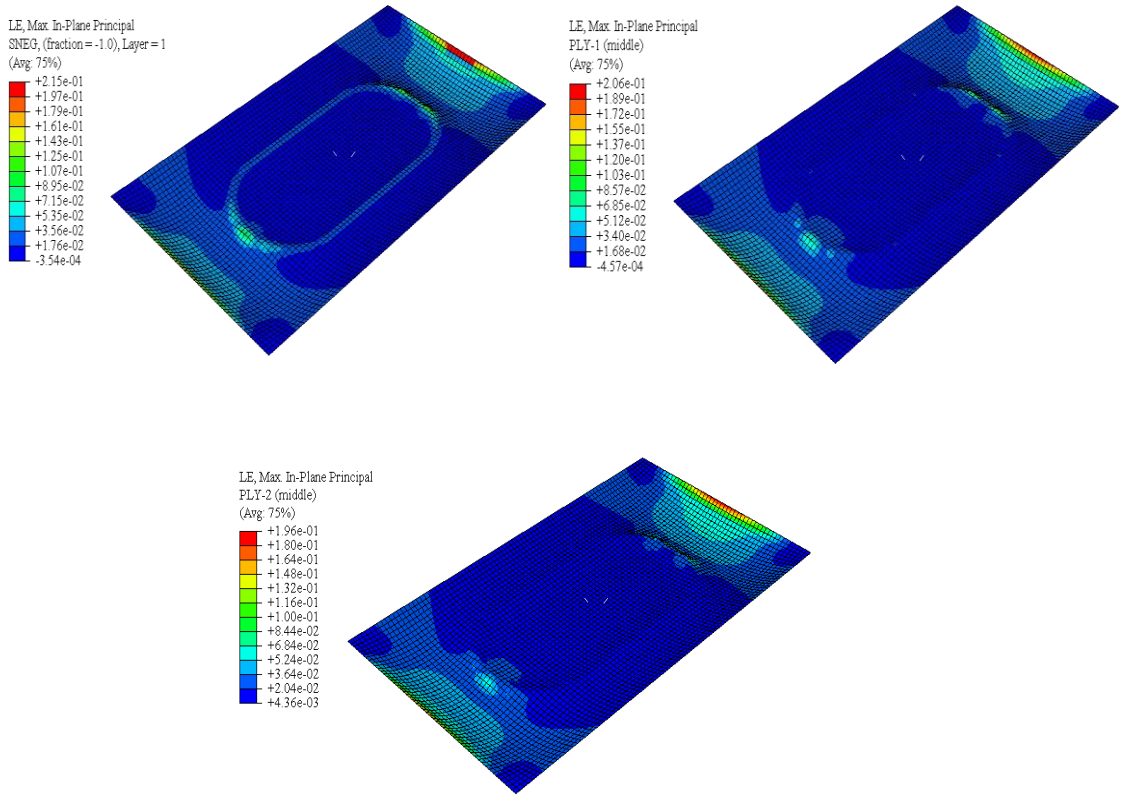

Figure 18. Maximum in-plane principal strain contours at 140 °C

The maximum in-plane principal strain (LE) stays about the same, reaching about 0.216 in the 1st ply. The 2nd ply, on the other hand, shows slightly lower values. This indicates that increasing the temperature from 120 °C to 140 °C does not significantly enhance stretching in either layer. Even the strain distribution contours are not significantly different from those recorded at 120 °C; plastic deformation occurs in the central cavity and wall transition zones. It can be concluded that because there is no significant increase in the LE factor, it cannot be further deformed in its current state. The stress concentration continues to be confined at the side wall transition zones and corners, while the center cavity and flange regions show no difference from the stress distribution at 120 °C.

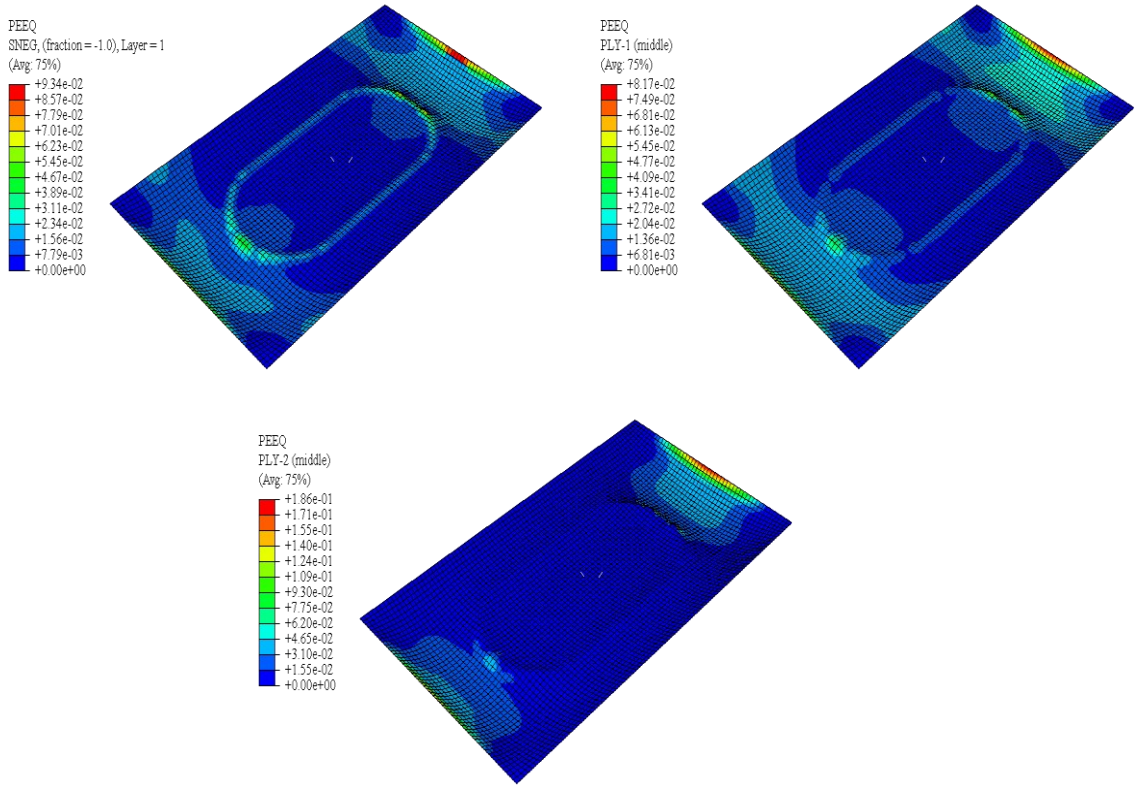

Figure 19. Equivalent plastic strain (PEEQ) contours at 140 °C

A similar tendency is observed in the equivalent plastic strain (PEEQ) results. In the 1st ply, the maximum PEEQ decreases slightly to approximately 0.093, while the 2nd ply continues to exhibit high plastic strain values, although without a meaningful increase compared to 120 °C. This indicates that the PETG coating layer still accommodates a large portion of the irreversible deformation, but that the overall plastic development has started to stabilise. In other words, the material does not gain further forming advantage from the additional heating, even though it remains softened. The contour distributions indicate that plastic deformation remains well distributed; however, the absence of further increase suggests that the material response is approaching its deformation limit.

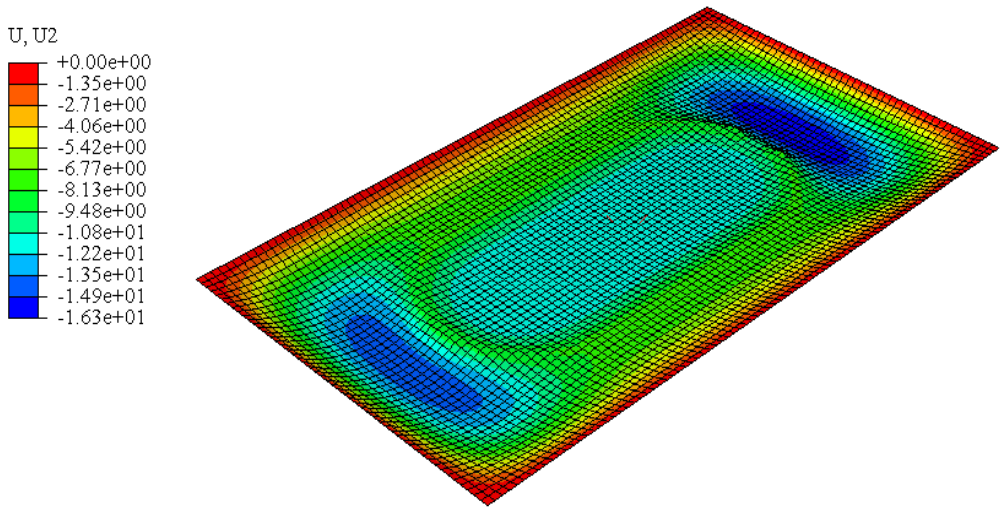

Figure 20. Vertical displacement (U2) contour at 140 °C

Vertical displacement (U2) shows this trend as well. The maximum value of vertical displacement is reduced slightly to -16.2 mm compared to -16.5 mm observed at 120 °C. This indicates a slight reduction in the forming depth. However, the pattern of the vertical displacement is still even as before. The sheet conforms well with the surface of the mold, but the slight reduction in the vertical displacement shows that the temperature rise will not be beneficial to the material with this applied force of 0.2 MPa.

As a result, it can be concluded that at 140 °C, the thermoforming operation has reached its peak value. This is demonstrated by the low stress values and stabilized strains, as well as a slight reduction in displacement. The operation has reached a saturation point, in which an increase in temperature has no positive effect on the deformation process. This suggests that increasing the temperature beyond 120 °C is not beneficial, as excessive heating may lead to thermal degradation of the PETG coating, affecting material performance and surface quality.

4.2 Quantitative Comparison Across Temperatures

The following figures show the overall trends by comparing the four temperatures directly using the highest values from each simulation.

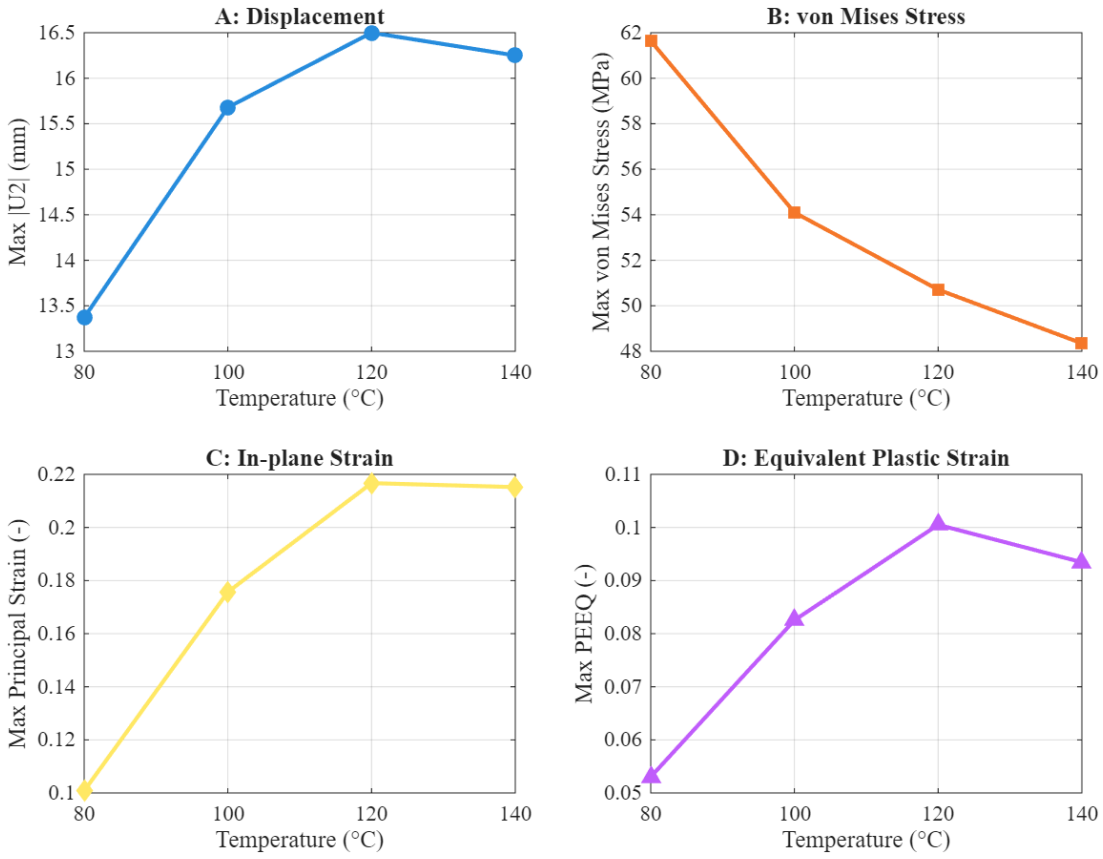

Figure 21. Overview of four primary thermoforming response variables versus temperature

The effect of temperature on thermoforming response (Figure 21) shows all four important variables for the thermoforming process at once: (A) maximum vertical displacement, (B) maximum von Mises stress, (C) maximum in-plane principal strain, and (D) maximum equivalent plastic strain. Subplot A shows that |U2| slowly rises to its highest point of 16.5 mm at 120 °C, up from 13.4 mm at 80 °C. After that, it drops slightly to 16.2 mm at 140 °C. This shows that formability gets a lot better up to 120 °C, but after that, more heat doesn't help as much.

As shown in subplot B, maximum von Mises stress decreases almost linearly, from 61.7 MPa at 80 °C to 48.4 MPa at 140 °C, indicating gradual thermal softening of both the paperboard substrate and the PETG coating layers.

According to subplot C, the maximum in-plane principal strain increases dramatically from 0.101 at 80 °C to 0.217 at 120 °C before remaining constant at 0.216 at 140 °C. As a result, it is possible to conclude that maximum strains occur around 120 °C. It should be noted that at higher temperatures, the maximum strains obtained in PETG coating layers were consistently lower than those obtained in paperboard layers.

Finally, subplot D shows the maximum equivalent plastic strain (PEEQ). As expected, the results are quite similar; however, maximum strain rises to 0.100 at 120 °C, up from 0.053 at 80 °C, before dropping slightly at 140 °C.

Thus, the overall analysis of (Figure 21) shows that 120 °C is the best temperature for current forming pressure and geometry. It ensures maximum drawing depth, strains, and plastic deformation, and a further reduction in stress level. However, additional thermal softening no longer provides significant formability benefits.

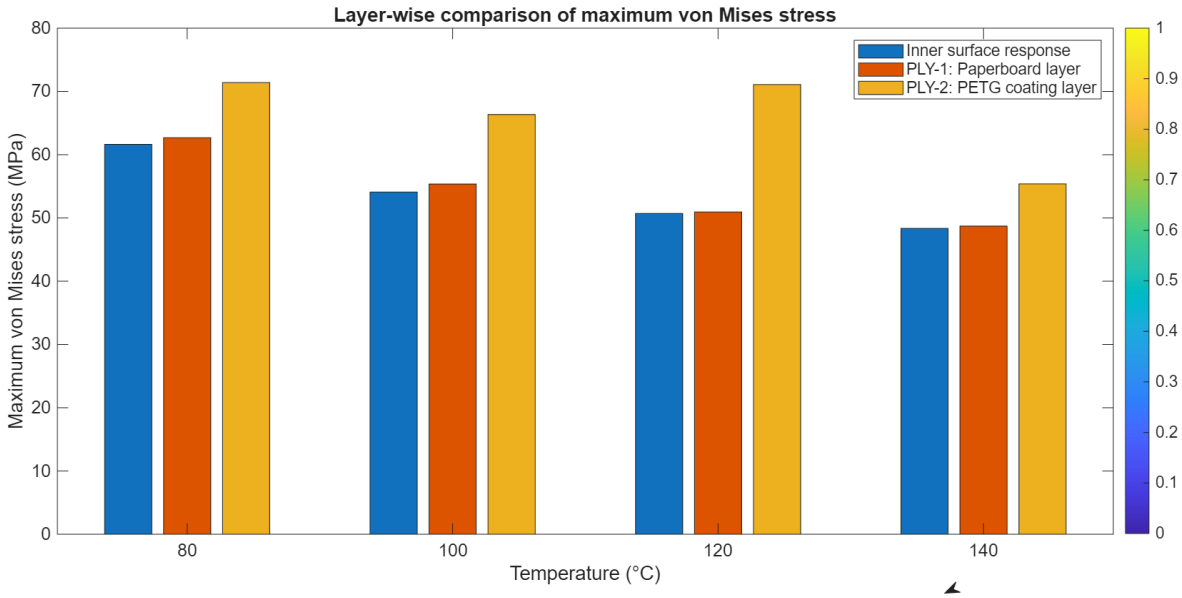

Figure 22. Layer-wise comparison of maximum von Mises stress

The layer-wise distribution of maximum von Mises stress across the inner surface, paperboard layer (1st ply), and PETG coating layer (2nd ply) is shown in (Figure 22). In any case, at any temperature, the PETG coating (yellow bars) exhibits the highest stress of the three layers. The inner surface response (blue bars) is the second most stressed layer, with values identical to those of the paperboard layer (orange bars). At 80 °C, the stresses are 61.7, 62.7, and 71.0 MPa, respectively. As the temperature rises, all bars drop, though the PETG layer continues to have much higher stresses than the others. For example, when the temperature is raised to 100 °C, the stress level for the coating is 66.35 MPa; at 120 °C, it drops to 71 MPa, whereas the values for both paperboard and inner surface are around 51 MPa. When the temperature rises to 140 °C, the difference decreases slightly, with the PETG coating having 55.5 MPa and the other two bars having 48.5 MPa each.

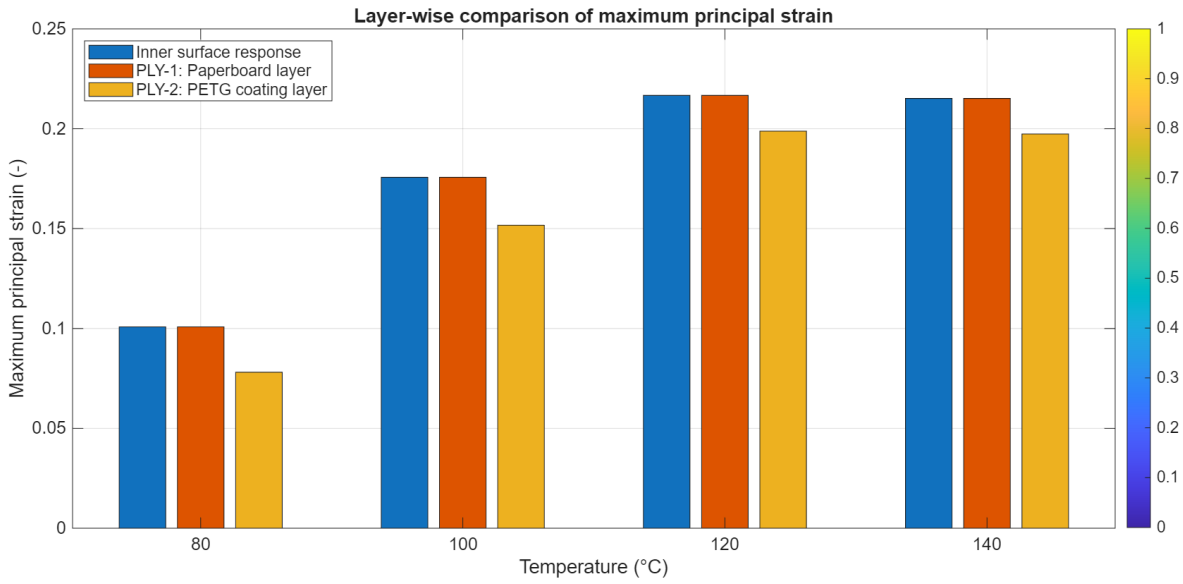

Figure 23. Layer-wise comparison of maximum in-plane principal strain

(Figure 23) presents the layer-wise comparison of the maximum in-plane principal strain. At 80 °C, the strains in all three responses are modest and relatively similar. With increasing temperature, the paperboard layer (1st ply) and the inner surface develop nearly identical peak strains (≈ 0.217 at both 120 °C and 140 °C), whereas the PETG coating layer remains

slightly lower. This indicates that the substrate experiences the largest deformation once the temperature exceeds 100 °C.

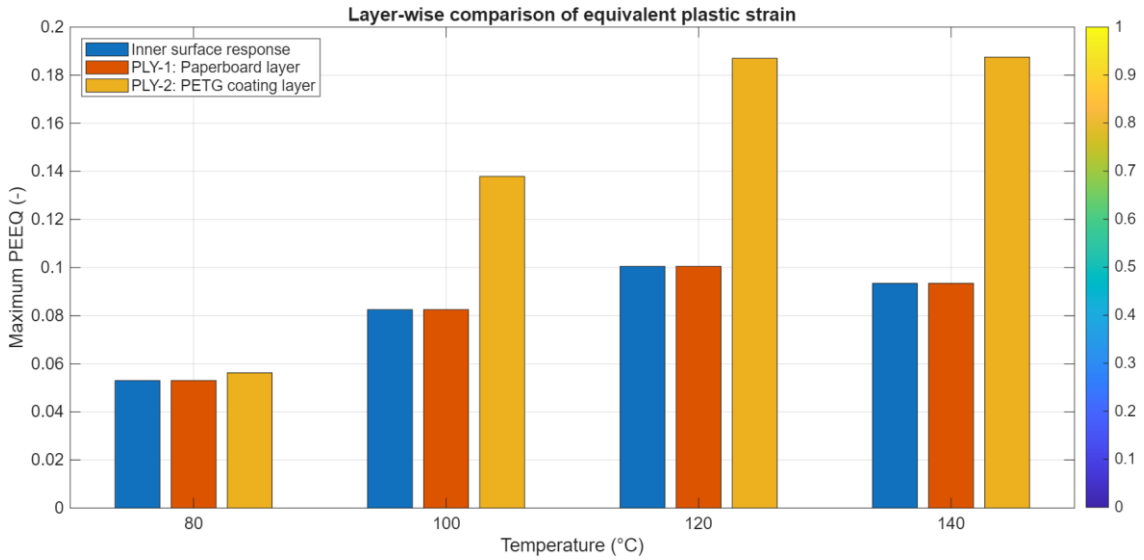

Figure 24. Layer-wise comparison of maximum equivalent plastic strain (PEEQ)

The layer-wise distribution of equivalent plastic strain is shown in (Figure 24). Here, the difference between layers is even more striking: the PETG coating undergoes significantly more plastic deformation than the paperboard layer once the temperature exceeds 100 °C, reaching nearly twice the substrate value at 120 °C and 140 °C. This is expected, since the PETG coating softens more readily than the fibre network in the paperboard.

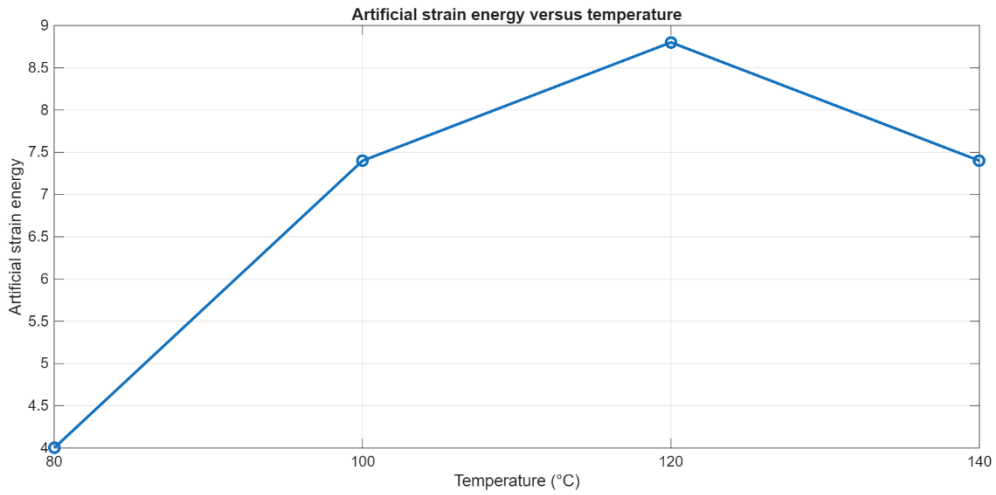

Figure 25. Artificial strain energy (ALLAE) versus temperature

(Figure 25) displays the artificial strain energy across the temperature range. The ALLAE value increases from approximately 4.0 at 80 °C to a maximum of 8.8 at 120 °C and then drops to 7.4 at 140 °C. In all cases, the artificial energy accounts for only a tiny fraction of the total internal energy, demonstrating that the automatic stabilization method proposed in the static steps did not result in any numerical artifacts.

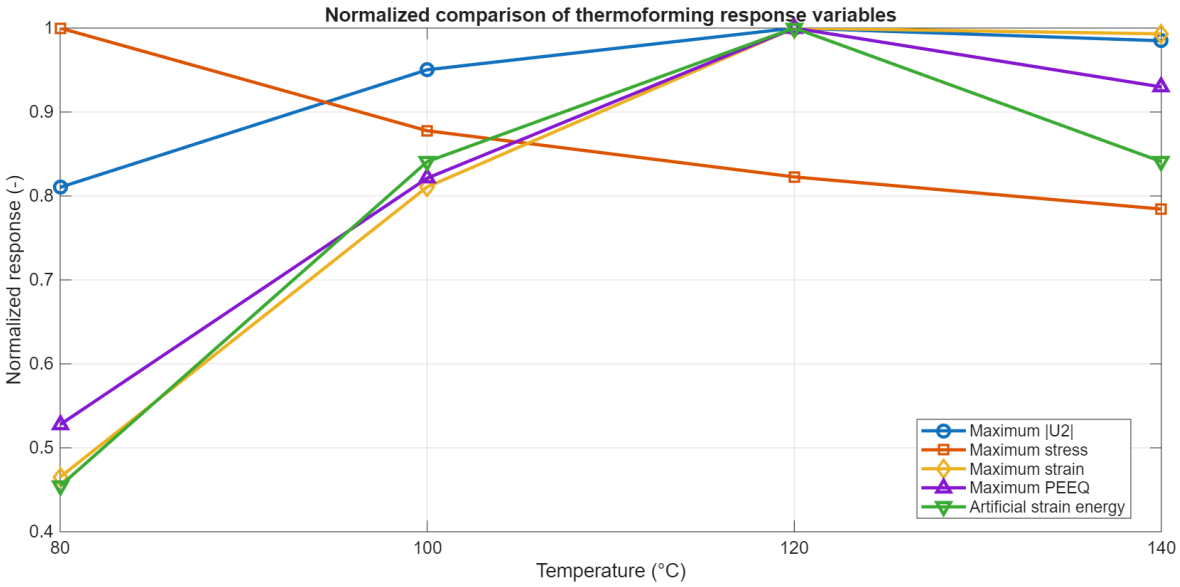

Figure 26. Normalised comparison of all thermoforming response variables

Finally, (Figure 26) depicts the normalized variation of all five response variables in relation to their individual maximum values. The graph shows that displacement, strain, and plastic strain peak at 120 °C, while stress decreases until 140 °C. As a result, 120 °C can be considered the optimal temperature for both deep drawing and proper material flow under the given pressure loading and shape.

In conclusion, increasing the temperature from 80 °C to 120 °C improves the component's formability due to increased plastic strains at higher temperatures, where the material softens due to decreased stiffness of both layers of paperboard substrate and PETG coating layer under the given pressure loading. Any additional temperature increases above 120 °C has no significant effect on formability and may even reverse the effect in the event of displacement. The PETG coating layer exhibits higher plastic strains and stress than the paperboard

substrate layer; thus, the thickness or type of PETG coating should be carefully chosen when applying industrial thermoforming to similar components.

The above analysis clearly shows that temperature has a significant impact on the thermoforming behavior of the PETG-coated paperboard sheet. The paperboard and PETG coating become more flexible as the temperature goes from 80 °C to 120 °C. This makes the sheet less rigid, which allows it to become more plastically deformable when the pressure stays the same at 0.2 MPa. This observation aligns with the established scientific principle that the stiffness of fibers and polymers diminishes with increasing temperature.

A key finding is that 120 °C represents the optimal forming temperature, corresponding to the maximum drawing depth (16.5 mm), as well as peak values of in-plane principal strain and equivalent plastic strain. But raising the temperature from 120 to 140 degrees Celsius does not make the material easier to shape. Instead, formability and plastic strain show a slight decrease. This means that the material has a limit to how much it can bend when it is under a constant load. Thus, making it softer won't make it easier to shape.

The outcomes of layer-wise stress and strain distributions offer further understanding of the distinct properties of the two materials. Under all conditions of temperature rise above 100°C, the stress and strain levels in the PETG coating layer (2^{nd} ply) are much higher than those in the paperboard substrate (1^{st} ply). This result is easy to understand because the polymer coating material has a lower modulus of elasticity than the fiber structure of the paperboard. So, the polymer coating is the main part that causes permanent deformation, while the substrate material is very resistant to deformation.

The results of the present model showed that the most favourable forming response for the studied PETG-coated paperboard sheet was obtained at 120 °C under the selected geometry, pressure load, and boundary conditions. At this temperature, there was the highest amount of forming, strain development, and plastic deformation at controlled stress levels. However, the optimum temperature cannot be directly transferred to all coated paperboard materials or thermoforming setups since it depends on the material composition, the coating thickness, the geometry, the pressure, and the contact conditions. The results suggest that an effective forming temperature should allow for deformation by providing adequate thermal softening but also maintain material stability to prevent too much softening or loss of forming efficiency. This temperature gives the lowest values for stress and strain, as well as low

artificial strain energy. Temperature control is essential for successful thermoforming, as excessive heating can reduce forming efficiency and may lead to material instability or thermal degradation. The results have shown how important temperature is as a processing parameter that affects the thermal-mechanical behavior of coated paperboard during thermoforming. The study employs a simulation-based methodology to examine the impact of temperature on stress, deformation, and plasticity. This information can help figure out process parameters and be used as a starting point for more research in the field.

5 Conclusion

This thesis presents a finite element analysis of a PETG-coated paperboard specimen to evaluate its performance and mechanical response under thermal and pressure loading conditions. For this purpose, a three-dimensional model has been created using ABAQUS/Standard to investigate the effects of temperature variations on mechanical properties, while maintaining constant other factors, including model geometry, boundary conditions, contact behavior, and pressure loading. The simulation was done at four different temperatures: 80°C, 100°C, 120°C, and 140°C.

The results indicate that temperature has a significant effect on the material's formability. The effect of temperature on deformation, stress, and plastic behavior can be clearly observed while other factors were kept constant, as temperature was the only parameter varied in this study. When the temperature goes from 80 °C to 120 °C, the material becomes less stiff, which means that it can deform a lot at pressures of 0.2 MPa. At 120 °C, where strains are very high, the maximum forming depth reaches 16.5 mm. However, increasing the temperature to 140 °C does not further improve the forming behaviour. While a slight reduction in stress is observed, there is no significant increase in deformation or plastic strain, indicating that the forming response has reached a saturation level. It should be noted that these findings are based on finite element simulations conducted in ABAQUS/Standard and reflect numerical trends under the defined modelling conditions, rather than experimentally validated outcomes. The analysis of each layer individually led to the conclusion about their complementary interaction. For instance, when the temperature was above 100°C, it could be inferred that the stress values of the PETG layer would be greater

compared to the paperboard layer. This happens because the polymer layer is more flexible compared to the fibre layer in the paperboard layer, which causes most of the plastic deformation. Such data can help improve the design process of paperboard applications produced on an industrial scale.

Taking the practical aspect into account, 120 °C is the most effective temperature for this material because it provides optimal conditions for deep drawing, stress distribution, and plastic deformation. The process was carried out at multiple temperatures, with 120 °C representing the most effective forming condition, resulting in the lowest possible stresses, the highest strain capacity, and the least amount of additional strain energy. This confirms the numerical stability of the calculation. In this regard, the results guide the selection of temperature process parameters

However, there are some limitations to this research. A simplified mechanical model was adopted in which temperature was applied as a predefined field, while rate-dependent and viscoelastic effects were neglected. Nonetheless, the careful analysis enabled a clear separation of the effect of temperature on the structure, resulting in consistent and reproducible numerical trends.

To summarize, this thesis successfully demonstrated the capability of a systematic finite element simulation in accurately simulating the thermoformability behaviour of PETG-coated paperboard. The findings will be extremely useful in establishing a foundation for future experimentation. Future research can broaden the scope of this thesis by utilizing coupled thermomechanical simulation, applying varying degrees of pressure or dies, and conducting actual lab experiments.

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