Measure, Digitise, Execute: Streamlining Sustainable Packaging Design

Dr R. Blair, Dr D. Papadimitrakis, A. McKee, R. Armstrong
(Blow Moulding Technologies, Northern Ireland);

Prof. G. Menary
(Queen's University Belfast, Northern Ireland).

Abstract

The plastic packaging industry is under increasing pressure to reduce its environmental impact, particularly from single-use PET bottles. This study presents a structured "Measure, Digitise, Execute" methodology for lightweighting 100% recycled PET (rPET) bottles while maintaining critical performance metrics. The approach involves: Material Characterisation (Measure) – experimentally characterising and calibrating a material model for accurate finite element simulation of the stretch blow moulding (SBM) process; Virtual Prototyping (Digitise) – parameterising preform design and SBM conditions, then using finite element analysis and design of experiments to generate performance data; and Design Optimisation (Execute) – employing surrogate modelling and multi-objective optimisation to reduce material usage while maintaining functional requirements. A case study on a 20.7 g rPET preform demonstrated a 13% weight reduction to 18.1 g, whilst meeting empty top load and burst pressure performance requirements. The optimised design reduces carbon footprint through material savings and energy-efficient heating profiles. This automated, simulation-driven approach provides a scalable solution for manufacturers seeking to accelerate sustainable packaging development while aligning with regulatory sustainability targets.

1. Introduction

1.1 The Problem

The plastic packaging industry faces a growing challenge: disposable plastic bottles have become a global symbol of environmental degradation. The increasing demand for convenience among end-users has driven a surge in the production and consumption of plastic packaging, yet this demand has not been matched by sufficient measures to ensure reuse or recycling. As a result, vast amounts of plastic waste accumulate in landfills or are discarded in natural environments. Globally, an estimated 525 billion plastic bottles are purchased annually [1]. Compounding this issue, plastic bottles can take approximately

450 years to degrade [2], exacerbating the severe and long-term impact of such waste on ecosystems.

Despite efforts to recycle, less than 10% of the world's plastic is effectively reused. As majority of plastics are derived from fossil fuels, the production process contributes significantly to greenhouse gas emissions. In response, nations like the UK have implemented policies to reduce plastic waste [3]. To mitigate environmental impacts, strategies include the use of biodegradable or recycled materials, optimising packaging designs, or transitioning to reusable packaging solutions.

1.2 The Need for Sustainable Packaging Design

Sustainable beverage packaging minimises environmental impact whilst maintaining its functional purpose. However, designing more sustainable packaging presents challenges. One significant barrier is the limited understanding of the mechanical properties of new materials, which complicates the design process and results in unpredictable performance outcomes and unnecessary material waste.

Simulation tools, such as finite element analysis (FEA), have the potential to reduce the number of physical trials, saving both material and resources. This study focuses on lightweighting a 20.7 g recycled PET (rPET) preform for a given bottle design. The goal is to reduce the preform's weight while maintaining critical performance metrics, such as top load and burst strength. By leveraging advanced simulation methodologies, this work aims to address gaps in current design approaches and support the transition to more sustainable practices.

1.3 Methodology and Objectives

This study aims to identify the lightest preform design that meets functional performance requirements. The methodology follows three key stages, each aligned with specific objectives:

1. **Material Characterisation (Measure):** Experimentally characterise a 100% rPET resin and calibrate it for accurate stretch blow moulding (SBM) and bottle performance simulations.
2. **Virtual Prototyping (Digitise):** Parameterise preform geometry and SBM process conditions, generating simulation data via design of experiments (DOE).
3. **Design Optimisation (Execute):** Apply surrogate modelling and multi-objective optimisation to reduce preform mass while maintaining performance.

2. Material characterisation

2.1 The Stretch Blow Moulding Process

Single-use plastic bottles are predominantly manufactured using polyethylene terephthalate (PET) via the SBM process. This process, illustrated in Figure 1, begins with the heating of a preform to a specific temperature (a). The preform is inserted into a mould and sealed (b), stretched longitudinally using a rod (c), and then expanded using pressurised air in two stages: pre-blow (0.6-1 MPa) and final blow (>2.5 MPa) [4] (d). Finally, the mould opens (e), and the finished bottle is removed (f).

The ability to simulate this process with accuracy depends on a comprehensive understanding of the material's behaviour during forming and the influence of processing history on its mechanical properties. To achieve this, experimental data is required. Digital image correlation (DIC) is employed during free stretch blow (FSB) testing to capture the material response and calibrate a material model for SBM simulations. Additionally, biaxial tensile testing is used to quantify how the SBM processing history affects the material's stiffness and, by extension, the blown bottle’s performance in terms of top load and burst strength.

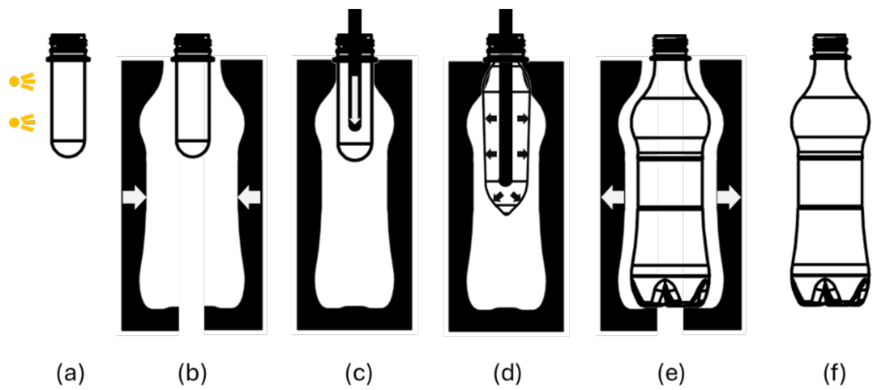
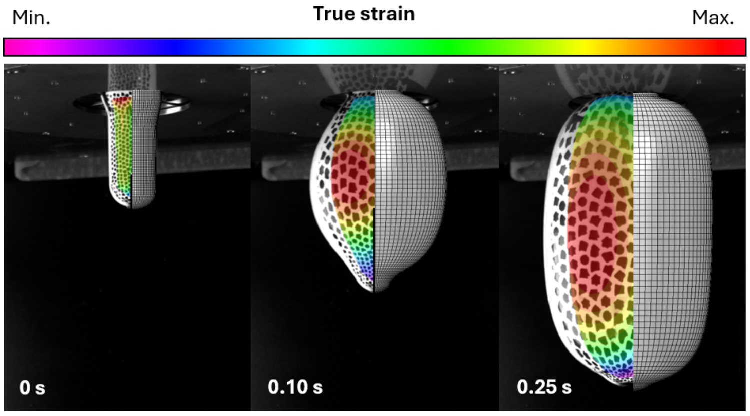


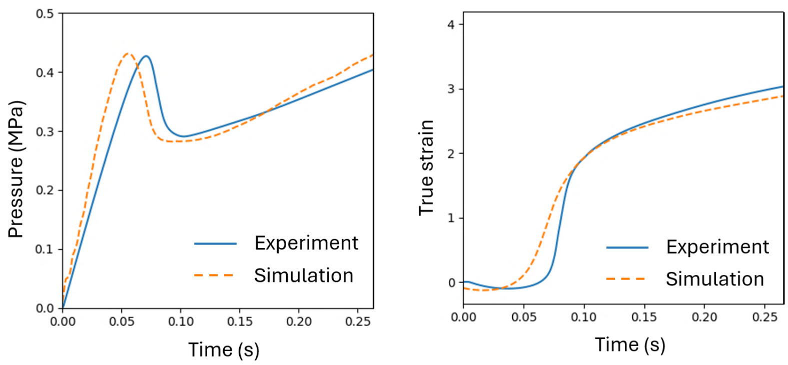
Figure 1: Key stages of the stretch blow moulding (SBM) process.

2.2 Digital Image Correlation and Free Stretch Blow Testing

Free stretch blow tests were performed for the 100% rPET 20.7g preform, with varying temperature (100, 105, and 110°C), flow rates, and stretch rod timing to capture temperature and rate-dependent stress-strain behaviour. In an FSB test, a preform is heated above its glass transition temperature—the point at which the polymer transitions from a rigid, glassy state to a softer, rubber-like state—allowing it to be stretched and formed. The preform is then stretched with a rod while pressurised air freely blows it without a mould. Digital image correlation measures strain by tracking surface deformation (Figure 2a), while an instrumented stretch rod records cavity pressure and reaction forces [4]. The strain and pressure data from FSB tests are compared to Abaqus/Explicit simulations to calibrate a custom constitutive (VUMAT) model (Figure 2b). Based on the work of Yan et al. [5] and Buckley et al. [6], this model accounts for polymer temperature, strain rates, and deformation modes. It uses a spring-dashpot assembly to represent linear elastic deformation, viscous flow, and non-linear elastic deformation.



(a) Strain evolution during free stretch blow testing (FSB), obtained from digital image correlation (DIC).

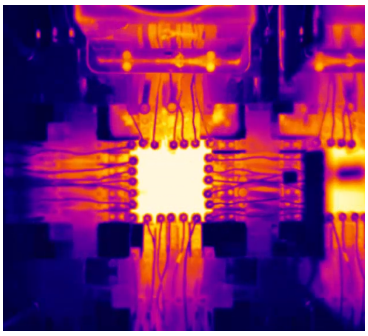


(b) Calibration of a representative constitutive model against FSB data.

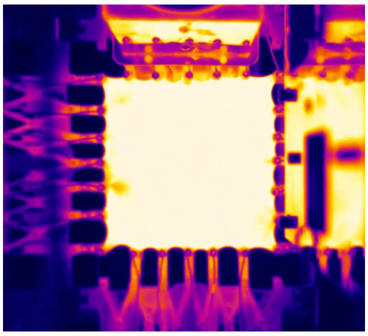
Figure 2: Calibration of a temperature and rate-dependent constitutive model for the stretch blow moulding (SBM) process.

2.3 Biaxial Testing and Influence of Processing History

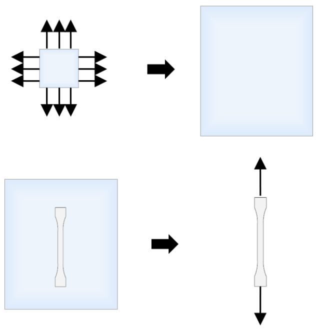
Complementing the FSB tests, biaxial tensile testing quantifies how the bottle's processing history influences its post-processing mechanical properties, particularly stiffness (elastic modulus). rPET sheets are injection moulded, heated above the glass transition temperature, and stretched to various equibiaxial stretch ratios (Figure 3a–b) [7]. Following biaxial stretching, dog-bone specimens are punched from the stretched sheets and subjected to uniaxial tension tests (Figure 3c). These tests measure the stress-strain response of the rPET material at different stretch ratios, enabling the calculation of elastic modulus (Figure 3d). These results offer critical insights into how stretching history affects the stiffness distribution along the bottle, which directly impacts its performance in terms of top load and burst strength.



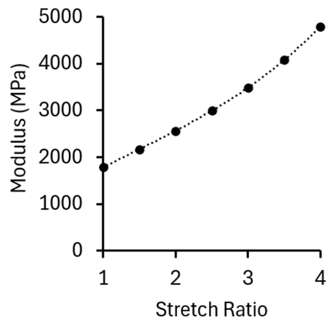
(a) Biaxial specimen pre-stretching.



(b) Biaxial specimen post-stretching.



(c) Uniaxial tensile specimens punched from biaxially stretched sheets.



(d) Elastic modulus as a function of stretch ratio.

Figure 3: Post-processing elastic modulus as a function of processing history.

3. Virtual prototyping

Benchmark SBM and performance simulations were established using the material model from Section 2 for a nominal 20.7 g preform and a given bottle design. The preform geometry and process conditions were systematically varied to explore a range of new, unique designs. SBM and performance simulations were then conducted, extracting key metrics such as maximum empty top load and burst pressure for each design.

3.1 SBM and performance simulations

The SBM simulations were developed by defining the geometry of the preform, bottle, and stretch rod, setting the preform's temperature profile, specifying process conditions, and selecting the material model calibrated in

Section 2. Dynamic explicit, non-linear finite element simulations were performed in Abaqus/Explicit to capture the high-speed, transient behavior of the SBM process (Figure 4a). Contact interactions and non-linear geometry were incorporated. To optimise computational efficiency, 2D axisymmetric shell models were used, taking advantage of the bottle's nearly axisymmetric shape. The simulations provided detailed insights into material flow, enabling the extraction of the blown bottle's thickness and modulus distributions. These distributions were then mapped onto a separate 3D quad-dominated shell mesh for performance simulations.

In the top-load simulation (Figure 4b), two rigid plates were used, with the bottle subjected to a displacement-controlled load from the upper plate. Contact interactions were included to ensure proper force transmission. The burst simulation (Figure 4c) involved applying internal cavity pressure to the bottle, constrained at the neck, and gradually increasing the pressure until the bottle burst (excessive mesh distortion). Maximum empty top load and burst pressure were extracted, which are critical for verifying that the design meets functional requirements.

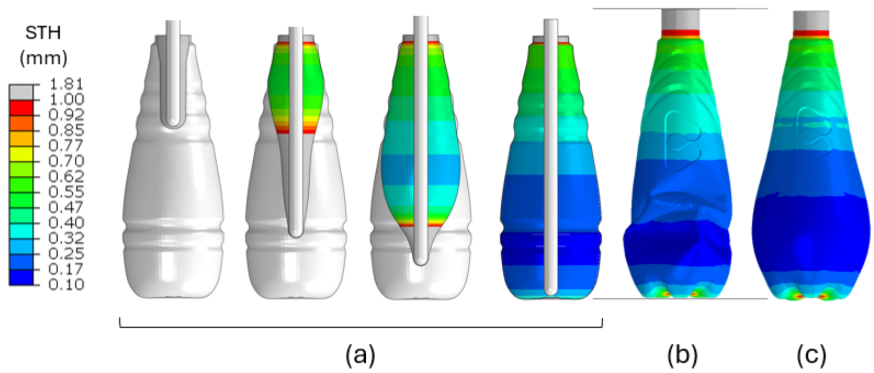


Figure 4: SBM and performance simulations for the BMT bottle.

3.2 Geometry and Process Parameterisation

The SBM simulation framework offers flexibility in tailoring preform geometry and process conditions. The geometry is parameterised following design rules [8], with the preform divided into four distinct sections: neck, taper, body, and dome (Figure 5). Each section is defined by parameters for radii (R), widths (w), and heights (h), ensuring the geometry is fully constrained. Manufacturability is integrated into the design through constraints like positive draft angles to allow easy demoulding. The temperature profile is represented using a dual Bezier curve with fixed points at the neck and tip, along with three adjustable control points. Temperature magnitudes are controlled by the neck temperature (T_n), midpoint temperature (T_m), and base temperature (T_b), while peak positions at the neck ($T_{p,n}$), middle ($T_{p,m}$), and base ($T_{p,b}$) determine the temperature distribution along the preform's length.

Processing conditions for the preblow and final blow phases are also parameterised, covering airflow variables such as preblow timing, preblow mass flow rate, and stretch rod speed, allowing for precise control of the forming process.

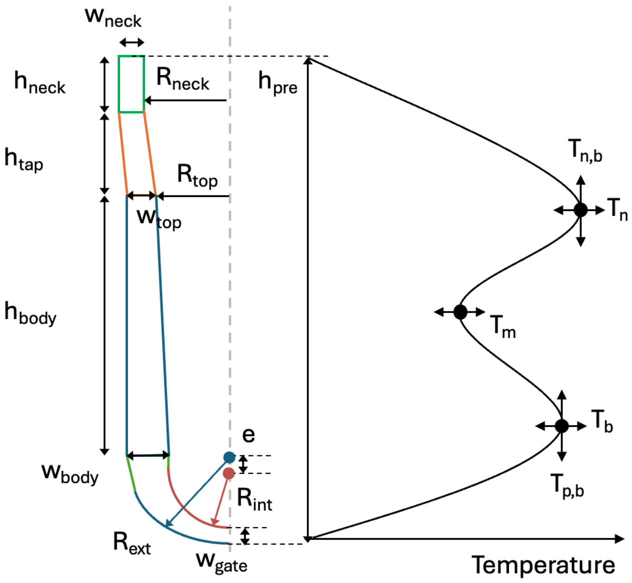


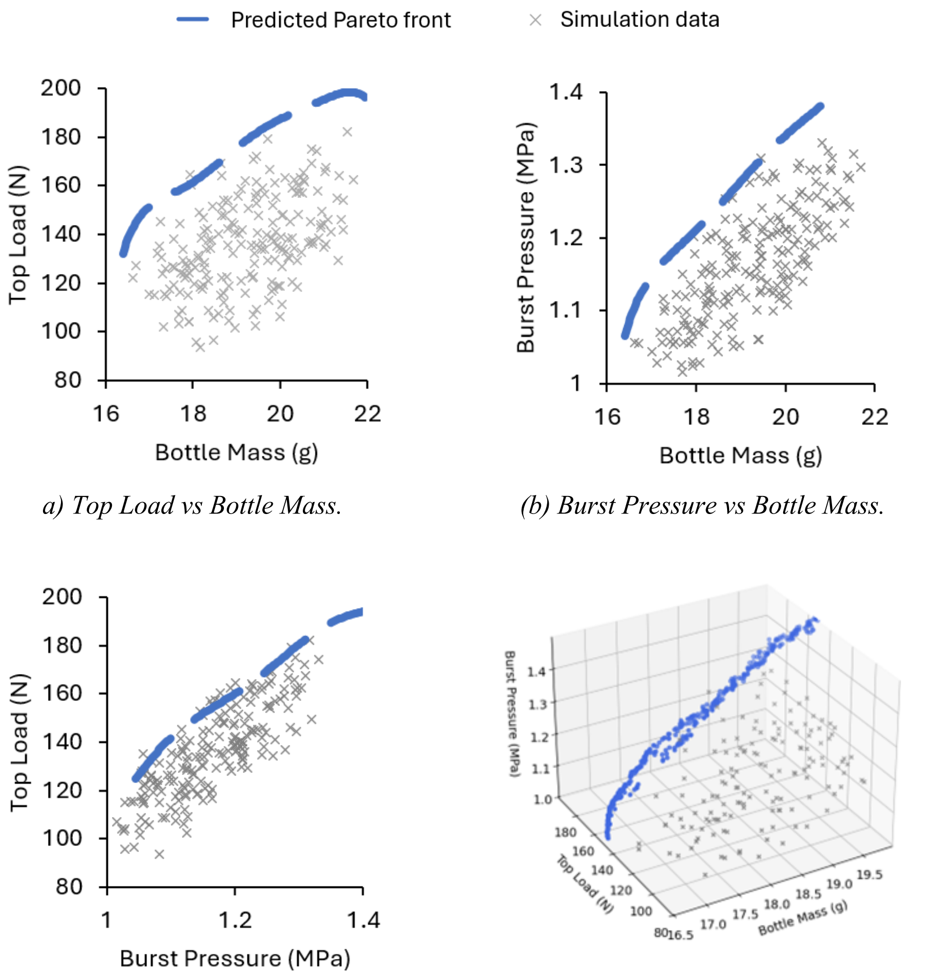
Figure 5: Preform geometry and temperature profile parameterisation.

3.3 Latin Hypercube Sampling

A Latin hypercube sampling (LHS) approach was used to create a DOE focused on reducing preform weight while exploring geometry, temperature, and process parameters. Based on sensitivity studies and historical data, key design parameters for the preform geometry and temperature profile were varied within approximately 10% to 20% of their nominal (initial) values. Latin hypercube sampling efficiently samples the parameter space by evenly distributing samples across each variable's range. This approach generated 200 unique combinations of preform designs and temperature profiles, resulting in preform masses between 16.6 g and 21.6 g. SBM simulations were performed for each combination, followed by performance simulations to evaluate burst pressure and empty top load.

4. Design Optimisation

Surrogate models, trained on simulation data using Kriging interpolation, were developed to predict top load, and burst pressure based on the geometry, temperature and process parameters with high accuracy (R^2 up to 95%). By approximating complex simulations, these models enabled rapid evaluation and optimisation. An 80/20 training and test split was used to validate the models, ensuring reliable predictions. These models were then applied in a multi-objective optimisation using an evolutionary algorithm (NSGA-II), aiming to maximise top load and burst pressure while minimising bottle mass. The optimisation process generated Pareto fronts (Figure 6a–d), illustrating trade-offs between objectives and providing non-dominated solutions for design selection. The results highlighted how mass reduction impacted achievable top load and burst pressure.



a) Top Load vs Bottle Mass. *(b) Burst Pressure vs Bottle Mass.*

(c) Top Load vs Burst Pressure. *(d) Top Load vs. Burst Pressure vs. Mass.*

Figure 6: Pareto fronts highlighting trade-offs between key metrics.

The optimisation process was guided by user-defined performance constraints of 150 N top load and 1.20 MPa burst pressure (Table 1). The lightest design meeting these requirements weighed 18.1 g and was validated through SBM and performance simulations, showing a 6.7% error in top load prediction and 1% error in burst pressure. Additionally, the preform's peak heating temperature was reduced by 5°C, lowering energy consumption during manufacturing. Compared to the initial 20.7 g preform, which achieved 205 N top load and 1.33 MPa burst pressure, the optimised design (Figure 7) maintained structural integrity with 165 N top load and 1.21 MPa burst pressure, demonstrating significant weight reduction of 13% while preserving performance.

Table 1: Performance comparison of initial and optimised lightweight design.

Preform	**Mass (g)**	**Top Load (N)**	**Burst Pressure (MPa)**
Functional Requirement	**-**	**150**	**1.20**
Initial Design (Simulated)	20.7	205	1.33
Optimised Design (Predicted)	18.1	165	1.21
Optimised Design (Simulated)	18.1	155	1.20

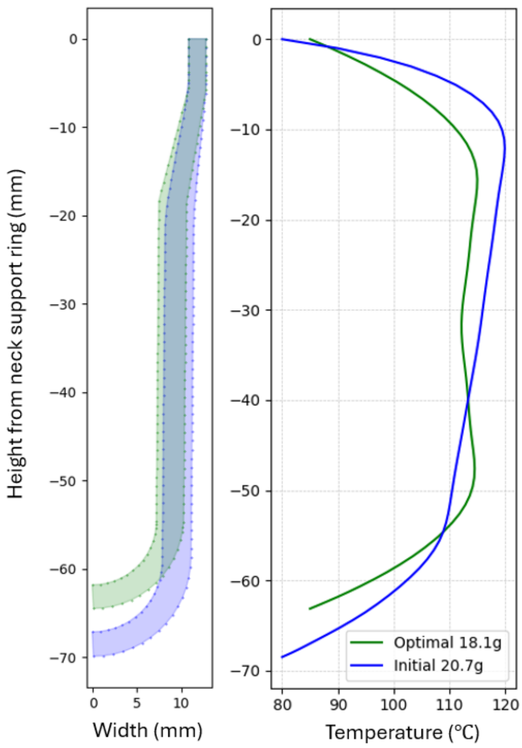


Figure 7: Comparison of initial and optimised lightweight designs, highlighting the differences between preform geometries and temperature profiles.

5. Discussion and conclusions

This study demonstrates how reducing preform mass by 13% and lowering heating temperatures by 5°C can significantly reduce the carbon footprint of bottle manufacturing. These changes not only minimise material usage but also reduce energy consumption, transportation costs, and plastic waste, contributing to lower environmental impact.

The workflow introduced in this study provides a transformative approach to accelerating sustainable bottle design. By combining simulation and surrogate modelling, it streamlines the design process while ensuring performance meets industry standards. This automated approach eliminates trial-and-error, embedding sustainability directly into the design process. As industries strive for net-zero emissions and sustainability, this workflow offers a scalable solution for improving environmental responsibility in packaging, making it a valuable tool for achieving broader sustainability goals.

6. References

[1] UNEP, ‘Beat Plastic Pollution’, UN environment programme. [Online]. Available: https://www.unep.org/interactives/beat-plastic-pollution/

[2] ‘Popping the Bottle’, UNDP. [Online]. Available: https://www.undp.org/popping-the-bottle

[3] M. Li and S. Zhang, ‘Tandem Chemical Depolymerization and Photoreforming of Waste PET Plastic to High-Value-Added Chemicals’, *ACS Catal.*, vol. 14, no. 5, pp. 2949–2958, 2024, doi: 10.1021/acscatal.3c05535.

[4] J. Nixon, G. H. Menary, and S. Yan, ‘Free-stretch-blow investigation of poly(ethylene terephthalate) over a large process window’, *Int. J. Mater. Form.*, vol. 10, no. 5, pp. 765–777, 2016, doi: 10.1007/s12289-016-1318-3.

[5] S. Yan, G. Menary, and J. Nixon, ‘A novel methodology to characterize the constitutive behaviour of polyethylene terephthalate for the stretch blow moulding process’, *Mech. Mater.*, vol. 104, pp. 93–106, 2017, doi: 10.1016/j.mechmat.2016.10.006.

[6] C. P. Buckley, D. C. Jones, and D. P. Jones, ‘Hot-drawing of poly(ethylene terephthalate) under biaxial stress: application of a three-dimensional glass—rubber constitutive model’, *Polymer*, vol. 37, no. 12, pp. 2403–2414, 1996, doi: 10.1016/0032-3861(96)85352-3.

[7] G. H. Menary, C. W. Tan, E. M. A. Harkin-Jones, C. G. Armstrong, and P. J. Martin, ‘Biaxial deformation and experimental study of PET at conditions applicable to stretch blow molding’, *Polym. Eng. Sci.*, vol. 52, no. 3, pp. 671–688, 2011, doi: 10.1002/pen.22134.

[8] O. Brandau, *Stretch Blow Molding*. William Andrew, 2016.