Modelling the Effect of Barrier Layers on the Tensile Properties of Paperboard Materials for Liquid Packaging

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Abstract. Investigations of the mechanical behaviors of the paperboard packaging materials has propelled to the forefront of the packaging industries owing to the anisotropic behavior of the paperboard materials. Paperboard materials undergo tensile forces during the creasing and folding operation. Therefore, the knowledge of the material tensile properties it is undeniably important to perform the operation without tearing the layers. Anisotropic behavior of the paperboard material is required to be addressed for the packaging material to be used effectively and efficiently. Paperboard material being anisotropic in nature have different properties in the Machine Direction (MD) and Cross Direction (CD). The paper focuses on the modelling of double layered paperboards with barrier elements either in aluminum or in Ethylene vinyl alcohol copolymers (EVOH). A numerical model of the packaging material was developed in LS-DYNA environment showing good fitting with the physical tests.

1. Introduction

The typical configuration of packaging paperboard is represented by a number of plies larger layered on each other. Each ply consists of a system of fibers, intertwined or bonded together through a chemical process. The outer plies which are composed of chemical pulp layers are generally stiffer than the inner plies that are made of mechanical pulp layers as they are softer [1]. Three main directions are typically considered in literature, namely the machine direction (MD) that concerns the fibers along the rolling direction, the cross direction (CD) referred to the fibers that lies the perpendicular direction of the ply plane with respect to MD and, finally, the through direction (ZD) that is through the abovementioned or at 45 deg with respect to the rolling direction [2]. Paperboard material are difficult to be characterized and simulated owing the anisotropic behavior and difficulty to obtain the out of plane properties of the material. Paperboard material can have up to 3 times the tensile strength in MD direction when compared to the CD direction and up to 2 times compared to the 45° [3]. As consequence of the complex material behavior, the design of all the processes to give the final shape to the packaging still represent an issue for engineers and robust and reliable tools and materials data are still missing [4].

The need to understand the paperboard mechanical behavior and the mechanisms that are activated during the deformation is increasingly demanding owing to the packaging industries which in turns require an accurate determination of the mechanical properties of the paperboard materials [5]. The previous literature available on the paperboard focuses on the prediction of in-plane properties with the tensile strength test of the material in the MD, CD and 45 deg direction: these values act as the base for obtaining the material information for the simulation material card to carry out the simulation [6]. The anisotropic behavior of the paperboard material is confirmed with the fact the tensile strength of the paperboard material in the machine direction is nearly 100% more when compared to the cross direction and also near to 50% more than the 45° direction [7].
The present paper aims at investigating the behavior of double layer ed paperboard with barrier elements either in aluminum or Ethylene vinyl alcohol copolymers (EVOH). A numerical model of the packaging material was developed in LS-DYNA environment showing good fitting with the physical tests.

2. Materials

The materials used in this study are commercially available paperboards for liquid packaging, layered respectively with (i) Ethylene Vinyl Alcohol Copolymers (EVOH) and (ii) with aluminum metal sheet. The properties of the as received materials are reported in Table 1.

Table 1. Nominal properties of the investigated paperboards.

| Properties/Weight (g/m²) | Aluminum paperboard | EVOH paperboard |
|--------------------------|---------------------|-----------------|
| Outer Polyethylene Layer | 18                  | 19.6            |
| Paperboard               | 240                 | 332             |
| Inner Polyethylene layer | 52                  | 47.3            |
| Barrier layer            | 17                  | 12              |
| Moisture %               | 6.2                 | 6.2             |
| Density                  | 570                 | 572             |

The materials thickness was investigated by using a Scanning Electron Microscope (SEM) and represented in Figure 1. From top to bottom the paperboard is made of several layers that can be identified as (i) printing inks, (ii) external Polyethylene (PE) layer, (iii) paperboard, and (IV) internal PE layer with barrier Layer. In the case of the aluminum paperboard, the layers distribution appeared similar, with the only difference of an inner aluminum layer instead of the EVOH.

3. Experimental

![Figure 1. SEM image of the paperboard cross section of the paperboard.](image-url)
The mechanical properties of the received materials were investigated by means of tensile tests, which were carried out on a MTSTM™ 322 servo-hydraulic dynamometer having a load capacity of 50kN. The specimens were cut from the paperboard with a dog-bone shape having a gauge length of 30 mm and 25 mm wide according to the ASTM D828 standard. To obtain the Lankford anisotropic parameters the paperboard was cut respectively in the MD, CD and 45 deg directions. All the tests were carried out at room temperature (approximately 20°C) and a test speed of 0.01mm/s, and repeated three times in each direction. To avoid the specimens tearing outside the gauge length, extra padding was provided by wrapping the same paper material and it was verified that no slippage happened during the tensile testing. The paperboards thickness was measured through a digital vernier caliper and validated through the SEM images, see Figure 2.

![Figure 2](image_url)

Figure 2. SEM images of the paperboards thickness: (a) aluminum and (b) EVOH paperboard.

With the aim of validation, the numerical model of the material, the following characteristics were calculated for the tensile tests:

a) in-plane tensile test in MD, CD and 45 deg direction.
b) out-of-plane shear test data,c) out-of-plane tensile test data.

The shear force is calculated with the experimental data by Nygård [8]. The experimental data were calculated based on Huang and Nygård [9]. The in-plane elastic moduli of the different paperboard material were calculated using the least fit curve method and the out of plane shear moduli were also calculated with the least fit curve method. Subsequently, the in-plane shear test data were calculated by doing the tensile test in MD, CD and 45 deg direction and then by using the Hook’s law.

### 4. Modelling

A numerical model of the tensile tests was developed by using LS DYNA [10] software. Table 2 shows the model with detail of the main properties. The paperboard was modeled by using the material card number 122: MATT_HILL_3R_3D. The boundary condition on the end nodes were defined for the tensile test to pull in one direction and rotation was restricted to simulate the tensile test conditions. The details of the thickness modelling are represented in Figure 3 in which the layers are represented.
Table 2. Main properties of the numerical model.

| Simulation Properties               |          |
|-------------------------------------|----------|
| Mesh Size                           | 0.4 μm (mixed type mesh) |
| Elements                            | PE       | Aluminum | Paperboard |
| Number of Elements                  | 1        | 1        | 2          |
| Dimension                           | 30 X 25 X 5 (mm) |

The yield model was obtained when the plasticity sets in, and Hill’s yield criteria was utilized for the present model. Hence, the yield surface was expressed in terms of stress components, $\sigma_{ij}$, according to equation

$$ f(\sigma) = \sqrt{F(\sigma_{yy} - \sigma_{zz})^2 + G(\sigma_{zz} - \sigma_{xx})^2 + M(\sigma_{xx} - \sigma_{yy})^2 + \frac{(\sigma_{xx})^2}{(\sigma_{yy})^2} + \frac{(\sigma_{yy})^2}{(\sigma_{zz})^2} + \frac{(\sigma_{zz})^2}{(\sigma_{xx})^2}} $$

(1)

where $\sigma_{ij}$ represents the initial yield stresses in the different direction and

$$ F = \frac{(\sigma_{xx})^2}{2} \left( \frac{1}{(\sigma_{yy})^2} + \frac{1}{(\sigma_{zz})^2} + \frac{1}{(\sigma_{xx})^2} \right) $$

(2)

$$ G = \frac{(\sigma_{xx})^2}{2} \left( \frac{1}{(\sigma_{zz})^2} + \frac{1}{(\sigma_{xx})^2} + \frac{1}{(\sigma_{yy})^2} \right) $$

(3)

$$ M = \frac{(\sigma_{xx})^2}{2} \left( \frac{1}{(\sigma_{xx})^2} + \frac{1}{(\sigma_{yy})^2} + \frac{1}{(\sigma_{zz})^2} \right) $$

(4)

The material starts to deform plastically once the yield criterion is fulfilled. The hardening was assumed to be isotropic, with a linear hardening modulus $H$. 

Figure 3. FEM model showing the mesh and model with different layer.
5. Results and Discussion

The values of the shear modulus were calculated as per the formulas used by Nygård (2009). The various values obtained for both the paperboard materials are tabulated in Table 3.

Table 3. Elastic constant obtained and calculated for the paperboard materials.

| Paperboard Material with Aluminum | Paperboard Material with Plastic (EVOH) |
|-----------------------------------|----------------------------------------|
| $E_x/\text{MPa}$                 | 5267                                   | 4998                                   |
| $E_y/\text{MPa}$                 | 1217                                   | 1210                                   |
| $E_z/\text{MPa}$                 | 127                                    | 187                                    |
| $G_{xy}/\text{MPa}$              | 987                                    | 921                                    |
| $G_{xz}/\text{MPa}$              | 51                                     | 48                                     |
| $G_{yz}/\text{MPa}$              | 51                                     | 48                                     |
| $v_{xy}$                         | 0.38                                   | 0.39                                   |
| $v_{xz}$                         | 0                                      | 0                                      |
| $v_{yz}$                         | 0                                      | 0                                      |

The isotropic hardening modulus, $H$, was determined from the linear slope of the curve between the yield point and the failure point of the MD tensile test. Hence, also after the experimentally observed failure point it was assumed that model had hardening modulus $H$.

Table 4. Continuum material properties for Hardening.

| Hardening and Initial yielding | Paperboard Material with Aluminum | Paperboard Material with Plastic (EVOH) |
|-------------------------------|-----------------------------------|----------------------------------------|
| $H/\text{MPa}$                | 3312                              | 2984                                   |
| $\sigma^0_{xx}/\text{MPa}$    | 38                                | 35                                     |
| $\sigma^0_{yy}/\text{MPa}$    | 12.8                              | 11.1                                   |
| $\sigma^0_{zz}/\text{MPa}$    | 12.8                              | 11.1                                   |
| $\sigma^0_{xy}/\text{MPa}$    | 24                                | 22                                     |
| $\sigma^0_{xz}/\text{MPa}$    | 3.8                               | 3.5                                    |
| $\sigma^0_{yz}/\text{MPa}$    | 3.1                               | 2.75                                   |
The stress distribution of the paperboard materials was calculated by the LS DYNA software according to the Von Mises stress theory. It was verified that the Ultimate Tensile Strength (UTS) of the paperboards was nearly equal to the values obtained from the physical testing of the materials. The paperboard material with coated barrier element as aluminum was tested and it was found that the ultimate tensile strength in the Machine Direction (MD) is $72 \pm 2$ MPa, in the Cross Direction (CD) it was measured as $40 \pm 2$ MPa and finally in the 45 deg direction it was measured to be $53 \pm 1$ MPa when it is compared to the simulated values for MD at $71 \pm 1$ MPa, for CD it was measured as $38 \pm 1$ MPa, and finally at 45 deg direction it was measured to be $51 \pm 1$ MPa. The paperboard material with coated barrier element as aluminum was tested and it was found that the ultimate tensile strength for MD is $64 \pm 2$ MPa, for CD it was measured as $30 \pm 2$ MPa and finally in the 45 deg direction it was measured to be $37 \pm 1$ MPa. When it is compared to the simulated values for MD at $64 \pm 1$ MPa, $36 \pm 1$ MPa for the CD, and finally at 45 deg direction it was measured to be $50 \pm 1$ MPa.

![Figure 4](image)

Figure 4. (a) and (b) shows the results of the numerical simulation respectively for the aluminum and the EVOH paperboard.

The results show that the values obtained from the physical and simulated methods are in conjunction and Figure 5 (a) and (b) show the comparison between the experimental results and the numerical simulations.
6. Conclusions

The present paper aims at investigating the behavior of double layered paperboard with barrier elements either in aluminum or Ethylene vinyl alcohol copolymers (EVOH). The results of the tests show that adding of coated barrier element aluminum has resulted in increase in the tensile properties of 72 (±2) MPa, as compared to other paperboard material which can be useful in packaging of high shelf materials which requires different filling conditions. The effect of plastic barriers was quite similar and there was significant difference between the tensile strength of that was recorded to be 63 (±2) MPa in MD direction.

A numerical model of the packaging material was developed in LS-DYNA environment. The material was modeled by using the material card number 122: MATT_HILL_3R_3D. The comparison with the experimental results, carried out in terms of stresses show a good fitting, demonstrating the capabilities of the software to simulate the material behavior.

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