Numerical optimization approach to modelling delamination and buckling of geometrically constrained structures

BY G. MULLINEUX1,*, B. J. HICKS1 AND C. BERRY2

1Department of Mechanical Engineering, University of Bath, Bath BA2 7AY, UK
2Pira International, Leatherhead KT22 7RU, UK

Understanding what happens in terms of delamination during buckling of laminate materials is of importance across a range of engineering sectors. Normally concern is that the strength of the material is not significantly impaired. Carton-board is a material with a laminate structure and, in the initial creation of carton nets, the board is creased in order to weaken the structure. This means that when the carton is eventually folded into its three-dimensional form, correct folding occurs along the weakened crease lines. Understanding what happens during creasing and folding is made difficult by the nonlinear nature of the material properties. This paper considers a simplified approach which extends the idea of minimizing internal energy so that the effects of delamination can be handled. This allows a simulation which reproduces the form of buckling–delamination observed in practice and the form of the torque–rotation relation.

Keywords: delamination; buckling; minimum energy method; cartons; carton-board

1. Introduction

Advances in manufacturing and materials have led to interest in the performance of materials and in particular composite materials and the potential effects of delamination under buckling [1–3]. A variety of analysis techniques have emerged, mainly based on finite-element methods.

When designing a structure, the engineer is usually interested in ensuring that strength is not adversely affected by delamination. There is, however, an application in which delamination to weaken a structure is actively encouraged. This is when carton-board is used to package fast moving consumer goods (FMCG) such as food products. Carton-board is produced by building up layers of fibres and hence is formed as a layered structure.

Cartons are usually produced from sheets of board which are initially printed and cut in the correct two-dimensional shape (net) by a company called a carton converter [4]. They are then taken to the user company (which is going to pack

*Author for correspondence (g.mullineux@bath.ac.uk).

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the product) in this two-dimensional form as this simplifies transportation. Each carton, therefore, has to be ‘erected’ into its three-dimensional form so that product can be introduced and the carton closed and sealed. This needs to be carried out at high speed. In order to ensure that the carton erects correctly, ‘creases’ are formed in the carton net by the carton converter. This has the effect of causing some delamination along the line of the crease as well as some initial deformation. During erection, the board naturally folds along this line of weakness and more delamination takes place. Ensuring that the crease is correctly formed so that good folding takes place (without splitting occurring) poses a challenge for carton converters. In particular, it is necessary to decide the appropriate depth and width of the initial crease for a given material and carton net.

It follows that there is interest in understanding what happens during the creasing and folding process, and how the properties of the board can be modified [5]. A number of empirical and computer studies have been undertaken. These have mainly concentrated on the torque needed to fold along a pre-defined crease [6–8]. If the behaviour for a single crease is known, then the forces needed to erect a complete carton can be determined [7,9,10], and the motion of more general paper-based structures can be investigated [11].

The interest of this paper is in representing the folding operation in a simplified way in terms of a collection of nodes running along the layers of the board. In the folding process, certain parts of the board are held fixed and others are forced to move. By considering states of minimal internal energy for the nodes, the motions of these can be simulated [12,13]. This type of approach has also been used to represent motions in layered geological structures [14].

The next section gives background information on the production and properties of carton-board and §3 considers the form of typical results of measuring the torque required to fold along a crease. The minimal energy formulation is discussed in §4 for layered structures with no adhesion between the layers, and the resultant model, based on numerical optimization, is given in §5. Section 6 considers how this can be extended to deal with the case where the layers are (partially) attached and delamination can occur. The results are discussed in §7 and conclusions presented.

2. Cartons and carton-board

Cartons are typically small- to medium-sized cardboard boxes made from carton-board material produced in a range of styles [15]. Folding cartons are one of the most popular methods of packaging available and are commonly used for all manner of FMCG. The popularity of cartons is due to their low weight and price compared with alternative methods of packaging. Unlike many other packaging methods, cartons can be economically produced in large or small batches, have a small environmental impact, and can be easily recycled or composted.

Carton-board materials are usually 250–1000 µm thick and consist of a number of layers or plies of cellulose fibres, plus a mineral coating which is used to provide a suitable surface for printing. The most commonly used cartoning materials are paper-boards, with modern materials being typically composed of three plies plus a mineral coating on the outer surface. The types of board produced are designed to fulfil a wide variety of applications and are available in a range of different
compositions, thicknesses and surface finishes. This allows carton producers and users to select a material that best suits the packaging required for their product.

Carton-board, like paper, is produced by forming a network of hydrogen-bonded cellulose fibres. At the start of production, these individual fibres are held in a suspension of almost 100 per cent water, which is then sprayed onto a forming wire, through which much of the water is drawn away. This high degree of dilution causes the fibres initially to be randomly oriented yet evenly distributed across the web (the continuous sheet of material formed on the paper machine). As the web is drawn through the machine, tension causes the web to stretch and this results in the fibres becoming more highly oriented in the direction of travel. This leads to significant differences in properties in the machine direction and cross direction (cf. [13]). With multi-ply boards, additional plies can either be formed on top of each other, or produced on separate wires which are then brought together before passing through a number of processing sections which dry, smooth, consolidate and coat the web.

After production of the board, the main stages in the creation of cartons are: conversion in which the board is cut and creased to create the main two-dimensional net of the carton; and filling where the carton is ‘erected’ into its three-dimensional form by folding along the pre-defined creases, product is introduced and the carton is closed and sealed.

Figure 1 shows the stages in the creation of cartons. Materials used for carton production are usually supplied from the board producer in sheet or reel form (part 1 of figure 1). They are typically sent to a carton converter who performs all the necessary steps required to produce a flat empty carton from the supplied board material. The first process is printing (part 2) in which the final design for the carton is applied to several carton nets on a single sheet.

The next operation is creasing and cutting (parts 3 and 4). Creasing involves pressing a metal edge (rule) onto the surface of the board causing it to deform. This is normally performed in an intermittent motion platen style press, into which a set of dies is mounted. Each die also holds cutting blades (as well as creasing rules) which separate each net from the main sheet.

The separate carton nets are then stacked (part 5), packed (possibly stored) and transported (part 6) to the company which uses the cartons to pack its products. When used, each carton is initially partially erected by machine (part 7), product is inserted (part 8) and the carton closed (part 9).

The objective of creasing is to form localized regions of lower board stiffness along the lines of fold [16] so that when the carton is subsequently folded into shape, the panels of the carton fold along the creases resulting in the carton forming with its intended shape and dimensions. The creases are obtained by creating permanent deformation in the board by means of forcing a radius-edged rule into the outer liner of the board which forces the inner liner into a cavity on the opposite side of the press (figure 2). This action leaves an impression of the rule on the outer liner and a raised rib on the inner liner.

The creasing rule and its corresponding cavity are shown as the crease is formed in figure 2. The creasing rule and cavity must be carefully selected to ensure that their combined height provides the required crease depth at the bottom of the stroke. The forces generated during creasing mean that the board plies and coating must be able to withstand the compressive and tensile loads involved, without excessive damage occurring.
Figure 3a shows the form of a section of board after the formation of a typical crease. The board is turned over compared with figure 2 so that the rib and groove of the crease point upwards. When folding takes place, it is in the directions of the arrows so that additional delamination is encouraged and the rib grows, as suggested in figure 3b. As this happens, the original groove ‘straightens out’ forming the roughly circular corner on the outside of the carton; the rib lies within the erected carton.
A common method [17] for determining suitable crease settings for a given material involves a visual assessment of the creases before and after folding for a range of settings.

An acceptable crease shows no external damage. However, internally some fibres and bonds are broken, owing to the elongation of the inner plies at the rib and outer plies at the edges of the rule impression. Despite the elongation of the board required to force it into the cavity, the fibre density of the board is increased at the edges of the crease owing to the compressive shearing action of the rule forcing the material into the cavity. In addition to the visual assessment of the folded crease, another standard test [18] can also be used to investigate the properties of the crease as it is folded.

3. Crease folding

A crease’s resistance to folding is typically recorded as the maximum torque and the angle at which it occurred. This is measured using a two point bending test.
Figure 4. Example torque–angle graphs: A based on Dai & Cannella [7], B based on Sirkett et al. [19], C and D based on Berry [20].

during which the test crease is folded through 90°. This property is of interest because the crease’s stiffness can be used to monitor and predict the performance of the carton through production operations.

A number of forms of torque–angle graphs have appeared and some of these typical forms are shown in figure 4. The variations are due to the type of board used, the form of the crease and the orientation of the material—whether the board is aligned in the machine or cross direction. As the interest here is purely in the generic form of the torque–angle relation, the graphs in the figure have been scaled in the vertical direction so that they fit conveniently together.

There is similarity between the graphs. Each has an initial rise and a flattening off (or even a decrease away from a peak occurring at an angle around 30°). During this process, some elastic deformation takes place and permanent damage in terms of further tearing apart of the layers occurs.

Figure 5 shows images of a crease during the folding process. As the angle of fold increases, the groove in the outer liner of the board, caused by the impression of the creasing rule, straightens and takes up a tensile load. This counteracts the compressive load, which arises in the centre and inner plies of the board owing to bending. The raised rib on the inner surface of the board then encourages the centre and inner plies to buckle and fully delaminate into the fold. This reduces the torque required to fold the board and prevents the outer liner from splitting. The folding torque increases as the angle increases. Most of the damage that occurs during folding involves the breaking of inter-fibre bonds through delamination within and between the plies and through bending. Some fibres are also broken but these are usually far stronger than their inter-fibre bonds.
4. Energy formulation

This section discusses an internal energy formulation for a nodal representation of a layered system. Consider a bending beam of elastic material of cross-sectional area $A$, second moment of area $I$ and Young’s modulus $E$. When this bends, it stores potential energy owing to bending and to stretching (or compression) in the axial direction. This energy $U$ is given by the following expression [12]:

$$U = \int \frac{1}{2} EI \kappa^2 \, ds + \frac{1}{2} EA \epsilon^2 \, s = U^{(b)} + U^{(s)}, \tag{4.1}$$

where $\kappa$ is curvature and $\epsilon$ is axial strain. The energy is the sum of the ‘bend energy’ $U^{(b)}$ and the ‘stretch energy’ $U^{(s)}$. (The original expression for $U^{(s)}$ involves an integral in the same way as $U^{(b)}$, but with the assumption that the strain is uniform; this can be evaluated leaving the expression given involving the total length $s$.)

Now consider material that is composed of a number of layers. Each layer in the material is represented by a number of nodes. For convenience, these are taken to be equally spaced with the same number of nodes in each layer. When this system is deformed, three forms of change for the layers are considered: they can bend; they can stretch (or compress), axially along their own length; and they can compress, across the thickness of a layer. Compression is regarded as being positive when the thickness of a layer is being reduced by the action of the other layers. It is assumed that compression cannot be negative: when this happens the layers start to separate (delaminate).

The nodes are assumed to be points in the neutral axis (under bending) of each layer. As the nodes lie in a single line in a layer, they cannot capture the full bending effect. Instead, for each node, the bending effect for its local region is used. The deformed geometry of the nodal array allows three ‘components’ of internal energy to be found. Deformation is only considered in two dimensions; it is assumed that the same effects happen across the width of the layers.

The nodes are allowed to move. Let $\mathbf{r}_{i,j}$ denote the position vector of the typical node, with the $i$ subscript running along the length of the layers (the axial direction) and the $j$ subscript across the layers (the transverse direction).
These position vectors are used for the typical configuration during simulation. The starting positions before movement takes place are denoted by \( r_{i,j}^{(0)} \).

A measure of internal energy is defined for any deformed configuration as now discussed. It is assumed that the system settles to a configuration in which this measure is minimized.

The strain at each node can be found in the axial and transverse directions. In the axial direction, there is a strain on either side of a node. These strains are as follows:

\[
\varepsilon_{i,j}^{(a-)} = \frac{|r_{i,j} - r_{i-1,j}| - |r_{i,j}^{(0)} - r_{i-1,j}^{(0)}|}{|r_{i,j}^{(0)} - r_{i-1,j}^{(0)}|}
\]

and

\[
\varepsilon_{i,j}^{(a+)} = \frac{|r_{i,j} - r_{i+1,j}| - |r_{i,j}^{(0)} - r_{i+1,j}^{(0)}|}{|r_{i,j}^{(0)} - r_{i+1,j}^{(0)}|}.
\]

During deformation, care is needed to try to ensure that nodes which are initially adjacent transversely remain so. Distance \( d_{i,j}^- \) is defined as the distance from node \( r_{i,j} \) to the next layer, that is the sequence of nodes with second subscript \( j + 1 \). This is determined by finding its distance to the line segment joining each pair of nodes in this second layer and finding the minimum. The distance is regarded as being positive when the node lies on the same side of the sequence as in the original configuration. Distance \( d_{i,j}^- \) is defined similarly with respect to the adjacent layer with second subscript \( j - 1 \). (These distances are taken to be zero when the node lies on the edge of the array and there is no appropriate adjacent layer.)

The strains in the transverse direction are given by the following expressions. These allow for the fact that if layers separate so that the strain would be positive, then it is taken to be zero.

\[
\varepsilon_{i,j}^{(t-)} = \begin{cases} 
0 & \text{if } d_{i,j}^- > |r_{i,j}^{(0)} - r_{i,j-1}^{(0)}| \\
\frac{d_{i,j}^- - |r_{i,j}^{(0)} - r_{i,j-1}^{(0)}|}{|r_{i,j}^{(0)} - r_{i,j-1}^{(0)}|} & \text{otherwise}
\end{cases}
\]

and

\[
\varepsilon_{i,j}^{(t+)} = \begin{cases} 
0 & \text{if } d_{i,j}^+ > |r_{i,j}^{(0)} - r_{i,j+1}^{(0)}| \\
\frac{d_{i,j}^+ - |r_{i,j}^{(0)} - r_{i,j+1}^{(0)}|}{|r_{i,j}^{(0)} - r_{i,j+1}^{(0)}|} & \text{otherwise}.
\end{cases}
\]

The curvature \( \kappa_{i,j} \) in the axial direction at the typical node can be approximated from the positions of it and its two neighbours. This is based on the Frenet–Serret formulae using finite difference approximations \( D_1 \) and \( D_2 \) for the first and second derivatives:

\[
\kappa_{i,j} = \frac{|D_1 \times D_2|}{|D_1|^{3/2}},
\]
where
\[
D_1 = \frac{r_{i+1,j} - r_{i-1,j}}{2h},
\]
\[
D_2 = \frac{r_{i+1,j} - 2r_{i,j} + r_{i-1,j}}{h^2}
\]
and
\[
2h = |r_{i,j} - r_{i-1,j}| + |r_{i+1,j} - r_{i,j}|.
\]

The three ‘components’ of energy can be found for each node. The first is that owing to bending, as in equation (4.1):
\[
U_{i,j}^{(b)} = \frac{1}{2} EI a_{i,j} k_{i,j}^2,
\]
where
\[
a_{i,j} = \frac{1}{2} |r_{i+1,j} - r_{i-1,j}|
\]
is the original length of an element centred on the node.

The next energy component is that owing to stretch in the axial direction, equation (4.1):
\[
U_{i,j}^{(s)} = \frac{1}{4} EA \left[ (\epsilon_{i,j}^{(a+)} - r_{i,0}^{(0)} - r_{i+1,j}^{(0)} + (\epsilon_{i,j}^{(a-)} - r_{i,j}^{(0)} - r_{i-1,j}^{(0)} \right].
\]

The third component represents compression across the thickness of the strip:
\[
U_{i,j}^{(c)} = \frac{1}{4} Ea_{i,j} w \left[ (\epsilon_{i,j}^{(t+)} - r_{i,j+1}^{(0)} + (\epsilon_{i,j}^{(t-)} - r_{i,j-1}^{(0)} \right],
\]
where \(w\) is the width of the strip.

These expressions simplify when it is assumed that the nodes are uniformly spaced in their initial state. Let \(a\) denote their distance apart along the length of each strip, and let \(w\) and \(t\) be the width and thickness, respectively, of the rectangular section of each layer. Then the cross-sectional area \(A\) and second moment of area \(I\) of the layers become
\[
A = wt \quad \text{and} \quad I = \frac{wt^3}{12}
\]
and the components of energy are as follows:
\[
U_{i,j}^{(b)} = \frac{1}{24} Eawt^3 k_{i,j}^2,
\]
\[
U_{i,j}^{(s)} = \frac{1}{4} Eawt \left[ (\epsilon_{i,j}^{(a+)} - (\epsilon_{i,j}^{(a-)} \right]
\]
and
\[
U_{i,j}^{(c)} = \frac{1}{4} Eawt \left[ (\epsilon_{i,j}^{(t+)} - (\epsilon_{i,j}^{(t-)} \right] .
\]

5. Numerical model

The idea of minimizing these forms of internal energy has been investigated. The numerical model used works with a rectangular array of points representing the region of the crease. Its layers are regarded as being the ‘rows’ of the array and

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each ‘column’ provides a line across the thickness of the material. Two additional columns, one at each end, are also introduced. This is partly so that the finite difference operations are always applicable in their symmetric form. It also enables the end positions and directions of the layers to be specified.

For given end conditions, the model seeks to move the remaining nodes to a configuration of minimal internal energy. This is carried out iteratively. For a given trial position of the nodes, the separations between them are calculated. From this, the three components of internal energy are found and combined. An optimization procedure is used to revise the positions of the internal nodes so as to minimize this combined value. Any of the standard optimization methods can be used. For the examples presented here, the method of conjugate gradients has been used [21]. This method was selected as it is a direct search method (not needing derivative information) and has been shown to be appropriate for related engineering problems [14].

Given the large number of degrees of freedom that are involved, the possibility of non-convergence or instability in the search process exists. Additionally, there are a number of different local minima. To try to avoid such issues, the approach used is to start in a known good configuration (such as the undeformed starting position) and then approach the required end conditions in gradual steps. Intermediate positions between the start and the required end ones are obtained by interpolation. Then minimal configurations for each of these intermediate stages are found in turn and each is then used as the starting configuration for the next.

Figure 6 shows stages in the motion obtained using this minimum energy approach. The nodes at the left end are held fixed and those at right are moved along an upward curving path and are rotated in the process. It is seen that the layers gradually separate as the motion progresses. A previous study [12] has shown good agreement with a finite-element model of the same situation and empirical tests carried out with strips of flexible material.

6. Incorporating delamination

The approach of the previous section deals with individual layers which are essentially assumed to be separate. This is not initially the case with carton-board. The layers are attached and while deformation takes place, they may locally become detached as delamination occurs. The aim of this section is to make allowance for the onset and progression of delamination so as to be able to represent what happens when folding takes place around a pre-defined crease.

When delamination occurs, the work done by the folding torque is partly used to separate the layers. What is required is a suitable measure of this work. It is assumed that delamination of carton-board occurs principally because of shearing

Figure 6. Simulation of bending of a layered structure.
between the layers [22,23]. As the layers move across each other, the inter-layer fibres distort and are broken causing the layers to become detached and hence able to move apart.

With the nodal model, the shear is measured in terms of internal angles. The node at position \( r_{ij} \) has (up to) four neighbours as shown in figure 7. There are associated four internal angles \( \alpha_k \), for \( 1 \leq k \leq 4 \), as shown in the figure (whose sum is \( 2\pi \) radians).

The work done against shearing is assumed to depend on the changes in these angles. If \( \alpha_k^{(0)} \) is the value of the angle in the initial state, then define

\[
 w_k = \begin{cases} 
 B \left( \frac{\alpha_k - \alpha_k^{(0)}}{T} \right)^2 & \text{if } |\alpha_k - \alpha_k^{(0)}| \leq T \\
 B & \text{if } |\alpha_k - \alpha_k^{(0)}| \geq T,
\end{cases} \tag{6.1}
\]

where \( B \) is a constant of proportionality, \( T \) is a threshold value for the angular change at which tearing has fully occurred, and the presence of the squared term ensures that there is no sudden motion away from the initial configuration. The measure of the delamination work done at the node is then formed as an average:

\[
 W_{ij}^{(d)} = \frac{1}{4} (w_1 + w_2 + w_3 + w_4). 
\]

Suitable adjustment is made in the case of nodes lying on the top or bottom layers. The total work \( W^{(d)} \) is then the sum of these values over all the nodes.

The previous energy model is now used to deal with folding of carton-board along a crease. It is only the recoverable internal energy that is minimized (as before). The work done in delaminating is assumed to be lost and, for any position
of the ends, the system settles to minimize the recoverable energy. The initial configuration of the nodes is that shown in the upper left of Figure 8. The region represented is simply that around the crease itself. As before the sets of end nodes are used to provide the end conditions and it is assumed that the region of delamination does not extend to these. The end nodes on the left in the figure are held fixed. Those on the right are driven to rotate about an axis representing a typical folding operation. In practice, the right-hand end is able to extend. So the block of right-hand nodes is allowed to slide along a radial line from the axis and the distance moved is used as an additional degree of freedom in the search process (together with the positions of the internal nodes as before).

The configuration with the initial crease is used as the starting point from which to measure the delamination work $W^{(d)}$ and so defines the start angles $\alpha_k^{(0)}$ used in equation (6.1). In doing this, the work done during creasing to cause the initial delamination is ignored. The rationale for this is that there is time between the initial creasing and the actual folding for the material to recover, and there is evidence [24] that over a long period changes in ambient temperature and humidity can cause carton-board to ‘lock’ into a deformed position.

Figure 8 shows the results of simulation as the crease is folded through $90^\circ$. It is seen that the inner layers buckle inwards as the fold angle increases in the same way as layers of the physical example shown in Figure 5. The initial geometry used for the simulation represents the minimum displacement found to be necessary to ensure that delamination occurred during the subsequent simulation. This
The solid curves in figure 9 are graphs of the work done in delamination and the stored internal energy (which is dominated by the energy owing to bending $U^{(b)}$). The delamination curve rises more steeply initially and then flattens as the various nodes reach the threshold angle at which complete shear-delamination is assumed to have taken place. The internal energy varies quadratically as its various parts depend on the squares of the relevant changes. The sum of the two graphs gives the total work done on the system as folding takes place. Since this is the integral of the product of the applied torque and the angle of rotation, its derivative with respect to the angle gives a representation of the torque. This is shown by the solid curve in figure 10.

The dashed curve in figure 10 shows the effect of reducing the threshold value associated with the shear angles. The corresponding delamination work is given by the dashed curve in figure 9. The reduction in the threshold means that full delamination occurs sooner. The graph of the delamination work rises more steeply initially, and this results in the initial sharp rise in the torque curve. The earlier flattening out of the delamination work leads to the drop in the torque seen after the first peak.

Figure 9. Delamination work and internal energy during folding.

This corresponds to what is found in practice with a real crease: if the crease depth is too small then no buckling–delamination occurs during bending and the crease acts like a simple hinge.
7. Discussion

Folding tests were performed using a test rig designed to fit into a universal tensile tester. The rig is shown in figure 11 with a schematic diagram of it given in figure 12. It consists of a flat plate fitted with an adjustable clamp and a rotating arm which is fitted with a bar that can be moved along the arm. The clamp holds a creased sample of carton-board against the flat plate and allows the crease to be aligned with the axis of rotation of the arm. The bar attached to the arm can then be used to push against the free side of the creased sample, causing it to be folded. This folding action is driven by a tensile tester which measures the folding force during the rotation of the arm.

The results shown as C and D in figure 4 are typical of the results obtained with the rig.

Comparison of figures 4 and 10 shows that the numerical model produces torque–angle graphs of the appropriate form. Furthermore, when the threshold for the effect of shearing is reduced, the numerical model shows the decrease in the torque that is required after the initial folding. This dip has been found to occur frequently in test results. The relation to the reduction in the threshold value suggests that the decrease in torque is a result of greater material damage occurring during the initial creasing.

There are naturally some limitations with the use of the numerical model. In particular, there are a number of local minimal energy configurations at each stage of folding. The sudden jumping between such states is likely to be the cause of the oscillations evident in the graphs of figure 10.
8. Conclusions

An energy formulation together with numerical optimization has been used to represent the behaviour of fully or partially geometrically constrained laminate structures. The layers are represented by nodes along their lengths, and the internal energy is considered in terms of axial stretching, bending and compression of the layers. This formulation has been extended to incorporate prediction of delamination based on consideration of the shear occurring between the layers. This allows a more complete representation of physical phenomena.
The approach has been applied to the case of carton-board used in the production of cartons. To allow successful erection of cartons into their three-dimensional forms, creases are introduced to the flat net. These cause initial weakening of the board and so encourage correct folding during erection. The numerical approach has been seen to give the appropriate buckling motion of the inner layers of the board. It also generates relations between the driving torque and fold angle of the form measured empirically. In this way, the model provides insight into how the magnitude and extent of shear influence the folding performance of cartons.

The results show how the torque characteristics can vary significantly with the shear parameters. In particular, they show that a drop in the required driving torque can occur after its initial rise. This effect has also been observed experimentally and the model suggests that it occurs when greater damage is induced in the carton-board during initial creasing. Although the aim was not to investigate the effect of the size (and geometry) of the initial crease, the simulation has confirmed the observation made in practice that insufficient crease depth results in no additional delamination during bending leading to poor fold formation.

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