Modeling the mechanical behaviour of some complex polymeric materials by relying on the nonlinear capability in Abaqus.

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Abstract: Polymeric materials are complex in their mechanical behaviour; inter alia, they exhibit large strain, anisotropic and irreversible response which is often accompanied by stable localized necking behaviour. When developing suitable computational models for such materials, one cannot do this without the underlying support of a FEM program that offers inherently non-linear solution capabilities.

Within Dow there has been some internal activity, concerned with the development of such a polymeric material computational model. Excellent agreement has been obtained in modeling simple tension tests of linear low density polyethylene (LLDPE) and polyethylene terephthalate (PET) films. In addition to showing the results of these model calibrating efforts, in the case of the LLDPE film, some simulation results from application areas for the developed model are presented. These application areas typically come from within advanced, flexible packaging applications where minimum usage of material has an environmental benefit. The severe deformation and generally complex behaviour able to be captured by the model, highlights how indispensible the core capabilities of Abaqus were in developing the Dow modeling capability.

Keywords: *Abaqus, Polymers, Consumer Packaging, Anisotropic, Necking, Non Linear, Fracture, Environmental, Wastage, Plastic*

1. Introduction

Modern polymers offer many advantages; this is especially true in consumer packaging applications. We, as consumers, have become accustomed to purchasing products that are well-protected from damage and/or appear attractive in see-through packaging. For products that may spoil, such as fruit and vegetables, remaining fresh on the shelves for a very long time is an advantage; less has to be discarded by the retailer and this in itself represents an environmental benefit. In both the developed and developing world ca. one-third of all plastics consumption goes into packaging. So, any reduction in ***wastage*** of packaging material would have a direct and beneficial impact on the environment. Much of packaging design and even material specification contains a significant trial-and-error component, relying heavily on the accumulated experience of those involved along the value-chain. Finite Element Method simulation can clearly enable new and economical possibilities in packaging design to be studied in advance, coupled to material specifications that are perhaps better-suited to resisting the externally-imposed environmental loads. Correctly applied and meaningful simulation can help reduce wastage and have a positive economic benefit for and on the environment. A generic packaging FEM example, with some important details for subsequent Abaqus analysis highlighted, is shown in Figure 1.

For the Finite Element Method simulation to be useful as a design aid, the material properties themselves must be meaningfully integrated into a computational model to the level of detail required of the analysis prediction; the computational model must enable the ***real materials*** to be represented. This is no easy task, since the challenges and complications are tough and many; some of these are noted in the following non-exhaustive list:

1. The computational model must deal with severely non-linear behaviour (thin films, very flexible, large strains of ca. 800%, ***with a large permanent plastic set*** and oftentimes exhibiting local material instability).
2. Failure and fracture needs to be represented in order to investigate misuse scenarios or intentional separation.
3. Individual films are laminated together, thus requiring a shell-type model; there is internal interaction between film layers via internal adhesive layers; all of these constituents have differing individual responses.
4. Film orthotropic behaviour needs to be sensibly modeled – not only in the film's small strain response.
5. A real laminated structure has imperfections, together with some mostly-unknown levels of internal stress.
6. There are theoretical shortcomings that have an impact on what can and cannot be modeled.
7. Often one is missing test data – this is usually why a simulation is required, else the test would suffice.

8. The analyst is usually severely time/resource constrained and cannot easily perform material model development and real problem analysis at the same time, unless the materials are very simple to describe.

Within Dow there has been an internal initiative to develop suitable material computational models for solving thin film, laminated structures using polymeric materials. Our initial candidate materials have been linear low density polyethylene (LLDPE) and polyethylene terephthalate (PET). The intent of the paper is not to discuss the detailed computational model development – this is proprietary to Dow, but rather to illustrate some of the analysis possibilities that are enabled by such a model. The paper shows some results from tensile test calibration of the developed model in the case of the far more-challenging LLDPE film and also some detailed applications thereof; we solve a pouch-dropping problem to demonstrate an intended future use, as well as a real-life bag handle application.

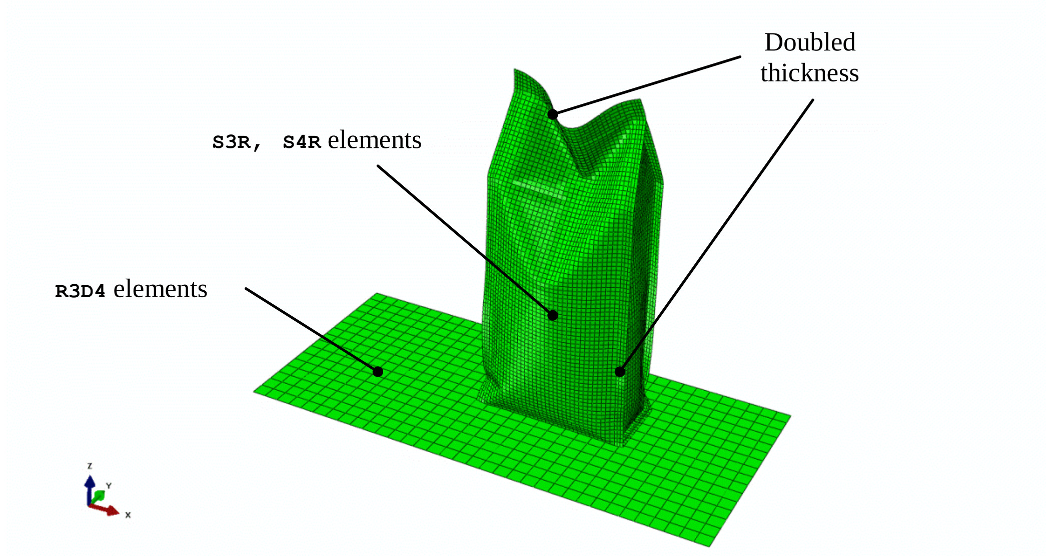


Figure 1. A FEM example of a modern, flexible package made from laminated polymeric materials.

2. Overview of pertinent capabilities offered by Abaqus

Abaqus has, in its suite of capabilities and procedures, much of what is required to solve our problem; our analysis requirements are listed in the Introduction. At its ***core***, Abaqus is a non-linear code; it is not a linear code that has some added-on features of non-linearity. In order to deal with failure and fracture during the rapid event of a bag impacting the floor, Abaqus/Explicit is used as the analysis development code.

Polymeric films are usually designated as having MD-orientation or CD-orientation; these mnemonics refer to the machine direction and cross-direction, respectively. The mechanical response is generally different along these directions and the nomenclature stems from the processes used to manufacture these films – they're typically manufactured on a blown film line in the case of LLDPE and cast film line in the case of PET. It is relatively-straightforward to specify such a composite shell, as illustrated in Figure 2, using the keyword-form:

```
**
** Define the LAMINATED Shell wall
**
*SHELL SECTION, ELSET = ALL_ELEMENTS, COMPOSITE,
ORIENTATION = REFERENCE_ALIGNED
<LLDPE_Shell_Thickness>,5,Material_DOWLEX_VUMAT,0.0,SHELL_LLDPE
<PET_Shell_Thickness>,5,Material_PET_VUMAT,0.0,SHELL_PET
**
```

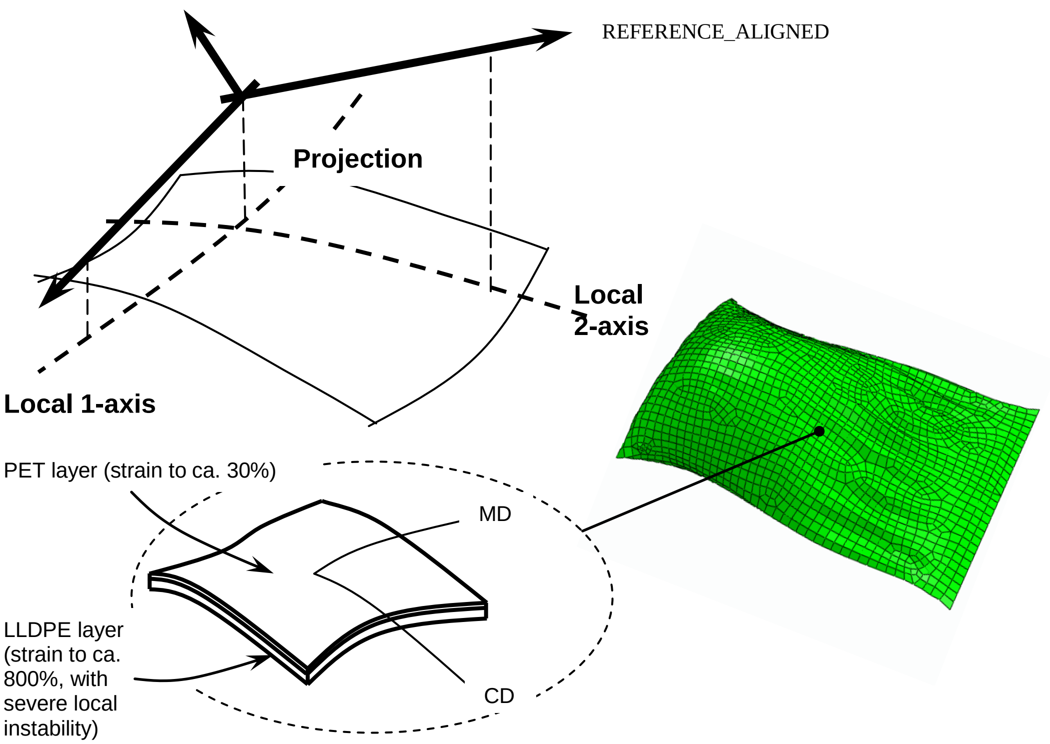


Figure 2. An example of using the projection of axes when specifying a laminated orthotropic film structure making up a pillow-pouch wall.

The alignment of the material is generally along some "axis" of the bag; in the case of a non-structured mesh it is not easy to specify these material orientations across the complicated mesh; Abaqus offers help here, in that the projections onto the shell surface from the REFERENCE_ALIGNED system, as illustrated in Figure 2, are used. Care must be exercised here – the projection swops around when the angle between the local element normal to the surface and the newly defined system with the axis labeled REFERENCE_ALIGNED is $\leq \cos 0.1°$ - see for example, in the case of small-strain shells, Sec. 3.6.3 in the Abaqus Theory Manual (Simulia, 2013).

Abaqus offers some considerable extensibility in its providing an interface, enabling the FORTRAN (or C) coding of material behavior falling outside that already represented in the material library. The keyword-form for invoking this is:

```
*MATERIAL, NAME = MATERIAL_DOWLEX_VUMAT
*DEPVAR
11
**
** Optional data lines to ease output interpretation
**
*USER MATERIAL, CONSTANTS = 7
<Material_DOWLEX_1>,<Material_DOWLEX_2>,<Material_DOWLEX_3>,
<Material_DOWLEX_4>,<Material_DOWLEX_5>,<Material_DOWLEX_6>,
<Material_DOWLEX_7>
```

The User Subroutine is called at every material point during the analysis and updates the stress tensor and the material state variables (11, in this case), from their initial values and from the kinematic increments passed into the routine. The User Subroutine then defines the generally complex behavior of the material that needs to be adequately represented.

Content-filled packages can be relatively-easily analyzed using the Eulerian or SPH analysis capability. The "Impact of a water-filled bottle" analysis example, documented as Problem 2.3.2 in the Abaqus Example Problems Manual (Simulia, 2013) illustrates the procedure very well for an analyst unaccustomed to dealing with these problems.

Geometric imperfections can be included by perturbing the perfect mesh with some fraction of the eigenmodes of the structure/package; these are first extracted in a frequency step in Abaqus/Standard. The general workflow, for an imperfection-seeded dropping of a package/structure onto the floor, in keyword-form is as presented below. Initial stresses can be included as initial model data; however the specification of this is less than trivial for a real bag or pouch structure.

2.1 Extracting frequencies

```
*HEADING
Extracting Layered Frequencies
*INCLUDE, INPUT = BAG_MODEL.INP
*STEP, NAME = EXTRACT_FREQUENCIES, PERTURBATION
*FREQUENCY, EIGENSOLVER=LANCZOS, NORMALIZATION=DISPLACEMENT
, <begin_frequency>, <last_frequency>, , ,
*NODE FILE, MODE = <BEGIN_MODE>, LAST MODE = <LAST_MODE>
U
*OUTPUT, FIELD, VARIABLE=PRESELECT
*END STEP
```

2.2 Adding imperfections and dropping

```
*HEADING
Dropping after adding imperfection
*INCLUDE, INPUT = BAG_MODEL.INP
**
*INITIAL CONDITIONS, TYPE = STRESS (DIFFICULT, IN PRACTICE)
**
*IMPERFECTION, FILE = EXTRACT_FREQUENCIES, STEP = 1
<mode_1>,<scale_factor_mode_1>
<mode_2>,<scale_factor_mode_2>
.
.
<mode_n>,<scale_factor_mode_n>
*STEP, NAME = DROP
*DYNAMIC, EXPLICIT
, .1
*END STEP
```

3. Model evaluation and partial calibration

3.1 Strip tension test

We present the results from our model in predicting the very large strain, slow-speed tensile stretching of a thin strip of DOWLEX™ LLDPE film; the strip is 100mm long by 15mm wide and the film thickness in this case is 130 microns (thinner films have been analyzed quite successfully). The analysis has been conducted in Abaqus/Explicit 6.13-3 using **S4R** elements and treating/modeling the problem as quasi-static, through suitable monitoring of the internal energy and kinetic energy after mass scaling. The test data collected from this test, inter alia, supplemented other input data for the model calibration and we use the average of 5 such tests as a representative curve for the experimental results; the agreement between all 5 curves was excellent, only deviating in the ultimate strain that each sample was able to sustain.

When pulled in the CD-orientation, the sample experiences significant localized necking; in the case of MD-orientation the neck is far more diffuse and tends to spread across the whole length of the sample; this is in agreement with what is observed in practice. In both cases, the neck is stable, but the degree of localization is significantly different, as shown in Figure 3.

Figure 3. Differences in tensile strip necking, aligned in CD- and MD-orientation.

The influence of imperfections for the two orientations is also different. There are not only geometric imperfections in such a film, but also some unknown distribution of internal stress from the manufacturing operation. Both of these effects have been accounted for by including only geometric imperfection; a reasonable scaling of the higher-frequency eigenmodes was applied. The MD-orientation tends to smooth out imperfections with increased stretch of the tensile strip, whereas the CD-orientation retains them and draws them into the stable necking region, as shown in Figure 4. This drawing-in of the imperfections, causes a marked wrinkling of the film in the neighbourhood of that zone, which can be quite clearly seen with the naked eye in the experimental tests. The computational model development and tuning was performed on the basis of assuming no imperfections in the film; any inclusions of imperfections in the analysis represents degradation that can be expected in its response, should the film deviate more severely from an accepted manufacturing norm.

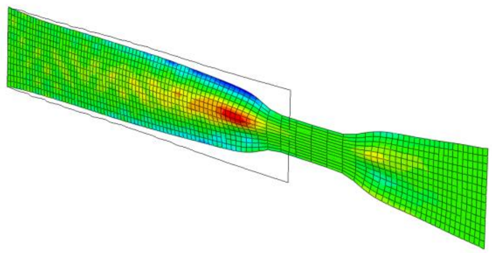


Figure 4. Local wrinkling of tensile strip when pulled in CD-orientation, after imperfections (eigenmode perturbations) have been included in the mesh.

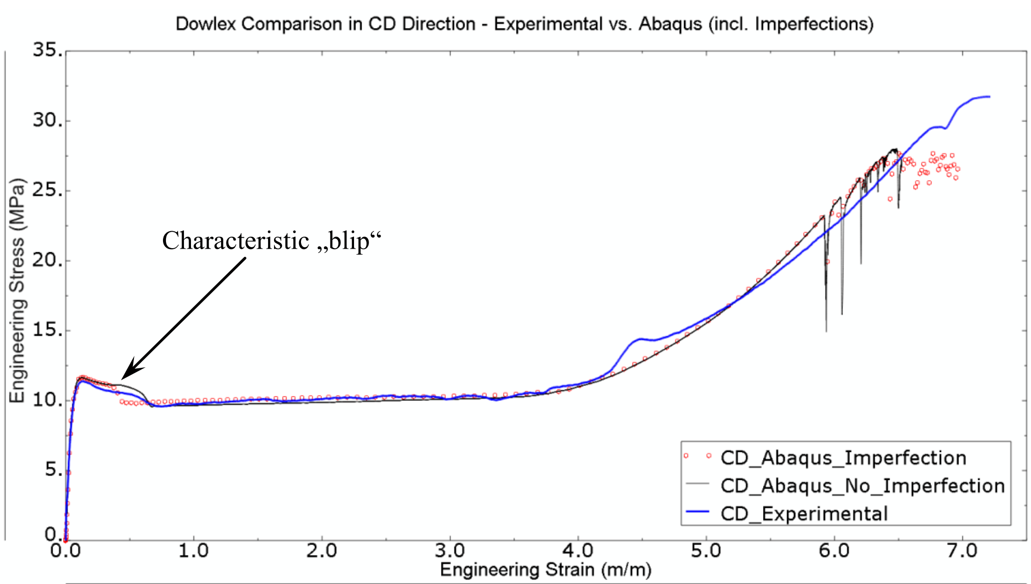


Figure 5. Analysis vs. Experiment when pulled in CD-orientation.

The predicted engineering stress vs. engineering strain for the tensile strip in comparison to the measured results is excellent; this is especially true in the early part of the curve up to an engineering strain of ca. 4.0 in the case of the CD-orientation and for virtually the whole extent in the case of MD-orientation. The introduced geometric imperfections have very little effect in the MD-orientation while for the CD-orientation, the extent of the stable necking zone in the curve in Figure 5 is influenced. The introduction of imperfections shortens the marked characteristic "blip", which is so typical of LLDPE materials. The engineering values were obtained from the analysis results of the "crosshead" displacement and force and suitably converting these, using the initial dimensions of the sample. In the model, the "crosshead" was a single node, tied to the free end of the tensile tab using a `*MPC` type `BEAM`. The results are compared to experiment in Figures 5 and 6.

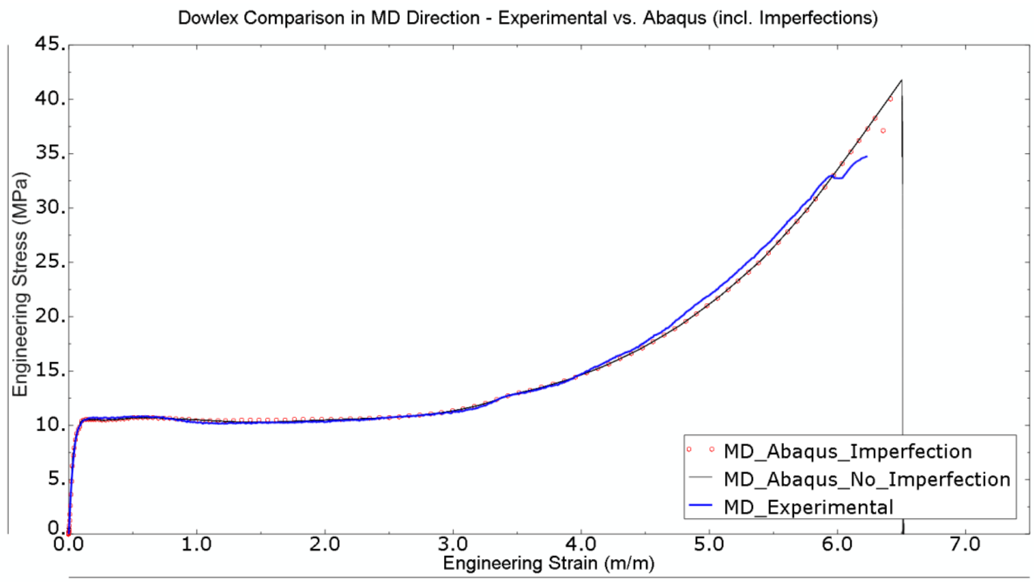


Figure 6. Analysis vs. Experiment when pulled in MD-orientation.

The same computational model, only suitably oriented is thus able to predict two different responses for such a DOWLEX™ LLDPE thin film; this is an important analysis result, since in a real bag or pouch with a complex stress field the internal load apportioning is moderated by the stiffness of the film. The degree to which external loading is absorbed along the two directions in turn affects the propensity for failure along that direction. In addition, the appearance of the neck and its marked difference along the two directions influences the internal stress distribution of any laminate made from these (and other) materials. The necking is clearly a complex, non-linear phenomenon that develops and extends as a function of strain and material orientation.

3.2 Elmendorf tearing test

The Elmendorf tearing test (ASTM D1922 : Propagation Tear Resistance of Plastic Film and Thin Sheeting) is a standard test used in industry for assessing the toughness of polymeric films or laminates having an initial crack; a sample is torn at high rate in a dynamic testing machine, similar to a Charpy test for toughness testing of metals. The test is used in a comparative sense, when ranking the performance of different candidates. The sample is torn, subjecting the crack area to mainly antiplane shearing/tearing; thus Mode III in the language of crack opening displacement measurements. The Abaqus model, used the “seam crack” feature in CAE with which to generate the initial crack; the outline of the model is shown in Figure 7.

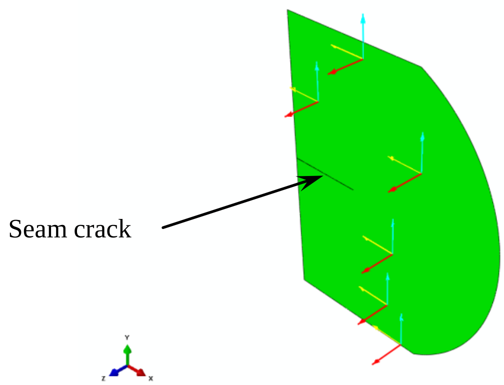


Figure 7. Elmendorf tearing test specimen, showing seam crack and reduced density plot of the material orientation vectors.

This test is a challenging numerical test; it is highly-dynamic, the films are thin and flimsy with significant failure. The problem is run with no form of mass scaling; thus the true dynamics in the problem apply. PET-film is usually co-laminated with LLDPE in practice, since the PET-film fails at a significantly lower strain than does the LLDPE. We can certainly predict improvements in resistance of the PET through lamination with LLDPE, as shown in Figure 8 but it is very difficult to get these models to run to completion. In this figure, the crack that originally ran for considerably longer was halted by the addition of the LLDPE-layer in the laminate. Remedies that have been tried, with varying degrees of success, is to treat the model as a membrane through permanent removal of degrees of freedom 4,5 and 6 and adjusting the hourglass stiffness to the maximum value recommended by Abaqus, using the keyword:

```
*SECTION CONTROLS, NAME = STABILIZER, HOURGLASS = RELAX STIFFNESS
1. , 3. , 3.
```

The error message encountered is either ***"Excessive rotation increment at one node"*** or perhaps ***"Excessive distortion of element"***, even in the case of using "standard" material descriptions. The standard diagnostic that is printed out by Abaqus, does suggest that the model may have failed completely. When the laminate is included into a bag or pouch containing a fluid, then it usually runs to completion; this is attributed to the far better energy absorption, say damping, of the fluid in that kind of problem and/or the lower degree of Mode III tearing in the laminate.

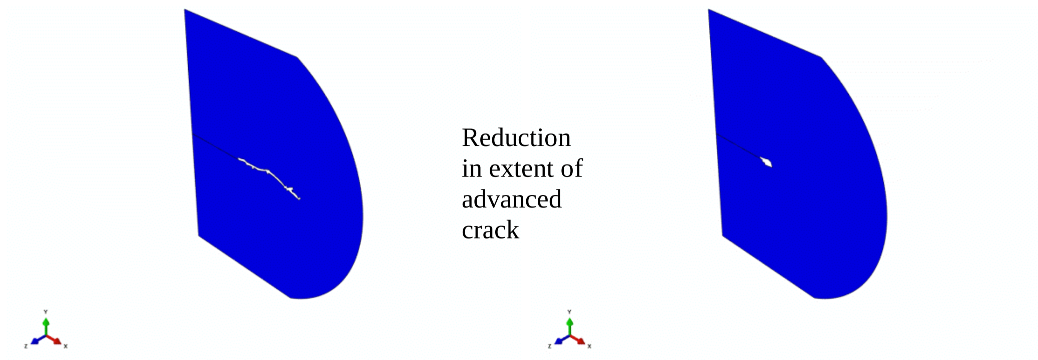


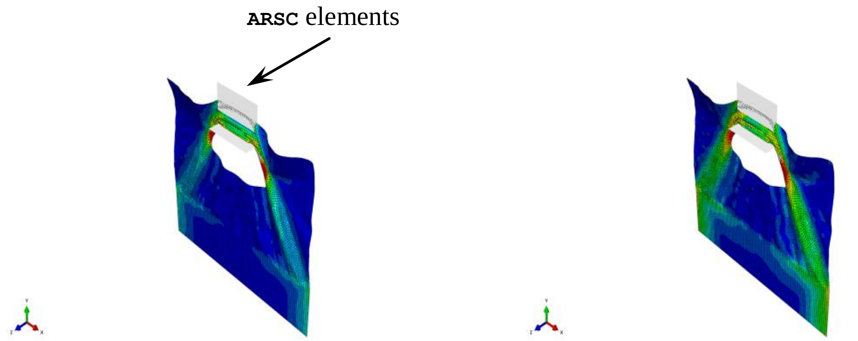
Figure 8. Improved resistance to tearing in PET-layer by addition of an LLDPE-layer in the Elmendorf tearing test; plotted on the *original, undeformed* mesh.

4. Application problems

As an initial test of the suitability of our general procedure and computational models, two industrially-representative problems have been analyzed.

4.1 Bag handle tearing

The bag-handle tearing test that has been modeled, mimics the overload that a packaging bag may sometimes be subjected to. The analysis has been conducted in Abaqus/Explicit 6.13-3 using **S3R** & **S4R** elements for the laminated bag wall and analytical rigid surface **ARSC**-elements to represent the load application device; geometrically simple rigid contact surfaces can be very easily represented using such **ARSC**-elements. General contact has been specified in the problem, with all surfaces included in the definition through usage of the parameter **ALL EXTERIOR**. All surfaces interactions were regarded as frictionless. One can view (post process) the results for any particular film within the laminate by selecting it from the **RESULTS** tab in Abaqus/Viewer and then choosing the relevant layer in the list that appears. The output of such a selection for the LLDPE layer and the PET layer is shown in Figure 9, with the **ARSC** elements having no contoured result.



LLDPE PET

Figure 9. Different Mises stress state in LLDPE layer and PET layer in laminate.

The bag-tearing analysis results show very good agreement with experiment; the location of severe tears and their development with crosshead displacement, as shown in Figure 10, mirrors the visual evidence from the test. The test has introduced an asymmetry into the loading of the bag which is not modeled; in practice there is some considerable geometric and (maybe) stress imperfection in the bag which may cause or exacerbate this asymmetry; the model is for an assumed-perfect bag handle.

Figure 10. Failed PET-layer in laminate highlighted by the remaining central red region that represents the LLDPE-layer in the contour plot.

4.2 Pouch dropping problem

The pouch measures 112.5mm by 50mm by 245mm and while no specific product is modeled, it is perhaps typical of a small "coffee-bean" pouch as illustrated in Figure 1. The thickness of plies in the laminate have been chosen to suit the analysis and for easy reference to the already developed data and model for the tensile test. The laminate, as modeled, consists of a 12micron PET-film and a 130micron DOWLEX™ LLDPE film; all the overlapping bonding edges of the pouch have had their thicknesses doubled, to represent a perfect bond. As a severe numerical test, it is fully-filled with an essentially incompressible fluid (water) and dropped onto a frictionless rigid floor; one expects significant strain energy to be absorbed by stretching of the pouch walls, since there is no free space in the pouch. The water model is the same as in Problem 2.3.2 in the Abaqus Example Problems Manual (Simulia, 2013), only converted to SI-units. The water is initially modelled/meshed as `C3D4` elements in CAE and converted to `PC3D` elements within the initial step of the analysis at time = 0.0, as has been illustrated in Example Problem Problem 2.3.2, by including the 4th line on the data of the **`*SECTION CONTROLS`** keyword:

```
*SECTION CONTROLS, NAME=EC-1, ELEMENT CONVERSION=YES, CONVERSION CRITERION=TIME, KERNEL=CUBIC
1., 1., 1.
[blank line]
[blank line]
1, 0.
```

While, in practice the pouch would exhibit imperfections, these have been neglected in the analysis presented in the paper; they can be easily added using the eigenmode perturbation technique as has been discussed and illustrated in the case of the tensile strip test.

The pouch has been given initial linear and rotational velocities, as it is on the point of striking the floor.

```
*INITIAL CONDITIONS, TYPE= ROTATING VELOCITY
FOUR_CORNER_BAG_SI.BAG_NODES, -0.1, -0.125,-0.125,-2.0
0.0,0.0,0.0,0.0,1.0,0.0
*INITIAL CONDITIONS, TYPE= ROTATING VELOCITY
WATER_SI.WATER_NODES, -0.1, -0.125,-0.125,-2.0
0.0,0.0,0.0,0.0,1.0,0.0
**
```

The acceleration due to gravity is also included, acting in the negative-z direction.

***DLOAD**
FOUR_CORNER_BAG_SI.BAG_ELEMENT**,GRAV**, 9.8, 0., 0., -1.
WATER_SI.WATER_ELEMENT, **GRAV**, 9.8, 0., 0., -1.

At the end of the analysis, the pouch is still intact. The four graphics in Figure 11 show the magnitude **U** of the deformed shape, **LE**, **MISES** and a computed indication **SEVERE** of the severity of potential failure of the laminate. The plot is for the envelope of the maxima through the shell wall. Interestingly, the peak contour values related to material performance - **LE**, **MISES** and **SEVERE** - do not occur at the same point on the bag. The points on the pouch that are the most **SEVERE**-ly close to failure are at the flopped-over neck region and the base that has contacted the rigid surface.

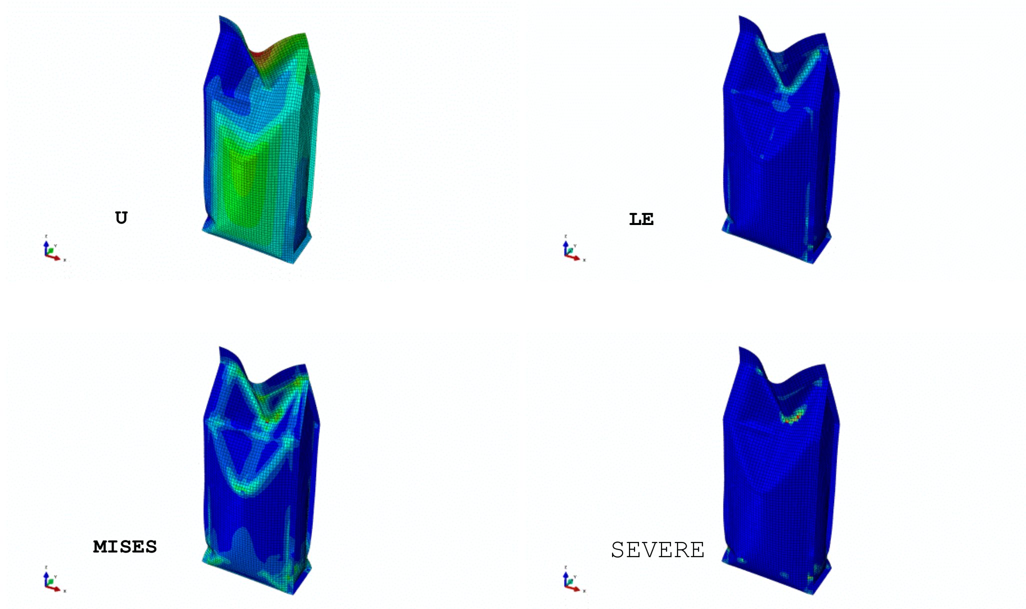


Figure 11. Pouch after impact with floor – envelope of contours of U, LE, MISES and SEVERE.

The differing degrees of orthotropy and thickness differences between the various film layers in the laminate is the cause of the shift in the peak values for the **LE,MISES** and **SEVERE** variables on the pouch wall-surface; hence the need for computing a failure **SEVERE**-ity. The necking differences along the CD- and MD-directions for the LLDPE, as well as the milder orthotropy of the PET-film all contribute to how the complex internal load-sharing in the laminate occurs.

5. Conclusions

The major effort in our work was the establishment of a computational framework for a thin film of LLDPE-type material, using Abaqus. This class of material can sustain very large strain of ca. 800% before failure, ***with a large permanent plastic set*** and exhibiting local and differentiated material instability along two directions. Our developed model shows excellent agreement with experiment for the low-speed tensile test cases for the particular grade of DOWLEX™ LLDPE film that has served as the basis for this paper. We have also investigated the usage of our approach to other grades of LLDPE and film thicknesses, with success.

By comparison, the PET film is not as extensible and does not exhibit the necking instability, although it also shows differentiated response along its MD- and CD-axes. The computational model has been used successfully within a laminate of these two film-types and the initial performance is very encouraging. We are able to compute the SEVERE-ity of failure envelope of the laminate and indeed for any film layer.

The continued development and extension of the capability is an on-going effort within Dow. We have identified improvements in our parameterization and improvements in our ability to extract information from test data; we are currently working on implementing these and correlating computations with experiments on dropping of pouches. We hope to be able to give feedback on these activities and additional packaging applications for the model at future SIMULIA Customer Conferences.

6. Acknowledgements

Acknowledgements go to Drs. M-A. Siddiqui and P. Shembekar from Dow for helping with the CAE creation of some of the analysis models for computer runs associated with this paper. Thanks to Dr. S. Bensason, also from Dow, for supplying the required material test data during the computational model development.

7. References

1. Abaqus 6.13 Documentation Collection, Abaqus Example Problems, Keywords & Theory Manuals, Simulia.