# Integrating Moldflow and Abaqus in the Package Simulation Workflow

Eskil Andreasson[a,b,*], Leo Persson[a], Henrik Jacobsson[c] and Johan Nordgren[d]

[a] Tetra Pak Packaging Solutions, Lund, Sweden
[b] Blekinge Institute of Technology, Karlskrona, Sweden
[c] FS Dynamics, Gothenburg, Sweden  [d] Altair Engineering, Lund, Sweden

[*] To whom correspondence should be addressed, eskil.andreasson@tetrapak.com

*Abstract: Tetra Pak has used numerical simulation tools for plastic injection molding (Moldflow) and structural analysis (Abaqus/Implicit and Abaqus/Explicit) for many years. Today these two simulation tools are used independently of each other without any coupling. How these two disciplines can be combined to better predict the mechanical response of a polymer component is presented in this work. The manufacturing process, in this case injection molding, creates the mechanical properties of the produced polymer part. Process settings, material selection and molding tool geometry affect the polymer flow, material orientation and rate of crystallinity. A method to build a layered finite element model in Abaqus using results from Moldflow simulations regarding crystallinity growth and molecular orientation is proposed. Relatively simple material models were utilized and assigned for each individual material layer through the thickness in the polymer part. These constitutive models were derived phenomenologically from experimental test results and could adequately capture both the microscopic and the macroscopic behavior in a more realistic way. The numerical results showed a good agreement with the experimental results, both regarding visual appearance and force/displacement response.*

*Keywords: Abaqus/Explicit, Moldflow, crystalline orientation factor, constitutive model, damage initiation, damage evolution, fracture mechanics, material modeling, polymer, injection molding*

## 1. Introduction

Today, many parts in a beverage package are made of polymer materials e.g. the top, neck and cap. The polymer parts are manufactured with injection molding technology. The mechanical properties in the polymer part, for instance a polymer top as shown in Figure 1, is not only dependent by material, it is also dependent on the geometry and settings used during the molding process. This will result in induced stresses and different mechanical properties in different directions, denoted anisotropy, in the manufactured part. Tetra Pak has a long history of using simulation tools for plastic injection molding (Moldflow) and structural analysis (Abaqus/Implicit and Abaqus/Explicit). Virtual analysis can be used to evaluate new polymer component early in the design process. These simulation tools have so far been used independently without any coupling in-between. The objective of this work is to present how these simulation disciplines can interact with each other to better predict the mechanical properties and behavior of a polymer part.

**Figure 1. Tetra Evero Aseptic package with the different parts (Tetra Pak, 2012)**

When a beverage package like the Tetra Evero Aseptic in Figure 1 is modeled in Abaqus, the geometry is based on the CAD geometry imported from Pro/ENGINEER. The material properties of the polymer are usually set to be equal in all directions, isotropy, as well as homogeneous, i.e. same material properties through the thickness. This modeling strategy has a disadvantage; it doesn't consider that the mechanical material properties vary through the thickness caused by the injection molding process as described in (Nordgren, 2012). In order to make more accurate and realistic simulations this deficiency has to be amended. If this new virtual prediction of the physical behavior is done successfully, the amount of required experimental tests will be significantly reduced. This will save money and time when developing new products.

Finally a method to build a finite element model using results regarding crystallinity growth and polymer chain orientation from Moldflow simulations was proposed. The new method showed a good agreement with the experimental tests, both regarding visual appearance and force displacement response. This was done by using the Moldflow simulations combined with experimental tensile tests to increase the knowledge and understanding of polymers morphology and microstructure regarding crystallinity and how the material react to mechanical loading. The sequence of deformation and failure processes was established for the polymer and it was possible to link these micromechanisms with the macroscopic behavior. This information was then used to build the layered composite material model in Abaqus. The described modeling approach will be presented in this paper and the procedure can further be used for package application simulations in new projects.

## 2. Injection molding of polymer parts

A comprehensive introduction and description of the injection molding technology and how polymer materials flow and reacts to mechanical loading could be found in several text books describing the specific subject. In this section is instead a brief introduction to how the injection molding process affects the morphology of the polymer orientation and crystalline growth presented. Injection molding of a polymer plate will result in several layers with orientation and rate of crystallinity that vary, as illustrated in Figure 2. This effect is due to shear forces originated from the event when the molten polymer fill the cavity and due to temperature gradients build up during the cooling phase. The surface layer is called skin, the middle layer is called core and between them there is a layer called shear zone. The molding tools, forces the skin to solidify fast, resulting in an orientation in the flow direction. The core, or the bulk, will have random orientation and hence similar mechanical properties in all directions, denoted isotropy. The shear zone will experience shear forces in one direction together with rapid crystallization giving the polymer chains strong orientation in this layer. A semi-crystalline high density polyethylene (HDPE) compound was used for the manufacturing of the experimental test specimens in this paper. These specimens were exerted to uniaxial mechanical tensile loading.
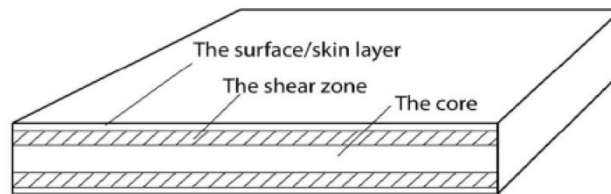


**Figure 2. Different layers created during injection molding (Lindgren, 2011)**

## 3. Experimental tensile tests

Tensile tests were performed to increase the knowledge of the mechanical properties and the associated failure processes and micromechanisms in a polymer top material used in a beverage package. A 2 mm thick plate, according to the standard ISO 294-5:2011, plate type F:80 mm x 90 mm, was injection molded in an Arburg 470 800-70S machine using a molding tool with a flood gate depicted in Figure 3. This result in two principal material directions in the molded plate, machine direction (MD) and cross direction (CD), due to the uniform polymer flow obtain in the flood gate. Dog bone shaped specimens were punched out in four different positions (CD1, CD2, CD3 and MD1) in the plate, according to Figure 3, to be tensile tested. This was done for varying thicknesses and different process settings, described in (Nordgren, 2012). The tensile test results showed that the injection molded specimen consisted of several layers with different mechanical behavior that responded quite differently under tensile load. The thickness ratio of these material layers depend on the total thickness of the specimen and the process settings used when molding. One of the results from the experimental tests is shown in Figure 4, the focus in this paper is the

specimen punched in the MD1 position. A thorough description of other positions, specific machine settings that were used and test results are presented in (Nordgren, 2012).
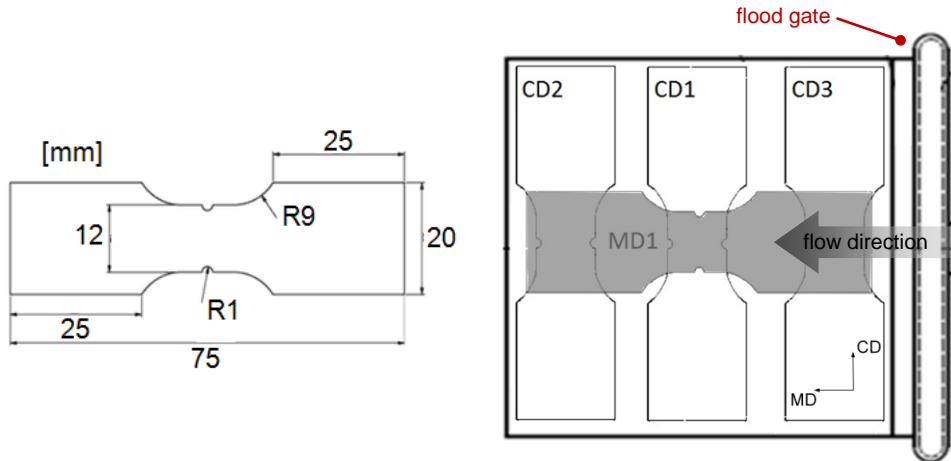


**Figure 3. Tensile test specimen geometry and the injection molded plate.**

Experimental results showed a small standard deviation, this concludes that the procedure of injection molding of plates and punching of dog bone specimens with a notch is a reliable method. Similar phenomenon found in experimental tests is expected to be found in the Moldflow analysis. One experimental test was therefore thoroughly examined with photos and video recording of the phenomenon involved in the deformation and fracture process. Tensile tests stopped at different incremental deformations are presented in Figure 4 and Figure 5 cf. (Nordgren, 2012). Including the manufacturing process of injection molded polymer details for structural analysis in Abaqus is important. This was accomplished by using the Moldflow simulations to get a better understanding of the micro mechanical structure and behavior in the polymer part.
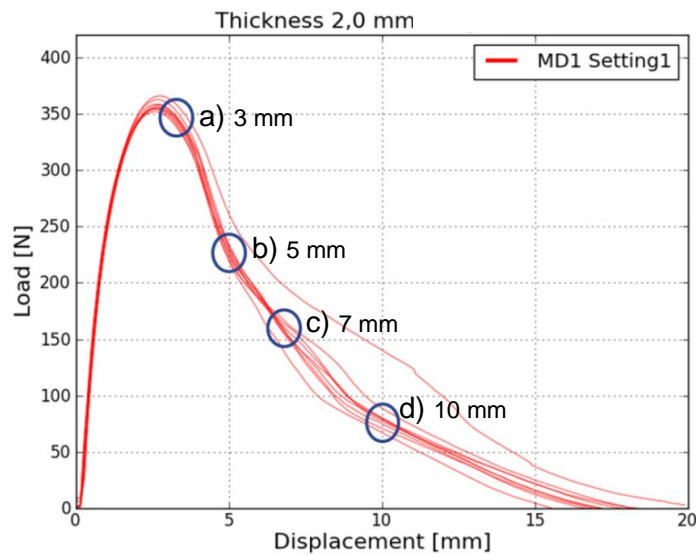
**Figure 4. Tensile test response of dog bone shaped geometry, 3-10 mm.**

The permanent or plastic deformation after unloading and dismounting the specimen is shown in Figure 5, both with front view to the left and side view to the right. Initial stress localization and necking is evident in Figure 5 a) at the notch when then maximum load is reached. The bulk zone, showing a more brittle material compared to the two shear zones, is fractured at both notch sides in Figure 5 b). The damage in the bulk zone material continues to propagate towards the centre of the specimen in Figure 5 c) until completely fractured in Figure 5 d). The skin/shear zone with a more ductile behavior is still holding the specimen together and is highly elongated.
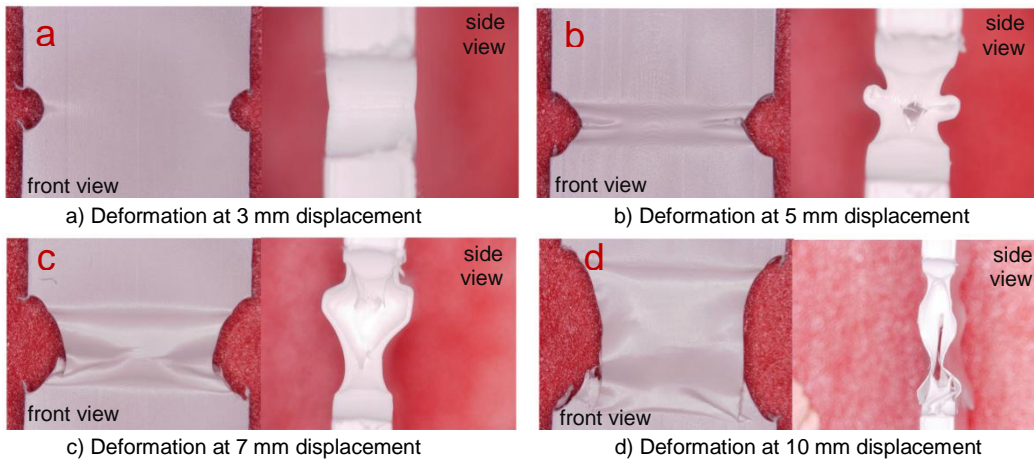


a) Deformation at 3 mm displacement



b) Deformation at 5 mm displacement



c) Deformation at 7 mm displacement



d) Deformation at 10 mm displacement

**Figure 5. Visual tensile test response of dog bone shaped geometry, 3-10 mm.**

## 4.  Moldflow analysis of the injection molding

The injection molding process was simulated with the software; Autodesk Moldflow Scandium Technology Preview 3. This pre-release is an extension of the Moldflow software that enables the Moldflow users to evaluate new technologies not yet released in the commercial release of the software. One of the new features available and of specific interested in this paper is the crystallization analysis option for Midplane and Dual Domain analyses. This functionality can model the flow-induced crystallization and morphological changes of semi-crystalline polymers. Therefore, the accuracy of predicting the mechanical properties of the molded part can be further improved. The growth of crystallinity in the structure and the orientation of the crystals are assumed to affect the mechanical properties of the part. How the process settings from the injection molding will affect the properties of the plate will be evaluated in this paper by running simulations with the same process settings as previously have been experimentally tested.

A fill and subsequent pack analysis was done for the HDPE compound which has been characterized by Moldflow for injection molding analysis. A Dual domain mesh has been used with approximately 70 000 elements. The analysis solution time for this type of analysis is a couple of hours. The result from a Moldflow simulation is a model of the polymer flow and the deformed geometry with induced stresses. These properties vary depending on tool geometry, injection locations as well as process settings, e.g. injection temperature and cooling time.  Figure 6 confirms and shows the uniform flow from the flood gate into the plate, from the right to the left in the figure. This results in a high orientation of the polymer chains in MD. The two principal directions, MD and CD were showing different results in the experimental tensile tests.
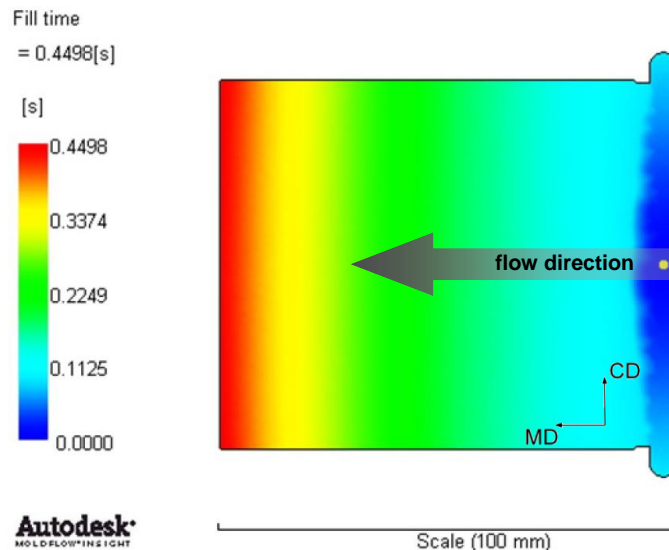


**Figure 6. Moldflow simulation showing the uniform flow front.**

It is possible to distinguish two types of zones, shear zone and bulk zone, through the thickness of the plate with high orientation from the surface to the center of the plate in Figure 7. The first zone originates during filling and is denominated the shear zone due to the shear forces enabling the strong orientation and high crystallinity growth in the polymer molecular structure. The second zone is created during packing. In the middle there is a bulk zone with random orientation.
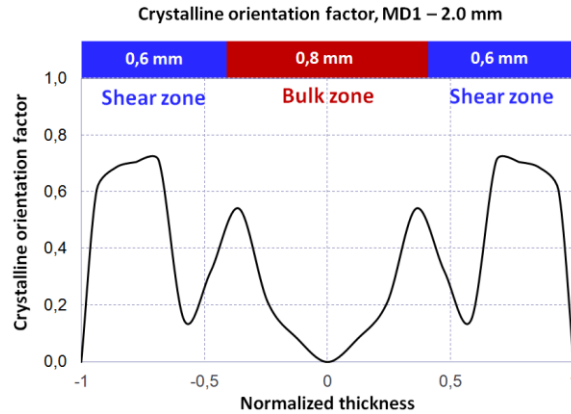


**Figure 7. Crystalline orientation factor through the thickness for MD1 specimen**

As mentioned before, Moldflow has the possibility to account for flow induced crystallization. The shear forces during injection molding will orient the polymer chains in the flow direction. These forces will facilitate growth of crystals in this material layer and this will influence the mechanical properties in the plate. Comparing the Moldflow results with the experimental results, for the 2 mm thick plate as discussed in this paper, it is possible to establish that the fracture mechanical behaviour in the different zones can also be connected to the crystalline orientation factor. There might be other parameters that influence the mechanical properties such as the size of the crystals and the orientation of the amorphous regions. Moldflow does not account for those parameters and thus they have not yet been considered, hence the conclusions below have been made based on the crystalline orientation factor:

- The bulk zone has random orientation *(crystalline orientation factor 0)*
- The bulk zone is isotropic, i.e. same material behaviour in all directions
- The shear zone has orientation in the flow direction (MD) *(crystalline orientation factor 0-1)*
- The shear zone is anisotropic, i.e. different material behaviour in different directions
- The shear zone show high displacement at fracture in MD and low displacement at fracture in CD

## 5. Coupling Moldflow with Abaqus

In order to transfer properties and in this case field variables and the material properties from Moldflow to Abaqus a coupling interface is needed or would be beneficial. Before identification of the available options it is important to state what information that is of interest:

- Run a Moldflow analysis that simulates the mold filling process of the polymer.
- Capture residual stresses in the structure and export them to Abaqus.
- Capture the orientations in the structure in order to use the directions to setup an anisotropic material model to analyze in Abaqus.

The mesh in Moldflow is created for a good performance in the simulation of the filling process. In Abaqus the most appropriate mesh to capture the structural behavior will not be the same as the Moldflow mesh, and thus a method to map the results from the Moldflow mesh to the Abaqus mesh is required. The material model used must have specified directions, i.e. three values of the mechanical constants E, G and ν, as well as the yield stress and plastic behavior. This means that the material orientation from Moldflow must be transferable, both for filled and non-filled materials.

Three different interfaces for coupling Moldflow results to Abaqus analysis have been evaluated AMSA 2012, Digimat and Abaqus interface for Moldflow described in (Nordgren, 2012). Coupled analyses were done with these three coupling interfaces, and it was concluded that they are more useful when simulating fiber filled materials. This is due to that the interfaces calculate the fiber orientation in the material, and not the material orientation due to direction of polymer chains and crystalline growth. These interfaces are also capable to map temperatures and residual stresses.

One of the key purposes with the use of coupling interfaces is to determine the anisotropy of an injection molded part. Common for all coupling interfaces is that the material orientations that can be imported from Moldflow are the fiber orientations. For analyses of fiber filled material, there are therefore benefits of using these coupling interfaces. For a fiber filled material, the fiber orientation is clearly what governs the anisotropy of the material. For an unfilled material it is harder to state, and a fictitious fiber orientation is maybe not that useful in such cases. For unfilled material, the benefits of these coupling interfaces are thus limited. As an example, in the semi crystalline material HDPE used in this paper, crystallinity growth is what governs the anisotropy and mechanical properties. The rate of crystallinity and orientation of crystals is what is important, not the fictitious fiber orientation. Although it is likely that the orientation of fibers will have the same direction as the crystals, the fictitious fiber orientation cannot be used as a measurement of the crystalline orientation. Today, the use of coupling interfaces for Moldflow and Abaqus is of primary use for fiber filled materials. For materials as HDPE presented in this paper, the benefits are restricted. In Moldflow 2013, a new feature to simulate crystallinity growth is available. If this feature could be employed in coming versions of the coupling interfaces, the potential benefits of using the coupling interfaces will be extended.

With the knowledge gained from the tensile tests and the Moldflow simulations a finite element model was created in Abaqus without using any of the three mentioned coupling interfaces. The objective with the Abaqus model was to see if the behavior seen in the experimental tests could be captured in a structural analysis, both visually and when comparing the force-displacement results from the tensile test.

The suggested procedure for creating the Abaqus simulation model of injection molded parts is given below:

- Perform experimental tests to determine material behavior for bulk and shear zone
- Fit an isotropic material model for the bulk zone
- Fit an anisotropic material model for the shear zone
- Use Moldflow simulations to determine the size of the different zones (skin, bulk and shear zone), shown in Figure 8 below
- Create an Abaqus model with different material layers, shown in Figure 8, corresponding to the different zones
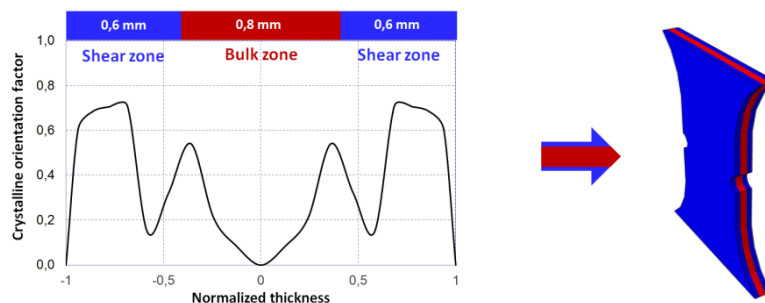- Assign appropriate material models in the different material layers.



**Figure 8. Identified zones in the Moldflow simulation to the left, transferred and used in the Abaqus simulations for shear zone and bulk zone to the right.**

## 6. Abaqus analysis of the tensile test

Abaqus/CAE 6.12 was used to create a structural solid 3D-model of the same dog bone shaped geometry, punched from the injection molded plate. Identical geometry of the specimen was used both for experimental and virtual tensile tests. SI-units (*m, s, kg*) were utilized consistently throughout the work in Abaqus. The main strategy was to use the zones identified in the Moldflow simulations to create a dog bone with different mechanical material properties in the respective material layers through the thickness. For this numerical model the 2 mm thick injection molded plate was studied in position MD1 as defined in Figure 3. The simulation was done with Abaqus/Explicit using a time step of 0.010 s for the loading step. The displacement was applied with a smooth step amplitude curve. Approximately 20 000 linear 8-node brick elements with reduced integration called C3D8R were used. In the upper and lower part a rather coarse mesh was utilized and the mesh was refined at the notch and through the thickness as shown in Figure 9.

The free gauge length of the dog bone during tensile testing was modeled in Abaqus. The bottom surface was locked in all degrees of freedom and the top surface was subjected to a displacement controlled loading. The dog bone was divided into three zones as shown in Figure 8. The middle zone is modeled as the bulk zone with a low displacement at fracture, hence brittle material, and the outer zones represent the shear zones with high displacement at fracture.
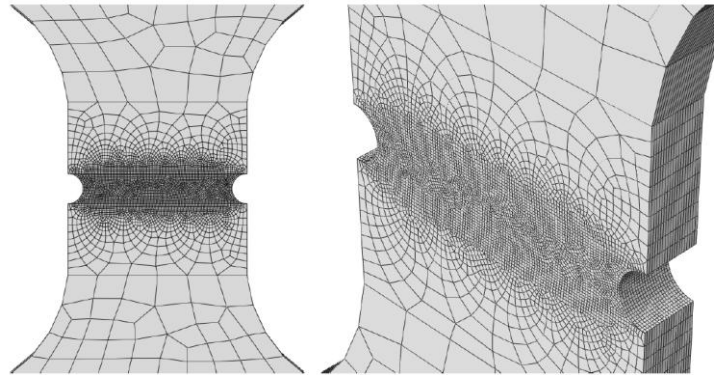
**Figure 9. Finite element mesh in the tensile test specimen.**

In order to incorporate the physical behavior seen in the experimental tests different factors had to be considered when creating the Abaqus model. One important factor is that obtaining similar response curve, force vs. displacement, is desired. Bulk zone material fractures first hence a more brittle- like material response is needed in this material layer. The two outer shear zones are held together, possible to extend more than the bulk zone, hence a ductile-like material behavior withstanding a larger displacement is needed in this material layer. These two different behaviors were experimentally shown and physically motivated in Figure 5. To achieve this, two different material models were used. An existing material model, already available for the HDPE compound at Tetra Pak, was slightly enhanced to facilitate these two types of material behavior. The constitutive continuum material model was modified and accompanied with a damage model. The damage criterion was defined in a way that enables the shear zone material to withstand higher displacement before fracture compared to the bulk zone material. The two material definitions for the bulk and shear zone are visualized in Figure 10. The plotted data in the figure is from one-element tensile tests on the actual material models in Abaqus/Explicit. To simulate the damage the options **\*Damage initiaion** and **\*Damage evolution** were used (Andreasson, 2012). **\*Damage evolution** uses a parameter called displacement at failure. Since this parameter has the dimension of length, the damage behavior is dependent of the element size Therefore, it is import-
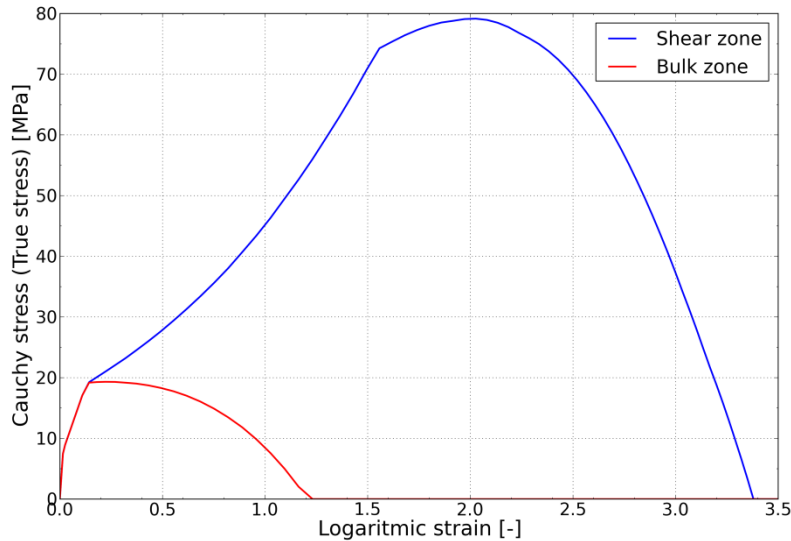
**Figure 10. The constitutive relation for bulk and shear zone material.**

ant to have equal element size in the regions of large deformations, i.e. in the notched region as depicted in Figure 9. Other damage parameters are often based on strain, and since strain is dimension free, a consistent element size is not as important in such cases. An extensive introduction to the field of constitutive modeling is presented by Ristinmaa et al., (Ristinmaa, 2015). In addition to this textbook and if you are not familiar with damage behavior, damage modeling or fracture mechanics a good reference book is (Anderson, 1995) for the general fracture mechanics and the Abaqus documentation (Abaqus, 2012) for the numerical material modeling aspects. The material model used for the bulk zone and shear zone in this paper is described in detail below with the corresponding Abaqus keywords.

```
********************************************************************************
**
** MATERIALS, two different material definitions, SI-units utilized (kg, m, s, Pa)
**
********************************************************************************
**
*Material, name=Bulk_zone, RTOL=0.0003, strain rate regularization=LOGARITHMIC
*Damage Initiation, criterion=DUCTILE
0.1,-5., 0.
0.1, 5., 0.
*Damage Evolution, type=DISPLACEMENT
0.00010,
*Density
950.,
*Elastic
500e+06, 0.42
*Plastic
8.00e+06, 0.000
10.7e+06, 0.003
```

```
13.1e+06, 0.008
...
373e+06,  3.098
543e+06,  3.298
793e+06,  3.448
*******************************************************************************
**
*Material, name=Shear_zone, RTOL=0.0003, strain rate regularization=LOGARITHMIC
*Damage Initiation, criterion=DUCTILE
1.4,-5., 0.
1.4, 5., 0.
*Damage Evolution, type=DISPLACEMENT
0.00015,
*Density
950.,
*Elastic
500e+06, 0.42
*Plastic
8.00e+06, 0.000
10.7e+06, 0.003
13.1e+06, 0.008
...
373e+06,  3.098
543e+06,  3.298
793e+06,  3.448
```

In the **\*MATERIAL** keyword there are several options, one optional parameters is **RTOL** (Abaqus manuals, 2012). This setting has a significant impact of the stress vs. strain response in the initial part of the material response curve. Below is an extract from the Abaqus Keywords Reference Manual. This parameter applies only to Abaqus/Explicit analyses. Set this parameter equal to the tolerance to be used for regularizing the material data. The default value of **RTOL** is **RTOL=0.03**. This default value was changed in this work to **RTOL=0.0003** for better curve fitting of the actual material response in the initial part of the curve. If strain rate dependent material data is utilized another optional parameter can be of interest, **SRATE FACTOR**. This parameter applies only to Abaqus/Explicit analyses. Set this parameter equal to the factor used for filtering the equivalent plastic strain rate for the evaluation of strain rate-dependent material data. The default value is 0.9.

Abaqus regulate the strain rate either by logarithmic or linear procedure:

**STRAIN RATE REGULARIZATION = [ LOGARITHMIC | LINEAR ]**

This parameter applies only to Abaqus/Explicit analyses and is used only to regularize strain rate-dependent material data. Set **STRAIN RATE REGULARIZATION=LOGARITHMIC** (default) to use a logarithmic regularization for strain rate-dependent material data. Set **STRAIN RATE REGULARIZATION=LINEAR** to use a linear regularization for strain rate-dependent material data.

After a couple of iterations the numerical results showed similar overall response as the experimental tensile test. Obtaining realistic and physically correct material responses in the bulk zone and shear zones was easily facilitated with the build in functionality of the current continuum and damage material models available in Abaqus. Both the visual fracture mechanical result and the response graphs from the tensile tests are shown in Figure 11 and Figure 12.
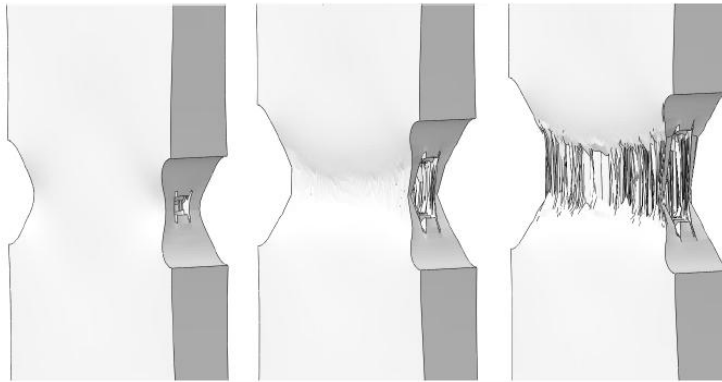
**Figure 11. Simulation results of the deformation in the dog bone at three different displacements. Bulk zone fractures first followed by stretching of the shear zone.**
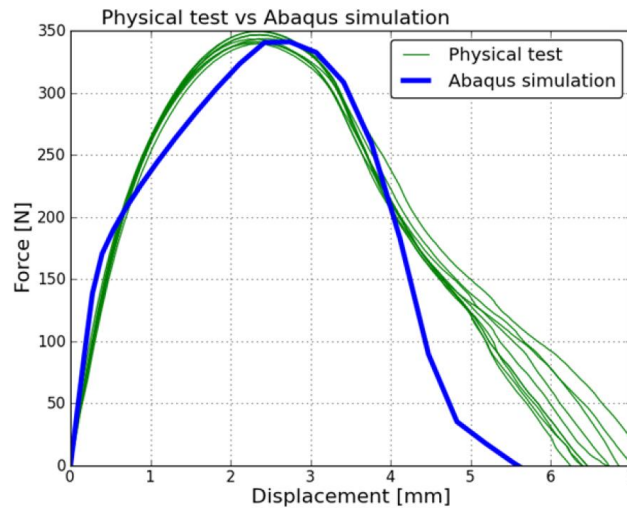


**Figure 12. Tensile test results; experimental vs. numerical.**

A comparison of the deformations at different load stages in the virtual and the experimental tensile tests are shown in Figure 13. Similar global or macroscopic behavior is shown but the microscopic behavior such as void nucleation, growth and finally coalescence is not accurately captured (Gurson, 1977). One of the reasons to the mismatch between the results is that in the current procedure was not a material model with this type of functionality incorporated. This can probably enhance the results further and several models are available for instance the GTN-model originally created by Gurson and later on modified by (Needelman and Tvergaard, 1984). But in the current stage is this current macroscopic result presented in this paper satisfactory.
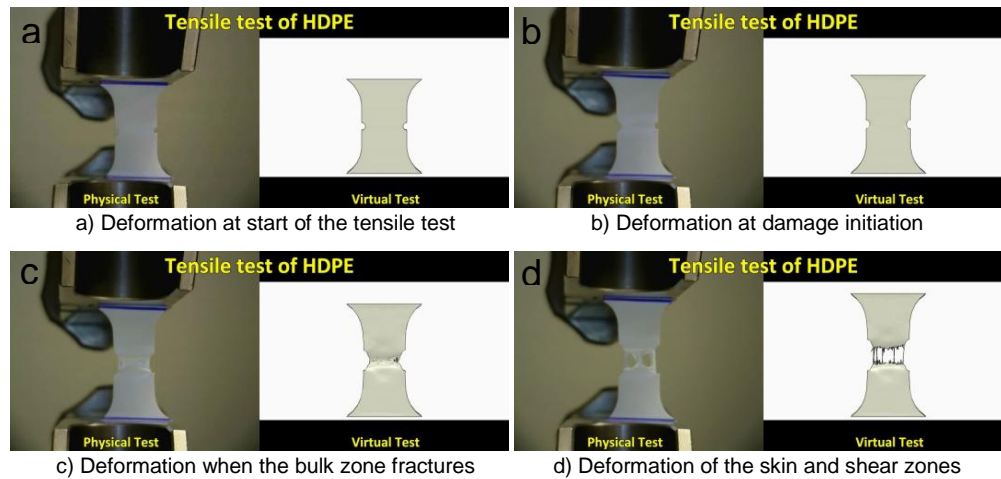
a) Deformation at start of the tensile test    b) Deformation at damage initiation

c) Deformation when the bulk zone fractures    d) Deformation of the skin and shear zones

**Figure 13. Experimental vs. Numerical results from tensile tests.**

## 7.  Discussion

The focus of this paper was not to find the perfect match and exact material models for the injection molded polymer material. Instead was the focus to understand the appropriate workflow to be able to capture the manufacturing processes of the injection molded part. Experimental testing is fundamental to increase the understanding of which material effects that is important to numerical implement and capture in the simulation models. Adopting an inverse calibration scheme would improve the automatization of the material parameter identification and also the accuracy of the numerical values but was not included in this work.

The conclusion from this paper is similar to the perky statement made by Albert Einstein:

> *"Computers are incredibly fast, accurate, and stupid. Human beings are incredibly slow, inaccurate, and brilliant. Together they are powerful beyond imagination."*

An engineering and physical motivated approach is needed to be able to do realistic simulations of the polymer parts in a beverage package. Including the injection molding technology, utilized for manufacturing of the polymer part, in the analysis workflow is important to be able to capture the physical behavior in the mechanical response. An experienced mechanical engineer with appropriate software's is needed to combining the polymer flow analysis in Moldflow with the structural analysis in Abaqus. By doing that it is possible to include the manufacturing of the polymer part and how these processes affects the mechanical behavior and functionality of the polymer part later on used in various applications. Therefore mixing the two numerical disciplines and the power of computers with accurate experimental tests and a "brilliant" engineer with vast knowledge of polymer behaviors and morphology is a fruitful symbiosis for future work.

# 8. Concluding Remarks

Experimental tensile test results of polymer parts with different process settings confirmed the hypothesis that the injection molding process settings have a great influence on the mechanical properties, and that the material properties are both anisotropic and vary through the thickness. In all experimental work, a HDPE based compound, was used. Since this material is semi-crystalline, crystalline growth is an important parameter creating the mechanical properties.

A new feature in Autodesk Moldflow Scandium Technology Preview 3 made it possible to simulate the crystalline growth during injection molding. The results of the crystalline growth in Moldflow, was unfortunately not possible to transfer to any available coupling interfaces. Our conclusion is that there is a limited usage of coupling interfaces for unfilled semi-crystalline polymers.

Moldflow simulations corresponding to the injection molding processes in which the test specimen had been produced were made. After studies of the crystalline growth and the crystalline orientation factor in the Moldflow results, a lot of the mechanical behavior in the experimental tests could be explained. The most important conclusions from the experimental tests and the Moldflow simulations are listed below:

- Material behavior is highly dependent of the process settings during injection molding.

- Mechanical material behavior is anisotropic and inhomogeneous.

- Crystalline orientation factor from Moldflow is a good way to identify different material zones through the thickness.

With the learning's listened above in mind, an Abaqus model was created. This virtually tested tensile test showed that the physical behavior could be captured satisfactory in a simulation model. A Moldflow simulation was used to identify the size of the different material zones through the thickness of the specimen, bulk and shear zone. These two zones were then assigned their own material definition, based on the learning's from the experimental tests. The simulation result was satisfying and showed that a rather simple numerical approach, with different material layers through the thickness assigned with an elastic material model accompanied with a continuum damage model, could capture the mechanical behavior really well. Therefore is the conclusion that it is possible and beneficial to couple the two disciplines, Moldflow analysis and Abaqus analysis. Next step is to start integrating Moldflow and Abaqus in the simulation workflow.

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