Proceedings of the ASME 2020
International Mechanical Engineering Congress and Exposition
IMECE2020
November 16-19, 2020, Portland, OR, USA

IMECE2020-22040

ON NUMERICAL MODELING OF EQUAL CHANNEL ANGULAR EXTRUSION OF ULTRA HIGH MOLECULAR WEIGHT POLYETHYLENE

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ABSTRACT

Ultra high molecular weight polyethylene (UHMWPE) is widely used in biomedical applications, e.g. as a bearing surface in total joint arthroplasty. Recently, equal channel angular extrusion (ECAE) was proposed as a processing method to achieve higher molecular entanglement and superior mechanical properties of this material. Numerical modeling can be utilized to evaluate the influence of such important manufacturing parameters as the extrusion rate, temperature, geometry of the die, back pressure and friction effects in the ECAE of polyethylenes.

In this paper we focus on the development of efficient FE models of ECAE for UHMWPE. We study the applicability of the available constitutive models traditionally used in polymer mechanics for UHMWPE, evaluate the importance of the proper choice of the friction parameters between the billet and the die, and compare the accuracy of predictions between 2D (plane strain) and 3D models.

Our studies demonstrate that the choice of the constitutive model is extremely important for the accuracy of numerical modeling predictions. It is also shown that the friction coefficient significantly influences the punch force and that 2D plane strain assumption can become inaccurate in the presence of friction between the billet and the extrusion channel.

Keywords: UHMWPE, ECAE, FEA, extrusion, friction.

1. INTRODUCTION

Equal channel angular extrusion (ECAE) was initially proposed as a method to deliver large amounts of uniform shear deformation to a metal specimen in order to influence the material microstructure and improve its mechanical and physical properties, see for example [1]. This technique is widely used for metal alloys processing and being actively developed and improved, see [2] , [3] and review [4].

Originally developed for metals, ECAE is also being considered for processing of polymer materials to form oriented structures and improve properties, see [5]. One of the earliest numerical modeling studies on extrusion of polymer material (polycarbonate) was published in [6]. The authors assumed 2D plane strain and used J2-Plasticity material model. More advanced 2D plane strain numerical simulations of the angular extrusion were performed in [7] and [8] for HDPE material. These publications implemented a hypoelastic visco-plastic constitutive model to take into account the deformation rate sensitivity of the polymer. The authors investigated how the die geometry and number of passes affect stress and strain fields within the polymer billet. The experimental study on how the angular extrusion affects mechanical properties of polypropylene (PP), supported by numerical modeling of the extrusion process, was reported in [9]. Similarly, numerical and experimental studies on the applicability and influence of ECAE process on the properties and behavior of high density polyethylene (HDPE) were presented in [10]. A set of parametric numerical studies on the extrusion rate, billet-die friction coefficient and back pressure sensitivity was performed for PP and HDPE showing that those parameters are crucial.

Recently, ECAE was proposed as a means of achieving higher molecular entanglement and thus superior mechanical properties of UHMWPE [11] and UHMWPE-based composites [12]. The numerical modeling of the process could be used to better understand its mechanics and how it influences physical

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and mechanical properties of the resulting material. In particular, it can be used to evaluate the importance of the processing parameters such as friction between the billet and the die, extrusion rate, extrusion angle, back-pressure and processing temperature. However, to the best of the authors' knowledge, there are no published results on the numerical simulations of the ECAE for UHMWPE material.

In this paper we consider several issues relevant for numerical modeling of ECAE of UHMWPE. First, we discuss the choice of the appropriate material model to account for material temperature and strain rate sensitivity. Then we investigate the applicability of the 2D plane strain assumption for ECAE simulations. Finally, the sensitivity of the process to the friction parameters is studied.

2. MATERIAL MODELS FOR UHMWPE

One of the important steps in numerical modeling of such a complex process as ECAE of a polymeric material is to pick a proper constitutive material model. The model has to be applicable to the large compressive and shear deformations of the polymer, allow for accounting of the rate and temperature sensitivity of the material, and has to be easy to calibrate based on limited experimental data (usually simple tension and compression tests). The J2-Plasticity (J2) model is often the simplest choice [6]. However, this material model was developed for metallic materials and hence is usually not suitable for highly rate and temperature dependent polymers [13].

A hypoelastic visco-plastic (HEVP) constitutive model presented in [8] can be considered as a candidate for the UHMWPE extrusion simulations. The advantages of the HEVP model are that it takes into account the strain rate sensitivity of the material and it has a reasonable number of material parameters to be obtained from the experiment. However, this model does not include temperature sensitivity of the material and hence requires additional experiments at each value of the temperature in order to be calibrated. It has also not been validated for UHMWPE.

Another potential candidate is Bergstrom-Boyce (BB) model [14]. This particular model was developed for elastomers, however it can be applied to UHMWPE as its high molecular weight causes the polymer chains to entangle and hence act like crosslinks producing pseudo-elastomeric response of the amorphous region. This model includes deformation rate sensitivity of the polymer and requires only two loading-unloading tests at different strain rates to be calibrated. The model is usually included in commercial FE software packages which makes it easy to implement. In addition, the Bergstrom-Boyce model was validated for UHMWPE [13] in simple mechanical tests. The major disadvantage of the model is its inability to take the temperature sensitivity of the material into account directly requiring additional experimental data for calibration.

Three Network Model (TNM) [15] explicitly includes dependence on both deformation rate and temperature sensitivity. It was developed specifically for UHMWPE and showed good agreement with the experimental data. The challenge for this model is that it is difficult to calibrate and implement due to a large number of material parameters.

3. FE MODEL OF ECAE

In this paper, we present FE simulations of right-angle ECAE for compression-molded UHMWPE specimens. Figure 1 provides schematics of the experimental setup used in our research. A billet is pushed through a steel angular channel of a 50mm × 50mm square cross section with a sharp right-angle connection. A set of heating cartridges is embedded into the channel walls to maintain constant temperature during the extrusion. An aluminum pressure punch which extrudes the material billet is velocity controlled and a back-pressure plate which delivers resistance to the billet motion in the horizontal part of the channel is force controlled in order to be able to prescribe desired extrusion rate and back-pressure. Before the extrusion, the virgin resin powder is compression molded (CM) at an elevated temperature in the vertical portion of the channel and then the specimen is extruded. The initial CM process consolidates the powder, so continuum mechanics material models can be used in numerical modeling of the extrusion. Once the extrusion is over, the billet is extracted from the horizontal part of the channel using a pressure-controlled extraction punch. More detailed description of the experimental set-up is given in [11].

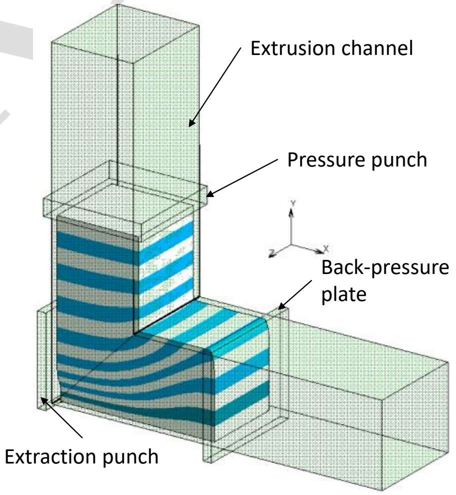

FIGURE 1: ECAE SCHEMATICS. THE LAYERS ON THE BILLET ILLUSTRATE THE NATURE OF DEFORMATION DURING EXTRUSION.

The extrusion channel, pressure punch, back-pressure plate and the extraction punch are modeled as rigid surface contact bodies. The extrusion channel is fixed, the pressure punch has its vertical displacement and velocity prescribed, the back-pressure plate is force controlled and the extraction punch is displacement controlled. The extrusion billet is modeled using ~15 thousand 2D plane strain Herrmann quadrilateral finite elements in the case of 2D plane strain assumption and ~190 thousand 3D Herrmann hexahedral finite elements in the case of 3D simulations. The contact interaction between deformable finite elements and rigid contact bodies is modeled as finite sliding with bilinear shear friction and friction coefficient μ. Two load cases are created to simulate extrusion and extraction separately. The extrusion takes 600 s which corresponds to the experimental extrusion time. All simulations are performed using MSC Marc Mentat software (https://www.mscsoftware.com/product/marc). The presented numerical models do not include the extrusion temperature influence as incorporation of this feature requires additional experimental data and is planned as future work.

Three constitutive models (J2, BB and TNM) were implemented in the simulations and calibrated for HDPE [7] and UHMWPE GUR 4150 [13]. To calibrate material models, we used MCalibration software (https://polymerfem.com/).

4. VALIDATION FOR EXTRUSION OF HDPE

Before simulating the ECAE for UHMWPE, we performed validation of our modeling approach by comparing with the published data for ECAE of HDPE [7]. Namely, we constructed a 2D plane strain finite element model based on the description provided in [7] and calibrated J2-Plasticity model for HDPE based on the published experimental data. Note that J2-Plasticity does not take into account the deformation rate sensitivity of HDPE which was modeled using HEVP in [7] and hence the agreement between the two models is not expected to be perfect.

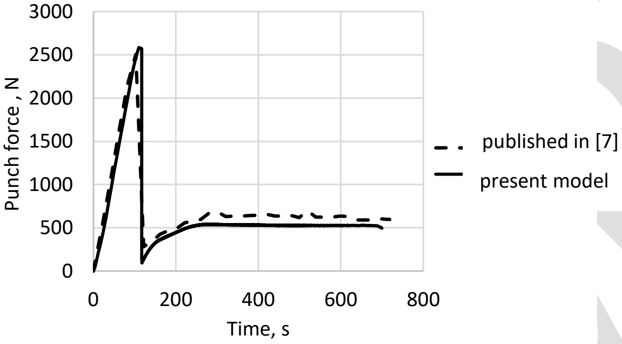

FIGURE 2: PUNCH FORCE VS. EXTRUSION TIME

Figure 2 shows comparison of the predictions for time history of the extrusion punch force in the experiment conducted at 60°C. The relative percentage difference as compared to the "published in [7]" peak load was calculated to evaluate the level of agreement. The difference between "present model" and "published" peak loads is 3.2% whereas the difference at the steady portion of the curves (at 400s) is 4.7%. Thus, it can be seen that the agreement between the two predictions is good despite the fundamental differences in the constitutive material models.

5. RESULTS AND DISCUSSION

We performed a set of parametric studies for numerical models of ECAE process for UHMWPE GUR 4150 material described in [13]. The first study provides an insight on the importance of the proper choice of the material constitutive model. The second study investigates the accuracy of the 2D plane strain assumption by comparing two-dimensional and three-dimensional modeling results. The third study presents results on sensitivity of the ECAE process to the billet-die friction parameters, namely the friction coefficient μ.

5.1 Sensitivity to the choice of the material model

A set of 2D plane strain finite element simulations was conducted to evaluate performance of three different constitutive models (J2, BB and TNM). The friction coefficient for this study was $\mu = 0.15$, the pressure punch velocity was $v = 0.17\ mm/s$ and back pressure was p = 36 MPa. All three material models were calibrated using experimental data from [13].

Figure 3 shows the actual and predicted deformed shapes of the UHMWPE billet extracted from the angular channel after extrusion. The deformed shapes predicted by BB and TNM models appear to be closer to the experiment than the J2-Plasticity model. However, there is still a noticeable discrepancy. The deviation from the experimental data might be caused by neglecting the temperature effects in the simulations while the actual extrusion is performed at elevated temperature and the polymer billet cools down after the extraction before the images are taken.

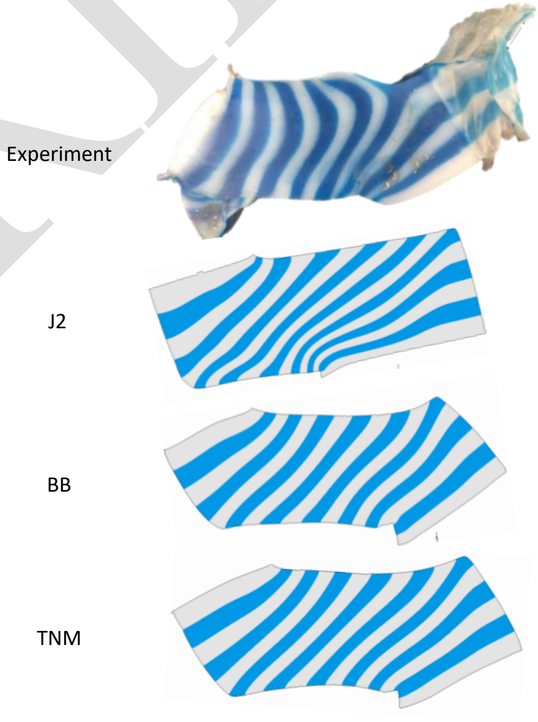

FIGURE 3: DEFORMED SHAPE OF THE BILLET AFTER THE EXTRUSION AND EXTRACTION

Punch force vs. displacement plot shown in Figure 4 supports the observations made based on the deformed shapes comparison. Namely, J2-Plasticity model performs differently from BB and TNM. It predicts significantly larger load needed to perform the extrusion which can be explained by linear hardening of the material in the model which is not the case for the considered polymer. At the same time, BB and TNM models have similar predictions for both the deformed shape and the punch force.

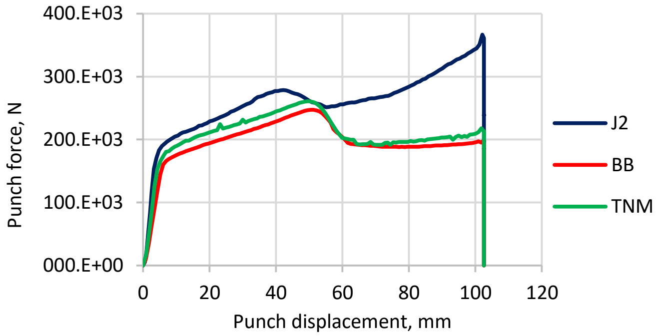

FIGURE 4: PUNCH FORCE VS. PUNCH DISPLACEMENT FOR DIFFERENT CONSTITUTIVE MODELS

We hypothesize that higher level of molecular entanglement of UHMWPE results in improved tribological properties of the material. The purpose of ECAE is to increase the entanglement by introducing severe shear deformations to the UHMWPE billet. Due to nonuniformity of the shear deformation in the material billet (see Figure 3) it is crucial to understand how shear strains (and hence increased molecular entanglement) are distributed through the specimen. Figure 5 shows maximum absolute value of shear strain experienced by the material during ECAE process as predicted by the J2, BB and TNM material models. Similarly to the force-displacement curves, BB and TNM models predict comparable levels of shear strain, while the strains predicted by J2 are lower and more uniform.

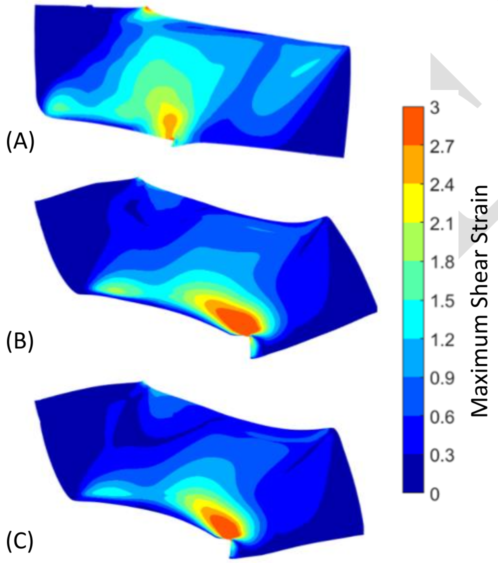

FIGURE 5: MAXIMUM SHEAR STRAIN DISTRIBUTION AS PREDICTED BY (A) J2, (B) BB AND (C) TNM MODELS

5.2 2D vs. 3D

This numerical study was performed to evaluate applicability of 2D plane strain assumption for ECAE of UHMWPE. In the presented simulations, the J2-Plasticity model was used because it is the simplest to implement. Since the plane strain assumption is geometrical and does not involve any constraints on physical behavior of the material, the obtained results will also be applicable to more complex material models. All the extrusion parameters were kept the same as in previous studies.

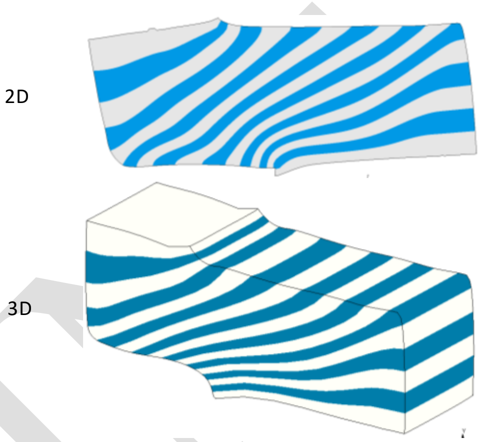

FIGURE 6: DEFORMED SHAPES USING J2-PLASTICITY, 2D VS. 3D

As seen in Figure 6, the predicted deformed shapes of the extracted billets are similar for 2D and 3D simulations. However, as shown in Figure 7, the punch force vs. displacement curves for 3D and 2D are not similar. The 3D model predicts larger punch force which can be explained by the contribution of friction between the billet and the side walls of the extrusion channel and also larger friction between the billet and bottom surface of the horizontal portion of the channel. This means that in the case of significant friction, the 2D assumption might become inaccurate and 3D modeling has to be considered.

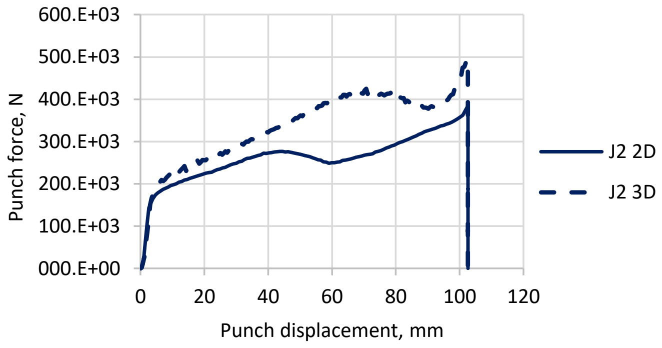

FIGURE 7: PUNCH FORCE VS. PUNCH DISPLACEMENT, 2D VS. 3D

5.3 Friction study

Based on the results of section 5.2, it becomes evident that friction effects are important in the simulation of ECAE of UHMWPE. Thus, a parametric study was conducted in order to investigate how friction coefficient μ influences the predicted ECAE results. A set of 3D FE simulations using J2-Plasticity model was performed with various values of friction coefficient μ = 0, 0.05, 0.1, 0.15 and 0.2. All other model parameters were kept the same as in section 5.2.

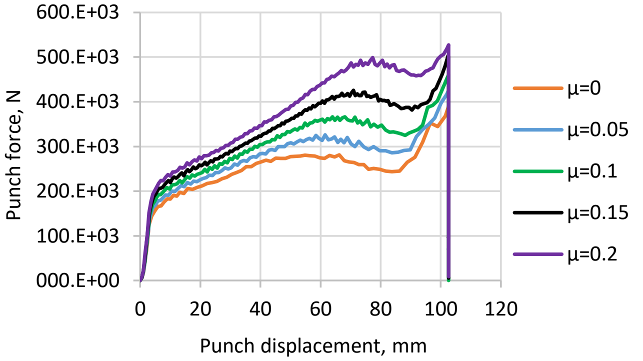

FIGURE 8: PUNCH FORCE VS. PUNCH DISPLACEMENT, FRICTION STUDY

Figure 8 confirms that the friction coefficient μ is an important parameter and must be identified from the experiments for accurate simulations of the extrusion process. A significant portion of the punch force is used to overcome friction (in addition to deforming the billet), so a significant increase in the punch force is observed for high friction coefficients.

6. CONCLUSION

An efficient numerical procedure was developed to simulate ECAE of UHMWPE material in order to better understand the mechanics of the process and improve the processing parameters with the goal of achieving superior mechanical properties of UHMWPE. The simulations show that the extrusion causes high shear strains in the material. It has been observed that the choice of the constitutive model is extremely important for the accuracy of numerical modeling predictions. It has been demonstrated that 2D plane strain assumption can become inaccurate if the friction between the billet and the extrusion channel is significant. The friction coefficient μ has been shown to be an important parameter which must be experimentally determined for accurate simulations.

ACKNOWLEDGEMENTS

This research is supported by a National Science Foundation EPSCoR award (#1757371).

The authors would like to thank Dr. Jorgen Bergström for his help with access to the constitutive material modeling software.

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