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BUCUREªTI, ROMÂNIA

- *materiale plastice*
- *elastomeri*
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CONTENTS

Analysis and Simulation of the Three-Dimensional Injection Moulding Process of Ultra-High Molecular Weight Polyethylene

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Ultra-high molecular weight polyethylene generally cannot be processed by injection moulding because of its high viscosity. In this paper, the formability of GUR-UHMW-polyethylene is numerically investigated during the injection moulding in an acetabulat cup. A number of numerical simulation tests have been performed on different acetabular cups to select the most appropriate process parameters and to optimize the injection moulding process. The numerical analysis demonstrates that the GUR-UHMW- polyethylene can be processed by injection moulding.

Keywords: injection moulding, finite element analysis, UHMW-PE

Each year, about 1.4 million joint replacement procedures are performed around the world. A combination of demographic factors and technological advances is poised to push the European hip and knee replacements market from an estimated USD 1.40 billion in 2004 to USD 1.83 billion in 2010. The 2005 revenues for hip implants in the US were $2 billion and $1.4 billion in Europe. The average prices for hip implants grew by 2-3% from 2004 to 2005 [1].

Introduced clinically in 1962 by Sir John Charnley, Ultra-high molecular weight polyethylene (UHMW-PE) articulating against either a metallic or a titanium-based alloys femoral head remains the gold standard bearing surface combination for total hip arthroplasty. UHMW-PE has over 40 years of clinical history as a successful biomaterial for use in hip, knee, and most recently, for spine implants. It has been estimated that more than 90% of total hip replacements implanted worldwide since the 1990s have incorporated UHMWPE inserts [2].

UHMW-PE is a linear polyethylene with outstanding physical and mechanical properties. It has extremely long chains, with an estimated weight-average molecular weight numbering in the millions, usually between 2 and 6 million which results in a very tough material, with the highest impact strength of any thermoplastic presently made. Outstanding properties include very low friction coefficient that results in self lubricating, biocompatibility, high resistance to abrasion and negligible water absorption. A very important property of the part is its creep resistance. For prosthetic devices, e.g. knee, hip, elbow joints, etc., any substantial creep can be devastating in the loss of the benefits of extremely expensive surgery.

At a conceptual level, three processing steps are needed to obtain an UHMW- PE component: (i) the ultra-high molecular weight polyethylene is polymerized from ethylene gas, (ii), the polymerized UHMW-PE, in the form of resin powder, is consolidated into a sheet, rod or near net-shape component, and (iii) the UHMW-PE component is manufactured into its final shape.

Each of these steps produces an alteration of the properties of the UHMW-PE implants. In some cases, such as machining, the change in the material may occur only at the surface. However, the quality of the final surface of the acetabular cup is crucial in the realization of the hip joint prosthesis that must have a high quality throughout the life cycle of the prosthesis [3, 4].

On the other hand, changes in polymerization and conversion of the UHMW-PE can impact the physical and mechanical properties of the entire implant [5, 6, 7]. In contrast to the low- molecular weight polyethylene, high molecular polyethylene does not melt without degradation on heating, but instead are converted into a viscoelastic state.

Because of its high melt viscosity, processing of UHMW-PE is not easy. Methods used currently are compression molding, ram extrusion, warm forging of extruded slugs, and machining. Historically, the UHMW-PE powder has been converted by compression moulding since the 1950s. In contrast with compression moulding, which originated in Germany in the 1950s, ram extrusion of UHMW-PE was developed by converters in the US during the 1970s. In the direct compression moulding, the resin is effectively converted to a finished part using individual moulds. The main advantage of the direct compression moulding of UHMW-PE is the extremely smooth surface finish obtained with a complete absence of machining marks at the acetabular cup surface.

Orthopedic manufacturers generally machine the UHMWPE components into their final form. Machining of UHMW-PE implants consists of milling and turning operations for both roughing and finishing steps. Sometimes, even components that are directed moulded may be machined [2].

Due to its high viscosity, UHMW–PE generally cannot be processed by injection moulding. Developmental work is being done on injection moulding of UHMW–PE resins. Recently, Ticona offers GUR UHMW – PE resins designed for injection molding instead of compression moulding or ram extrusion. These grades are solid in pellets and are FDA compliant. However, clinical studies will be critical to determine if this new UHMW–PE is biocompatible and can be used for orthopedic implants.

As for the injection moulding process, the quality of acetabular cups is greatly influenced by several factors, i.e., shape of the part, processing parameters, and moulding machine [8, 9]. Due to time and costs associated with experimental testing of the factors that influence the injection process computational methods have been developed. The numerical simulation of the injection

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moulding is useful at different levels. The firs level is the part design. At this level one has to prove the feasibility of the part concept. Thus, one has to check if the melt front progression will be smooth, if the unavoidable weld lines are away from area of high external stress, the distribution of the air traps. At the injection moulding level, numerical simulation of the injection process offers a lot of predicted data which normally are not available by experimental investigation and, thus, allows the evaluation of the moulding conditions with a high level of accuracy [9].

In this paper, the formability of GUR-UHMW-polyethylene is numerically investigated during the injection moulding in three different acetabulat cups. The simulations are carried out using Moldflow software. The influence of different acetabular cup shapes on the injection moulding process of GUR- UHMW - polyethylene is investigated. Based on the numerical results accurate prediction of the air traps and weld lines is carried out.

Governing equations

The injection moulding process can be broken into three phases: filling, packing phase, and cooling phases, respectively.

During the filling phase, plastic is pushed into the cavity until the cavity is just filled. A mathematical representation of the mould filling phase requires solution of the equations governing the conservation of mass and momentum along with constitutive equations that describe the behaviour polymer melt through its shear viscosity [10].

Fluid flow in injection molding is assumed to behave as Generalised Newtonian Fluid. The melt is a non-Newtonian fluid experiencing a phase change with its physical and transport properties changing with location in the cavity, temperature, and time.

The non-isothermal flow motion is mathematically described by the following equations [10]:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho u = 0 \tag{1}$$

$$\frac{\partial}{\partial t}(\rho u) + \nabla \cdot (\rho u - \sigma) = \rho g \tag{2}$$

$$\sigma = -pI + \eta(\nabla u + \nabla u^T) \tag{3}$$

$$\rho C_p \left(\frac{\partial T}{\partial t} + u \cdot \nabla T \right) = \nabla(k \nabla T) + \eta \dot{\gamma}^2 \tag{4}$$

where:

u is the velocity vector;

T - is the temperature;

t -the time;

p - the pressure;

σ - the total stress tensor;

C_p - the specific heat;

$\dot{\gamma}$ - the shear rate.

In this paper, in order to describe the viscosity of the polymer melt, the Cross-WLF viscosity mode is employed [11]

$$\eta = \frac{\eta_0}{1 + \left(\frac{\eta_0 \dot{\gamma}}{\tau^*} \right)^{1-n}} \tag{5}$$

with

$$\eta_0 = D_1 \exp\left[\frac{-A_1 + (T - T^*)}{A_2 + (T - T^*)} \right] \quad 6)$$

where *:*

n is the power law index,;

η_o - the zero shear viscosity;

τ^*- related to the relaxation time of the material and represents the parameter that describes the transition region between zero shear rate and the power law region of the viscosity curve;

D_1, A_1 and A_2 - data-fitted coefficients.

The packing phase begins after the cavity has just filled. This involves the further application of pressure to the material in an attempt to pack more material into the cavity in order to produce uniform shrinkage at reduced levels and consequently reduce component warpage [11].

If one region of a part is less densely packed than an adjacent one, then polymer will flow into the less dense region until equilibrium is reached. This flow will be affected by the compressibility and thermal expansion of the melt in a similar way to which the flow is affected by these factors in the filling stage.

The modified Tait equation is used to describe the material PVT characteristics and to provide the necessary information (density variation with pressure, temperature, compressibility and thermal expansion data) so that when combined with the material viscosity data accurate simulation of the material flow during the packing phase is possible [9, 11]:

$$V(P,T) = V(0,T)\left[1 - C \cdot \ln\left(1 + \frac{P}{B(T)}\right)\right] + V_t(P,T) \tag{7}$$

If

$$T > T_t,\ V_0(T) = b_{1m} + b_{2m}(T - B_5) \tag{8}$$

then

$$B(T) = b_{3m} \exp(-b_{4m} T), \tag{9}$$

$$V_t(P,T) = 0. \tag{10}$$

If

$$T < T_t,\ V_0(T) = b_{1s} + b_{2s}(T - B_5) \tag{11}$$

then

$$B(T) = b_{3s} \exp(-b_{4s} T), \tag{12}$$

$$V_t(P,T) = b_7 \exp(b_8 T - b_9 p) \tag{13}$$

where

T_t is the transition temperature,

b_1 to b_9 - the PVT model coefficients,

C=0.08494 is a universal constant.

Numerical simulation of the injection moulding process

The numerical simulation during the injection moulding of the UHMW-polyethylene in three different acetabular cups was considered in this paper. The finite element analysis is carried out using Moldflow software. The mould flow solver is based on the Hele-Shaw flow mode [11].

The UHMW-polyethylene under the trade name GUR EP4221 has been used for the injection moulding of the acetabular cups. The material properties (chosen from the Moldflow database) are presented in table 1 while the Tait PVT model coefficients are presented in table 2. The variation of the specific volume as a function of temperature is presented in figure 1.

The acetabular cup is modelled using a fusion representation of the three-dimensional cup (standard

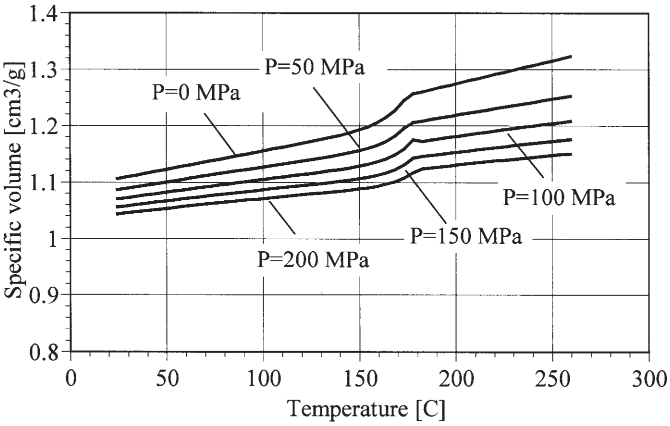
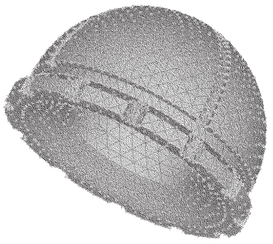


Fig. 1. Specific volume as a function of temperature

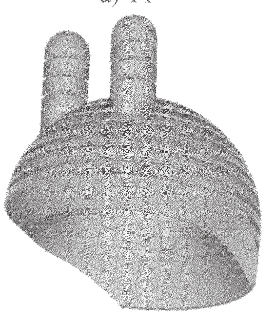
3D STL model format). The fusion technique creates a shell mesh on the two outside surfaces of the 3D model; the element on the opposite surfaces of the wall are matched and aligned on the two outside surfaces. The distance between the elements on the opposite sides of the wall defines the part thickness [11, 12].

To maintain consistency between the external surfaces of the mesh and ensure reliability of filling pattern, each pair of facing elements is bound with an extra element, i.e., connectors [11]. Within the fusion mesh, the flow and temperature profiles are evaluated over several positions through the thickness of the cavity. The fusion meshes of the three cups under consideration consist of 15582, 18776 and 32492 triangular elements for cups T1, T2, and T3, respectively (fig. 2). We have chosen different mesh densities in order to obtain the minimum percentage of matched elements (at least 85%) that can provide good quality of the mesh.

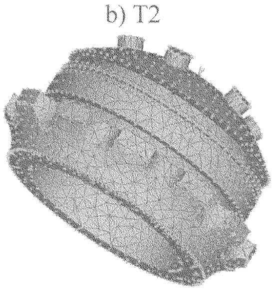
The simulations were carried out with the same process parameters, and the mould and melt temperature were



a) T1



b) T2



c) T3

Fig. 2. Fusion mesh of the acetabular cups

Table 1

MATERIAL PROPERTIES OF UHMW - PE

Modulus of elasticity	MPa	1100
Poisson's ratio		0.43
Shear modulus	MPa	385
Melt density	g/cm^3	0.77691
Solid density	g/cm^3	0.9052
Transition temperature	°C	119
Melting temperature	°C	190
Thermal conductivity	W/m °C	0.29
Heating/cooling rate	°C/s	-0.333
Specific heat	J/kg °C	3200

Table 2

TAIT PVT MODEL COEFFICIENTS

b5	K	448.65
b6	K/Pa	3.25 10^{-8}
b1m	m^3/kg	1.252 10^{-3}
b2m	m^3/kg	8.2 10^{-7}
b3m	Pa	8.81754 10^{+7}
b4m	1/K	4. 466 10^{-3}
b1s	m^3/kg	1.202 10^{-3}
b2s	m^3/kg	6.494 10^{-7}
b3s	Pa	1.11864 10^{+8}
b4s	1/K	4. 706 10^{-3}
b7	m^3/kg	4.98 10^{-5}
b8	1/K	0.09378
b9	1/Pa	5.36 10^{-9}

Table 3

PROCESS CONDITIONS

Mold surface temperature	°C	106
Melt temperature range	°C	176-260
Mold temperature range	°C	79-107
Ejection temperature	°C	112
Maximum shear stress	MPA	0.22
Maximum shear rate	1/s	65000

chosen according to the recommendation of the Moldflow database (table 3). To obtain an initial process evaluation, filling and packing analyses were carried out for each cup using only one mould with one cavity, the cavity being filled from a single gate at a constant volumetric flow rate [12, 13].

Figure 3 shows the predicted fill time distribution for the three cups. The pressure distributions through the flow path inside the mould, at the end of the filling phase are presented in figure 4. In case of T3 acetabular cup, at the transition between thin and thick sections, the melt front reaches the channel location at the end of filling which is practically impossible. Thus, it is recommended that the channel to be obtained by machining.

The pressure at injection location from the fusion flow at various times during the filling and packing phases of the analysis is presented in figure 5. The pressure at injection location result is very useful for checking whether there are any pressure spikes. This result can also be used to determine the pressure distribution in the cavity at the change-over point in the analysis. The variation of the polymer melt volume and clam force versus time to fill is presented in figure 6. and 7, respectively.

Generally speaking, air traps occur when converging flow fronts surround and trap a bubble of air. The trapped air can cause incomplete filling and packing, and will often

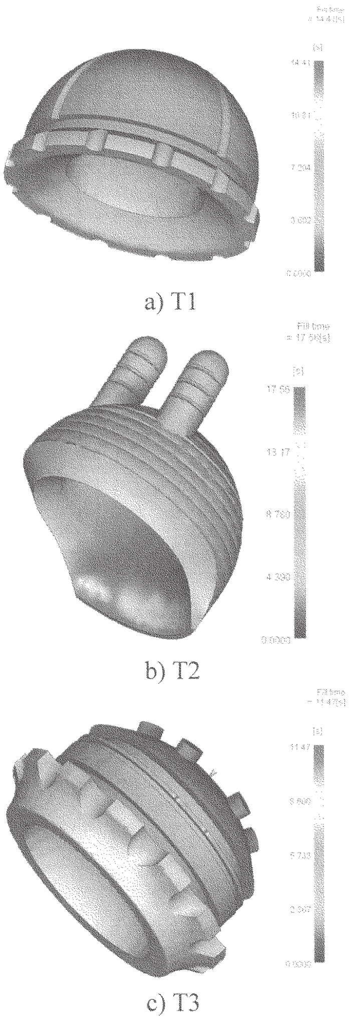


Fig. 3. Predicted fill time distribution

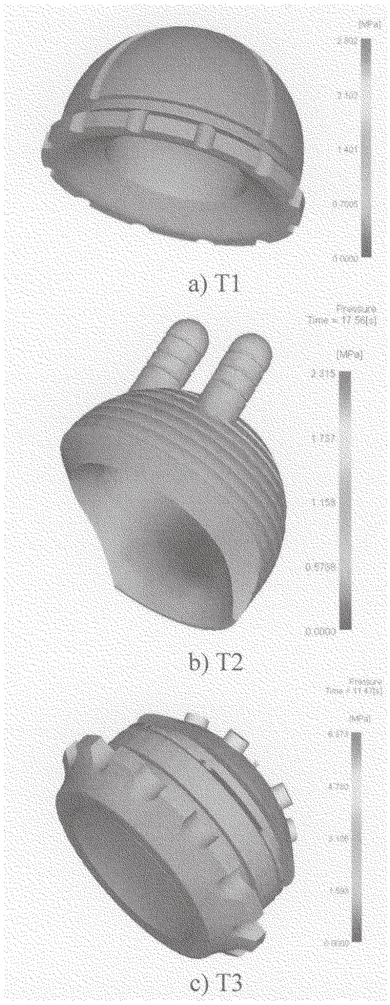


Fig. 4. Pressure distributions at the end of filling

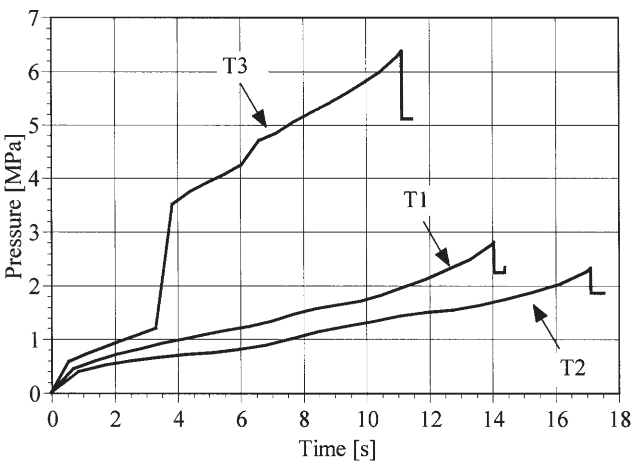


Fig. 5. Pressure vs. time to fill the acetabular cups at the entrance of the cup

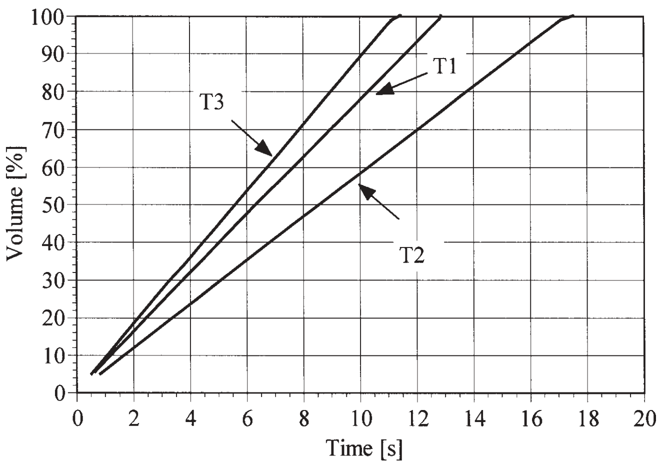


Fig. 6. Volume vs. time to fill

cause a surface blemish in the final part. In computational model, the air traps are located as single, empty nodes that are surrounded by filled nodes or cavity wall.

The predicted air traps for the three acetabular cups are presented in figure 8. The air traps are generated at the end of the fusion flow analysis, and shows a red line wherever an air trap is likely to occur [11]. This may be where the melt stops at a convergence of at least 2 flow fronts, or at the ends of flow paths.

The weld lines are generated at the end of a filling analysis, and shows where weld lines are likely to occur on the model (fig. 9). Weld lines are a weakness or visible flaw created when two or more flows meet and converge while filling a part. The weld lines are formed by flows meeting at higher angles, often head-on. The presence of weld lines may indicate a structural weakness and/or a surface blemish [10, 11].

Weld lines can cause structural problems, and they can also make the part visually unacceptable. However, some weld lines are unavoidable, so one needs to look at the processing conditions and the weld/meld line position to decide if they will be of a high quality [11]. However, if the weld line is positioned on a non-critical part surface, this may not be a problem.

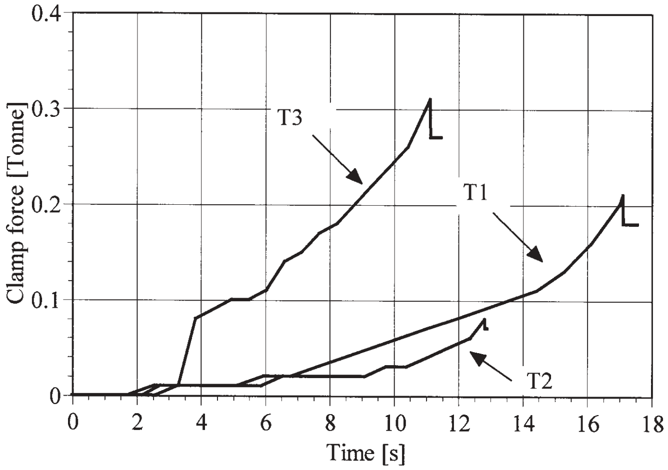


Fig. 7. Clamp force vs. time to fill

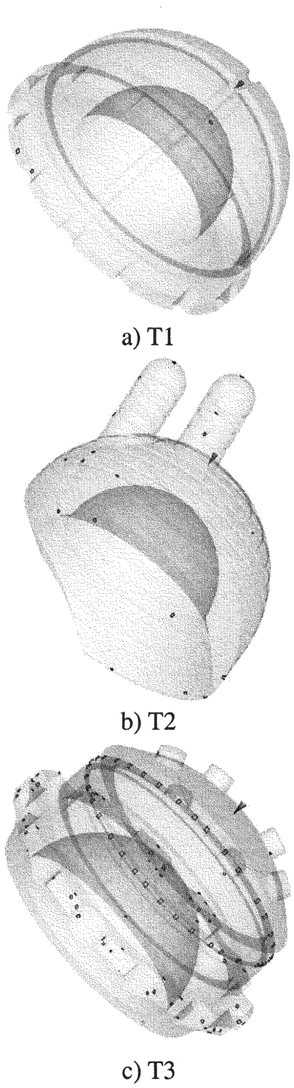


Fig. 8. Air trap prediction

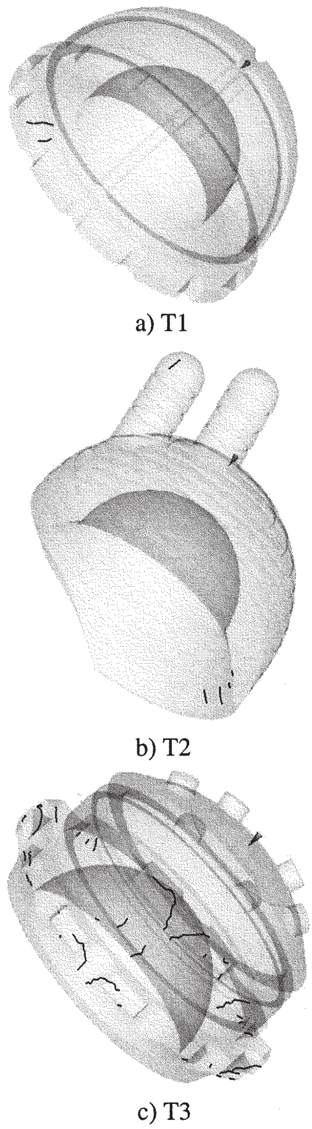
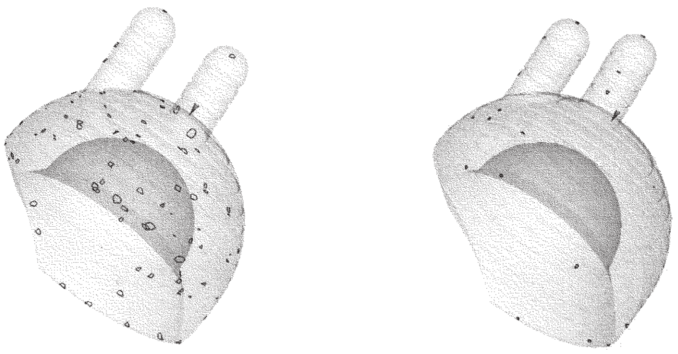


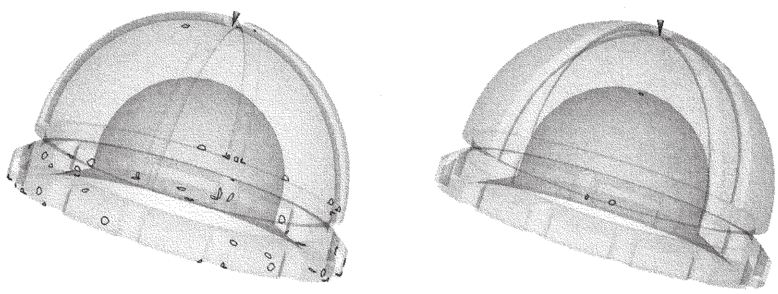
Fig. 9. Weld line prediction



a) 9152 elements

b) 18776 elements

Fig. 10. Air trap prediction with different mesh densities



a) 6476 elements

b) 15582 elements

From figures 8 and 9, it has been observed that the number of the defects (air traps and weld lines) is smaller in cup T1 than those in cups T2 and T3, respectively.

Accurate air traps and weld lines prediction depend on the mesh quality. Refining the mesh one can improve the air traps and weld line prediction, especially around holes or channels. In this sense, we have considered the case of T1 and T2 acetabular cups, respectively. Figure 10 presents the air traps predicted for two different meshes: first mesh (fig. 10(a)) is a low density mesh and consists of 9152 and 6476 elements, respectively; the second mesh (fig. 10(b)) is a high density mesh and consists of 18776 and 15582 elements, respectively. It can be seen that high mesh density can predict better the air traps.

Conclusion

In this paper, the formability of GUR-UHMW-polyethylene was numerically investigated during the injection moulding in three different acetabulat cups. The numerical analysis demonstrates that the UHMW-polyethylene can be processed by injection moulding. The simulations of the injection moulding process allow to (i) optimize the moulding conditions such as injection time, injection velocity profile, melt temperature, packing pressure, packing time, and cycle time; (ii) predict weld line locations and either move, minimize, or eliminate them; (iii) identify potential air traps and determine locations for proper mould venting. These results can be further used to select the appropriate injection moulding technology and to proper design the part and the mould.

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