Multiphase, Dual Polymer Injection Molding and Cooling of an Open Cavity to Form both Distinct and Graduated Material Properties within a Complex Three-Dimensional Body

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Abstract: With the advancement of medical devices and implants, many now require more advanced nonlinear, hyper-elastic materials such as elastomers to be extensively utilized in the body. This combined with the need to allow for considerably different, varying and graduated material responses within the three-dimensional device, poses a difficult challenge to manufacturing an elastomeric implant in a single process. A method of producing a complex three-dimensional, homogeneous body with distinct and graduated material properties is assessed using a multi-polymer injection process into an open cavity mold at elevated temperatures. COMSOL multiphysics is used to assess the multiphase, dual polymer injection and cooling process to form the required material properties across an implantable body, which is highly dependent on the flow and the mixing of two polymer blends at elevated temperatures.

Keywords: Injection Molding, Open Cavity, Multiphase, Co-injection Elastomer, Hyper-elastic, Implant.

1. Introduction

Frequently, more devices are using hyper-elastic, polymeric materials to produce biomimetic implants which duplicate, or augment the natural response of body tissues. Unfortunately, soft tissue mechanics and material responses are described as hyper-elastic and anisotropic, and vary considerably from one end to the other, through the body. Thus to produce an anisotropic, hyper-elastic, homogeneous, biomimetic implant, is no easy task in a single production process.

This paper looks at overcoming this problem through the use of COMOSL to model the injection of multiple elastomeric materials with specific injection rates, time and temperature dependent profiles to control the formation of an anisotropic, hyper-elastic body, with distinct regions and graduated material properties across its domain.

The implant assessed is a novel rotator cuff, Ligament Replacement and Augmentation System (LARS) for use in shoulder arthroplasty. The term, rotator cuff refers to the group of muscles and tendons in the shoulder region that help to stabilize the shoulder joint. Although current rotator cuff repair techniques offer excellent results in most cases, there are many instances where massive rotator cuff tears occur and tendon repair is not possible and a LARS is required to maintain anatomical integrity. Figure 1, illustrates the use of an embroidered/braided LARS for massive rotator cuff repair.

Figure 1. Ligament Replacement and Augmentation System (LARS), shown in shoulder joint, for massive rotator cuff repair [1]

The novel LARS described is made from two different hyper-elastic elastomers and designed to dynamically interact with joint function, where it augments and realigns the joint and brings the shoulder back to normal anatomical function. Figure 2, illustrates the shape and size of the homogeneous rotator cuff LARS.

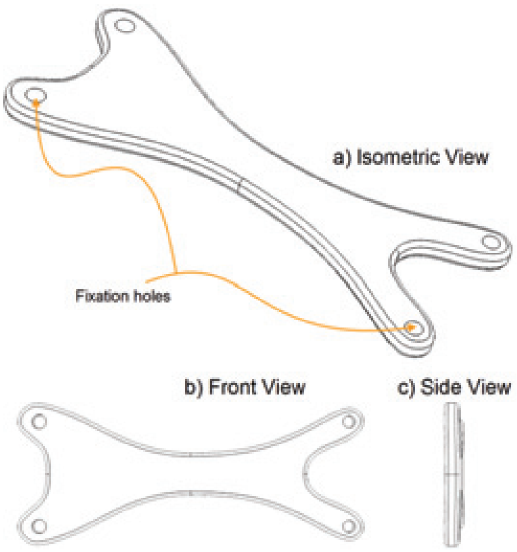

Figure 2. Novel elastomeric, homogeneous, rotator cuff LARS

2. Use of COMSOL Multiphysics

A three-dimensional, transient, multi-phase, fluid flow model is used to simulate the filling and the co-injected slow curing polymers which are heated during the injection process and allowed to cool and cure. The COMSOL model will then be used to optimize the injection rates, time-dependent profiles and mold temperature over time, to obtain a controlled, homogeneous body with distinct and graduated material properties and regions, within the mold cavity for various sized LARS.

The model assesses the interaction of the two slow curing polymers during the injection process, including, change in density and viscosity due to thermal effects. The multiphysics model was validated against physical test data where the dynamic air-fluid boundary (liquid flow front), the dual-polymer boundary and graduated region, and thermal profiles at specific locations and time points were assessed for two injection profiles on a single three-dimensional open cavity, body.
The problem was set up with three domains, a solid region representing the mold cavity walls, a liquid region representing the two dual injected polymers and a gas region representing the air within the cavity prior to injection of the two polymer solutions. Due to the symmetry of the problem, only one half the model was assessed and symmetry enforced on the mid-plane. Figure 3, illustrates the model geometry, domains and boundary conditions used in the model.

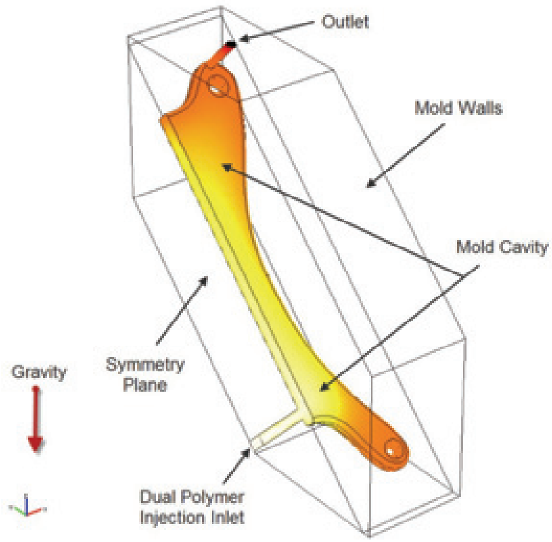

Figure 3. Model Geometry, Domains and Boundary Conditions

Three transient COMSOL multiphysics application modes were utilized and coupled in the study, namely, two multiphase flow modules [a Two-Phase Flow (Laminar) Phase Field (chns) and a Phase Field (mmpf) module], and a Convection & Conduction (cc) module.

The Two-Phase Flow (Laminar) Phase Field (chns), was used to model the liquid-air flow front, the second Phase Field (mmpf) module, was used to model the two dual injected polymer solutions in the fluid phase of the Two-Phase Flow (Laminar) Phase Field (chns), while the Convection & Conduction (cc) module was used to model the thermal changes in the model. All three modules implemented were coupled.
Velocity profiles of the Phase Field (mmpf) and Convection & Conduction (cc) modules, were coupled to the velocity profiles of the Two-Phase Flow (Laminar) Phase Field (chns), while the density and viscosity profiles of the polymer region in the Two-Phase Flow (Laminar) Phase

Field (chns), were coupled to the density and viscosity profiles of the Phase Field (mmpf) module, which were dependent on the temperature related functions for viscosity and density and the Convection & Conduction (cc) module, transient temperatures.

The temperature dependent functions for dynamic viscosity (μ) and density (ρ) of the polymer solutions used in the injection mold process are graphically illustrated in Figure 4 below.

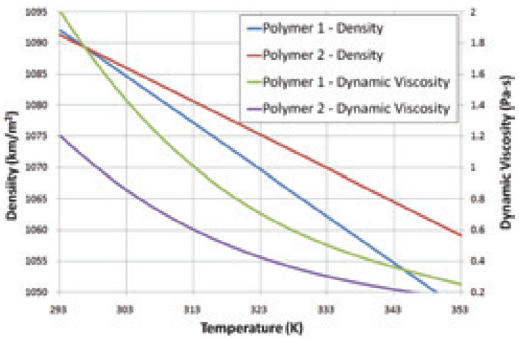

Figure 4. Change in dynamic viscosity & density with temperature for the two polymer solutions used in the injection mold process.

The implementation of the coupled density and viscosity values for the polymer flows was done with scalar expressions in terms of volume fraction, while the velocity fields and density of the second Phase Field (mmpf) module, and the Convection & Conduction (cc) module were equated to the Two-Phase Flow (Laminar) Phase Field (chns) modules, velocity field. These coupled scalar and field functions are described by Equations [1] to [4] below.

The heat capacity (C_p) and the thermal conductivity (k) of the Convection & Conduction (cc) module were coupled to both the air and fluid regions through functions utilizing the phase field function (*phi*) from the Two-Phase Flow (Laminar) Phase Field (chns) module. These functions are described by Equations [5] and [6] below, where, A, B, D and E are material dependent constants.

The injection process is achieved through a single inlet port and two outlet ports, as indicated in Figure 3 (NB: only a single outlet port is illustrated, due to symmetry). The co-injected polymers are mixed prior to entry into the mold cavity inlet port. This mixing process, prior to the inlet port is not modeled in COMSOL. Instead, a simplified inlet boundary condition is imposed, where an ideal mix of the two polymer solutions as a function of volume fraction is applied. Figure 5 gives an example of the injection profiles of the two polymer solutions injected into the inlet port over time. This figure also indicates the regions, where there is discontinuity in the injection profiles due to the switching of the polymer port control valves. Figure 6, shows the equivalent simplified COMSOL model inlet boundary condition, where a smooth inlet flow function is implemented in terms of combined flow rate and volume fraction of the second polymer solution.

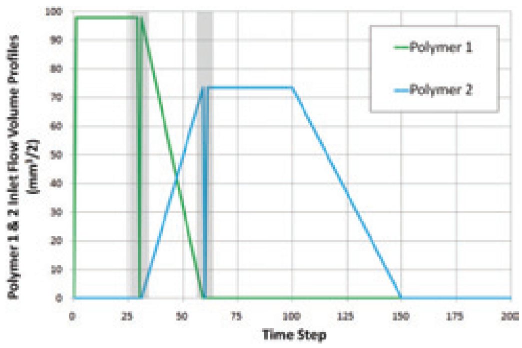

Figure 5. Mold machine polymer 1 & polymer 2 injection flow profiles vs. time.

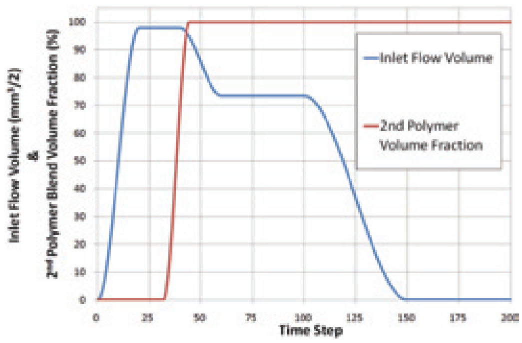

Figure 6. Equivalent, simplified COMSOL model inlet boundary condition, where a smooth inlet flow function is implemented in terms of combined flow rate and volume fraction of the second polymer solution (represented as a percentage).

Equations & Boundary Conditions

[1] $\rho(T_{cc})^{fluid}_{chns} = \rho(T_{cc})^{poly\,1} + \{[\rho(T_{cc})^{poly\,2} - \rho(T_{cc})^{poly\,1}] \times Volume\ Fraction^{poly\,2}_{mmpf}\}$

[2] $\mu(T_{cc})^{fluid}_{chns} = \mu(T_{cc})^{poly\,1} + \{[\mu(T_{cc})^{poly\,2} - \mu(T_{cc})^{poly\,1}] \times Volume\ Fraction^{poly\,2}_{mmpf}\}$

[3] $\rho_{cc} = \rho_{chns}$

[4] $\boldsymbol{u}_{cc} = \boldsymbol{u}_{mmpf} = \boldsymbol{u}_{chns}$

[5] $k_{cc} = A \times phi_{chns} + B$

[6] $C_{p\_cc} = D \times phi_{chns} + E$

[7] $T^{air}_{cc}(t = 0s) = 293.15K$

[8] $T^{solid}_{cc}(t = 0s) = 353.15K$

[9] $T^{fluid}_{cc}(t = 0s) = 353.15K$

Where:

Subscripts = the COMSOL Multiphysics module the equation parameter applies
Superscripts = the material phase or state: solid, gas, fluid
Poly 1 = 1st Polymer material/solution
Poly 2 = 2nd Polymer material/solution
A, B, D & E = Various material dependent constants
k = Thermal Conductivity
C_p = Heat Capacity
$\boldsymbol{u}$ = Velocity Field
μ = Dynamic Viscosity
ρ = Density
T = Temperature
t = Time

3. Model Validation

The COMSOL model was validated against quantitative thermal data and sectional views of a number of molded bodies, and qualitatively against captured video footage of the liquid-air flow front during the filling process of an open cavity mold. The validation work was done on a different three-dimensional body and cavity which cannot be fully represented here.

Figure 7 illustrates the comparison between the temperature profiles obtained from physical tests verses the model solutions with time, at three different locations across the body. From Figure 7, it can be seen that the model solution gives a good fit to the physical data. It should be noted that the COMSOL is an ideal smooth function solution and the results do not follow the physical data ideally, this is particularly true, where the discontinuity in the physical injection profiles due to the switching of the polymer port control valves is observed. These regions are indicated in Figure 7 for reference.

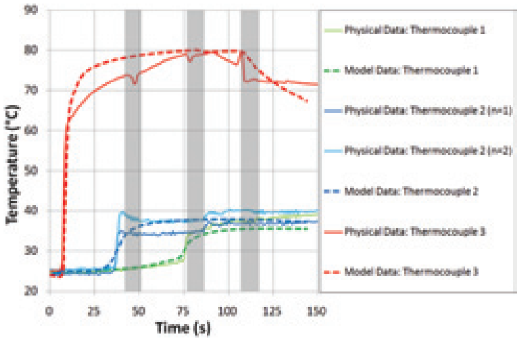

Figure 7. Time dependent thermal response curves of validation model vs. physical data at three different locations (NB: Grayed sections indicate discontinuous profiles due to the switching of the mold polymer port control valves; refer to Figure 5 for more details).

Additionally, it should be noted that there was a spread in the thermal data collected, as illustrated by the two temperature curves collected at thermocouple location 2.

Figure 8, shows a partial view of a cured section of a molded body, illustrating the boundary between the two polymer regions. The boundary for the 2nd polymer region in the equivalent model is also shown for a direct comparison. (NB: the model shows a partial view only of a different three-dimensional device to that of the rotator cuff LARS).

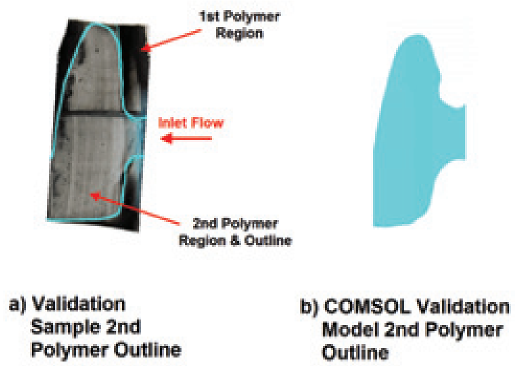

Figure 8. Partial view of a cured section of a molded device, illustrating the distinct cured polymeric regions (1 & 2) and comparison to the equivalent COMSOL model.

Although the full three-dimensional body cannot be disclosed, it can be seen from Figure 8, that the model solution obtained, gives a very good estimation of the final cured 2nd polymer region boundary. It is sufficient to say, even though further quantitative and qualitative data, such as air-fluid flow front video footage cannot be disclosed, it should be noted that the COMSOL model solutions obtained, adequately represented the physical data observed.

4. Model Results for Rotator Cuff LARS

Using the validated COMSOL model, a rotator cuff LARS three-dimensional mold cavity model was implemented as illustrated in Figure 3. A number of polymeric injection flow rates vs. time were assessed. For the purposes of this paper, only the data obtained for the flow vs. time profiles as illustrated in Figures 5 will be illustrated and discussed.

The model assessed, consisted of 51795 elements with a minimum element quality of 0.275. The total number of degrees of freedom solved for was 295068. The model was solved within 18hrs on a desktop computer with a 2.83GHz Intel® Core™ 2, Quad Processor Q9550 and 8GB memory, running on the 64-bit Windows Vista operating system.

Figure 9 illustrates the interface surface profiles or isosurfaces for 1) the air-fluid boundary, 2) the graduated polymer region with a volume fraction of 0.5 for the 2nd injected polymer and 3) the flow front where the 2nd injected polymers volume fraction is equal to 1, within the liquid region, and the thermal subdomain plots of the liquid and air regions at various time points during the mold cavity filling process.

As can be seen from the isosurface profiles in Figure 9, that the LARS is molded to form both distinct polymer 1 and polymer 2 regions with a graduated "mixed" blended region between, of which the volume fraction value of 0.5 is highlighted to indicate the mid surface of the graduated 'mixed' polymer solution.

Once the injection process comes to a stop at time step 150, the filled cavity is allowed to cool and the polymer regions assessed during the cooling process. During the cooling process the density and viscosity of the polymeric materials changes, as illustrated in Figure 4. Thus, continued fluid motion occurs until high viscosities values are reached, which then prevents further fluid motion and the polymer is allowed to cure fully.

Figure 10 below shows the comparison between the isosurface polymer regions obtained at time steps 100, 150, 750, and 5000. It can be seen that the distinct and mixed graduated polymer regions and boundaries continue to move and change from the end of the injection process at time step 150. At time step 5000, the temperature of the mold cavity falls below 43.5°C, and no further fluid motion is observed in the mold cavity. This figure demonstrates the gradual and continued flow of the polymer due to, a) the elevated temperatures and change in density and viscosity while cooling, and, b) gravitational forces.

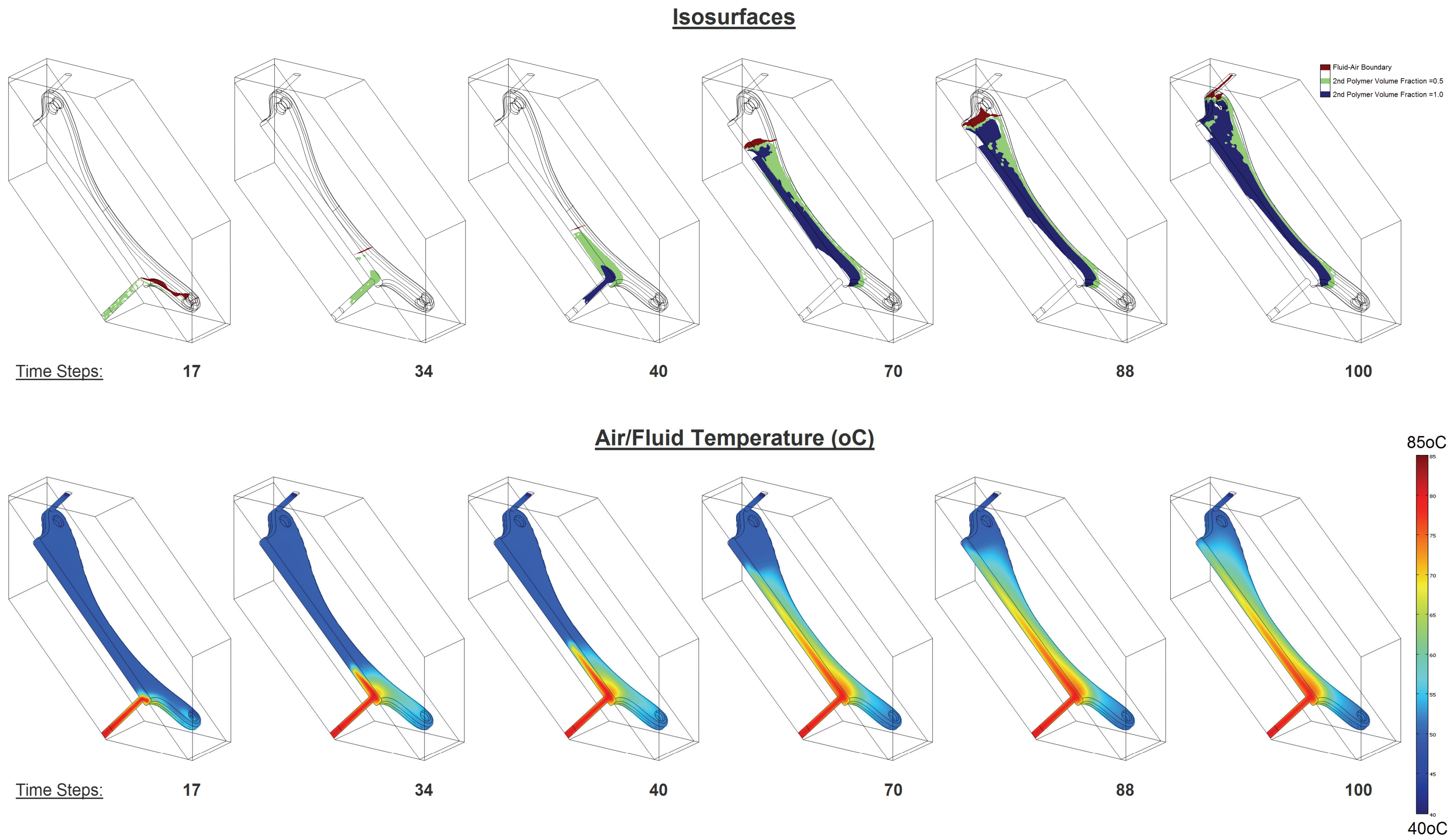

Figure 9. Isometric views illustrating the isosurfaces for the air-fluid boundary & volume fractions of 0.5 & 1 for the 2nd injected polymer and the mold cavity temperature values at various time steps during injection process

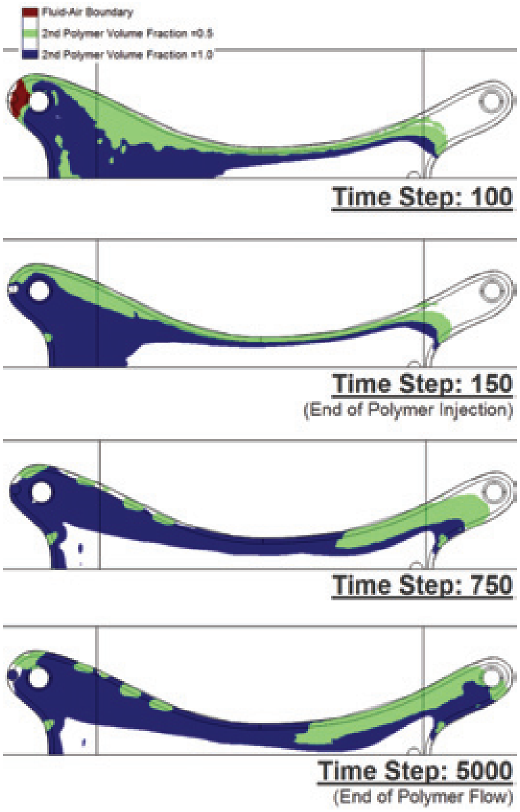

Figure 10. Front view of rotator cuff LARS illustrating the change in the distinct & 'mixed' graduated blend of polymeric regions from the end of the injection process at time step 150 to 5000.

5. Conclusions

In conclusion COMSOL was successfully used to model the coupled multiphysics problem of multiphase, dual polymer injection molding and cooling of an open cavity to form both distinct and graduated material properties within a complex three-dimensional body.

The model was validated against both quantitative and qualitative data. Only a section of the validation data is presented, as not all the data could be disclosed. However, a partial sectional view of a single sample is demonstrated, and the model solution versus the final cured sample compared. This demonstrated the close comparisons obtained between the model boundaries and the physical molded samples. Additional video footage of the air-fluid flow front was qualitatively assessed, and the model showed good comparative results.

The coupled multiphysics model is now ready to be used further for optimization of the injection profiles and the control of the mold temperature, to obtain specific and controlled graduated material regions. Thus, non-linear, anisotropic, hyper-elastic material properties across the three-dimensional implantable device can be achieved in a single production process.

The COMSOL multiphysics model is to be developed further to include:

a) additional polymer solutions,

b) multiple inlet and outlet locations across the mold cavity,

c) a polymer curing function to include the change in polymer properties due to the time dependent curing process,

d) multi-parameter optimization of the injection flow inlet profiles and temperature, including; injection velocities, rates, volume fractions and mold wall and inlet temperature with time.

Once these additional features are implemented in the model, the coupled multiphysics model will be used further to find a number of single production process solutions, to produce a variety of anisotropic, hyper-elastic, homogeneous, three-dimensional implantable bodies which are biomimetic.

6. References

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7. Acknowledgements

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