CFD EVALUATION OF POLYMER CHAINS ORIENTATION IN STYRENE BLOCK COPOLYMERS PROCESSED BY INJECTION MOULDING

POLITECNICO DI MILANO UNIVERSITY OF CAMBRIDGE

F. De Gaetano[1], M. Serrani[2], J. Stasiak[2], J. Brubert[2], G. Moggridge[2], and M. L. Costantino[1]

[1] LaBS, Department of Chemistry, Materials and Chemical Engineering "Giulio Natta", Politecnico di Milano, Milan, ITALY

[2] Department of Chemical Engineering & Biotechnology, University of Cambridge, Cambridge, UK

Introduction

Polymeric Heart Valve (**PHV**) prostheses aim at combining the hemodynamic advantages of biological valves with the durability of mechanical valves [1]. Styrene Block Polymers (SBPs) appear as the best materials to this purpose, because of their excellent biocompatibility, chemical stability and fatigue resistance. In addition, these materials can be processed by **injection moulding**, a technique that allows controlling the alignment of the **polystyrene micro chains** [2,3] with the purpose to replicate the same **circumferential** orientation of the fiber of collagen in the natural heart valve leaflets (Fig.1). The aim of this work is the investigation of the micro domains orientation within the PHV leaflets produced by injection moulding technique in order to optimise the PHVs manufacturing.

Fig. 1 Natural heart valve leaflet. Collagen's fiber are circumferentially oriented within a protein matrix.

Materials and Methods

In order to evaluate the polystyrene micro chain orientation during the injection moulding technique, a numerical model was developed. Numerical steady fluid dynamic simulation of the injection moulding of the valve were performed using ANSYS Fluent (ANSYS Inc., Canonsburg, PA, USA) with hexahedral elements mesh. Only one third of the valve was considered due to the valve's geometric periodicity (120°) (Fig. 2). Different polymer outlets (Fig.3a), inlets (Fig.3b) and flow rate have been simulated to investigate the best configuration leading to a predominantly circumferential orientation of the polymer chains.

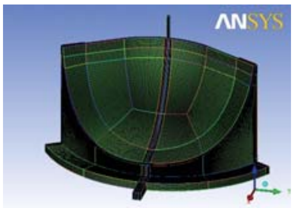


Fig. 2 Model of the valve discretized with hexahedral elements.

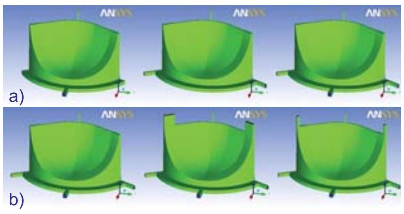


Fig. 3 Fluids domains with different Outlet (a) and Inlet (b) location.

The rheology of poly-(Styrene-Isoprene-Butadiene- Styrene) containing 19 wt% styrene at 160°C was described by the Carreau Model (1).

$$\eta = \eta_\infty + (\eta_\infty - \eta_0)(1 + \dot{\gamma}^2\lambda^2)^{(n-1)/2} \qquad (1)$$

The parameter used to describe the Carreau Model are reported in Tab.1 while Fig.4 show how this model well fits the experimental data.

Tab. 1 Parameter used into the Carreau Model.

η_∞	4234,91 Pa s
η_0	70346,28 Pa s
λ	38,614 s
n	0

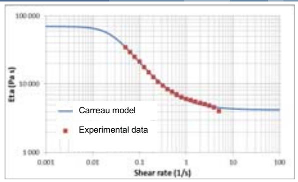


Fig. 4 Experimental data and by injection moulding of the SBP

Spatial coordinates and velocity data obtained by the computational analysis were processed with Matlab (The MathWorks Inc., Natick, MA, USA), to calculate from the deformation tensor **D** a stretch rate ε and the shear rate γ. These vectors describe the directions along which the extensional flow and the shear flow align the polymer chains. When the stretch and the shear vector were not aligned the dominant vector for the micro domains orientation was determined by comparing the ratio $\psi_v = |\gamma| / |\varepsilon|$ whit a threshold ψ_{vc}. This threshold has been determined by comparing the polymeric chain orientation in a thin injection moulded membrane of SI\BS19 measured by Small Angle X-ray Scattering Analysis (SAXS) (Fig.5) and the output of a simplified numerical model.

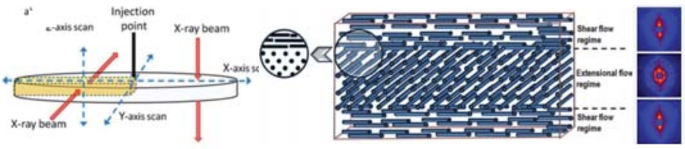


Fig. 5 SAXS analysis of an anisotropic cylinder orientation obtained by injection moulding of the SI\BS19

Results and Discussion

Different injection inlet/outlet were simulated with the same mass flow rate equal to **5.3·10^{-6} kg/s**. In the leaflet, no significant effects on the streamline were obtained (Fig.6).

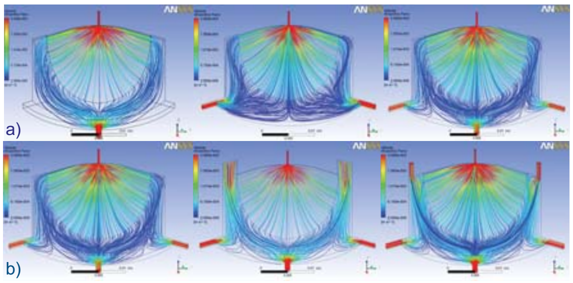


Fig. 6 Streamline of the configuration characterized by 1 inlet and different outlet (a) and 3 outlet and different inlet (b). The color scale range from 0.02 mm/s (blue) to 2 mm/s (red).

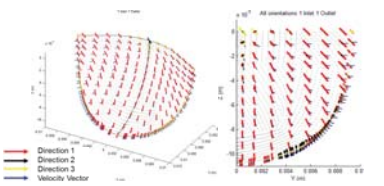


Fig. 7 Typical orientations of the polymer chains predicted by the model for the configurations characterized by a single inlet located in the middle of the leaflet free edge and a single outlet channel. a) 3D view of the entire leaflet. b) 2D view of one half of the leaflet.

The differences in the polymeric chains orientations resulted negligible and for that reason the results obtained in the configurations shown in Fig. 7 are representative also of cases not reported. Modelling prediction of the SI\BS19 microstructure averaged in the thickness of the leaflets show a micro domains mainly in the circumferential orientations (Fig. 7).

Furthermore, even if the phenomena that leads the polymer chains orientation is the same, differences in the orientation directions were seen among the point located near the mould walls (30 μm) and the ones at the middle of the leaflet thickness (Fig.8)

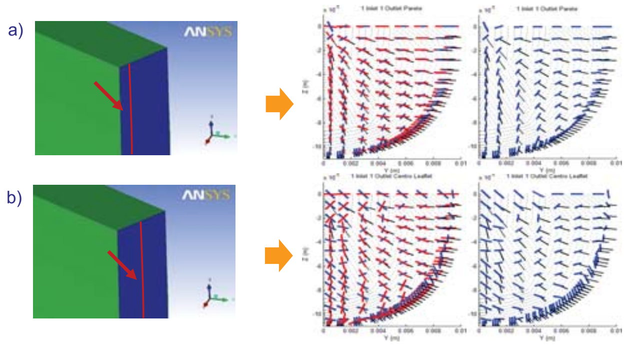
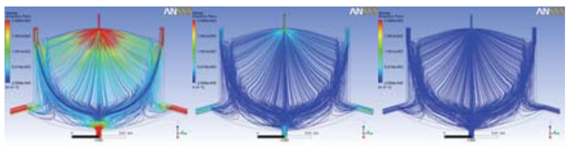


Fig. 8 2D view of the results of one half of the leaflet in planes at different position in the thickness located 30μm from the mould walls (a) and in the middle (b).

The analysis performed on different configurations allowed to highlight how the orientation of the polymer chains achieved in the leaflet is not affected by inlet and outlet locations that were tested. Therefore, it is possible to focus the mould's design to optimize the distributions of the polymer in the structure.



5,3 10-5 kg/s 5,3 10-6 kg/s 5,3 10-7 kg/s

Fig. 9 Streamline of the configuration with 3 inlet and 3 outlet. Different mass flow rate were considered (ten times higher and ten times lower than the standard condition).

In conclusion, the comparison of the different location of the injection points that were considered showed the same alignment of the polymer chains of the SBP. In particular, the micro domains are mainly oriented circumferentially, with negligible differences induced by the different inlet and outlet positions as well as by different polymer mass flow rate (Fig.9).

References

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Corresponding author: francesco.degaetano@polimi.it