USING COMPUTATIONAL MODELLING TO IMPROVE THE INSIGHT REGARDING MULTI-LAYER POLYMER FLOWS IN CO-EXTRUSION

M.M. MARTINS[1,2], O.S. CARNEIRO[1], C. FERNANDES [1], J.M. NÓBREGA [1]

INTRODUCTION

Polymer multilayer co-extrusion is a manufacturing process wherein two or more polymers feed a common extrusion die to form a layered product, aiming to combine in a synergic way the properties of the individual polymers comprising each layer [1]. The usual manufacturing approach starts by co-extruding two layers which are duplicated in each Interfacial Surface Generator Module (ISGM) employed, see Figure 1. This is achieved by dividing the flow of the two inlet layers (AB) in the division region, deforming and overlapping the two individual streams, which are subsequently joined in the junction region to reach a 4 layer structure (ABAB) [2]. In this way, each ISGM employed allows duplicating the number of layers in the final product.

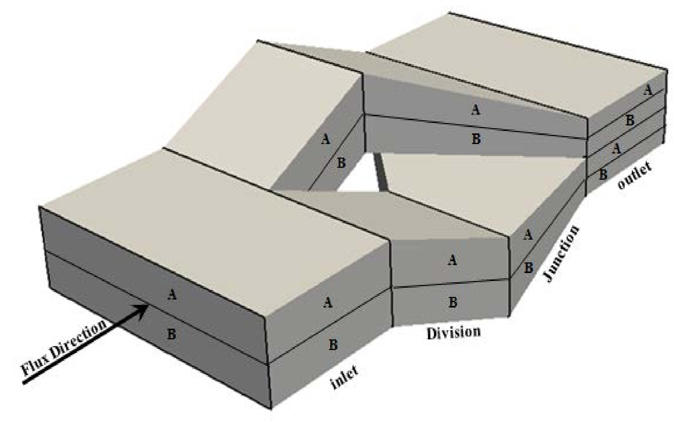


Figure 1. Interfacial surface generator module.

In this work we resort to computational modelling, aiming to improve the knowledge related to the design of these multiplexing devices, which was done with the support of the multiphase flow solvers from OpenFOAM computational library. Each ISGM comprise several geometrical transformations (effects), which could be done simultaneously or sequentially. The simultaneous combination of geometrical transformations, allows reducing both the device length and, in general, the total pressure drop. For this purpose, we studied several configurations for the ISGM, aiming to identify the details of the geometry that promote a non-uniform layer distribution.

MATHEMATICAL MODELLING

Numerical simulations of the phenomena are performed using a free-surface capturing model based on a two-fluid formulation of the classical volume-of-fluid (VOF) model in the framework of the finite volume numerical method. In the conventional VOF method the transport equation for an indicator function, representing the volume fraction of one phase, is solved simultaneously with the continuity and momentum equations,

$$\nabla\cdot\mathbf{U}=0 \qquad \frac{\partial\alpha}{\partial t}+\nabla\cdot(\mathbf{U}\alpha)=0 \qquad \frac{\partial(\rho\mathbf{U})}{\partial t}+\nabla\cdot(\rho\mathbf{U}\mathbf{U})=-\nabla p+\nabla\cdot\mathbf{T}+\rho f_b \qquad (1)$$

where $\mathbf{U}$ represents the velocity field shared by the fluids throughout the flow domain, α is the phase fraction, ρ is density, p is pressure, f_b are body forces per unit mass. For the constitutive equation the Newtonian fluid model is employed, where $\mathbf{T} = 2\eta\mathbf{S}$ is the deviatoric viscous stress tensor, η is fluid viscosity and $\mathbf{S} = 0.5[\nabla\mathbf{U}+(\nabla\mathbf{U})^{T}]$ is the rate of strain tensor. In VOF method [3] the transport equation for an indicator function is solved and phase fraction can take values within the range $0<\alpha<1$, with the values of 0 and 1 corresponding to regions accommodating only one phase. As a consequence, gradients of the phase fraction are found only at the interface region. In this way the two immiscible fluids are considered as one effective fluid throughout the domain. For the effective fluid the physical properties are calculated as weighted averages based on the distribution of the liquid volume fraction. In momentum equation the body forces considered are gravity and surface tension effects at the interface and rearranged according by [4],

$$\frac{\partial(\rho\mathbf{U})}{\partial t}+\nabla\cdot(\rho\mathbf{U}\mathbf{U})-\nabla\cdot(\eta\nabla\mathbf{U})-(\nabla\mathbf{U})\cdot\nabla\eta=-\nabla p_d-\mathrm{g}\cdot\mathrm{x}\nabla\rho+\sigma\kappa\nabla\alpha \qquad (3)$$

where $p_d = p - \rho\mathrm{g}\cdot\mathrm{x}$, being $\rho\mathrm{g}$ the hydrostatic component, x is the position vector, σ is the surface tension coefficient and κ is the mean curvature of the free surface.

NUMERICAL METHOD

The OpenFOAM was used in this study. The code is based in a cell-center finite volume method on a fixed unstructured numerical grid. The coupling between pressure and velocity fields is done by PIMPLE algorithm. The transient and source terms are discretized using the midpoint rule and integrated over cell volumes. The implicit Euler scheme is used for the discretization of the time derivative terms. The spatial derivatives terms (diffusion and convective) are converted into surface integrals bounding each cell making use of the Gauss theorem. The cell faces values are obtained by interpolation and then summed up to obtain the surface integral. For the evaluation of gradients a linear face interpolation is used. The time step is adjusted based on the maximum Courant number, which was considered 1 in this work. Consequently the time step values was varying along the calculations, ranging from 10^{-5} s to 10^{-4} s. The boundary conditions were applied as illustrated in Figure 2 and described in Table 1. The sets of linear equation were solved using a preconditioned conjugate gradient with diagonal incomplete-cholesky for pressure with tolerance 10^{-8} and preconditioned bi-conjugate gradient with diagonal incomplete-LU for velocity with tolerance 10^{-8}.

Table 1. Boundary conditions.

Patch	U (m.s-1)	p (Pa)	α
inlet_1	(0 0 0.1)	zerogradient	0
inlet_2	(0 0 0.1)	zerogradient	1
walls	non-slip	zerogradient	zerogradient
outlet	zerogradient	0	zerogradient

RESULTS

The cases have the base geometry presented by Figure 2. Polymers behavior was considered Newtonian and some properties is shown in Table 2. The surface tension coefficient was considered zero, since the polymers are the same. The mesh independence studies were performed with the geometry presented in Figure 2. The number of cells for each mesh is shown in Table 3. Figure 3, Figure 4 and Figure 5 show, respectively, the convergence of velocity, pressure and phase fraction in relation to the variation of the mesh refinements. Figure 3 and Figure 4 show the convergence of velocity and pressure, respectively, considering the center line through the channel defined in Figure 2.

The agreement of the velocity results between the M2 mesh and the M3 mesh is very good, with Root Square Mean error equal RMS = 0.022%. Figure 5 shows the convergence of the phase fraction by graphs obtained in specific vertical lines, given in detail in Figure 2. Then, the cell size is defined by the M2 mesh and this mesh will be used in all cases.

Table 2. Fluid Properties.

Property		Value
Density	$\rho\,(kg.m^{-3})$	1000
Kinematic Viscosity	$\eta\,(m^{2}.s)$	0.577

Table 3. Meshes.

Meshes	Number of Cells
M1	254170
M2	2003302
M3	16065457

Two effects situations are evaluated to verify the consequence in the layers uniformity. Figure 6 shows a case referring to only one effect (contraction – Effect_C) and the layers remain uniform. Figure 7 shows a case considering three effects (Lateral-Vertical-Contraction – Effect_LVC) and uneven layers can be seen.

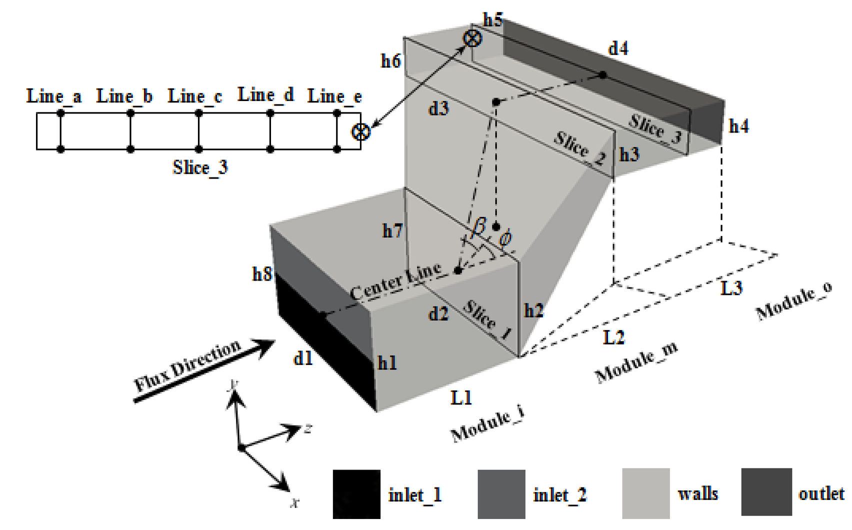


Figure 2. Base geometry for effects study.

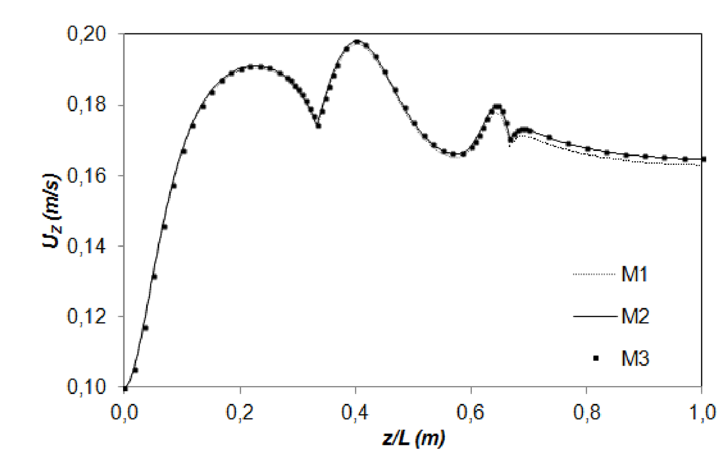


Figure 3. Axial velocity convergence.

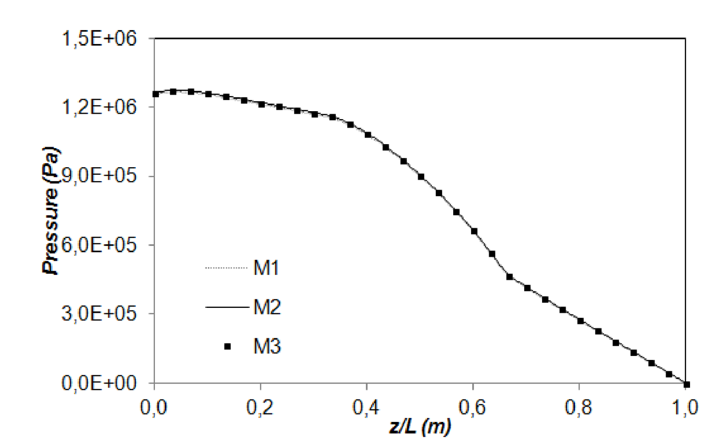


Figure 4. Pressure convergence.

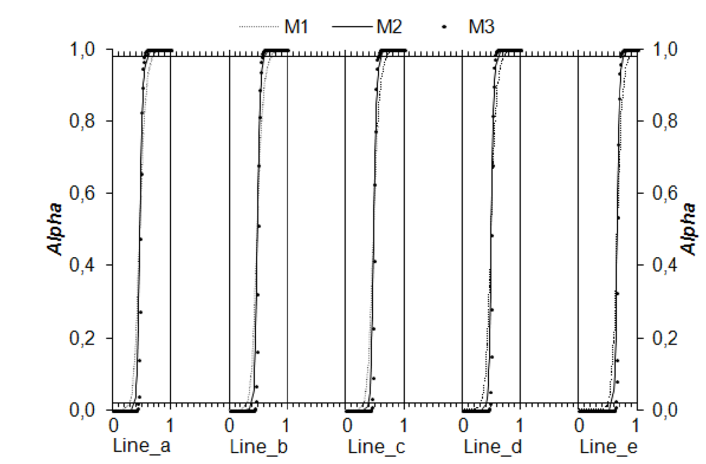
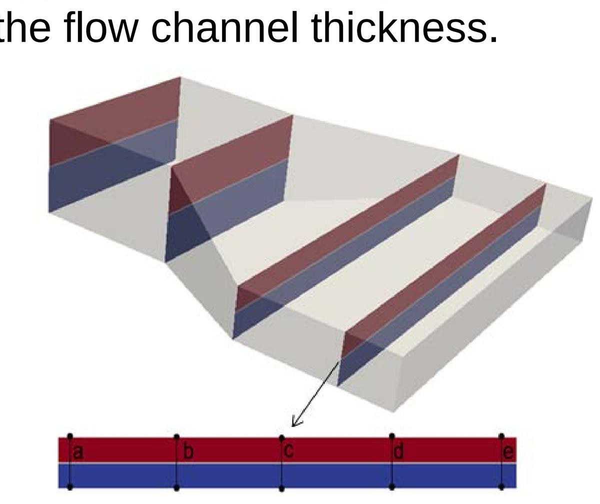


Figure 5. Phase fraction convergence by graph comparison.

Figure 8 shows phase factor results through graphs plotted on the vertical lines shown in the slice 3 of Figure 2. The results allow to realize that uneven layers appeared for some geometries. This is linked to an asymmetric velocity field along the flow channel thickness.



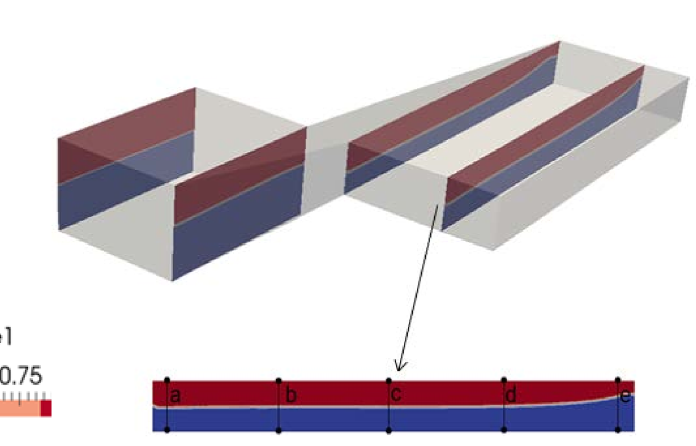


Figure 6. Effect_C. **Figure 7**. Effect_LVC.

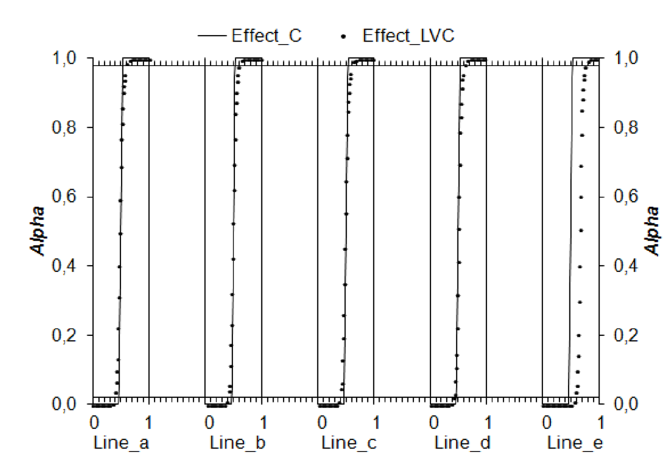


Figure 8. Results of layers uniformity by graphs of phase fraction for specific lines.

CONCLUSIONS

The results obtained showed that the simultaneous combination of specific geometrical transformations might have a negative impact on the uniformity of the polymer layer thickness distribution at the device outlet. It was possible to conclude that uneven layers are formed, when the velocity contour in the flow channel cross section is unsymmetrical along the perpendicular direction to the fluid interface. This information can be used to guide the design of duplicators, capable of producing coextruded parts with uniform layer distribution.

ACKNOWLEDGEMENT

This work is funded by National Funds through FCT - Portuguese Foundation for Science and Technology, Reference UID/CTM/50025/2019. The authors would like also to thank the support of the Search Cluster, Project TSSIPRO - Portugal and University Centre - Catholic of Santa Catarina - Brazil.

REFERENCES

[1] Tadmor, Z., Gogos, C. G., 2013. Principles of Polymer Processing. John Wiley & Sons.

[2] Dooley, J., 2002. Viscoelastic ow eects in multilayer polymer coextrusion. Ph.D. thesis, Technische Universiteit Eindhoven, Eindhoven.

[3] Hirt, C., Nichols, B., 1981. Volume of uid (VOF) method for the dynamics of free boundaries. Journal of Computational Physics 39.

[4] Rusche, H., 2002. Computational fluid dynamics of dispersed two-phase flows at high phase fractions. Ph.D. thesis, Imperial College of Science, Technology and Medicine, London.

[1]University of Minho/IPC – Guimarães/Portugal

{demaram@gmail.com, olgasc@dep.uminho.pt, cbpf@dep.uminho.pt, mnobrega@dep.uminho.pt}

[2]University Centre– Catholic of Santa Catarina – Joinville/Brazil

demaram@gmail.com