Int J Mater Form (2010) Vol. 3 Suppl 1:607–610
DOI 10.1007/s12289-010-0843-8

NUMERICAL MODELLING OF THE POLYMERS REPLICATION IN MICRO-CAVITIES BY THE ROLL EMBOSSING PROCESS

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ABSTRACT: The objective of the work is related to the modelling of micro-cavities replication in polymer plates by the roll embossing process. Finite element simulations are set up and performed to analyse the polymer deformation and flow leading to the filling of micro-cavities engraved on the moving roll system in the roll to roll (R2R) process. In the proposed approach, the roll engraved with micro-cavities is assumed to be undeformable, whereas the polymer plate rigid exhibits a viscoelastic or a coupled viscoelastic-viscoplastic material behaviour depending on the experimental processing conditions. The flow behaviour of the selected materials (cyclic olefin copolymer, COC) depends on the experimental processing parameters (rolling velocity, applied pressure and temperature) that are considered. The numerical simulations are performed using LsDyna® finite element software in order to analyse the filling of the micro-cavities vs. the rolling velocity and temperature, as a function of friction and sliding conditions. The results lead to the choice of roll embossing conditions in order to get the micro-cavities with the required geometries and properties.

KEYWORDS: Roll embossing process, Flow behaviour, Simulation, Polymers.

1 INTRODUCTION

Among the micro-forming processes that consist to replicate the surface topography of a die cavity mould during the filling of imprints, micro-injection moulding and hot embossing [1,2] stands out as interesting processes for the manufacturing of components with reduced size. The protocols associated with these technologies, as shown in Fig. 1, need to guarantee both the dimensional accuracy, even for complex shapes, and the replication of topographical surface states [1].

Injection moulding process is regarded as one of the well appropriate mass-production method to replicate micro-components with high productivity. However, the mould and equipments are expensive. The hot embossing is another method to replicate microstructures onto thermoplastic substrates [1,3]. The roll embossing process is also a very simple manufacturing process which addresses the needs for the increasing demand for low cost manufacturing of polymeric components [4,5]. This process is used to generate proper quality microstructures by pressing a rigid micro-structured roll on a thermoplastic polymer substrate/film. It is a continuous forming process in which a long polymer plaque passes through shaped rolls (see Fig 1a). Roll embossing is ideal for producing small size parts in large quantities, with complex shape, excellent mechanic properties and proper quality surface (see Fig 1b).

Today, products obtained by roll forming are used in numerous applications, for example optical systems, micro-fluidics and micromechanical components [2,6], Figure 1b.

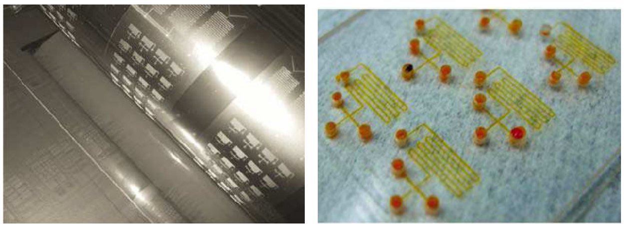

Figure 1: *(a) Hot roller embossing process, (b) capillary electrophoresis separator manufactured by hot roller embossing [7].*

The polymer plaque is unrolled and fed between the forming rolls. There are few research works in the literature. Tan et al. [8] performed roller nano-imprint lithography on thin photoresist coatings with hundreds nanometers in thickness. They reported the advantage of using lower force covering a large substrate. However, the size was limited to a couple of centimeters and the setup was not performed continuously. Other tests were successfully conducted by Ng et al. [7], for the processing of micro-fluidic devices by hot roller embossing process. The results revealed that the embossing depth increased with increasing the applied load or decreasing the roll speed. From our knowledge, no simulations have been performed on roll-to-roll embossing processes.

In our approach, a roll is wound on thermoplastic sheet preheated before to come in contact into the roller. Heat is supplied to the embossing interface through the mould and a clamping pressure is applied by the roll. The roll embossing enables a way to replicate complex shape at

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high speed. These microstructures are either in relief above or below the surface of the mould (see Fig 2). One considers here the first case of a roller with different cavities.

In the proposed study, the finite element method has been used for modelling of roll embossing process using the LsDyna® software to describe the filling of micro-cavities during the forming process of the material. The simulations were carried out to evaluate the filling of the cavities taking into account the mechanical behaviour of the selected polymer into the model.

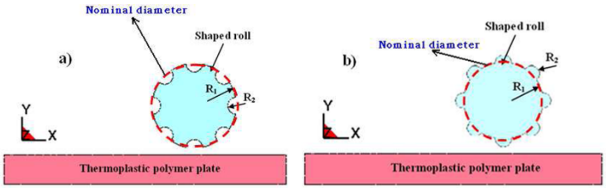

***Figure 2:** Schematic representation of the two different forming modes that can be obtained by roll embossing: (a) negative forming; (b) positive forming*

2 ASSESSMENT OF CONSTITUTIVE MATERIAL MODELS

In the last decades, important efforts have been devoted to establish models for the behaviour of solid polymers. As example one can the Johnson-Cook model, G'Sell-Jonas model, Brooks model or Matsuoka model. In the present analysis, the Johnson-Cook model has been used to describe the filling of mould cavities during the forming process of the polymer through roll embossing.

2.1 JOHNSON-COOK CONSTITUTIVE MODEL

The Johnson-Cook model is a robust constitutive material model that is highly used in modelling and simulation analyses. It is a phenomenological model that allows reproducing several important material responses observed in impact and penetration of ductile metals. The mains physical variables are strain hardening, strain-rate effects, and thermal softening. These three effects are combined, in a multiplicative manner, to establish the Johnson-Cook constitutive model expressed as:

$$\sigma_p = \left[A + B(\varepsilon_p)^n\right]\left(1 + C\ln\dot{\varepsilon}\right)\left[1 - (T_H)^m\right] \qquad (1)$$

As related in eq. (1), σ_p depends on the plastic strain ε_p, plastic strain rate $\dot{\varepsilon}$, and temperature T. A, B, C, n, and m are material parameters; T_H is achievement temperature is expressed as:

$$T_H = T - T_{room} / T_{melt} - T_{room} \qquad (2)$$

where T is the current temperature, T_{room} is the ambient temperature, and T_{melt} is the melt temperature.

2.2 MATERIALS

The experiments have been performed with thermoplastic polymers provided in pellet shape by Ticona® company (cyclo-olefin copolymer). Table 1 relates the properties of the selected COC copolymers.

***Table 1:** Main characteristics of the COC polymers*

Polymer grades	5013	6013
Young modulus (MPa)	3200	2900
Coeff. linear thermal expan. ($\times 10^{-4}$ K^{-1})	0.6	0.6
Thermal conductivity (W/m.K)	0.15	0.15

2.3 TENSILE TESTS

Tensile test specimens have been injected with an hydraulic injection moulding equipment. The injection temperature was first varied from 230°C to 260°C from hopper to nozzle (in steps of 10°C) to optimize the filling of the mould cavity. Then, the injection pressure was varied between 8 and 10MPa (with steps equal 0.5MPa). Tensile tests have been realized on an Instron® 6025 testing electrical machine operating with axial speed control (1mm/min). The experimental results were used for the identification of constitutive material model parameters. The equipment is instrumented with an isothermal furnace providing test temperatures from 20 to 300°C with an accuracy equal ± 2%. Four temperatures have been considered: 100, 120, 140 and 160°C. Two strain rates are used, ie. 10^{-3} and 10^{-1} s^{-1}. A schematic view of the experimental setup is releted in Fig. 3.

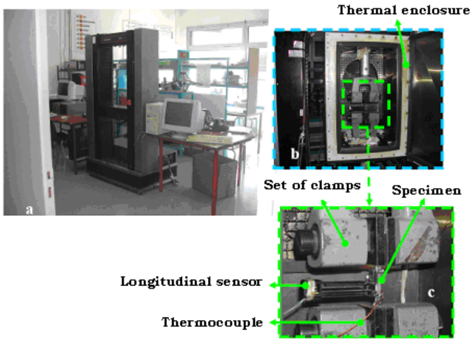

***Figure 3:** Experimental set-up for the tensile tests: a) global view of the tensile test equipment; b) enlarged view of the set-up at the level of the thermal enclosure; c) enlarged view of the set-up at the level of the specimen*

2.4 IDENTIFICATION OF CONSTITUTIVE MATERIAL MODEL PARAMETERS

From the stress/strain relationships, it is possible to identify the material parameters of the model related in eq.1 (Table 2). The validation of the thermo-mechanical behaviour of the polymer was verified afterward by computers numerical tensile tests. As an example, the stress/strain curve of the specimens at 160°C presented in figure 4 illustrates a proper agreement between the experimental results and proposed viscoplastic model.

Table 2: *Material parameters of the power law associated to COC*

Polymers	n	m	A	B	C
COC5013	0.27	0.7	0.25	1.1	0.08
COC6013	0.25	0.7	0.10	0.8	0.04

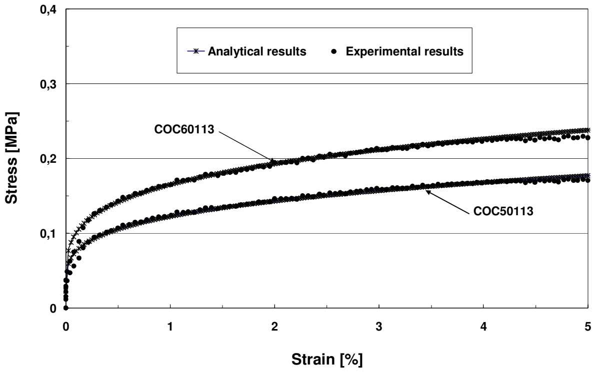

Figure 4: *Comparison of the uniaxial tensile test curves*

3 FINITE ELEMENT SIMULATION

In this finite elements investigation, attention is focused on the filling rate for the different cavity shapes during the forming of polymer film by undeformable roll. The FE modelling is used to simulate the roll embossing process through a rigid roll in contact with a polymer plate. The finite-element model was therefore set up to include important features of the experiments while reducing computation time as few as possible. Several assumptions were proposed to describe boundary conditions. First of all, the polymer plate is fixed while the roller rotates and moves forward. Moreover, one considers that the polymer material exhibits the viscoplastic behaviour presented in the preceding section. It has been said before in this study, two geometries for die cavities were tested: a triangular cavity shape and a circular shape. One typical geometry considered in this investigation is related in Fig. 5.

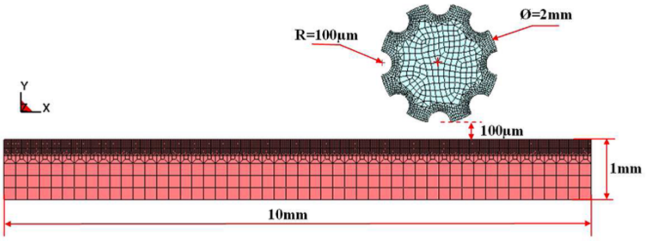

Figure 5: *Complete 2D mesh of FE model used for the numerical simulations of roll embossing associated to circular shape for the second analysis*

4 SIMULATION RESULTS

4.1 CAVITY WITH OF TRIANGULAR SHAPE

The filling rates for different cavity shapes are investigated in the proposed applications. Figure 6 relates the contour plot of von-Mises stress in the polymer substrate during roll embossing. The simulation data permit to get the rate of filling in percentage. During forming, the cavities are correctly filled (see Fig.6). The filling rate of the lower part of the cavity is consistent with expectations (see Fig.7b).

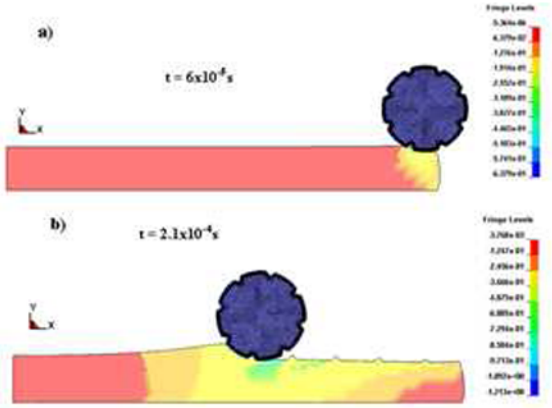

Figure 6: *Stresses contours obtained by FE simulation during roll embossing process at different instants*

The development of defects form has been evaluated predicted during roll embossing process linked to problems related of material flow. The filling of the summits of cavities corresponds to truncation more or less important vs. imposed displacement. The filling rate of the die mould cavities is indeed higher when the penetration increases in the roll (see Fig.8). It can be noted that the trend is consistent with those reported in the literature.

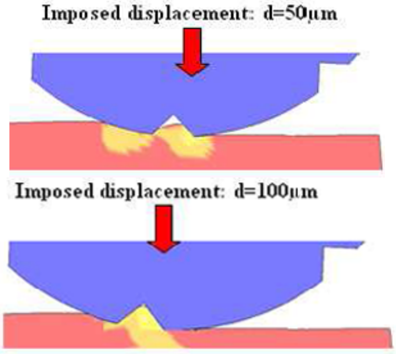

Figure 7: *Filling of the mould cavity with triangular shape for different imposed displacements*

Different simulations have been carried out in order to optimize the filling of cavities. Figure 8 relates the evolution of the filling rate vs. the imposed displacement of rigid roll in the case of triangular shaped cavities. One remarks that higher the imposed displacement is increased, the filling rate increases, too leading to replicas of the geometric shapes corresponding to the original beyond 100µm. Figure 8 shows well progressive filling of cavities that takes place in appropriate conditions.

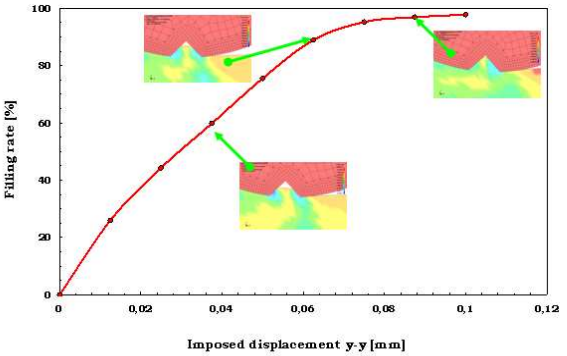

Figure 8: *Filling rate vs. imposed roll displacement during roll embossing process*

4.2 CAVITY WITH CIRCULAR SHAPE

A similar numerical approach was applied for the replication of cavities of circular shape as specified in Figure 5. Figure 9 shows the filling corresponding to the different stage of the roll embossing process for an imposed displacement equal to 100µm. One found that the cavity profiles are almost equivalent. As an example, the final filling time is 1.5 times higher in this first case (triangular cavity) than in this second one (circular cavity). The contours of cavities filling after replication of polymeric materials are given Fig.10. One observes that the result leads to almost the same value of filling of roll engraved cavities. The overall results show also that the filling rate of cavities is largely influenced by side-effect. Moreover, the values at the final filling time in the case of a semicircular cavity are distinctly higher than for a conical cavity because of the difference in volume. Finally, these results help to understand and analyse the various aspects resulting from the shaping of thermoplastic polymers by roll embossing.

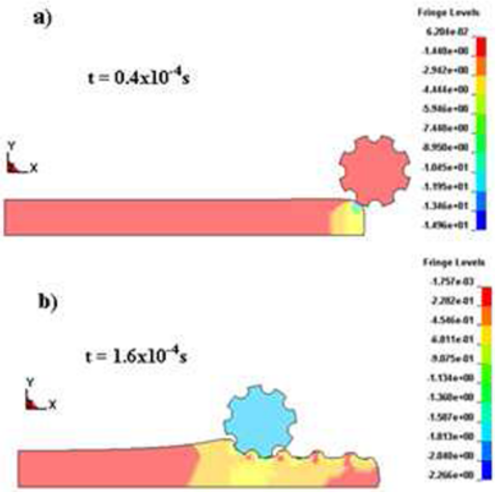

Figure 9: *Stress contours obtained by FE simulation during roll embossing process at different instant*

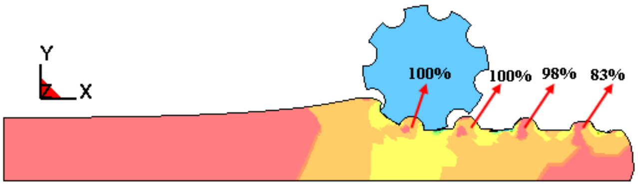

Figure 10: *Filling rate values obtained by FE simulation during roll embossing process*

5 CONCLUSIONS

The paper clearly demonstrates through numerical simulations based on properly determined mechanical properties, that the continuous embossing of polymer plates through the roll embossing process, is a technology that can be industrially used. The viscoplastic thermo-mechanical properties have been indentified by tensile test experiments, and then fitted with an appropriate mechanical model accounting strain, strain rate and temperature. Then 2D extensive simulations of the embossing have been carried out accounting the geometrical, physical and technological aspects of plates roll embossing. The simulation results clearly indicate that the ability to perform shape replication depends of processing parameters as well as physical behaviour of the polymer plaques.

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