



# Molecular dynamics simulation method applied to nanocavities replication via injection moulding



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## ABSTRACT

Injection moulding is a promising manufacturing process for obtaining cost-effective plastic parts with nanostructured surfaces. However, replication of nanocavities is not a straightforward method because the large heat transfer that takes place at the nanoscale tends to solidify the polymer before it has replicated all the cavities. This behaviour has been studied by different authors by means of Computational Fluid Dynamics simulations; in this way, factors such as process parameters (mould and melt temperatures, filling time, injection pressure limit, holding time, etc.) and geometric parameters (cavity geometry, cavities location in the mould, etc.) have been quantified. However, such investigations have found a roadblock when aiming to evaluate the replication of nanocavities with dimensions smaller than 100 nm. The reason is that the continuum hypothesis in which Computational Fluid Dynamics is based is not valid anymore. The purpose of this work is to overcome the scale limitation of Computational Fluid Dynamics and expose a Molecular Dynamics based algorithm to foresee the replication of nanocavities.

## 1. Introduction

The interest in manufacturing parts with nanostructured surfaces by means of injection moulding is increasing because of the cost-affordable mass production and the obtainable wide field of applications like lab-on-chips devices [1], optical antireflectivity [2], optical transmission enhancements [3], antimicrobial surfaces [4], etc.

Manufacturing a nanostructured surface by means of injection moulding is an industrial challenge. The reason is that the nanoscale stands out for its large surface to volume ratio, that leads to a large heat transfer and tends to solidify the polymer prematurely. In order to overcome this, a good knowledge of both process and geometric factors is indispensable. Various researchers (Rytka [5,6], Oh [1], Choi [7], Tofteberg [8], Pina [9]) have studied nanostructure replication by means of Computational Fluid Dynamics. The results are sometimes contradictory and based on parameters that cannot be known in advance, like the Mushy constant, as proved by Pina [10].

The purpose of this paper is to develop a model valid for dimensions smaller than 100 nm (approximately the length of three aligned polyethylene chains of degree of polymerization 100). For such dimensions, the continuum approach is not valid anymore and, hence, the Computational Fluid Dynamics modeling based on the Navier-Stokes

equations is no longer valid. The Molecular Dynamics simulation method is chosen in order to study the replication at that scale, considering the replication of the nanocavity an N-body simulation.

## 2. Methods

### 2.1. Submodeling approach

This work is based on the submodeling strategy. This model consists in carrying out a first injection moulding simulation of the full part with a commercial CFD software (e.g. Moldflow, Solidworks Plastics, CoreTech Moldex3D, etc.) and in using the results of this simulation as inputs of the subsequent MD simulation. In Fig. 1 the process is shown along with the inputs and outputs of each simulation.

The submodeling is based on the hypothesis that the nanocavity replication can be considered a two-step process. The first step consists of the polymer going through the nanocavity without noticing its presence and, a second one, in which the polymer gets into the nanocavity due to the pressure profile. This hypothesis was experimentally proved by Pina [9].

The nanoscale simulation finishes when the polymer reaches the No Flow Temperature (NFT), which is considered to be  $T_g + 30^\circ\text{C}$  as stated

*Abbreviations:* BC, Boundary condition; CFD, Computational Fluid Dynamics; DP, Degree of polymerization; E, Energy; MD, Molecular Dynamics; NFT, No flow temperature; N, Number of atoms; P, Pressure; PE, Polyethylene; T, Temperature;  $T_g$ , Glass transition temperature; V, Volume

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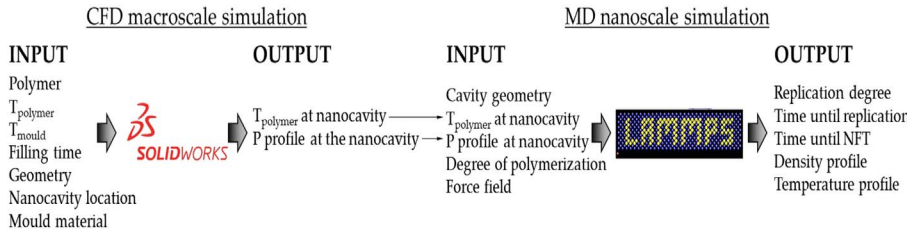


Fig. 1. Submodeling approach for coupling CFD macro-simulation with MD nanosimulation.

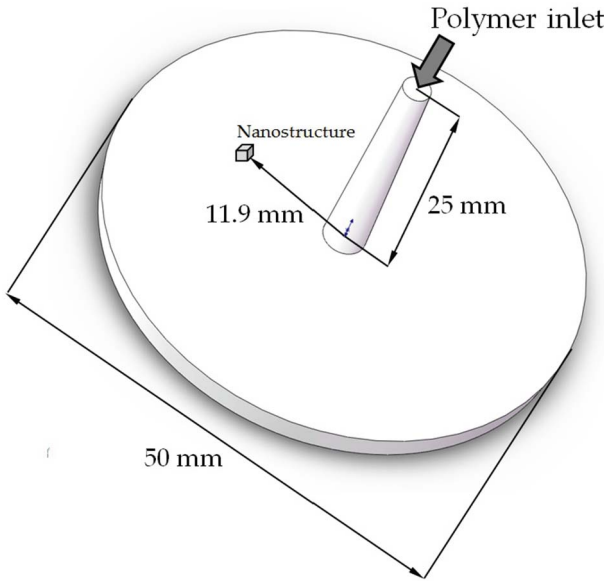


Fig. 2. Geometry used for the macroscale simulation.

by Mannella [11]. Plastic deformations, once the polymer reaches the solid state ( $T < \text{NFT}$ ), are not considered in the present work.

Hereunder, both the CFD macrosimulation and the MD nanosimulation details are exposed.

### 2.1.1. CFD macrosimulation

This article is based on a macroscale simulation carried out with polyethylene (PE-MD BASELL LUPOLEN 2410 T),  $T_{\text{polymer}} = 230^\circ\text{C}$ ,  $T_{\text{mould}} = 45^\circ\text{C}$ , filling time 2 s and injection pressure limit of 134 MPa in the geometry of Fig. 2.

If the nanocavity is considered to be at 11.9 mm of the center, its pressure profile is the one on Fig. 3. A second order polynomial is adjusted to the first three points and the equation  $P/\text{MPa} = 1.0643t^2 + 0.1202t$  is obtained, where time  $t = 0$  s is defined when the polymer flow front first reaches the nanocavity. This equation and the temperature at which the polymer reaches the nanocavity ( $227^\circ\text{C}$ ,  $3^\circ\text{C}$  less than the inlet temperature) will be used as input data of the MD nanosimulations.

### 2.1.2. MD nanosimulation

LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) [12] software is used for the nanoscale simulations. In order to avoid the overestimation that Pina [10] proved that takes place when 2D simulations are carried out with cavities with length/width  $> 4$ , all MD simulations of this work are run in 3D.

All the input details are shown hereunder:

- Force field

In MD simulations, the force field is used to calculate the potential energy of a system of atoms. In the present work, the generic DREIDING force field is used. A force field has 2 parts: the formulas that define it and the coefficients used for the studied system. The DREIDING

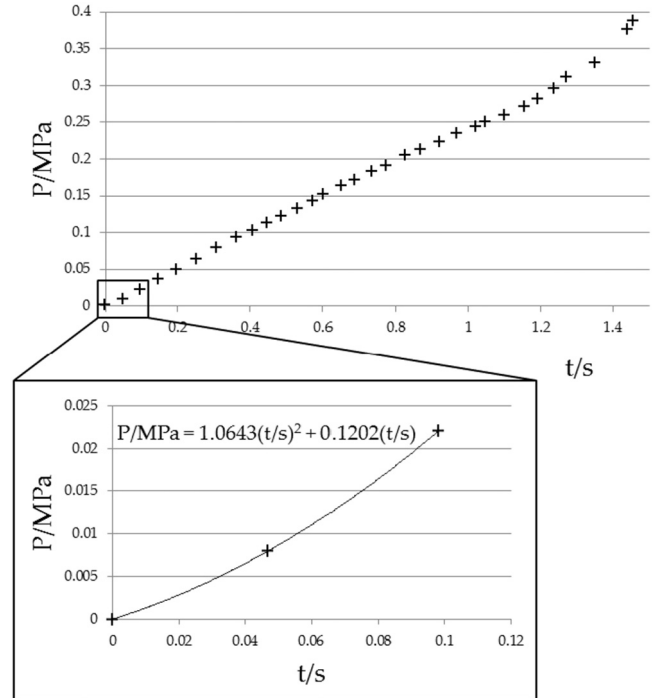


Fig. 3. Pressure profile at the nanocavity located at 11.9 mm of the center.

formulas are integrated into LAMMPS and will be exposed for completeness. The coefficients are obtained from the original Mayo publication of 1990 (Mayo [13]) where the DREIDING force field was first announced.

DREIDING force field considers that the system energy is the superposition of valence (or bonded) interactions ( $E_{\text{val}}$ ) and nonbonded interactions ( $E_{\text{nb}}$ ):

$$E = E_{\text{val}} + E_{\text{nb}} \quad (1)$$

The valence interactions consists on bond stretch ( $E_{\text{bond}}$ , two body), bond-angle bend ( $E_{\text{angle}}$ , three-body) and dihedral angle torsion ( $E_{\text{torsion}}$ , four-body). The non-bonded interaction consists on van der Waals ( $E_{\text{vdw}}$ ) forces, modeled by means of Lennard-Jones 12-6 model.

$$\begin{aligned} E &= E_{\text{bond}} + E_{\text{angle}} + E_{\text{torsion}} + E_{\text{vdw}} \\ &= k_b(r - r_0)^2 + k_a(\theta - \theta_0)^2 + k_t(1 + \cos(n\phi - \phi_0)) \\ &\quad + 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right) \end{aligned} \quad (2)$$

where  $k_b$ ,  $k_a$  and  $k_t$  are constants of bond stretching potential, angular bending potential and torsion potential, respectively.  $r$  is the bond radius and  $r_0$  the equilibrium bond radius.  $\theta$  is the bond angle and  $\theta_0$  the equilibrium bond angle.  $\phi$  is the dihedral angle and  $\phi_0$  the equilibrium dihedral angle.  $\epsilon$  is the depth of the potential well and  $\sigma$  is the finite distance at which the inter-particle potential is zero, both parameters of the Lennard-Jones 12-6 model.

The cutoff distance of the nonbonding interaction is set to 1.25 nm in order to neglect the interactions between atoms at distances larger than 1.25 nm. This approach is valid when the cutoff distance is larger

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