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Two-Phase Flow Simulations for Injection Molding Applications: Comparison between COMSOL Multiphysics and XNS In-House Solver

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ABSTRACT

Injection molding is a manufacturing process for plastic components where precise geometries and part properties, such as local strength and stiffness, are critical. The mold filling phase, during which the hot molten polymer is rapidly injected into the cooled mold cavity, presents significant simulation challenges due to steep temperature and velocity gradients, as well as the nonlinear visco-elastic behavior of polymers. In this work, we present a comparative study using a widely known commercial simulation tool, COMSOL Multiphysics, and our in-house-developed solver, XNS, with a specific focus on the treatment and impact of wall boundary conditions. For the comparison, we use a 2D macroscale test case. For both solvers, stabilized linear finite elements are used, and they utilize a two-phase flow formulation, with the level-set method to capture the interface. The two solvers differ in their definition of the level set function and in their variable Navier-slip algorithms as boundary condition. The results indicate that variations in the treatment of wall boundary conditions lead to differences in both the advancing profile of the interface and the width of the frozen layer. This study highlights the critical role of accurately modeling wall boundary conditions in predicting the onset of solidification and subsequent part quality. Moreover, our findings demonstrate that the in-house solver achieves accuracy comparable to that of COMSOL Multiphysics with a drastically reduced computational time, while offering more flexibility for the wall boundary conditions and the potential for a more physical representation of them.

1 | Introduction

Injection molding is a key method for producing plastic parts in large volumes. The process demands precise control over product geometry and material properties, often relying on a combination of experimental trials and simulation-based approaches. Although established simulation software provides valuable insights, the need for computational efficiency typically leads to the adoption of simplified physical models, which may not meet the requirements for high-resolution applications. This highlights the need for a simulation approach that is both accurate and

efficient, ultimately leading to better part quality and lower production costs.

In the present work, the numerical simulation of one of the first stages of the process is analyzed: the mold cavity filling. In this stage the molten polymer is injected into the cooled mold cavity. The hot polymer immediately contacts the cooled surfaces, triggering rapid solidification. This contact not only initiates the solidification process but also induces complex fluid dynamic phenomena governed by steep temperature gradients and significant shear stresses. Such interactions at the mold walls

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are especially critical, as they directly influence the evolution of the flow front, the subsequent packing phase, and ultimately, the final part geometry and part properties.

Several experimental studies have analyzed the flow front behavior typical in injection molding applications [1–4]. In the numerical simulations, this behavior has been modeled following different approaches, which will depend on the numerical methods used, for example, finite volume method [5–7] or finite element method [8–10]. Wide variety of solvers are used for injection molding simulations, from in-house developed solvers, to open-source research codes, to commercial solutions. Some of the most popular commercial software for injection molding simulations include: Moldflow (Autodesk, Inc., Mill Valley, CA, USA), Moldex 3D (CoreTech System Co., Ltd., Zhubei City, Taiwan), Sigmasoft (SIGMA Engineering GmbH, Aachen, Germany), Cadmould (Simcon kunststofftechnische Software GmbH, Würselen, Germany), and COMSOL Multiphysics (COMSOL Inc., Stockholm, Sweden). Even with the high number of existing solvers, there is still a gap between numerical simulations predictions and reality [11–14]. This is, in general, due to the model simplifications applied to meet the requirement of realistic computational times, as well as to the numerical treatments used to address the complexities of the physical model. This motivates the research toward a robust, efficient, and accurate numerical model.

Following the work in [15, 16], this study compares the numerical models in the in-house solver XNS with the well-established COMSOL Multiphysics. Both solvers are commonly used for fluid and heat transfer problems in a wide range of applications [17–21]. Both solvers can use stabilized linear finite elements and a two-phase flow formulation with the level-set method for capturing the interface between polymer and air in the fixed domain. Using the same spatial mesh and material modeling, simulations differ only in the time discretization, semi-discrete in COMSOL and discontinuous-prismatic space-time in XNS [10], and, most relevantly, in the boundary conditions. We assume that both solvers solve their models within a certain tolerance, so that the equation system solver is only relevant for timing.

After a description of both models and methodology, in the results section we will compare the simulation outcomes from using COMSOL and XNS solver. The simulation with XNS compares two cases, using a weaker and a stronger imposition of the wall no-slip condition for the polymer phase. The difference between both boundary conditions approaches are analyzed and the relevance of the wall boundary condition in accurate cavity filling simulations are outlined.

2 | Governing Equations

To model the flow problem in this work, we use a two-phase flow formulation, modeling both the air and the polymer in a fixed domain representing the rigid cavity. To capture the polymer–air interface, the two phase level-set method is employed. To model the flow, the general Navier–Stokes equations have been simplified. From the polymer’s properties, it is considered that the flow is incompressible and viscous dominated, $Re \ll 1$, therefore, the Stokes formulation is used. To compute the shear

rate and temperature-dependent polymer’s viscosity, the heat transfer equation is also solved.

The considered computational domain $\Omega \subset \mathbb{R}^2$ encloses the immiscible subdomains representing the air $\Omega_1(t)$ and polymer phases $\Omega_2(t)$, where $\Omega_1(t) \cup \Omega_2(t) = \Omega$. The interface between both phases is defined as $\Gamma_{int}(t) = \Omega_1(t) \cap \Omega_2(t)$, while the boundary of the entire domain is $\Gamma = \partial\Omega$.

The unsteady Stokes equations define the velocity $\mathbf{u}(x, t)$ and pressure $p(x, t)$ at each time $t \in [0, t_{final}]$:

$$\rho_i \frac{\partial \mathbf{u}}{\partial t} - \nabla \cdot \boldsymbol{\sigma}_i = \mathbf{0}, \quad (1)$$

$$\nabla \cdot \mathbf{u} = 0, \quad (2)$$

$$\boldsymbol{\sigma}_i = -p\mathbf{I} + \mu_i (\nabla \mathbf{u} + (\nabla \mathbf{u})^T), \quad (3)$$

for indices $i = 1, 2$ corresponding to air and polymer phases. ρ corresponds to the density. Notice that no body forces are considered in our formulation. The stress tensor $\boldsymbol{\sigma}$ includes viscous and pressure contributions and depends on the dynamic viscosity μ . The dynamic viscosity is modeled as shear and temperature dependent; the model is described in Section 4.

The temperature $T(x, t)$ is governed by the heat transfer equation:

$$\rho_i c_{p,i} \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) - k_i \nabla^2 T - \Phi_i = 0, \quad (4)$$

where c_p is the isobaric heat capacity, k the thermal conductivity, and Φ viscous heat dissipation.

To capture the interface between air and polymer $\Gamma_{int}(t)$ different approaches are followed by the XNS and COMSOL.

2.1 | XNS

The XNS solver solves the transport equation of the function ϕ_X , which represents initially the signed distance to $\Gamma_{int}(t)$:

$$\frac{\partial \phi_X}{\partial t} + \mathbf{u} \cdot \nabla \phi_X = 0. \quad (5)$$

Every time step, the level-set function is reinialized to conserve the property of a signed distance function.

2.2 | COMSOL

In COMSOL Multiphysics, the level-set function does not represent a distance function but a smooth step function that equals zero in Ω_1 and one in Ω_2 . Across the interface, there is a smooth transition from zero to one [22]. The interface $\Gamma_{int}(t)$ is defined by the 0.5 isocontour, in contrast with the XNS definition, where $\Gamma_{int}(t)$ is defined by the isocontour 0. The transport equation of

the level set is, in this case, the following:

$$\frac{\partial \phi_C}{\partial t} + \mathbf{u} \cdot \nabla \phi_C = \gamma \nabla \cdot (\epsilon \nabla \phi_C - \phi_C(1 - \phi_C) \frac{\nabla \phi_C}{|\nabla \phi_C|}). \quad (6)$$

Here, ϵ determines the region of smoothing and by default is equal to the largest value of the mesh size in the domain Γ . γ determines the amount of re-initialization or stabilization of the level-set function [22]. This parameter is set to $\gamma = 0.2ms$ for the simulations presented in this work. No volume correction technique is applied to any of the simulations.

3 | Solution Technique

3.1 | XNS

XNS is the finite-element in-house solver at the Chair for Computational Analysis of Technical Systems. With this solver, Equations (1)–(5) are discretized using P1P1 finite elements, that is, linear interpolation for all degrees of freedom. For the stabilization, the Galerkin/Least-squares approach is used [23]. The level-set equation, Equation (5), Stokes equations, Equations (1) and (2), and the heat equation Equation (4), are solved iteratively at each time-step, until convergence is reached. For the domain, the discontinuous-prismatic space-time formulation is used [24].

A relevant aspect of the simulation is the transition of the material properties at the interface between the air and polymer phases. This transition has a direct influence on both the numerical convergence and the solution accuracy. In both COMSOL and XNS, an arithmetic mean weighted by a smooth step function is used to smooth the material properties near the interface $\Gamma_{int}(t)$:

$$X_\phi = x_1 + (x_2 - x_1)H_{s,\phi}, \quad (7)$$

where X_ϕ is the resulting material property at the level-set ϕ , x_i the material property at phase i , and $H_{s,\phi}$ is the smoothed Heaviside function for the transition between phases. $H_{s,\phi}$ is defined differently for COMSOL and XNS. For XNS, the smoothed heaviside function is defined as follows:

$$H_{s,\phi} = \frac{1 + \frac{\phi}{\epsilon} + \frac{\sin(\frac{\pi\phi}{\epsilon})}{\pi}}{2} \quad (8)$$

with ϵ set to 0.8 for this work. Notice that here the level-set function corresponds to the distance function.

3.2 | COMSOL

Similarly to XNS, COMSOL uses P1P1 finite elements, but streamline upwind Petrov–Galerkin stabilization is used [23]. The system of equations is solved sequentially and a backward Euler scheme with adaptive time stepping is utilized. The time step ranges from 0.09 to 0.28ms.

Regarding the material weighting between phases, the smoothed weighted arithmetic mean is used as in Equation (7). However, the smoothed Heaviside function, $H_{s,\phi}$ corresponds to the integrated smoothed step function, defined by piece-wise 5th-degree

polynomials [22]. The mixing parameter that defines the size of transition between phases is set to 0.8 for this work, and is referring to the level set function. Notice that for COMSOL, the level-set function does not correspond to a distance function.

4 | Simulation Model

The simulation performed in this study corresponds to the one described in [15]. The domain is defined by the 2D rigid cavity channel and has been shortened with respect to the one defined in [15]. The spatial mesh used is the same for all simulations, and has 18 576 elements, 9831 nodes, and an element size $h \sim 0.25mm$; see Figure 1.

The cavity is initially filled with air at mold temperature of 303 K, and the hot molten polymer compound is injected through the 6 mm wide inlet (see Figure 1) with a ramped velocity of

$$u = -50 \frac{1}{1 + e^{-100t+4}} y \quad mm/s,$$

at a temperature of 513 K. A traction-free boundary condition is imposed at the outlet, that is, rightmost wall in Figure 1, to let the air escape. The wall boundary conditions are defined in the next section.

Regarding the temperature boundary conditions, we prescribe a Neumann boundary, where the heat flux q represents the convective heat transfer at the mold walls Γ_{wall} , when in contact with cold steel plates, at T_{ext} :

$$q = -\mathbf{n} \cdot (k \nabla T) = h \cdot (T_{ext} - T), \quad \text{on } \Gamma_{wall}. \quad (9)$$

The heat transfer coefficient for the walls of the cavity, h , is set to 700 W/(m²K).

The polymer is modeled as an isotactic polypropylene PP505P by Saudi Basic Industries Corporation, Riyadh, Saudi-Arabia. The Cross–Williams–Landel–Ferry model [25] with the formulation in [8] is used to model the shear-thinning behavior of the polymer. The specific material properties used for both material phases are described in Tables 1 and 2 in [15]. In XNS, the air is modeled with constant properties independent of temperature and pressure. In COMSOL the air is modeled as an ideal gas, with a dynamic viscosity of $2.66 \cdot 10^{-5} Pa \cdot s$ and a constant density of $0.784kg/m^3$.

5 | On the Wall Boundary Conditions

Boundary conditions on the wall play a crucial role in the cavity filling problem with melted polymers. Different authors use different approaches to model them, depending on the problems characteristics, that is, capillarity, and the numerical methods used. In general, the molten polymer will solidify after contacting with the cooled mold walls. This effect will cause the so-called “frozen layer” of solidified polymer stick to the mold walls. In this area, a no-slip condition can resemble the physical behavior $\mathbf{u} = 0$. Depending on the wall shear stresses, especially in microfluidic flows, there can be some slippage in this region [4]; it is,

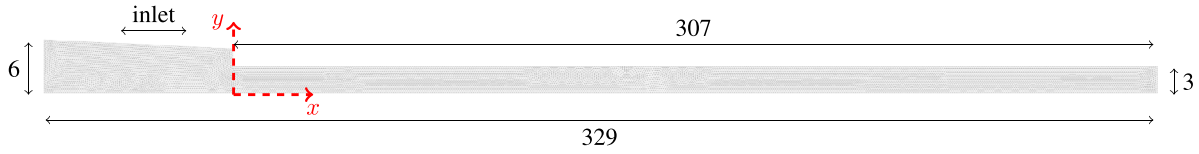


FIGURE 1 | 2D testing geometry and spatial mesh. Dimensions in mm.

TABLE 1 | Wall boundary condition parameters for XNS simulations, with $h = 0.25\text{ mm}$.

	$\alpha_{\infty}(\text{Pa} \cdot \text{s}/\text{mm})$	$\delta_1(\text{mm})$	$\delta_2(\text{mm})$
Soft BC	$3 \cdot 10^4$	$-80h$	$-3h$
Strong BC	$1 \cdot 10^3$	$-4h$	$-h$

however, not considered here. For the air, both slip and no-slip wall boundary conditions can be used and will not influence the polymer solution. Therefore, a slip boundary condition is preferred for better numerical convergence.

When dealing with finite-elements and the level-set interface capturing method, if we apply a no-slip condition for the polymer phase, the interface-wall contact point will be solidified, preventing the flow from moving. This problem has been studied by several authors, in a broader context [26–28]. The treatment of this triple dynamic contact point can be treated by adding a wetting condition, allowing it to slip with a certain $\mathbf{u}_{\text{slip}}$, determined by the surface tension, capillarity effects, and so forth. [9, 29].

Given the high capillary number of our problem, $Ca \gg 1$, the surface tension and capillarity effects can be neglected. The flow will be driven by the viscous forces and not the surface tension. Therefore, $\mathbf{u}_{\text{slip}}$ will not be determined by the wetting phenomenon, and simply some slip will be allowed near the triple contact point. For the treatment of the different boundary condition at the wall, from no-slip to slip at the interface, different numerical approaches are used [5, 8, 9]. In this study, the slip condition at the contact point will be treated with different approaches for COMSOL and for XNS.

5.1 | XNS

The XNS solver achieves the transition between slip and no-slip condition in the polymer phase by using a variable Navier-slip formulation. The variable Navier-slip condition relies on applying a variable tangent stress at the wall opposing the fluid movement, using a coefficient α to control the slip behavior:

$$K_{nt} = \mathbf{n} \cdot \boldsymbol{\sigma} \cdot \mathbf{t} = \alpha u_t, \quad (10)$$

where $\mathbf{n}$ and $\mathbf{t}$ are the normal and tangent vectors at the boundary, $\boldsymbol{\sigma}$ the stress tensor, u_t the tangential component of the fluid velocity, and α a variable coefficient defined as follows:

$$\alpha = \begin{cases} \alpha_{\infty} & \phi_X < \delta_1 \\ -(\phi_X + \alpha) \frac{\alpha_{\infty}}{\delta} & \delta_1 < \phi_X < \delta_2 \\ 0 & \phi_X > -\delta_2[3pt] \end{cases} \quad (11)$$

The α coefficient upstream of the front flow, α_{∞} , should be a sufficiently high value to restrict completely the fluid movement, resembling the no-slip condition. δ_1 and δ_2 are the limits for the slip transition area, where α is linearly ramped from 0 to α_{∞} . The smallest the area is the quicker the physical boundary condition is recovered. However, the transition length needs to be sufficiently big to be solvable and represented for at least one mesh element.

Two different simulations have been performed with XNS. In the first one, XNS—soft BC, the α_{∞} coefficient and limits have been adjusted to imitate the COMSOL simulation. In the second simulation, XNS—strong BC, the parameters have been adjusted to emulate a more physical behavior. In Table 1, the parameters used for both simulations are defined:

5.2 | COMSOL

In COMSOL, a different formulation is used for the wall boundary condition. Again, a Navier-slip condition is applied, but in this case, the tangential stress varies with the viscosity and a fixed slip length

$$K_{nt} = \mathbf{n} \cdot \boldsymbol{\sigma} \cdot \mathbf{t} = -\frac{\mu}{\beta} u_t. \quad (12)$$

In this formulation, the slip length β is set to 0.1 and 10 mm for the air, with a transition region from $\phi_C = [0.5 - 0.52]$, linearly ramped. In general, COMSOL documentation [22] recommends a β equal to the mesh element size. In this case, the beta is set even smaller, for a stricter no-slip condition.

6 | Results

The resulting polymer flow front advancement from COMSOL and XNS simulations is represented in Figure 2.

In Figure 2 it can be observed that the interface profiles strongly depend on the imposed boundary conditions. Soft imposition of the no-slip condition leads to a less sharp profile, since some slip is allowed along the interface, while stronger imposition of the no-slip condition leads to a sharper profile. Regarding the filling time, we observe that, independently of the boundary conditions imposed, both XNS solutions have the same filling pace, since the distance between the interfaces is constant in all time steps. In contrast, the filling pace of the COMSOL solution is slightly quicker, the polymer reaches the end of the mold faster. One possible explanation of this difference could be the inlet condition, since some differences were observed near the inlet flow. At the same time, there could be some volume loss for the XNS simulations, since no volume conservation technique is applied and the level-set method is not inherently

TABLE 2 | Numerical simulation performance: computational effort and time.

Solver	Mesh size ($n_{elements}$)	Element size (mm)	Time step (ms)	Computational time (hours)
COMSOL	18,576	~ 0.25	0.09 – 0.28	2.65 on 32 cores
XNS—strong BC	18,576	~ 0.25	5	0.32 on 32 cores
XNS—soft BC	18,576	~ 0.25	5	0.34 on 32 cores

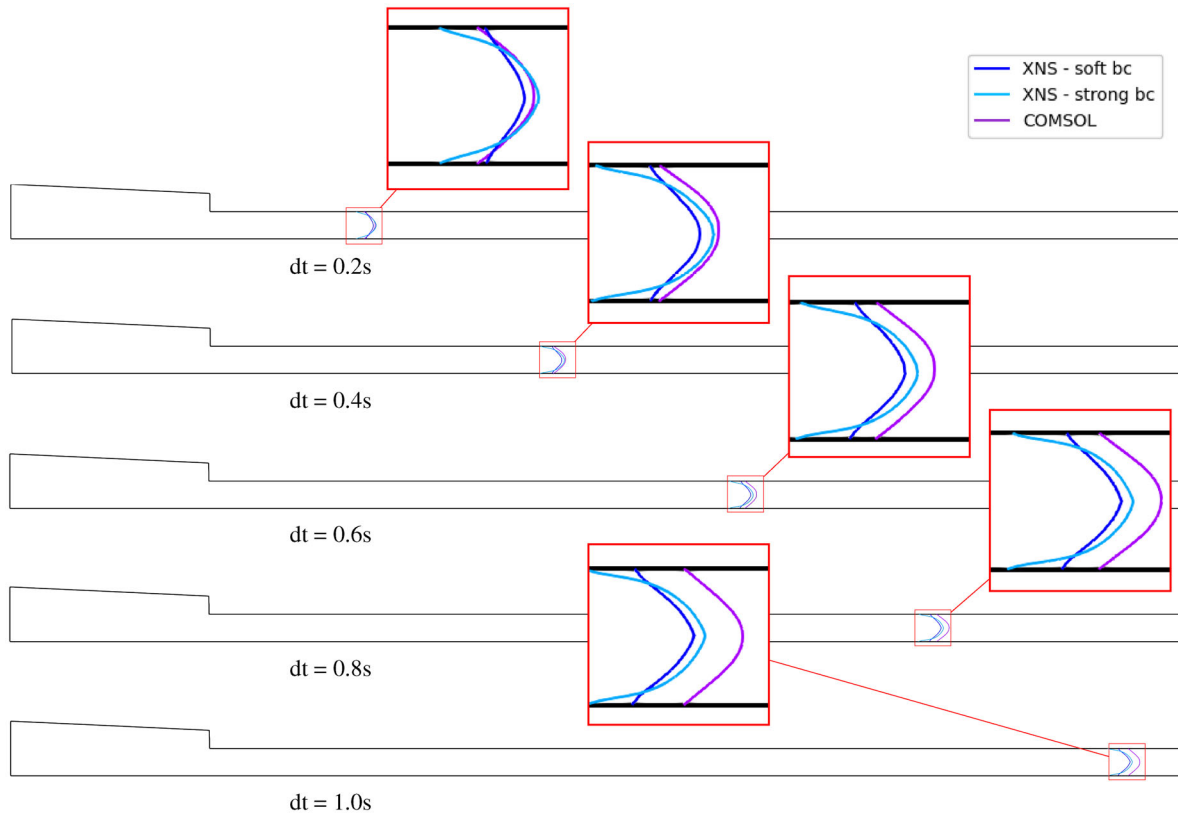


FIGURE 2 | Polymer–air interface Γ_{int} at different times for XNS and COMSOL solutions.

volume conservative. This effect could have been overcome in the COMSOL simulation by the use of an adaptive very small time step.

Figure 3 shows the velocity profiles along the channel walls, for an intermediate time, $dt = 0.4s$, and the final time, $dt = 1.05s$. From Figure 3a, we can observe that the velocity at the channel walls in the polymer region ($\phi_x < 0$, $\phi_c > 0.5$) is almost near 0 when imposing the strong boundary conditions with XNS. The change from the slip to the pseudo-no-slip condition is smooth but steep, as required. On the other hand, both the XNS—soft BC and the COMSOL simulations have a smoother transition, having more total slip on the channel walls. Specially, in the COMSOL simulation, we observe some non-negligible, non-desired, velocity at the beginning of the channel. The velocity at the boundary walls affects the velocity profile and it shows a higher peak velocity for XNS—strong BC, compared with the other simulations. In the air region ($\phi_x > 0$, $\phi_c < 0.5$), the slip boundary condition produces a flat uniform profile; the velocity in the middle of the channel and at the walls is equal.

Figure 3b shows the velocity profile once the polymer has filled the channel. Regarding the velocity at the wall, for the COMSOL results we notice some slip at the beginning of the channel, already present at time $t = 0.4s$ and a new slip in the upper wall between the 40 and 50 mm channel length. For both XNS simulations, with strong and soft boundary conditions, the final velocity at the walls is near 0, as required. The influence of the velocity at the walls to the velocity at the center line of the channel can be also observed here. Notice that both XNS simulations have nearly the same center line velocity.

In Figure 4, the temperature, pressure, and velocity fields from COMSOL and XNS—strong BC are compared. The temperature field differs near the interface. This seems to be an effect from the air properties and the difference in transition zone description between simulations. Regarding the pressure profile, both simulations seem to have the same values, but shifted. This shift, however, seems to coincide with the interface position difference. In Figure 3c, the velocity transition between the wall and the center line positions is shown. Here, we see again a

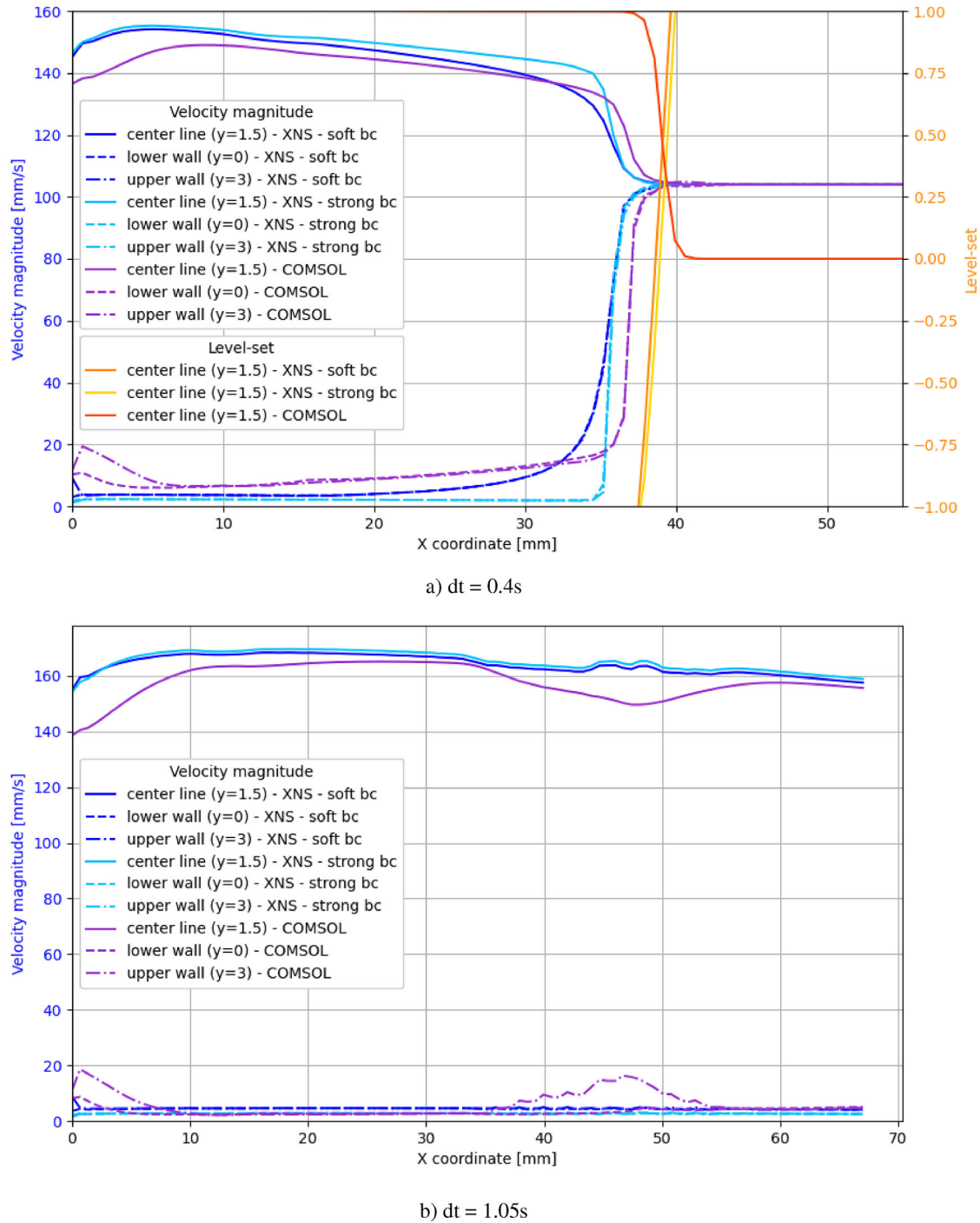


FIGURE 3 | Velocity magnitude and level set along the channel length at the walls and center line.

higher velocity in the center for the XNS simulation. We can also observe some asymmetry in the COMSOL velocity profile near the interface, which could be related to the slip in the upper wall observed in Figure 3. Additionally, a difference in the frozen layer thickness is visible; in the XNS simulation, this layer is thicker and we have steeper velocity gradients along the channel width, that is, higher shear rate. In case of semi-crystalline polymers, this difference in the shear rate can have a direct impact on the polymer microstructure, influencing the final part properties. This can result in high residual stresses in the part walls, which will finally lead to part warpage.

Even though XNS—strong BC simulation has the desired no-slip condition for the polymer phase, it comes with some drawbacks. First, is the choice of the parameters α_∞ and δ_1 , which are selected by trial. Second, since the tangential force is only dependent on the fluid velocity but not in its viscosity, this might result in applying more tangential force than required, having too restrictive boundary conditions causing unnecessary more computational efforts and even leading to divergence. In Figure 5, the viscosity and shear rate from the XNS—strong BC simulation are plotted. We observe the shear-thinning behavior of the material: high shear rates reduce the viscosity. Here, the effect

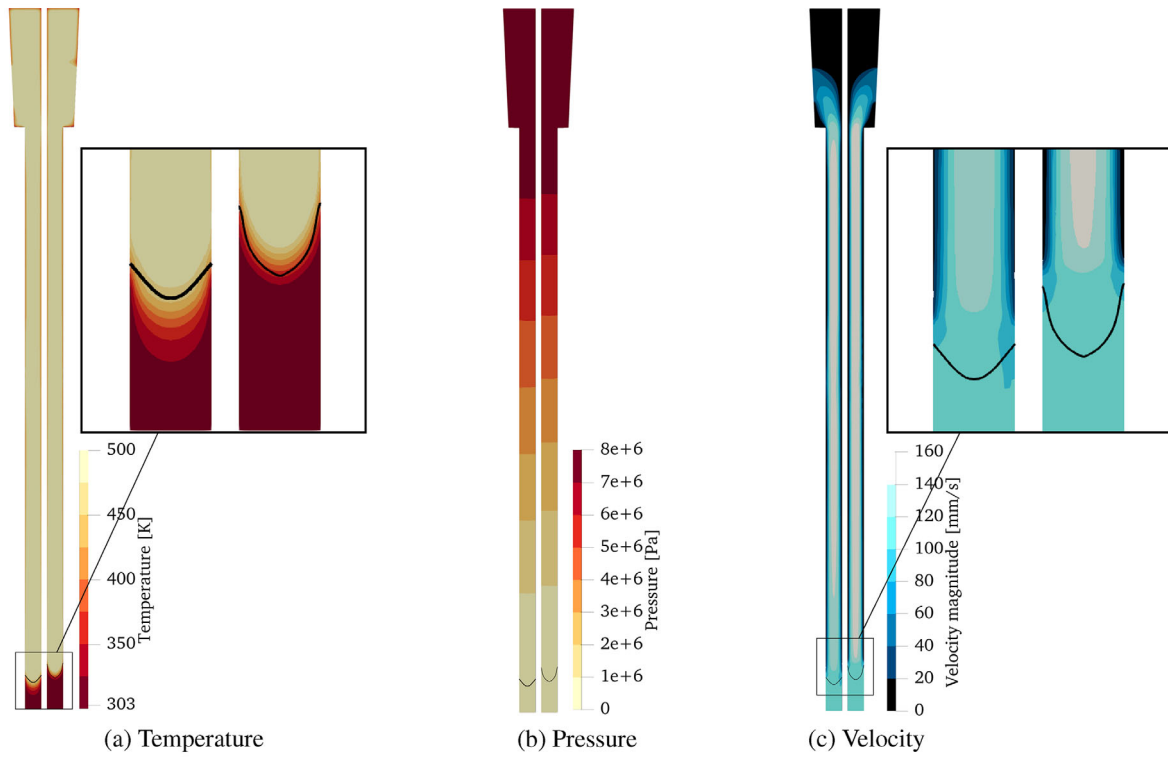


FIGURE 4 | Comparison between COMSOL (left mirrored geometry) and XNS—strong BC (right geometry) simulation results, at $t = 1$ s. In black the polymer-air interface.

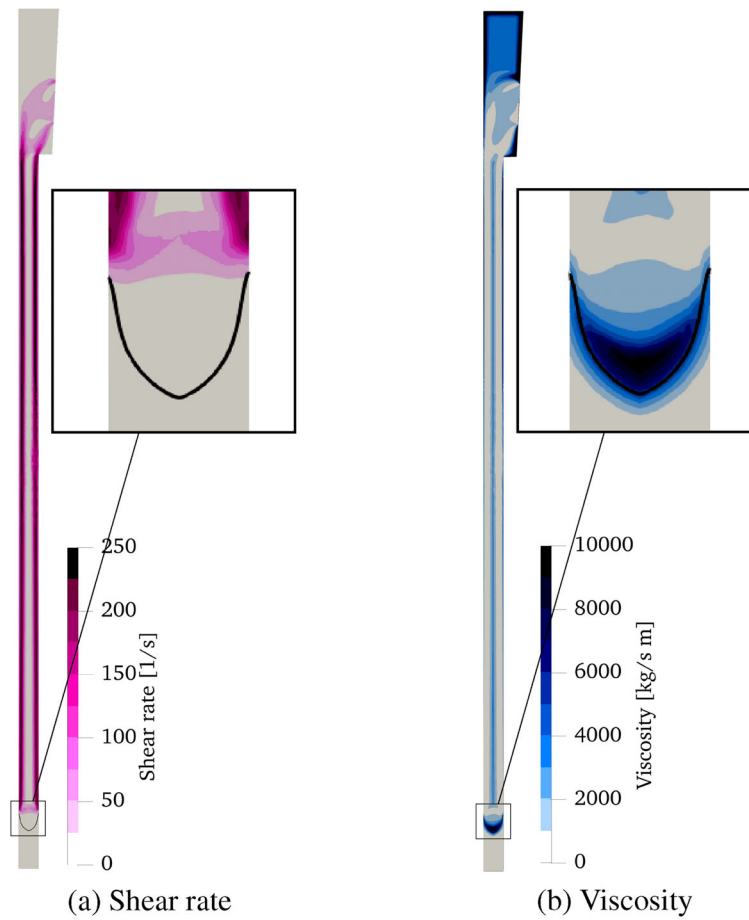


FIGURE 5 | Results from XNS—strong BC simulation. In black, the polymer-air interface.

of the temperature gradients on the viscosity is not as relevant as the shear rate, since the temperature is rather constant and far beyond the melt temperature of the polypropylene ($\sim 433\text{K}$). On the walls, we observe the highest shear and lowest viscosity values. Both, shear rate and viscosity, determine the shear stress, which influences the boundary conditions.

The comparison of computational effort is especially important if the geometry is elevated to a full 3D model of the part, while achieving high accuracy. As shown, during the injection phase the flow front behavior is largely dependent on boundary conditions; therefore the elements at the boundary should be as small as possible to have less effect on the bulk material. In order to have small elements at the boundary, a generally high number of elements must be considered for large meshes. Comparing the simulation times on similar but not identical computers while employing an identical mesh, the XNS space-time discretization leads to a significant reduction in computational time, see Table 2.

7 | Summary and Outlook

Three simulations have been compared, using the commercial tool COMSOL Multiphysics, and the in-house solver XNS. All simulations result in qualitatively similar results in terms of filling time, temperature, and pressure. However, we could observe that the difference on the application of the boundary conditions, that is, different formulation and coefficients for the variable Navier-slip condition, influences the velocity and the interface profile. For high-precision applications with semi-crystalline polymers, this can have a direct influence on the final properties, since the solidification through crystallization is directly influenced by the flow shear rate.

XNS boundary conditions show better agreement with the desired no-slip behavior of the polymer phase. However, the parameters defining the boundary conditions are not unique, allowing flexibility but not robustness. The COMSOL formulation depends on the viscosity and the velocity, making the formulation more robust, but the results show some undesired slip behavior along the channel.

The computational effort is drastically reduced while maintaining identical mesh accuracy by the space-time discretization of the XNS solver compared to the dynamic time stepping of COMSOL.

To complete this study and get a more general insight, more geometry configurations, for example, different ratio inlet/outlet, should be tested. Additionally, further efforts will be invested in the investigation toward a consistent variable Navier-slip formulation, adapting the imposed tangential stress to the simulation, recovering the 0 velocity at the wall with the minimum computational effort. The experimental validation of this numerical approach is also planned.

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