We show how to use and extend OpenFOAM’s incompressible two-phase flow solvers for the simulation of injection molding with short fiber reinforced thermoplastics in a laminar flow regime. Second order fiber orientation tensors are computed using the Folgar-Tucker equation (FTE) with quadratic closure. The FTE is coupled to the viscosity-term of the Navier-Stokes equations for the non-Newtonian flow in a segregated manner. Phase dependent boundary conditions are implemented to simulate wall heat transfer, stickiness of the melt to the wall and to prevent air-traps close to the wall.

1 Introduction

Nowadays, injection molding (IM) can be considered one of the economically most important processes for the mass-production of plastic products. To increase the strength of such parts, fillers such as glass or carbon fibers, are added to the polymer matrix. Today, such fiber reinforced thermoplastics (FRTs) parts, produced by IM become increasingly attractive for the mass-production of lightweight structures in the automotive industries. The part quality such as part warpage and mechanical properties are highly influenced by the IM process variables, such as flow temperature, flow rate and injection location. Furthermore, fill and cooling times are often of economical interest. Commercial software is readily available for the simulation of IM. However, due to the complex nature of the process, most of the software does not allow the integration of customized models for the flow rheology, which is particularly important at high fiber volume fractions and the characterization of weld lines. In the following sections we present a basic model for IM with FRTs and we discuss the topics given in the abstract.

2 Governing Equations

For brevity we explain here an incompressible model, which consists at first of the Navier-Stokes equations, which include equations for conservation of momentum, incompressibility and conservation of energy (incl. heat transfer)

\[
\frac{D\rho u}{Dt} = \nabla \cdot \sigma + \rho g, \quad \nabla \cdot u = 0, \quad \rho c_p \frac{DT}{Dt} = \sigma : \nabla u + \nabla \cdot (k \nabla T), \quad \sigma = -p I + 2\mu (D + N_p A D).
\] (2.1)
Here \( \rho \) denotes the density, \( \mathbf{u} \) the unknown velocity and \( \mathbf{g} \) the gravity. The term \( \frac{D \mathbf{A}}{Dt} \) denotes the material derivative, i.e. \( \frac{D \mathbf{A}}{Dt} := \frac{\partial \mathbf{A}}{\partial t} + \nabla \cdot (\mathbf{A} \mathbf{u}) \), for some variable \( \mathbf{A} \). The specific heat at constant pressure is denoted by \( c_p \) and \( k \) is the thermal conductivity. The quantity \( \sigma \) denotes the stress of the fluid, which contains the unknown pressure \( p \). The viscosity \( \mu \) is further dependent on the shear-rate, which is described by a Carreau-WLF type law. The \( N_p \) term describes the anisotropy of the viscosity, caused by different fiber orientations, which are described in terms of the second and fourth moment

\[
\mathbf{A} = \int_{S^2} \mathbf{p} \otimes \mathbf{p} \Psi (\mathbf{p}) \, dS \quad \text{and} \quad \mathbf{A} = \int_{S^2} \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \Psi (\mathbf{p}) \, dS
\]

of the probability density function \( \Psi (\mathbf{p}) \) of fiber orientations on the sphere \( S^2 \). The change of \( \Psi \) in terms of the moments \( \mathbf{A} \) and \( \mathbf{A} \), caused by the flow velocity is described by the FTE [1]

\[
\frac{D \mathbf{A}}{Dt} = (\mathbf{W} \mathbf{A} - \mathbf{A} \mathbf{W}) + \lambda (D \mathbf{A} + AD - 2AD) + D_r (I - 3A), \tag{2.2}
\]

where \( \lambda = \frac{r_e - 1}{r_e + 1}, r_e = \frac{4}{3} \) are scalars accounting for the geometry of the fibers with length \( \ell \) and diameter \( d \). The diffusion coefficient \( D_r \) describes the strength of fiber-fiber interactions, which is relevant in concentrated regimes only. \( \mathbf{A} \) is approximated here by the quadratic closure \( \mathbf{A} = \mathbf{A} \otimes \mathbf{A} \). Finally \( D = \frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \) is the rate-of-strain tensor and \( \mathbf{W} = \frac{1}{2} (\nabla \mathbf{u} - (\nabla \mathbf{u})^T) \) accounts for the rotation of the fluid. The flow consist of two phases: the polymer melt and air. We use a phase field function, indicating the phase fraction of each phase, i.e. \( \alpha (\mathbf{x}) = 1 \) inside the polymer, \( \alpha (\mathbf{x}) = 0 \) inside the air and \( \alpha (\mathbf{x}) = \frac{1}{2} \) at the interface. The phase field has to be transported with the flow, i.e. \( \frac{D \alpha}{Dt} = 0 \). All phase dependent material properties, such as density, viscosity, specific heat and thermal conductivity have to be formulated in terms of \( \alpha \), i.e. \( q = \alpha q_1 + (1 - \alpha) q_2 \), where \( q_1 \) and \( q_2 \) describes the material properties of each individual phase.

### 3 Implementation

The implementation, called injectionMoldingFoam (IMF), is based on OpenFOAM, which is a flexible C++ toolbox/library based on the finite volume method (FVM), which allows to solve a range of problems in engineering and science, especially in the field of computational fluid dynamics (CFD) involving multiple phases. Since OpenFOAM is released under the GNU General Public License (GPL), development of customized numerical solvers is possible. The available interFoam solver for incompressible two phase flows was extended to the specific needs for injection molding simulations, such as the specification of injection points and phase dependent boundary conditions. In particular for the velocity, pressure and phase we used the following boundary conditions:

\[
(1 - \alpha_c) \frac{\partial \mathbf{u}}{\partial n} + \alpha_c \mathbf{u} = (1 - \alpha_c) \mathbf{u}_0 \quad \text{and} \quad \alpha_c \frac{\partial p}{\partial n} + (1 - \alpha_c) p = (1 - \alpha_c) p_0 \quad \text{and} \quad \alpha = \begin{cases} \frac{1}{2} \alpha_i \text{ on walls}, \\ 1 \text{ at injection points}, \end{cases}
\]

where \( \mathbf{u}_0 \) denotes the injection velocity (zero at wall sections) and \( p_0 \) denotes the external air pressure. The parameter \( \alpha_c \) is defined as \( \max \{ \alpha, \alpha_i \} \), where \( \alpha_i \) is the patch internal value. This definitions leads to \( \alpha = \frac{1}{2} \) at wall sections adjacent to completely filled cells, which results in a more realistic interface position at interface reconstruction. To avoid outflow of the polymer (\( \alpha = 1 \)) through the boundary as long as the adjacent cell is not completely filled, it is particularly important to set positive (outgoing) face fluxes of \( \alpha \) explicitly to zero at the boundary. However this introduces the risk of overshooting \( \alpha \) above 1. Such overshoots are therefore set to 1 and the arising mass defect is recorded. The fiber orientation tensor \( \mathbf{A} \) in (2.2) is normalized to have trace one after each time step. Due to large jumps of the material coefficients \( \mu, \rho, c_p \) at the interface, often numerical difficulties (velocity or temperature spikes) may arise. These difficulties may be relaxed by setting for example \( \mu_2 = 10^{-3} \mu_1 \). For the heat equation it is favorable to have \( \rho_1 c_{pl} = \rho_2 c_{p2} \) at the interface, which avoids heat generation at the interface. Such conditions may also be imposed directly to the corresponding equations. Large values of the parameter \( N_p \) also introduce stability issues, since OpenFOAM does not allow an implicit discretization of the \( \nabla \mathbf{u}^T \) terms. Therefore additional terms for stabilization has to be added to the
equations. The simulation is stopped when \( \max\{\phi|\Gamma\} > 0.98 \), in which case the mold is filled and the system becomes almost singular.

4 Numerical Results

IMF was tested for several real world CAD geometries. An example for an FRP fill simulation is shown in Fig. 4.1. The mesh consists of 87 286 cells and the simulation runtime was about 15 minutes on 10 cores. The time step is limited by the CFL number to be less than 1. The largest velocities of the flow usually occur at the injection point and depend on the diameter of the latter. The fill simulation and computed fiber orientations are in good agreement with the results of Moldflow.

5 Conclusion and Outlook

In this paper we presented a basic model for FRP injection molding. However, for a more realistic simulation there are several more issues to be addressed, such as compressibility, viscoelasticity [2],
crystallization and frozen layers, exact closure approximation (cf. [3]), velocity-pressure switchover, holding and cooling, residual stress formation, fiber concentration and distributions models.

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