MATHEMATICAL MODEL AND NUMERICAL ANALYSIS OF POLYMER MELT FLOW AND HEAT TRANSFER IN A COOLING EXTRUDER

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Abstract

This paper presents a mathematical model and numerical analysis of momentum transport and heat transfer of polymer melt flow in a standard cooling extruder. The finite element method is used to solve the three-dimensional Navier–Stokes equations based on a moving barrel formulation; a semi-Lagrangian approach based on an operator-splitting technique is used to solve the heat transfer advection–diffusion equation. A periodic boundary condition is applied to model fully developed flow. The effects of polymer properties on melt flow behavior, and the additional effects of considering heat transfer, are presented.

Introduction

A tandem extrusion system is an extrusion line with a secondary extruder for cooling and homogenizing to produce high volume quality foam. Optimization of both the equipment (specifically, the second extruder) and the process would enable more efficient use of raw materials and energy. This goal can best be achieved by developing a mathematical model, based on physical laws and assumptions, to predict the melt flow and heat transfer behaviors in response to a given screw geometry, material properties, and process conditions. This, however, is a difficult task. A standard cooling extruder is a solid screw with a three-dimensional, naturally curved and naturally twisted flight, rotating at low speed, which means that the flow channel (in which the polymer melt is flowing) is three-dimensional, curved, and twisted as well. Furthermore, the polymer melt consists of large molecules composed of many small, simple chemical units; as a result, the most important characteristic of a polymeric melt is its shear-rate-dependent (or non-Newtonian) viscosity. The complex geometry and the rotation of the screw, when combined with the properties of the polymer melt, make the prediction of flow and heat transfer a challenging task.

There are three usual approaches to studying such complex phenomena: analytical, experimental and numerical. Theoretical analyses have severe limitations in their ability to handle complex geometries and complex boundary conditions. And, although experimental approaches can provide valuable and direct information on the extrusion process, they are usually costly to set up and difficult to perform. Therefore, as three-dimensional flow simulation is within the capabilities of modern computer technology, numerical modeling is an attractive choice for investigating polymer melt flow and heat transfer behavior within an actual extruder.

As the use of tandem extrusion lines to produce quality structured foams has expanded, there has emerged an increasing interest in modeling the polymer melt flow through a cooling screw, and designing more efficient screws. At the moment, there are few published simulation results of flow and heat transfer in a cooling screw, and designs are still more art than science. This paper presents a precise mathematical model to simulate polymer melt flow and heat transfer in a standard cooling screw, which makes possible the efficient optimization of screw geometry taking into consideration the many mutually interacting parameters.

Methodology

Flow conservation laws

A polymer melt in a cooling extruder is assumed to be incompressible, and its flow is assumed to be steady-state and compliant with conservation laws for mass, momentum and energy. These laws are expressed by the following three partial differential equations:
the continuity equation,

$$\nabla \cdot u = 0 \tag{1}$$

the momentum equation,

$$\rho \frac{Du}{Dt} = \nabla \cdot \sigma + \rho g \tag{2}$$

and the energy equation,

$$\frac{\partial T}{\partial t} + u \cdot \nabla T = \nabla \cdot (D \nabla T) + \Phi \tag{3}$$

In these equations, u is the velocity vector, σ is the stress tensor, ρ is fluid density, g is gravitational acceleration, T is the scalar temperature, D is the thermal diffusivity, and Φ represents the viscous reheating. The stress tensor is required to obey the constitutive equation

$$\sigma = -PI + \tau \quad (4)$$

where

$$\tau = 2\mu(\dot{\gamma})d \quad (5)$$

and P is the fluid pressure, I is the identity tensor, $\mu(\dot{\gamma})$ is the dynamic viscosity, and d is the rate-of-deformation tensor:

$$d = \frac{1}{2}[(\nabla u) + (\nabla u)^T] \quad (6)$$

The local shear rate, $\dot{\gamma}$, is defined as:

$$\dot{\gamma} = \sqrt{2tr(d \cdot d)} \quad (7)$$

The polymer melt is modeled as a purely viscous fluid, where the shear-rate- and temperature-dependent viscosity of the polymer melt is described via a modified power-law model:

$$\mu(\dot{\gamma}) = m(\dot{\gamma})^{n-1} e^{-b(T-T_b)} \quad (8)$$

Where m is the consistency index (unit of Pa·s^n), n is the power-law index, b is a constant parameter and T_b is a reference temperature.

Equations (1), (2) and (3) can be simplified by introducing the following scaling parameters: the characteristic length L, velocity U, temperature T_0, and viscosity μ_0. These parameters then allow us to define the following non-dimensional variables (indicated with overbars): $\bar{x} = x/L$, $\bar{u} = u/U$, $\bar{T} = T/T_0$, $\bar{\mu} = \mu/\mu_0$, $\bar{P} = PL/\mu$ (if $\mathrm{Re} << 1$), $\bar{t} = Ut/L$, Reynolds number $\mathrm{Re} = \rho UL/\mu$, Peclet number $Pe = UL/D$, and $\bar{f} = fL/(U\Delta T_0)$. For a typical molten polymer flow, the Reynolds number is usually in the range 10^{-4} to 10^{-2} [2]. We neglect the gravitational effect and drop the overbar notation so that equations (1), (2) and (3) in non-dimensional form become:

$$\nabla \cdot u = 0 \quad (9)$$

$$\frac{\partial u}{\partial t} + u \cdot \nabla u = -\nabla P + \frac{1}{\mathrm{Re}} \nabla \cdot [\mu \cdot (\nabla u) + (\nabla u)^T] \quad (10)$$

$$\frac{\partial T}{\partial t} + u \cdot \nabla T = \frac{1}{Pe}(\nabla^2 T) + f \quad (11)$$

Numerical algorithm

The governing equations (9), (10) and (11) are spatially discretized using a Galerkin finite-element approach in conjunction with P2-P1 tetrahedral Taylor–Hood elements, with ten nodes for velocity and temperature, and four nodes for pressure. A finite element solver for three-dimensional non-Newtonian fluid flow and advection-diffusion heat transfer has been developed. The unknown velocity, pressure and temperature fields can be expressed in terms of the shape functions ϕ_j and ψ_j, and nodal velocity, pressure and temperature values u_j, p_j, and T_j:

$$u\,(or\ \mathrm{T}) = \sum_{j=1}^{N} u_j\,(or\ T_j)\,\phi_j \quad (12)$$

$$p = \sum_{j=1}^{N_p} p_j \psi_j \quad (13)$$

where there are $N = 10$ degrees of freedom for velocity and temperature in each coordinate direction, and $N_p = 4$ degrees of freedom for pressure.

After the Galerkin spatial discretization, the governing equations can be written in semi-discrete form as:

$$[M]\frac{d\{u\}}{dt} + [S]\{u\} + [L]^T\{p\} = \int_\Gamma (-p\vec{n} \cdot \vec{x} + \frac{\partial u}{\partial n})\,d\Gamma \quad (14)$$

$$[L]\{u\} = 0 \quad (15)$$

$$\frac{\partial \{T\}}{\partial t} = D\{T\} + C\{T\} + f \quad (16)$$

where $\{u\}$ is the vector of nodal velocity values, $\{p\}$ is the vector of nodal pressure values, $\{T\}$ is the vector of nodal temperature values, $[M]$, $[S]$ and $[L]$ are elemental matrices, $D = \frac{1}{Pe}\nabla^2 T$ is the diffusion operator, $C = -u \cdot \nabla$ is the advection operator, Γ is the boundary of the elemental volume Ω, and $\vec{x}$ is the unit vector in the x_i direction, where $i = 1, 2, 3$ represent the *x*, *y*, and *z* directions, respectively.

Coupled system

The velocity and temperature fields are coupled by viscosity and shear-reheating terms in the governing equations, and so the fully coupled system must be solved iteratively. An approach that exploits operator integration factors to reduce the multiple operator equation to an associated series of single-operator sub-problems has been adopted for the time-splitting scheme. This time splitting is described in detail by Maday et al. [4].

Moving barrel and periodic inflow/outflow condition

In the simulations, the frame of reference is attached to the screw, so that the screw root and flights appear motionless and the barrel moves in a direction opposite to that of the actual screw rotation. In this way, the complexity associated with applying boundary conditions induced by the rotation of the screw is removed.

Since a standard screw geometry within a cooling extruder has a periodic flow channel, a periodic inflow/outflow boundary condition is applied to simulate fully developed flow. Validation tests showed that a single pitch of the screw with periodic boundary conditions is sufficient to model polymer melt flow behavior in the whole cooling screw geometry.

Results and Discussion

The material considered in this study is WB130HMS polypropylene (PP), and the flow geometry is one pitch length of a standard cooling screw (Killion's Extruder) channel. The standard cooling screw geometry is shown in Figure 1, and one pitch length of the screw channel (the flow domain) is shown in Figure 2.

The effect of polymer melt properties on the flow field

In order to investigate how polymer melt properties affect flow behavior, the flow is assumed to be isothermal. Three simulations were carried out, for a pure PP melt, and a PP/CO_2 mixture with 5% CO_2 by weight, at two different melt temperatures. The non-dimensional flow velocity and pressure, and the normalized screw wall shear stress, were calculated. A summary of geometrical and material data and the operating conditions used in the calculations are listed in Table 1. The cross-section tangential and axial velocity distributions along the screw channel from the screw root to the barrel are shown in Figures. 3 and 4, respectively. A comparison of the three cases shows that the gas content (which varies between Case I and Case II) does not significantly affect the flow behavior, because for both of these cases the power-law index is the same, and it is the power-law index that describes the degree of shear-thinning behavior. On the other hand, Case III shows that melt temperature influences flow behavior, because at a lower temperature, the mixture of melt and gas has a smaller power-law index, and so the degree of shear-thinning is larger. Finally, the polymer melt properties affect the pressure drop along the axial direction. Figure 5 shows a comparison of the pressure drop for the three cases. Under extrusion conditions, the pressure gradient increases with increasing power-law index at the same flow rate.

Wall shear stress

The wall shear stress is the shear stress exerted by the screw on the fluid. Figure 6 shows the wall shear stress for Case I. From the figure, it can be seen that the highest shear stress occurs along the edge between the barrel and the flight. This is because the shear rate is much higher between flight tips and the barrel.

Temperature field

Figure 7 shows the modeled temperature profile in a cross-section of a typical screw channel. The figure shows that the temperature is higher in the center of the screw channel, since this inner region is insulated from the screw and barrel surfaces and heat removal from this region is ineffective. This high-temperature region is the major problem with the standard cooling screw; improved mixing, leading to the elimination of these high temperatures, is one of the most important factors when considering screw design.

Conclusions

A finite-element solver of three-dimensional polymer melt flow and heat transfer in a standard cooling screw geometry has been developed based on a moving barrel formulation. The velocity, pressure, wall shear stress, and temperature profiles were calculated and presented for several melt conditions. The effect of polymer melt properties on the flow field was investigated; results indicate that the degree of shear thinning is the major factor that influences the flow behavior. The heat transfer results show that for a standard cooling screw geometry, that cooling is not sufficient and that the temperature distribution is far from uniform, which implies that a novel screw design is required to obtain better cooling and temperature uniformity, in order to more efficiently use raw materials to produce high quality foam.

This solver and simulation results such as the ones presented here will be used as an extruder design tool, to allow a designer to repeatedly modify a screw geometry and easily perform simulations, in order to determine an optimal technical solution for the elements of an extruder. The next step in this work will be the design of an advanced cooling screw.

Acknowledgments

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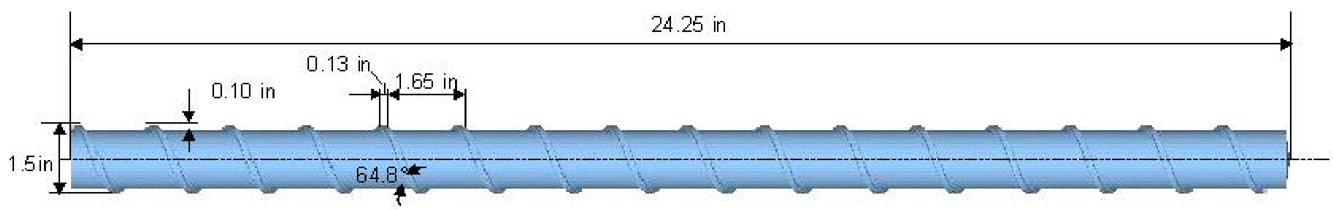

Figure 1. A standard cooling screw geometry (Killion's Extruder).

Table 1. Material data and operating conditions.

Parameter	Case I	Case II	Case III
Gas content (% CO_2)	0 %	5 %	5 %
Melt Temperature T_b (^oC)	190	190	155
Density (g/ml)	0.910	0.910	0.910
Power-law index n	0.41	0.41	0.25
Power-law consistency m	7150	5400	40000
Flow rate (g/min)	19.9		

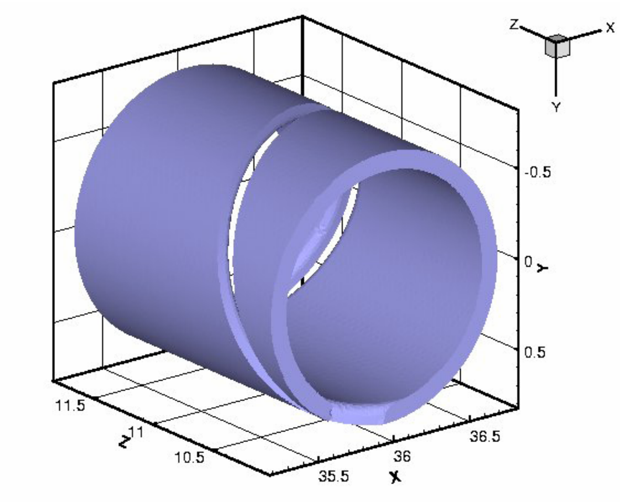

Figure 2. One pitch length of the flow channel

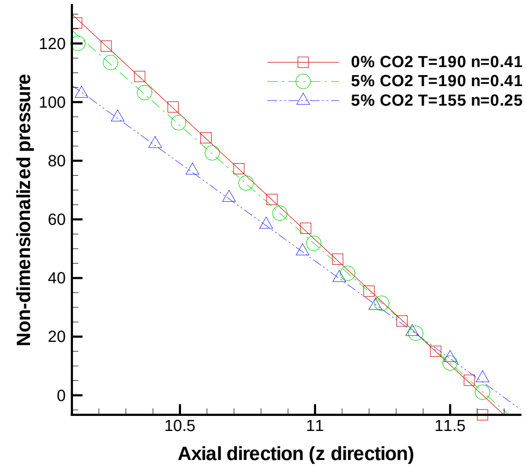

Figure 5. Axial pressure profiles

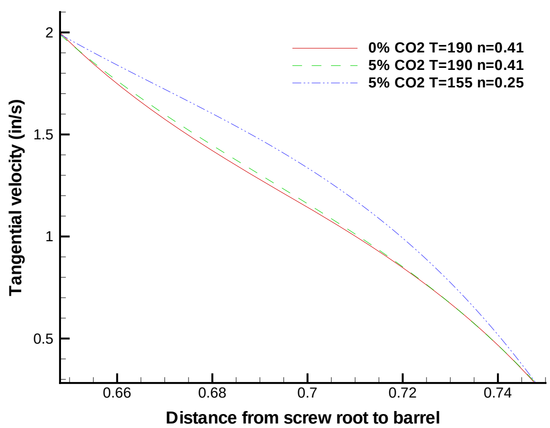

Figure 3. Tangential velocity profiles

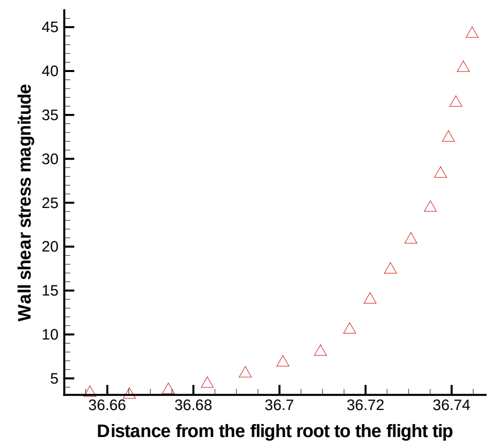

Figure 6. Wall shear stress distribution

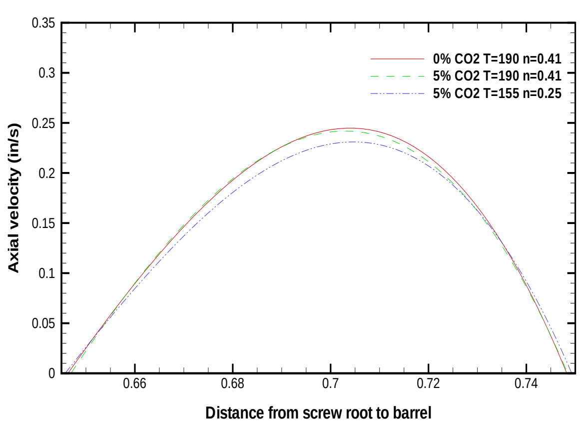

Figure 4. Axial velocity profiles

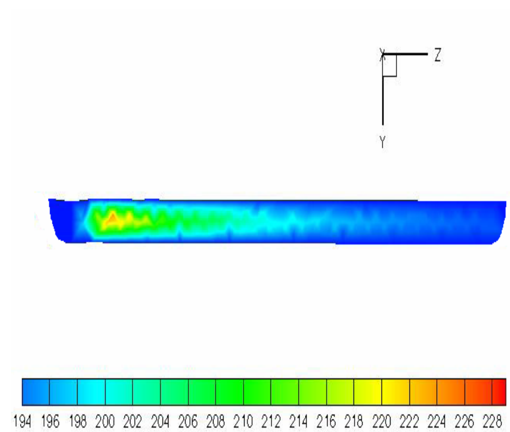

Figure 7. Screw channel cross-section temperature profile