

## Research Paper

## Development and validation of a model for the temperature distribution in the extrusion calibration stage



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## HIGHLIGHTS

- New model to calculate the temperature distribution in two phase systems.
- The approach is able to deal with temperature discontinuity at the phases interface.
- The methodology was implemented in OpenFOAM® computational library.
- The developed code is able to model the profiles extrusion cooling stage.

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## ABSTRACT

A new model to calculate the temperature discontinuity between two phases is derived in detail and implemented in the *OpenFOAM*® computational library. The derivation of the model is based on the local instantaneous conservation equation for energy. With the conditional volume averaging technique a single equation that governs the temperature distribution, valid in both phases, is obtained. The order of convergence of the solver is determined using the Method of Manufactured Solutions (MMS), which also allows to identify eventual coding bugs. To verify the developed code, 2D problems, namely the heat transfer between two slabs in contact and between two concentric hollow cylinders, are considered. For the same purpose, the solution for a complex two-dimensional layout, which consists of a polymeric sheet and a calibrator, is compared with benchmark solutions. Finally, the developed code is used to study the behavior of a complex 3D calibration system. All results show good agreement with benchmark ones or, in case of the realistic calibrators, are in line with our expectations.

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## 1. Introduction

Fig. 1 shows a typical extrusion line for the production of thermoplastic profiles that consists of an extruder, a die, a calibration unit, a haul-off and a saw. The hopper is used to feed the extruder barrel with polymer pellets; while inside the extruder, the plasticizing screw melts and homogenizes the polymer and pumps it toward the extrusion die, which shapes the polymer melt into the desired cross-section geometry. The calibration/cooling zone is intended to cool down the polymer and to impose the extruded profile outer-dimensions. In the last steps of the extrusion line the haul-off is used to set the profile linear extrusion speed and the saw cuts

the polymer profile in the specified length [1]. Due to the viscoelastic nature of polymeric materials, it is difficult to produce polymer profiles with the required cross section dimensions [1]. At the calibrator, uniform cooling is intended to minimize temperature gradients along the profile contour and thickness, in order to induce the adequate morphology and to minimize the residual thermal stresses level induced during cooling [2,3].

In practice, and due to the geometric complexity of some profiles and to the high number of variables involved, the optimization of these tools is quite difficult to accomplish. Therefore, numerical simulation of the heat transfer in the calibrator is helpful and desirable to facilitate the design task. That would be further improved if the modeling code is coupled with an optimizer.

The use of numerical simulations in the field of fluid flow and heat transfer phenomena increased significantly in the last decades, due to the development of better and faster computers that allow the employment of more realistic models. However, few works are

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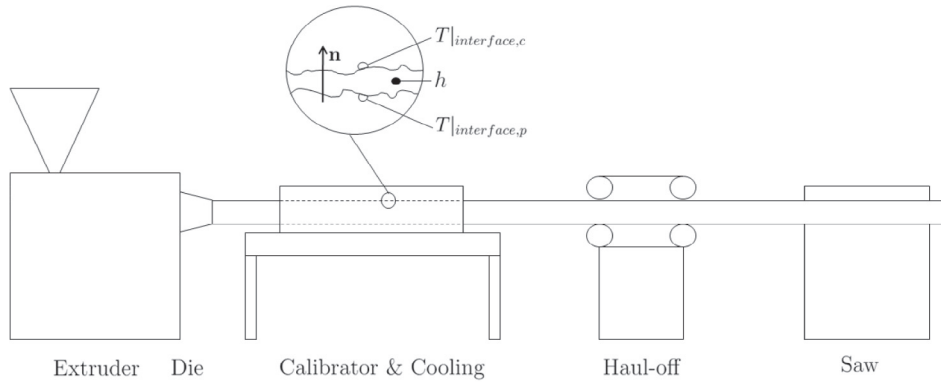


Fig. 1. Schematic view of a thermoplastic profile extrusion line.

available in the literature concerning the design of calibration/cooling system assisted by numerical modeling codes. The proposed models covered 1D [4,5], 2D [6–8], hybrid 2D [9] and 3D [10] problems. The effect of the boundary conditions was studied in Szarvasy et al. [7], Szarvasy and Sander [8] and Nóbrega et al. [10].

A detailed numerical code was developed by Nóbrega et al. [10,11,12], Nóbrega and Carneiro [13] and Carneiro et al. [14] in addressing the thermal design of calibrators. The developed code framework comprised geometry and mesh generators, that coupled with an optimization routine, allowed to determine automatically the optimal cooling conditions. The main limitation for the developed modeling code is that it is limited to structured computational meshes, and therefore it cannot be extended to complex (i.e. realistic) geometries.

In this paper a new numerical code is developed to describe the heat transfer between the two phases present in the profile extrusion cooling process (polymer and calibrator) that allows the assumption of contact resistance at the polymer–calibrator interface. The devised model uses a single equation that is valid in both phases, which can predict the temperature for any two-phase set up, whether 2D or 3D. Furthermore, the model can handle a wide range of physical properties and contact resistances and is not restricted to structured meshes or sharp interfaces. To verify the developed codes, the results are compared with analytical solutions, tested with the Method of Manufactured Solutions (MMS), and with results of a similar model for polymer cooling [11].

The remainder sections of the paper are organized as follows. First, the numerical procedure and the discretization process will be presented. Then, the code is verified using the MMS and compared against both analytical solutions and numerical solutions obtained from Nóbrega et al. [11]. Finally, the robustness of the numerical code will be assessed using a real life case study of the cooling stage of a thermoplastic matrix composite deck profile, where the developed code is coupled with an optimizer [15]. The paper ends with the main conclusions obtained.

## 2. Numerical procedure

### 2.1. Development of a calibrator model

In this work we aim at predicting the temperature field in the calibration/cooling unit and polymeric profile. Under incompressible conditions, constant pressure (specific heat capacity at constant pressure  $c_p$ ) and absence of volumetric heat sources and sinks (e.g. due to dissipation, etc.), the energy conservation holding in phase  $i$  ( $i = p, c$  for polymer and calibrator, respectively) can be cast into an equation for temperature  $T$ :

$$\frac{\partial(\rho_i c_{p,i} T_i)}{\partial t} + \nabla \cdot (\mathbf{U}_i \rho_i c_{p,i} T_i) - \nabla \cdot (k_i \nabla T_i) = 0 \quad (1)$$

Eq. 1 is a generic scalar transport equation (transient convection-diffusion).  $\rho$  is density,  $t$  is time,  $\mathbf{U}$  is velocity and  $k$  is thermal conductivity. In Fig. 1 an enlarged view of the polymer/calibrator interface is depicted. In case of perfect thermal contact between polymer and calibrator, temperature  $T$  and heat flux  $\mathbf{q}$  are continuous at the interface

$$T|_{interface,p} - T|_{interface,c} = 0 \quad (2)$$

$$(\mathbf{q}_p - \mathbf{q}_c) \cdot \mathbf{n} = (k_p \nabla T|_{interface,p} - k_c \nabla T|_{interface,c}) \cdot \mathbf{n} = 0 \quad (3)$$

where  $\mathbf{n}$  denotes the interface normal vector pointing from polymer to calibrator (see Fig. 1). However, under real processing conditions there is an imperfect contact between polymer and calibrator resulting in a thermal resistance at the interface, which is why temperature is discontinuous [16], and thus Eq. 2 must be replaced by

$$T|_{interface,p} - T|_{interface,c} = \frac{\mathbf{q}_c \cdot \mathbf{n}}{h} \quad (4)$$

where  $h$  denotes the heat transfer coefficient. The inverse,  $\frac{1}{h}$ , is called contact resistance.

A common approach is to solve Eq. 1 sequentially for both phases  $i = p, c$  until convergence. The coupling between the two phases is achieved by imposing the heat flux based on either Eqs. 2 or 3 (or Eqs. 3 or 4 for contact resistance), as described in Nóbrega et al. [11]. The main drawback of this approach is the long computation time required to achieve convergence, due to the sequential iterative solution. To overcome these limitations, mixture quantities can be introduced:

$$T_m = \alpha_p \bar{T}^p + \alpha_c \bar{T}^c \quad (5)$$

$$\mathbf{U}_m = \alpha_p \bar{\mathbf{U}}^p + \alpha_c \bar{\mathbf{U}}^c \quad (6)$$

$$\rho_m = \alpha_p \bar{\rho}^p + \alpha_c \bar{\rho}^c \quad (7)$$

$$c_{p,m} = \alpha_p \bar{c}_p^p + \alpha_c \bar{c}_p^c \quad (8)$$

$$k_m = \alpha_p \bar{k}^p + \alpha_c \bar{k}^c \quad (9)$$

In these equations  $\alpha_p$  is the volume fraction according to  $\alpha_p = \frac{V_p}{V_p + V_c} = \frac{V_p}{V}$  ( $\alpha_c = 1 - \alpha_p$ ), where  $V$  denotes the volume of a

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