A new energy conservation scheme for the numeric study of the heat transfer in profile extrusion calibration

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Received: 29 August 2016 / Accepted: 16 March 2017 / Published online: 3 April 2017
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Abstract In this work, a new second-order conservative finite volume scheme using the cell-to-vertex interpolation is proposed to solve the heat transfer problem involving discontinuous solution and discontinuous materials properties. We apply the method to a thermoplastic extrusion process where a dry calibration is used to cool down a polymer tape. One of the major difficulties in the modelling is to prescribe the adequate value for the heat transfer coefficient between the polymer and the calibrator. To this end, we define an optimization procedure coupled with the new finite volume method to evaluate the heat transfer coefficient at the polymer–calibrator interface from experimental data.

1 Introduction

Numerical simulations of the extrusion process turns to be a fundamental tool to design and develop extruders, extrusion dies and calibrators, to optimize the production and to provide high quality products [1, 2]. One of the most challenging extrusion processes concerns the production of profiles, as illustrated in Fig. 1, since the geometry can be very complex and varied, making difficult to generalize the design process of the required forming tools, namely the extrusion die, used to shape the polymer melt, and calibrator, used to cool down the profile.

To properly model the heat exchange that takes place at the cooling stage, special attention has to be paid to the interface between the polymer and the calibrator, depicted in Fig. 2, where temperature discontinuities take place. Such discontinuities are relied on the imperfect contact between the two domains (profile and calibrator) deriving from the irregularities on the two surfaces in contact and is usually characterized by the so-called interface heat transfer coefficient ($h_{int}$).

As any other industrial process, the main objective is to shape the profile extrusion for increasing the production rate and the quality of the produced profiles [3, 4]. However, these two goals are antagonistic since the increase of the production rate generally leads to a reduction of the product quality. Indeed, the low thermal conductivity of polymers is one of the major reasons for quality damaging, since the thermal gradients developed during the temperature drop give rise to internal residual stresses, which decrease the profile performance. Consequently, the cooling stage plays a crucial role in the entire extrusion process, since it is generally the limiting factor governing the maximum production rate. The solidification of the outer layers of the profile should be as fast as possible and, at the same
time, it should preserve an homogeneous temperature to minimize the internal thermal induced stresses.

Due to its intrinsic measurement difficulties, the number of studies available in the literature concerning the evaluation of the heat transfer coefficient at the polymer–calibrator interface are very scarce. Mousseau et al. [5] developed a prototype system to characterize the heat transfer coefficient, but for specific profile whereas the cooling conditions are difficult to characterize. More recently Carneiro et al. [6], developed a more flexible measurement system that combines experimental and numerical approaches to assess the same coefficient. The methodology comprises mainly two steps: (1) experimental tests to measure the temperature evolution of a polymeric tape along the cooling system; (2) model the process to identify the heat transfer coefficient value that better fits the experimental observations. Consequently, both the measurements performed and the accuracy of the modeling code play a major role on the approach effectiveness. However, the limited performance of the numerical code employed, make the calculation process rather difficult to undertake, which reduces the accuracy of the heat transfer coefficients evaluation.

Numerical methods such as the finite element method (FEM) [8–11] or finite difference hardly provide a good approximation when dealing with solutions involving discontinuities since, by construction, continuity across the contact boundary is mandatory. Moreover, local energy conservation in the cells is not fulfilled and may lead to unrealistic evaluation of the heat transfer process. On the contrary, finite volume method (FVM) is a well-adapted technique due to its built-in conservative property [12], simplicity, and versatility. This turns the FVM to be very competitive when compared with the traditional FEM [13] or its recent extension, the finite pointset method [14, 15].

Recent progress in the FVM enables to easily handle discontinuous solutions or discontinuous material coefficients [16] still preserving both the local energy conservation and the accuracy. The method Cell-to-Vertex coupling with nodal values on the interfaces provides an excellent treatment of the discontinuity and extensions for three-dimensional problems as well as non-isotropic problems have been successfully experimented [17]. A complete state-of-art review of the technique is given in [16, 17] where an extensive set of benchmarks has been tested to demonstrate the accuracy and the stability of the method.

This work proposes a novel methodology to obtain the heat transfer coefficient, $h_{\text{int}}$, at the polymer–calibrator interface in profile extrusion, using the experimental prototype system presented in [6]. This coefficient highly depends on extrusion conditions such as the roughness of the calibration material, the extrusion velocity, and the degree of vacuum. Notice that to assure a good contact between the calibrator and the thermoplastic profile, vacuum is imposed at the interface between both domains. The “degree of vacuum” corresponds to the vacuum level imposed, which affects the quality of the contact between both domains and, thus, the interface heat transfer coefficient [7]. Due to the sensitivity of the cooling process with respect to the heat transfer coefficient at the interface, an accurate model and numerical scheme are mandatory to provide approximations leading to a correct evaluation of this coefficient [18] with regards to data collected in extrusion experiments. Based on the above, the proposed methodology requires the following developments: (1) to provide and implement a numerical scheme to couple the Cell-to-Vertex technique, and an optimization algorithm to numerically evaluate the heat transfer coefficient, presented in Sect. 3. The developed numerical scheme robustness is verified in Sect. 4; (2) The fitting of the experimental measurements (presented in Sect. 5.2), which is preceded by the necessary mesh sensitivity study, given in Sect. 5.1; (3) in Sect. 5.3 the system behavior is studied to evaluate the
relevance of the main process parameters, aiming to guide the carefulness that has to be taken during the experimental characterization when measuring them.

2 Modelling

As described in [6] and illustrated in Fig. 3, the prototype calibration system developed to characterize \( h_{\text{int}} \), and modeled in this work, is modular and has several functionalities. However, in the context of the present work, the important component is the metallic insert (or calibrator), in contact with the polymer tape, which temperature is monitored by 35 thermocouples in contact with its lateral and upper surfaces. In such conditions, for heat transfer modelling purposes it will be sufficient to consider the metallic insert (and its surface temperature distribution, as boundary condition), the polymer tape and the surrounding air.

A two-dimensional convection–diffusion model of the multi-domain polymer–calibrator system is considered. Figure 4 displays the geometry of the subdomains where \( \Omega_c \) and \( \Omega_p \) stand for the calibrator and polymer (the subscripts c and p refer to the calibrator and polymer, respectively) while the boundaries are defined as:

- calibrator: \( \Gamma_c = \Gamma_{\text{sup}} \cup \Gamma_{\text{lat}} \cup \Lambda \),
- polymer: \( \Gamma_p = \Gamma_{\text{air}} \cup \Gamma_{\text{in}} \cup \Gamma_{\text{out}} \cup \Lambda \).

For each of the two domains, the energy conservation equation reads

\[
\nabla \cdot (C_\alpha U_\alpha T_\alpha - k_\alpha \nabla T_\alpha) = f_\alpha \quad \text{in} \Omega_\alpha \quad \alpha \in \{c, p\},
\]

(1)

where \( k_\alpha \) is the thermal conductivity, \( C_\alpha \) is the volumetric heat capacity, \( T_\alpha \) is the temperature distribution, \( U_\alpha \) is the velocity vector, and \( f_\alpha \) is the source term. For the particular problem under study, we assume the reference associated to \( \Omega_c \) to be fixed and \( U_c = (0, 0)^T \) whereas \( U_p = (u, 0)^T \) with \( u \) being the extrusion speed.

The heat transfer between the calibrator and the polymer is defined as a thermal contact resistance, which originates a discontinuity in the temperature domain, and the flux of energy across the interface is assumed to be linear with respect to the difference of the temperatures. The energy conservation equation can then be written as

\[
k_c \frac{\partial T_c}{\partial n_c} = -k_p \frac{\partial T_p}{\partial n_p} = h_{\text{int}} (T_p - T_c) \quad \text{on} \Lambda,
\]

(2)

where \( n \) denotes the unit vector normal to the interface boundary.

A polynomial temperature distribution given by Eq. (3) was prescribed for the upper surface of the calibrator, which depends on the variable \( x_1 \)

\[
T_{\text{sup}} = a_1 x_1^5 + a_2 x_1^4 + a_3 x_1^3 + a_4 x_1^2 + a_5 x_1 + a_6 \quad \text{on} \Gamma_{\text{sup}},
\]

(3)

where real values \( a_1, a_2, a_3, a_4, a_5, \) and \( a_6 \) are the polynomial coefficients and will be determined experimentally in order to fit the data provided by thermocouples embedded in the calibrator block [6]. The choice of the polynomial order was done in order to reduce the differences between the measurements and the temperature.
\[
-k_c \frac{\partial T_c}{\partial n_c} = h_{air}(T_c - T_{air}) \quad \text{on } \Gamma_{lat},
\]

where \( T_{air} \) is the constant temperature of the air and \( h_{air} \) is the natural convection heat transfer coefficient. As regards to the polymer, natural convection is also prescribed for the bottom and the upper surfaces, namely

\[
-k_p \frac{\partial T_p}{\partial n_p} = h_{air}(T_p - T_{air}) \quad \text{on } \Gamma_{air}.
\]

A constant prescribed temperature is given on the polymer inflow boundary (left) corresponding to the extrusion temperature

\[
T = T_{in} \quad \text{on } \Gamma_{in},
\]

while we prescribe the energy flux on the outflow polymer boundary (right)

\[
-k_p \frac{\partial T_p}{\partial n_p} = g_N \quad \text{on } \Gamma_{out}.
\]

### 3 Numerical scheme

To provide a generic expression for the discretization of the numerical scheme, we consider the Eq. (1) on an open bounded polygonal domain \( \Omega \) of \( \mathbb{R}^2 \) with boundary \( \Gamma \) (we skip the index \( \alpha \) for the sake of simplicity). We seek the temperature distribution \( T = T(x_1, x_2) \) as a solution of the steady-state convection–diffusion equation

\[
\nabla \cdot (VT - kV T) = f \quad \text{in } \Omega,
\]

where \( VT \) is the convective term with \( V = CU \), \( kV T \) is the diffusive term and \( f \) is the the source term. All the parameters in the equation were already described in Sect. 2. The boundary domain is partitioned into four subsets \( \Gamma_D, \Gamma_N, \Gamma_R, \) and \( \Lambda \), where different types of conditions may be prescribed, namely:

- **Dirichlet:** \( T = T_D, \text{on } \Gamma_D \) [Eq.s (3) and (6)];
- **Neumann:** \( -kVT \cdot n = g_N, \text{on } \Gamma_N \) [Eq. (7)];
- **Transference (Robin):** \( (VT - kV T) \cdot n = h(T - T_R), \text{on } \Gamma_R \) [Eq.s (4) and (5)];
- **Interface:** \( k_c V T_c \cdot n_c = -k_p V T_p \cdot n_p = h(T_p - T_c), \text{on } \Lambda \) [Eq. (2)],

with \( T_D \equiv T_D(x_1, x_2), g_N \equiv g_N(x_1, x_2), \) and \( T_R \equiv T_R(x_1, x_2) \) given regular functions.

### 3.1 Mesh

We denote by \( T \) a mesh consisting of \( I \) non-overlapping convex polygonal cells \( c_i, i = 1, \ldots, I, \) and \( K \) vertices \( v_k, k = 1, \ldots, K. \) We highlight that \( T \) composes two meshes, \( T_c \) and \( T_p, \) for the subdomains \( \Omega_c \) and \( \Omega_p, \) respectively, and are conformed with \( \Lambda \) such that if \( \hat{\epsilon} \cap \Lambda \neq \emptyset \) then \( \epsilon \subset \Lambda. \) We adopt the following conventions (see Fig. 5):

- the mesh \( T_c \) consists of \( I_c \) non-overlapping convex polygonal cells \( c_{i_c}, i_c = 1, \ldots, I_c, \) and \( K_c \) vertices \( v_{k_c}, k_c = 1, \ldots, K_c; \)
- the mesh \( T_p \) consists of \( I_p \) non-overlapping convex polygonal cells \( c_{i_p}, i_p = I_c + 1, \ldots, I_c + I_p, \) and \( K_p \) vertices \( v_{k_p}, k_p = K_c + 1, \ldots, K_c + K_p; \)
- for any cell \( c_i, \partial c_i \) represents its boundary and \( |c_i| \) its area; we denote by \( m_i \) the mass centre of \( c_i; \)
- two cells \( c_i \) and \( c_j \) share a common edge \( e_{ij} \) whose length is \( |e_{ij}| \) and the midpoint is \( m_{ij}; n_{ij} \) is the unit normal vector to \( e_{ij} \) outward to \( c_i, \) i.e. \( n_{ij} = -n_{ji}; \) if an edge of \( c_i \) belongs to the boundary \( \Gamma \), we replace the index \( j \) by \( D, N, R, \) or \( \Lambda \) if \( e_{ij} \) belongs to \( \Gamma_D, \Gamma_N, \Gamma_R, \) or \( \Lambda, \) respectively;
- for any cell \( c_j \) belonging to \( \Omega_c \) or \( \Omega_p \) we associate the index set \( \nu(i_c) \subset \{1, \ldots, I_c\} \cup \{D, N, R, \Lambda\} \) or \( \nu(i_p) \subset \{I_c + 1, \ldots, I_c + I_p\} \cup \{D, N, R, \Lambda\}, \) respectively, such that \( j \in \nu(i) \) if \( e_{ij} \) is a common edge of \( c_i \) and \( c_j, \) or with the boundary \( \Gamma_j \) if \( j = \{D, N, R\}, \) or with the interface \( \Lambda; \)
- for any vertex \( v_k \) belonging to \( \Omega_c \) or \( \Omega_p \) we associate the index set \( \mu(k_c) \subset \{1, \ldots, I_c\} \) or \( \mu(k_p) \subset \{I_c + 1, \ldots, I_c + I_p\}, \) respectively, such that \( i \in \mu(k) \) if \( v_k \) is a vertex belonging to the cell \( c_i. \)

![Fig. 5 Mesh notation](image-url)
Remark 3.1 If \( v_k \) is a vertex at the intersection of \( \Gamma_D \), and \( \Gamma_N \), \( \Gamma_D \) and \( \Gamma_R \), or \( \Gamma_D \) and \( \Lambda \), we assume that \( v_k \) belongs to \( \Gamma_D \) and will be treated as a Dirichlet point.

Remark 3.2 On the interface \( \Lambda \), each node considers two vertices, \( v_{k_c} \) and \( v_{k_p} \), which share the same position but are evaluated separately.

3.2 Generic finite volume scheme

To provide the finite volume scheme, Eq. (8) should be integrated over cell \( c_i \)

\[
\int_{c_i} \nabla \cdot (VT - k \nabla T) \, dx = \int_{c_i} f \, dx, \tag{9}
\]

and applying the divergence theorem we get an integral over the surface

\[
\int_{\partial c_i} (VT - k \nabla T) \cdot nds = \int_{c_i} f \, dx, \tag{10}
\]

and then,

\[
\sum_{j \in \mu(i)} \int_{e_{ij}} (V \cdot n_j T - k \nabla T \cdot n_j) \, ds - \int_{c_i} f \, dx = 0. \tag{11}
\]

The numerical integration of Eq. (11), based on a quadrature method, introduces consistency second-order errors and provides the following approximation

\[
\sum_{j \in \mu(i)} |e_{ij}| \left( V(m_{ij}) \cdot n_j T(m_{ij}) - k(m_{ij}) \nabla T(m_{ij}) \cdot n_j \right) - |c_i| f_i \approx 0. \tag{12}
\]

Let \( T_i \) be an approximation of \( T \) at \( m_i \). We gather all the approximations in two vectors \( T_c = (T_i)_{i=1,...,I_c} \) and \( T_p = (T_i)_{i=K_c+1,...,I_p} \), and we recall that \( \theta_c \) and \( \theta_p \) is an approximation of the mean temperature where we use the node \( v_k \) for the data belonging to \( \Omega_c \), and the node \( v_k \) for the data coming from \( \Omega_p \) (see Fig. 6). Consistency of the mapping with linear functions implies that coefficients \( \beta_{ki} \) have to fulfill the following restrictions

\[
\sum_{i \in \mu(k)} \beta_{ki} \equiv 1, \quad \sum_{i \in \mu(k)} \beta_{ki} m_i = v_k, \tag{15}
\]

except if vertex \( v_k \) belongs to a boundary where the temperature is prescribed (Dirichlet condition) where we have

\[
\theta_k = T_D(v_k) \quad \text{on} \Gamma_D. \tag{16}
\]

For the Neumann boundary condition, vertex interpolation can be obtained in two ways: we introduce ghost cells where the temperature is evaluated using the Neumann condition; or we consider a stencil for the interpolation gathering cells around the vertex. We refer to [16] for further details of the method.

3.3 Cell-to-vertex interpolation

The key of the method is a new accurate computation of diffusive flux across the edges. To this end, we use both approximations at the cell points and at the vertices to provide a good approximation of the temperature gradient, following [19–24] but introducing some weights in order to optimize the stencil and the accuracy [16, 17]. Since the unknowns are only located at the cell centers, a mechanism is introduced for linking the cell values with the vertex values to provide an accurate evaluation of the vertices temperature based on the cells temperature.

Let \( \theta_{k_c} \) and \( \theta_{k_p} \) be approximations of \( T \) at vertices \( v_{k_c} \) and \( v_{k_p} \), respectively, and let us gather all the approximations in two vectors \( \Theta_c = (\theta_{k_c})_{k_c=1,...,K_c} \) and \( \Theta_p = (\theta_{k_p})_{k_p=K_c+1,...,K_c+K_p} \) while \( \Theta = (\Theta_c, \Theta_p) \) stands for the global vector. We introduce the generic linear mapping \( T \rightarrow \Theta(T) \)

\[
\theta_k = \sum_{i \in \mu(k)} \beta_{ki} T_i, \tag{14}
\]

where \( \beta_{ki} \) are the interpolation coefficients for vertex \( k \) and we recall that \( \mu(k) \) is the index set of the cells having vertex \( v_k \). For \( v_k \in \Lambda \), one has to consider two different temperatures, \( \theta_{k_c} \) and \( \theta_{k_p} \), whether the temperature is associated to the calibrator or to the polymer. Two different stencils for the same location are introduced to estimate the temperature where we use the node \( v_k \) for the data belonging to \( \Omega_c \), and the node \( v_k \) for the data coming from \( \Omega_p \) (see Fig. 6). Consistency of the mapping with linear functions implies that coefficients \( \beta_{ki} \) have to fulfill the following restrictions

\[
\sum_{i \in \mu(k)} \beta_{ki} \equiv 1, \quad \sum_{i \in \mu(k)} \beta_{ki} m_i = v_k, \tag{15}
\]

except if vertex \( v_k \) belongs to a boundary where the temperature is prescribed (Dirichlet condition) where we have

\[
\theta_k = T_D(v_k) \quad \text{on} \Gamma_D. \tag{16}
\]

For the Neumann boundary condition, vertex interpolation can be obtained in two ways: we introduce ghost cells where the temperature is evaluated using the Neumann condition; or we consider a stencil for the interpolation gathering cells around the vertex. We refer to [16] for further details of the method.

3.4 Polynomial reconstructions

Based on the data stored in the two vectors \( T \) and \( \Theta \), we carry out the computation of several linear functions for the flux evaluations. For each cell \( c_i \) (resp. edge \( e_{ij} \)), we associate an index set \( S_i \) (resp. \( S_{ij} \)) of vertices and we consider affine functions on the cells and edges based on the information of vectors \( T \) and \( \Theta \). The first reconstruction concerns the conservative one. For each cell \( c_i \) we define the affine function

\[
T_i^l(x_1, x_2) = T_i + C_{i, 1} (x_1 - m_{i, 1}) + C_{i, 2} (x_2 - m_{i, 2}). \tag{17}
\]
where $C_{i,1}$ and $C_{i,2}$ are the coefficients to be determined. With the associated stencil $S_i$, we consider the quadratic functional

$$E_i(C_{i,1}, C_{i,2}) = \sum_{k \in S_i} \left( T_i^1(v_k) - \theta_k \right)^2$$

(18)

and we denote by $\tilde{C}_{i,1}$ and $\tilde{C}_{i,2}$ the unique coefficients that minimize the quadratic functional and $T_i^1(x_1, x_2)$ the associated polynomial function, which corresponds to the best approximation in the least squares sense of the data of the stencil.

The second reconstruction deals with polynomial functions associated to the edges. For a given inner edge $e_{ij}$, we consider the following expression for $T_i^1$ and $T_j^1$ given by

$$T_i^1(x_1, x_2) = T_i + C_{ij,1}(x_1 - m_{i,1}) + C_{ij,2}(x_2 - m_{i,2}),$$

(19)

and the symmetric expression for $T_j^1$, where $C_{ij,1}$ and $C_{ij,2}$ are the coefficients to be determined. We denote by $\tilde{C}_{ij,1}$ and $\tilde{C}_{ij,2}$ the unique coefficients such that the associated polynomial function $\tilde{T}_{ij}^1(x_1, x_2)$ interpolates $T_i$, defined at $m_i$, and $\theta_k$, defined at $v_k$, $k \in S_{ij}$. We perform the same operation to build $\tilde{T}_{ji}^1(x_1, x_2)$ and define the resultant polynomial

$$\tilde{T}_{ij}^1 = \tilde{T}_{ji}^1 = \sigma_g \tilde{T}_{ij}^1 + \sigma_j \tilde{T}_{ji}^1,$$

(20)

where $\sigma_g = \frac{|g|}{|g| + |g|}$ and $\sigma_j = \frac{|j|}{|g| + |g|}$.

At last, for an edge $e_{ID} \subseteq \Gamma_D$, we proceed in the same way to provide polynomial $\tilde{T}_{ID}^1(x_1, x_2)$.

3.5 Second-order scheme

Based on local affine reconstruction for $T$ based on vectors $T$ and $\Theta$ we compute the numerical approximations $F_{ij}$ in the following way. Five situations are identified:

- for an inner edge $e_{ij}$, the numerical flux at the midpoint $m_{ij}$ can be written as

$$F_{ij} = \left[ (m_{ij} \cdot n_{ij}) \tilde{T}_i^1(m_{ij}) + (m_{ij} \cdot n_{ij}) \tilde{T}_j^1(m_{ij}) \right] - k(m_{ij}) \nabla \tilde{T}_i^1(m_{ij}) \cdot n_{ij},$$

(21)

with the notations $\Phi^+ = \max(0, \Phi)$ and $\Phi^- = \min(0, \Phi), \Phi \in \mathbb{R}$.

- for a Dirichlet boundary edge $e_{ID}$, the numerical flux at the midpoint $m_{ID}$ can be written as

$$F_{ID} = \left[ (m_{ID} \cdot n_{ID}) \tilde{T}_i^1(m_{ID}) + (m_{ID} \cdot n_{ID}) \tilde{T}_j^1(m_{ID}) \right] - k(m_{ID}) \nabla \tilde{T}_i^1(m_{ID}) \cdot n_{ID};$$

(22)

- for a Neumann boundary edge $e_{IN}$, the numerical flux at the midpoint $m_{IN}$ can be written as

$$F_{IP} = V(m_{IN}) \cdot n_{IN} \tilde{T}_i^1(m_{IN}) + g_N(m_{IN});$$

(23)

- for a heat transfer boundary edge $e_{IR}$, the numerical flux at the midpoint $m_{IR}$ can be written as

$$F_{IR} = h \left( \tilde{T}_i^1(m_{IR}) - T_R(m_{IR}) \right);$$

(24)

- for an interface edge $e$ we have to distinguish two cases regarding to the side where the flux comes from. If we consider the calibrator side such $e = e_{i,A}$, the numerical flux at the midpoint $m_{iA}$ can be written as

$$F_{iA} = h \left( \tilde{T}_i^1(m_{iA}) - \tilde{T}_{ij}^1(m_{jA}) \right);$$

(25)

and, for the polymer side, a similar expression can be derived.

Since $F_{ij}$, and $f_i$ are linearly dependent on vector $T$, we define the affine operator $T \to G_i(T)$ for each cell $c_i$, $i = 1, \ldots, I$, as

$$G_i(T) = \sum_{j \in v(i)} |e_{ij}| F_{ij}(T) - |c_i| f_i.$$  

(26)

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Gathering all the components $\mathcal{F}_j(T)$ of the residual in vector $G(T)$, we seek the solution vector $T^*$ such that $G(T^*) = 0$. We obtain a matrix-free scheme and the affine problem is solved by applying a preconditioned GMRES procedure.

4 Numerical tests

Several numerical tests from manufactured solutions are presented to assess the robustness and accuracy of the implemented numerical scheme. Firstly, smooth solutions were tested for pure diffusion and convection–diffusion problems, with low and high Péclet number (Pe), and different types of boundary conditions. Heat transfer problems with discontinuous diffusion coefficients are then tackled in the context of convection–diffusion problems. To measure the accuracy of the obtained solution for a single mesh, two error estimators are introduced, namely

$$E_1(T) = \sum_{i=1}^{l} \frac{|c_i||T^*_i - \bar{T}_i|}{|\Omega|}, \quad E_{\infty}(T) = \max_{i=1}^{l} |T^*_i - \bar{T}_i|,$$

where $T_i$ is the exact mean value of $T$ over cell $c_i$. The first norm gives the average evaluation of the error in all the domain, while the second norm indicates the highest local error. These error estimators can also be applied to the values interpolated on the vertices of the mesh. To study the convergence order, successive finer unstructured triangular Delaunay meshes were considered. The convergence order between two different meshes $T_1$ and $T_2$ with $I_1$ and $I_2$ cells, respectively, is computed by

$$O(T_1, T_2) = 2 \frac{\log(|E(T_1)/E(T_2)|)}{|\log(I_1/I_2)|}.$$

4.1 Convection–diffusion problem

We deal with the full convection diffusion process and assess the capability of the scheme to compute an accurate solution for low and large Pe. Assuming constant diffusion coefficient, $k = 1$, and velocity, $V = (u, v)$, the Péclet number is given by $Pe = \frac{|V|}{k} L$ with $L$ the characteristic length of the domain (here $L = 1$) and $|V|$ the velocity norm. We consider a solution of the form $T(x, y) = C \alpha(x) \beta(y)$, $C \in \mathbb{R}$, with

$$\alpha(x) = \frac{1}{u} \left( x - \frac{e^{ux} - 1}{e^x - 1} \right), \quad \beta(y) = \frac{1}{v} \left( y - \frac{e^{vy} - 1}{e^y - 1} \right)$$

with homogeneous Dirichlet boundary condition, while the source term is written as $f(x, y) = C(\alpha(x) + \beta(y))$. We take $V = (3, 3)$ for the low Pe = 4.24 number case, and $V = (10, 10)$ for the large Pe = 14.14 case. $C$ is calculated in such a way that the solution is normalized, that is, $C = 80$ for low Pe (Fig. 7-left), and $C = 223$ for large Pe (Fig. 7-right). Table 1 shows the errors and convergence rates for the low and large Pe, respectively. The results obtained show that second-order convergence for different Pe is obtained. No oscillations are reported while the maximum principle is preserved, i.e. the solution ranges between 0 and 1, which highlight the robustness of the method.

4.2 Discontinuous solution at the interface

This section is dedicated to the critical part of the problem. Discontinuities of material properties or discontinuity of the solution require a specific treatment to preserve the optimal order. Such a point is crucial since a degradation of the flux evaluation across the interface $\Gamma$ leads to a rough evaluation of the heat transfer coefficient at this location. We present several numerical tests to prove that the new

Fig. 7 Computed temperature fields corresponding to low (left) and high (right) Pe
proposed technique correctly handles such discontinuities and provides accurate approximations.

### 4.2.1 Pure diffusive case

We consider two domains \( \Omega_1 = ]0, 1[ \times ]0, \frac{1}{2} [ \) and \( \Omega_2 = ]0, 1[ \times ]\frac{1}{2}, 1[ \) which share a common interface \( \Lambda = ]0, 1[ \times \{ \frac{1}{2} \} \) where a linear heat transfer condition is prescribed

\[
k_1 \nabla T_1 \cdot n_\Lambda = k_2 \nabla T_2 \cdot n_\Lambda = h(T_2 - T_1)
\]

with \( k_1 \) and \( k_2 \) being the constant diffusion coefficients. We first tackle the case where the convective contribution is null for both domains, an adiabatic boundary condition \( k\nabla T \cdot n = 0 \) is assumed on the lateral side, while constant Dirichlet conditions \( T = T_1 \) on \( y = 0 \) and \( T = T_2 \) on \( y = 1 \) were set. The exact solution is composed by two functions,

\[
T_1(x, y) = \frac{A}{k_1} \left( \frac{1}{\pi} \right)^2 \sin(\pi y) + \frac{a}{k_1} + T_1
\]

and

\[
T_2(x, y) = \frac{A}{k_2} \left( \frac{1}{\pi} \right)^2 \sin(\pi y) + \frac{a}{k_2} (y - 1) + T_2,
\]

with

\[
a = \frac{h}{1 + \frac{h}{2k_1} + \frac{h}{2k_2}} \left( \frac{A}{\pi} \right)^2 \left( \frac{1}{k_2} - \frac{1}{k_1} \right) + T_2 - T_1
\]

with \( A \) being a free parameter associated to the source term \( f(x, y) = A \sin(\pi y) \).

The simulations for this case study were carried out with \( A = 10, k_1 = 1, k_2 = 0.1, T_1 = 1, T_2 = 10, \) and \( h = 1 \). The solution is displayed in Fig. 8, left panel, and the errors and convergence rates are presented in Table 2. Again the results indicate an effective second order of convergence.

### 4.2.2 Convection–diffusion case

For this problem both velocity and diffusion coefficients are discontinuous across the interface \( \Lambda \), where the continuity of normal velocity is required for sake of conservativeness. In the present test, null velocity is set in domain \( \Omega_2 \), and a constant velocity \( V_1 = (u, 0) \) is used in domain \( \Omega_1 \). In this case, the exact solution is given by

\[
T_1(x, y) = A_1 e^{\frac{\pi^2}{h_1^2} y} + a_1 y + T_1,
\]

and

\[
T_2(x, y) = e^{\frac{\pi^2}{h_2^2} y} \left[ A_2 (y - 1) + B_2 (y - 1)^2 \right] + a_2 (y - 1) + T_2.
\]

While the conservation of the flux at the interface yields

\[
k_1 A_1 = k_2 A_2 - k_2 B_2, \quad k_1 a_1 = k_2 a_2,
\]

and the linear heat transfer condition (30) on \( \Lambda \) provides

\[
4k_1 A_1 = h(B_2 - 2(A_1 + A_2)),
\]

and

\[
2k_1 a_1 = h(2(T_2 - T_1) - (a_1 + a_2)).
\]

After some algebraic manipulation, we get

### Table 1 Errors and convergence rates for low and high Pe

| | Cells | Vertices |
|---|---|---|
| | \( E_1 \) | \( O_1 \) | \( E_\infty \) | \( O_\infty \) | \( E_1 \) | \( O_1 \) | \( E_\infty \) | \( O_\infty \) |
| Low | 1054 | 5.30e–04 | NA | 3.82e–03 | NA | 1.93e–03 | NA | 6.62e–03 | NA |
| | 4262 | 1.43e–04 | 1.88 | 1.14e–03 | 1.73 | 4.65e–04 | 2.03 | 1.53e–03 | 2.10 |
| | 16778 | 3.69e–05 | 1.98 | 3.19e–04 | 1.86 | 1.18e–04 | 2.00 | 4.18e–04 | 1.89 |
| | 67862 | 9.27e–06 | 1.98 | 8.83e–05 | 1.84 | 2.90e–05 | 2.01 | 1.10e–04 | 1.91 |

### Table 2 Errors and convergence rates for heat transfer problem with discontinuous solution (pure diffusive case)

| | Cells | Vertices |
|---|---|---|
| | \( E_1 \) | \( O_1 \) | \( E_\infty \) | \( O_\infty \) | \( E_1 \) | \( O_1 \) | \( E_\infty \) | \( O_\infty \) |
| 1014 | 6.83e–03 | NA | 2.80e–02 | NA | 1.23e–02 | NA | 7.01e–02 | NA |
| 4126 | 1.24e–03 | 2.43 | 6.58e–03 | 2.07 | 2.72e–03 | 2.15 | 2.14e–02 | 1.69 |
| 17020 | 3.29e–04 | 1.88 | 1.81e–03 | 1.83 | 6.87e–04 | 1.94 | 1.14e–02 | 0.89 |
| 67620 | 8.55e–05 | 1.95 | 5.08e–04 | 1.84 | 1.79e–04 | 1.95 | 2.85e–03 | 2.01 |
where $A_1$ is a free parameter which can be defined arbitrarily. From this exact solution, we derive the source term $f_1(x,y) = 0$, $f_2(x,y) = -k_2e^{\frac{u}{k_1}}x \left[ 2B_2 + \left( \frac{u}{k_1} \right)^2 (y-1)(A_2 + B_2(y-1)) \right].$

(34)

Dirichlet condition is prescribed on the boundary using the exact solution. Simulations are carried out with parameters $A_1 = 1$, $k_1 = 0.18$, $k_2 = 23$, $u = 1$, $T_1 = 1$, $T_2 = 10$, and $h = 1$ and the associated solution is displayed in Fig. 8, right panel. Table 3 shows that we obtain once more an effective second-order convergence. As in the previous case, no oscillations are reported even in the vicinity of $\hat{W}$, which demonstrates the capability of the scheme to handle such field discontinuities.

### Table 3 Errors and convergence rates for the heat transfer problem with discontinuous solutions (convection–diffusion case)

| I | Cells $E_1$ | Vertices $E_1$ | $O_1$ | $E_\infty$ | Vertices $O_\infty$ |
|---|---|---|---|---|---|
| 1014 | 1.38e−01 | 8.65e−02 | 1.08e+00 | 1.46e+00 |
| 4126 | 3.10e−02 | 2.13 | 3.28e−01 | 1.70 |
| 17026 | 7.37e−03 | 4.91e−03 | 2.07 | 1.56e−01 | 3.37 |
| 67718 | 1.88e−03 | 1.26e−03 | 1.97 | 4.41e−02 | 1.83 |

5 Application to the polymer/calibrator heat transfer

The study case consists in a polymer tape cooled by a unique calibrator. Figure 9 displays the quadrangular mesh geometry, while $N_{tp}$, $N_{tc}$, and $N_{th}$ denote the number of elements on polymer and calibrator on $x_2$ direction and the number of elements on $x_1$ direction on calibrator, respectively.

The dimensions of the setup are given, according to Fig. 4, by $L_{in} = 0.17$ m, $L_{c} = 0.3$ m, $L_{out} = 0.13$ m, $t_{p} = 1.45 \times 10^{-3}$ m, and $t_{c} = 0.012$ m (see Fig. 9). We followed the setup developed in [6] to obtain the experimental data.

Numerical simulations are carried out with $k_{p} = 0.17$ W/(m K), $k_{c} = 123$ W/(m K), $\rho_{p} = 1040$ kg/m$^3$, $c_{p_{p}} = 2050$ J/(kg K), $U_{p} = (0.0175, 0)$ m/s, $U_{c} = (0, 0)$ m/s, $h_{air} = 50$ W/(m$^2$K), $T_{air} = 18^\circ$ C, and $T_{in} = 229.5^\circ$ C. The temperature distribution on $\Gamma_{sup}$ was approximated by a polynomial function deriving from the temperature measured by seven thermocouples uniformly distributed at the top calibrator surface. The polynomial approximation is plotted in Fig. 10 along with the experimental data, and is given by the analytical expression.

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Fig. 8 Exact solution for the heat transfer problem with discontinuous temperature at the interface. Pure diffusive case (left) and convection diffusion case (right)
5.1 Mesh analysis

To provide an accurate approximation with low computational time, several tests were performed with different kinds of mesh to assess the accuracy of the approximation with respect to mesh parameters. All the experiences were carried out with $h_{\text{int}} = 500 \text{ m/sW/(m}^2\text{K)}$. We assess the accuracy by plotting the temperature distribution along the polymer tape upper surface, since it corresponds to the critical location where the heat transfer takes place.

We report in Fig. 11 the curves obtained with three different meshes to assess the impact of the mesh cell number following the $x_1$ direction. We note small differences at the inlet and the outlet of the calibrator and observe the convergence in mesh as $N_h$ increases.

We also analyse the accuracy with respect to the number of cells following the $x_2$ direction in the polymer. Figure 12 shows that the approximations converge to a limit.

$$T_{\text{sup}} = 26399x_1^5 - 29434x_1^4 + 11403x_1^3 - 1848.9x_1^2 + 100.99x_1 + 39.581 \text{ on } \Gamma_{\text{sup}}. \quad (35)$$

5.2 Optimization

We have developed a numerical tool to identify the heat transfer coefficient value at the interface ($h_{\text{int}}$) that promotes the best fitting of the experimental measurements.

The impact of the cell number on the $x_2$ direction of the calibrator was also considered and the results are shown on Fig. 13. We conclude that this last parameter has a small influence on the temperature distribution hence a coarse mesh can be used for the calibrator.
To do so, we consider the function \( h \rightarrow T^h \) where we substitute Eq. (2) by

\[
k_c \frac{\partial T^h}{\partial n_c} = -k_p \frac{\partial T}{\partial n_p} = h(T_p^h - T_c^h).
\]

To compute an approximation of \( h_{\text{int}} \), the least squares method is carried out where the optimal solution is found through the minimization of functional

\[
F(h) = \sum_{\ell} \frac{1}{2} \left[ T_p^h(q_\ell) - T_{p\ell} \right]^2.
\]

Here, \( T_p^h(q_\ell) \) stands for the temperature of the polymer located at \( q_\ell \), obtained by the numerical simulation, while \( T_{p\ell} \) is the temperature of the polymer measured experimentally at the same point.

The nonlinear problem is solved with the Newton-Raphson iterative method where the condition \( \frac{\partial F}{\partial h} = 0 \) should be verified. Hence the updated value for heat transfer coefficient is calculated as follows

\[
h^{n+1} = h^n - \frac{F'(h^n)}{F''(h^n)},
\]

using the following approximations for the first and second derivatives

\[
F'(h^n) \approx \frac{F(h^n + \varepsilon) - F(h^n - \varepsilon)}{2\varepsilon}, \quad \text{and} \quad F''(h^n) \approx \frac{F(h^n + \varepsilon) + F(h^n - \varepsilon) - 2F(h^n)}{\varepsilon^2},
\]

with \( \varepsilon > 0 \) being a small parameter with respect to \( h^n \).

A determination of the heat transfer coefficient has been performed using the temperature measured on the polymer surface downstream the contact interface (calibrator outlet). The Newton-Raphson method converges in few steps and gives \( h_{\text{int}} = 390.5 \text{ W/(m}^2\text{K)} \), while temperature at the upper side of the tape is plotted in Fig. 14.

Table 4 presents the temperature measured experimentally (the input data in the optimization process) and the associated approximation obtained from the numeric approximation. We observe that the approximation fits very well with the experimental data since the difference between both temperatures presents a small relative deviation. Moreover, as also shown in Table 4, if perfect contact boundary condition was considered at the polymer calibrator interface, there would be a significant difference between the measurement and the numerical predictions. In this case, as expected, the numerical code would anticipate a more effective cooling and, thus, lower temperatures.

### 5.3 Sensitivity Studies

Measurements suffer of small deviations depending on the sensors quality leading to small errors. Consequently, the sensitivity analysis with respect to some input parameters is important to assess the impact of the sensor deviation on the heat transfer coefficient evaluation. Parameters were divided into two groups, namely: (1) the parameters that have a direct influence on the energy of the system, such as the polymer velocity and inlet temperature, \( u \) and \( T_{\text{in}} \), respectively; (2) the parameters which deals with the environmental conditions such as the natural convection heat transfer coefficient of the air and the room temperature, \( h_{\text{air}} \) and \( T_{\text{air}} \), respectively.

### Table 4 Comparison between the temperature from experimental measurements and the numeric approximation (considering polymer-calibrator contact resistance)

| Coordinate (m) | Experimental \( ^\circ\text{C} \) | Numerical contact resistance \( ^\circ\text{C} \) | Error (%) | Numerical perfect contact \( ^\circ\text{C} \) |
|---------------|------------------|-------------------|-------|-------------------|
| 0.485         | 58.5             | 58.7               | 0.27  | 42.0               |
| 0.527         | 59.6             | 59.6               | 0.30  | 43.5               |

Last column: temperatures predicted considering perfect contact...
5.3.1 Direct parameters

The influence of small variations of velocity and input temperature on the computed heat transfer coefficient is displayed in Figs. 15 and 16. We observe that the velocity of the polymer has a huge influence on the heat transfer evaluation with a nonlinear dependence. On the other hand, variations of the input temperature results into a linear variation of the heat transfer coefficient. The two figures provide the information to quantify the deviation of the coefficient with respect to the error measurements. For example assuming that the real velocity is $u = 1.8$ and that we measure $u_m = 1.85$, i.e. a 2.7% of relative deviation, we deduce from Fig. 15 a 4.7% relative deviation for the heat transfer coefficient.

5.3.2 Indirect parameters

Equations (4) and (5) introduce convection heat transfer with the calibrator and the polymer characterized by two different coefficients, namely $h_{\text{air},c}$ and $h_{\text{air},p}$. Figure 17 shows that the convection heat transfer coefficient for the calibrator has no significant impact on the temperature distribution, hence $h_{\text{int}}$ remains almost constant. The convection coefficient for the polymer produces, on the contrary, significant variations on the computed heat transfer coefficient at the interface which means that the environmental condition strongly affects the cooling process and should be controlled to provide reliable results.

The room temperature influence on the heat transfer coefficient at the interface is indicated in Fig. 18. Room temperature parameter provide an affine relation and we observe significant impact on $h_{\text{int}}$. A variation from 12 °C
(morning) to 20 °C (afternoon) generates a 15% relative deviation of the \( h_{\text{int}} \) evaluation, far away from the disturbances created by the sensors deviations.

6 Conclusion

We have presented a new second-order finite volume method for the heat transfer problem involving discontinuous solution and discontinuous material properties. The scheme is based in a cell-to-vertex reconstruction, being the vertex values computed via linear combinations of the closest cell values where the coefficients are determined by a functional minimization. The verification tests performed demonstrated the robustness and the accuracy of the procedure. Based on the solver, an optimization algorithm has been developed to compute the heat transfer coefficient at the interface between the calibrator and the polymer. Influence of the input data such as the velocity, the energy transfer to air, and the environmental temperature has also been assessed to highlight the most significant parameters.

Acknowledgements This research was financed by FEDER Funds through Programa Operacional Factores de Competitividade — COMPETE and by Portuguese Funds through FCT — Fundação para a Ciência e a Tecnologia, within the Projects PEst-OE/MAT/UI0013/2014, PTDC/MAT/121185/2010, and UID/CTM/50025/2013. The second author was also financed by project FCT-ANR/MAT-NAN/0122/2012.

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