This paper describes the application of the Radial Functions Method to model and simulate polymer processing. The coupled system of energy and motion equations for laminar two-dimensional flows in steady state of incompressible non-Newtonian fluids is considered. The results delivered by RFM are compared with numerical results of other methods, and with analytical solutions based on simplified mathematical models. The cases presented are: non-isothermal pressure flow through a slit for non-Newtonian fluids, non-isothermal power law flow in the calendering process and non-isothermal disc flow.

Introduction

Mathematical modeling attempts to mimic the actual process with equations by means of material, energy and momentum balances, along with a series of assumptions that simplify the model. The more complex the mathematical model, the more accurately it represents the actual solution. Eventually, the complexity is so high that we must resort to numerical simulation to model the process.

For the particular case of polymer flows, the modeling results in highly non-linear partial differential equations due to the non-Newtonian and viscoelastic behavior of polymers. Additionally, in many processes, energy and motion equations are strongly coupled, due to high Brinkman ($Br$) and Péclet ($Pe$) numbers, obtaining models that are difficult to solve.

Numerical solutions for the partial differential equations that describe polymer flows have been studied by means of four widely known methods: Finite Differences (FDM), Finite Volumes (FVM), Finite Elements (FEM) and Boundary Elements (BEM). However, these methods have not been completely satisfactory to solve polymer processing models, requiring the exploration of other alternatives.

In the last 15 years, meshless methods based on radial basis functions have attracted attention to solve PDEs. In the beginning, the radial basis functions were developed to interpolate multivariate data and multidimensional problems. In 1990, Kansa [12] proposed the use of RBFs for the solution of partial differential equations. An unsymmetrical coefficients matrix is obtained when this method is applied. The computational implementation of Kansa’s method is rather straightforward due to the simple structure of the RBF formulation, making it useful not only to mathematicians, but to other users as well [26]. Mai-Due and Tanner [18] used the technique to model non-Newtonian fluid flow or shear thinning and viscoelastic liquids.

The main advantage of the radial functions method (RFM) is that it is a technique that does not need domain nor boundary meshes as required with FEM and BEM, or homogeneous grid points as FDM, to solve partial differential equations. Essentially, it is a meshless technique based on collocation methods. The method has proven to be very accurate compared to other numerical techniques, even for a small number of collocation points [12].

The Radial Functions Method

Collocation techniques are based on the fact that a field variable in a continuous space can be approximated with linear interpolation coefficients and basis functions evaluated on discrete points sprinkled within the domain. In this way, if some values of the field are known, any value at any point of the domain can be estimated [5]. The basis functions of Kansa’s method are the radial basis functions (RBF) [20, 3, 12, 13]. The formulation is:

$$ F(x_i, y_i) = \sum_{j=1}^{N} \phi(r_j) \alpha_j $$

(1)
where \( r_{ij} \) is the distance between the nodes \( i \) and \( j \), \( N \) represents the number of collocation points and \( \phi(r_{ij}) \) is the radial basis function. If we apply a differential operator \( L \) on eq. (1) we can interpolate the solution for the operated field:

\[
L\{F(x_i, y_i)\} = \sum_{j=1}^{N} L\{\phi(r_{ij})\} \alpha_j \tag{2}
\]

In this way, operated fields can be interpolated allowing the solution of partial differential equations (PDEs), and hence problems that are modeled by means of PDEs\([7, 8, 22, 5, 26, 16]\).

There are many types of radial basis functions of global support that can be used, such as Polyharmonic Spline (SP), Polyharmonic Thin - Plate Spline (TPS), Multiquadrics (MQ), Wedlands, Gaussian and others \([2, 3, 20]\). Franke \([11]\) evaluated some radial basis functions from the interpolation accuracy point of view, finding the best results using the Polyharmonic Thin - Plate Spline (TPS). TPS is given by:

\[
\phi(r_{ij}) = r_{ij}^{2a} \ln(r_{ij}) \tag{3}
\]

When solving the energy and motion equations that define a polymer flow, four different primary state variables must be simultaneously solved for: temperature, pressure and the two components of velocity, as shown respectively in (4), (5), (6) and (7).

\[
T_i = \sum_{j=1}^{N} \phi_T(r_{ij}) \alpha_j \tag{4}
\]

\[
p_i = \sum_{j=1}^{N} \phi_p(r_{ij}) \beta_j \tag{5}
\]

\[
u_x = \sum_{j=1}^{N} \phi_u(r_{ij}) \lambda_j \tag{6}
\]

\[
\nu_y = \sum_{j=1}^{N} \phi_u(r_{ij}) \xi_j \tag{7}
\]

Additionally, the radial basis functions can be used to estimate the derivatives of properties that are a function of the primary variables. In this particular case, the viscosity field depends on the temperature and the deformation rate, therefore, we can write:

\[
\eta(x_i, y_i) = \eta_i \approx \sum_{j=1}^{N} \phi_{\eta}(r_{ij}) \delta_j \tag{8}
\]

\[
\frac{\partial \eta_i}{\partial x} \approx \sum_{j=1}^{N} \frac{\partial \phi_{\eta}(r_{ij})}{\partial x} \delta_j \tag{9}
\]

\[
\frac{\partial \eta_i}{\partial y} \approx \sum_{j=1}^{N} \frac{\partial \phi_{\eta}(r_{ij})}{\partial y} \delta_j \tag{10}
\]

In the above equations \( \phi_p, \phi_T, \phi_u, \phi_{\eta} \) are the radial basis functions to interpolate unknown fields, that may not be the same with the aim of better accuracy. This depends on the differential operators involved in the governing equations \([6]\). \( \alpha, \beta, \lambda, \xi, \delta \) are the interpolation coefficients for temperature, pressure, x-component of velocity, y-component of velocity and viscosity, respectively. Finally, \( N \) is the number of points on the boundary and within the domain and \( Np \) is the number of points within the domain and on the Dirichlet pressure boundaries.

The energy and motion equations have nonlinear terms. Their representation by means of RBF, allows their linearization in such a way that the resulting system of equations can be solved using any method for the solution of linear systems for each step in an iterative process.
Results and Discussion

**Rheological models**

The Newtonian, eq.(11), Power Law, eq.(12) and Carreau, eq.(13) models are used to represent the fluid viscosity in the simulations.

\[
\eta = a_T \eta_0 \quad (11)
\]

\[
\eta = (a_T)^n m \dot{\gamma}^{n-1} \quad (12)
\]

\[
\eta = \frac{a_T A}{(1 + B a_T \dot{\gamma})^c} \quad (13)
\]

The Arrhenius model is used to calculate the temperature shift factor:

\[
a_T = e^{\frac{U}{R} \left( \frac{1}{T} - \frac{1}{T_{ref}} \right)} \quad (14)
\]

**Non-isothermal pressure flow between parallel plates of Newtonian and non-Newtonian fluids**

In many flows in polymer processing, viscous dissipation is significant \((Br > 1)\), with a resulting temperature rise that affects the flow through a temperature dependent viscosity. To simulate this phenomenon, the coupled motion and energy equations of a slit flow were solved, considering the heat generation for viscous dissipation within a domain of size \(0.015 \text{m} \times 0.015 \text{m}\). In Fig.1 the geometry and the location of the coordinate system are illustrated. For the simulation, two different types of node distributions were used: a triangular distribution and a random distribution, both with 740 nodes, as depicted in Fig.2. The random distribution is actually a semi-random distribution because a minimal distance between nodes is imposed in order to avoid linear dependences between the equations of very close nodes, and to guarantee a good distribution over the whole domain. For this particular case, the minimum distance between nodes is \(2.8 \times 10^{-4} \text{m}\).

Non-slip boundary conditions are assumed in the walls. The flow is considered completely developed and the pressure difference between the outflow and inflow boundaries is 105000 Pa. The temperature of the plates is 200 °C.

The solution was obtained using a second-order TPS to interpolate the pressure and temperature fields, and a third-order TPS to interpolate the velocity field. To compare the results, a solution using the FDM is formulated. The FDM solution is considered as the reference, because it uses a one-dimensional formulation and a high number of nodes to approach the solution (10000 nodes).

The thermal conductivity of the polymer is \(k = 0.280 \text{ W/m-K}\). For the rheology, four different cases are considered:

**CASE 1:** \(\eta = \mu\). The value of the viscosity is assumed equal to a constant, in this case \(\eta = 2859.4 \text{ Pa-s}\).

**CASE 2:** \(\eta = f(T)\). The viscosity has a Newtonian behavior and the temperature dependence is described by the Arrhenius equation, eq.(14), with \(U = 42048.3 \text{ J/mol}\), \(\mu_0 = 2859.4 \text{ Pa-s}\) and \(T_{ref} = 493 \text{ K}\).

**CASE 3:** \(\eta = f(\dot{\gamma})\). The viscosity presents non-Newtonian behavior, which is represented by means of the Carreau model, eq.(13), with: \(A = 2859.4 \text{ Pa-s}\), \(B = 0.077 \text{ s}\) and \(c = 1 - n = 0.661\).

**CASE 4:** \(\eta = f(\dot{\gamma},T)\). The viscosity depends on temperature and rate of deformation. The shear thinning behavior is modeled by means of the Carreau equation and the temperature shift factor is estimated using the Arrhenius model. The parameters are the same as in cases 2 and 3.

The results of the velocity fields and the temperature fields for the different cases are presented in Figs. 3 and 4. The solutions of FDM and RFM are very similar, indicating that RFM gives a correct approach to the solution of non-isothermal flow, obtaining the biggest difference when the viscosity is a function of both temperature and rate of deformation. The arranged and random distributions delivered good results, indicating that the random distribution is feasible as long as a minimum distance between nodes is kept.

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Calendering process for Newtonian and shear thinning polymer melts

In the calendering process, variables such as the final thickness of the sheet and the force exerted by the melt on the rolls are important to calculate. Solutions using lubrication approximation have been proposed with good results for isothermal Newtonian and power-law flows. However, for more accurate solutions and in order to consider viscous heating, numerical approaches are required.

This problem is an excellent example of application of RFM in polymer processing compared with traditional numerical methods. The complexity of the geometry makes a Finite Difference implementation difficult. The high ratio between the bank size or fed-sheet thickness and the nip between rolls makes the generation of an acceptable FEM difficult. The convective transport of energy during calendering requires upwinding techniques for the solution using FEM and FDM. The non-linear behavior of viscosity makes the implementation of a boundary elements solution difficult since it requires a mesh. RFM is a good alternative because it does not require meshes nor upwinding techniques and it works well with highly non-linear problems.

To compare with lubrication approximation, the same dimensions and process conditions used by Agassant et al. [1], schematically depicted in Fig. 5 are considered. The problem was solved for a power law fluid with a consistency index, \( K \), of \( 10^6 \) Pa-s\(^2\) and several power law indices, \( n \), of 0.7, 0.5 and 0.3. A nip ratio, \( h_r/h_b \), of 50 was considered. The boundary conditions are given by the velocity on the roll surfaces, a zero pressure at the entrance and exit surfaces as well as a zero normal stress at the entrance surface given by \( \partial u/\partial n = 0 \). This boundary condition is imposed by setting the velocity of the first two collocation points of each row equal to each other. Furthermore, this problem must be manually iterated, since the final sheet thickness is not known a priori. Hence, a sheet separation and thickness is assumed for the first solution. This results in a pressure field with unrealistic oscillations close to the end of the sheet indicating that the guessed sheet separation point does not coincide with the actual one. After the first solution, the separation point is moved looking for the reduction of the oscillation. After some iterations the correct sheet thickness and separation point are achieved, along with a smooth pressure distribution. The pressure distribution along the \( x \) -axis for the shear thinning melt is presented in Fig. 6 for various power law indices and in Fig. 7 for a power law index of 0.3. Again, the RFM results were compared to solutions using lubrication approximation. As can be seen, the agreement is excellent. The FEM results presented by Agassant [1] are also in agreement with the RFM. The FEM results predict a slightly higher pressure than the lubrication approximation prediction, whereas the RFM pressure predictions are slightly lower.

Finally, the non-isothermal case is considered. The same collocation points and geometry for a bank-to-nip ratio, \( h_r/h_b \), of 50 were used to solve for velocity, temperature and pressure distributions for non-Newtonian shear thinning polymer melts, including viscous dissipation and considering the viscosity as a function of temperature. A power law model with a consistency index, \( K \), of \( 10^6 \) Pa-s\(^2\) and a power law index, \( n \), of 0.5 was used. The temperature-viscosity dependence was modeled using Arrhenius equation, eq.(14) with \( U = 4000 \) J/mol and \( T_{ref} = 473 \) K. The convective term as well as the heat generated by viscous dissipation are considered for the solution of the energy equation. Fig. 8 depicts the temperature field delivered by RFM for the non-isothermal case. Due to viscous heating, the temperature increases 5.5K in the region of the nip. The increase of heat reduces the viscosity magnitude and therefore, decreases the pressure. Figure 9 presents a comparison between the non-isothermal and isothermal solutions for pressure distribution along the \( x \) -axis. The effect of viscous heating on the solution can not be represented using the lubrication approximation for cases where the viscosity is considered as a function of temperature.

Non-isothermal disc flow (injection molding)

In injection molding, the lubrication approximation is widely used due to the high aspect ratio between the lengths of injected parts and their thicknesses. However, when a deeper study of the flow and the changes of variables across the thickness is required, that kind of approximation is no longer useful, and the complete geometry must be considered. The high aspect ratio of injection parts makes the creation of good meshes difficult, which is an important obstacle to get a solution using a mesh dependent method such as Finite Elements. Lopez-Gomez and Osswald [17] developed an approach to simulate high aspect geometries using the Radial Basis Function Method by means of different scale factors for the different coordinates. In the present work the same approach was used to simulate the non-isothermal disc flow.

For the simulation the axis-symmetrical system composed of the sprue and the disc is considered. The radius of the sprue is 4 mm and its length 5.68 cm. The thickness of the disc is 2 mm and its radius 8.2 cm. The Carreau model eq.(13), was used to calculate the viscosity (PA66) with: \( A = 892.7 \) Pa-s, \( B = 0.002 \) s and \( c = 1 - n = 0.71 \). The
temperature shift factor is estimated using the Arrhenius model eq.(14) with $U = 98025 \text{ J/mol}$ and $T_{ref} = 593 \text{ K}$. The flow is assumed in steady state. The wall temperature is 280 °C and the pressure difference 19Mpa.

In this simulation we are interested in the temperature behavior of the melt that is affected by the combined effect of viscous heating and convective transport. The solution for the temperature field is presented in Fig.10. The melt temperature increases 11 °C due to viscous dissipation. The temperature rise is critical in the disc gate. The temperature is not uniform across the disc thickness leading unsymmetrical behavior of the flow in the disc because the fluid is faster on the left side where the polymer temperature is higher.

**Figures**

![Geometry of the pressure flow between parallel plates](image1)

**Figure 1:** Geometry of the pressure flow between parallel plates

![Distribution of nodes for pressure flow between parallel plates](image2)

**Figure 2:** Distribution of nodes for pressure flow between parallel plates
Figure 3: Velocity field for a non-isothermal pressure flow between parallel plates for Newtonian and non-Newtonian fluids

Figure 4: Temperature field for a non-isothermal pressure flow between parallel plates for Newtonian and non-Newtonian fluids

Figure 5: Schematic diagram of a calendering process fed with a finite sheet.
Figure 6: Comparison of lubrication approximation solution and RFM solution of the pressure profiles between the rolls for a bank-to-nip ratio of 10, and several power law indices using power law viscosity model.

Figure 7: Comparison of lubrication approximation solution and RFM solution of the pressure profile between the rolls using a power law viscosity model with a power law index, $n$, of 0.3.

Figure 8: RFM temperature profile between the rolls using a power law viscosity model with a power law index, $n$, of 0.5, considering viscous heating.
Figure 9: Comparison of non-isothermal and isothermal RFM solutions of the pressure profile between the rolls using a power law viscosity model with a power law index of 0.5.

Figure 10: Temperature field in a disc-sprue system

Conclusion

The results of this work allow us to consider RFM as a promising technique to solve polymer processing problems. The Radial Functions Method can solve adequately non-isothermal, Non-Newtonian flows, including the phenomenon of
heating by viscous dissipation and the convective transport of energy. Those characteristics are common in polymeric flows which involve highly non-linear behavior and strong dependence between energy and momentum balances. RFM has the advantage of being relatively easy to implement, because it allows formulating the governing equations in terms of the primitive variables making the computational model more understandable. It does not require the generation of meshes or grids and can use random distribution of nodes as long as a minimum distance between nodes is kept. The method has proven to be stable for highly non-linear problems. The implementation is the same independently of the number of dimensions of the problem, due to the fact that it is only based on the distance between nodes. The interpolation and extrapolation of fields can be done with the same coefficients delivered by the solution of the PDEs, yielding easier post-processing steps.

The biggest disadvantage of the method is that it solves PDEs with full unsymmetric matrices requiring high computing resources. Several alternatives have been developed to improve this limitation, such as the symmetric formulation [22, 8, 16], the use of subdomains [29], the use of compact support radial basis functions [24] and the use of special distribution of nodes that generates matrices that are easy to simplify [15].

References


[16] Larsson, E., and Fonberg, B. A numerical study of some RBFs based solution methods for elliptics PDEs.


