Modeling of a Multilayered Propellant Extrusion in Concentric Cylinders

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Abstract: A novel propellant technology of interest involves in simultaneously extruding two formulations to form a multilayered propellant stick configuration. This propellant is processed into a concentric cylinder configuration, in the form of slow-fast-slow burning rate layers with a single perforation. The material flows through different path lengths between the inner and outer sections of the die, both coming from the same pressurized inlet. This study optimizes the die design to enable a wide range of materials, while keeping balanced flow conditions for each layer. The model recalls to the Computational Fluid Dynamics (CFD) Module and Heat Transfer Module to study the non-isothermal steady state flow of non-Newtonian fluids, including viscous heating and heat transfer. The simulations shed light on the interaction between the power law index “n” and the viscous heating in the die design.

Keywords: Coextrusion, multilayer, Fluid, thermal, shear-thinning

1. Introduction

To establish the criteria that render possible the extrusion of multilayered propellants in concentric cylinders, this study optimized a die design that enables the widest possible range of material rheology while keeping the flow balanced. The main challenge originated from the different path lengths between the inner and outer sections of the die, both coming from the same pressure driven flow as shown in Figure 1.

The mid section of the geometry is filled with a low viscosity fluid whose flow rate can easily be set to match the flow in the other adjacent sections. This study uses COMSOL Multiphysics® simulations for extrusion die optimization. It recalls to the CFD Module (Computational Fluid Dynamics) and Heat Transfer Module to study the non-isothermal steady state flow behavior, including viscous heating and heat transfer between each layer of extruded materials.

2. Die optimization using COMSOL Multiphysics®

Several die geometry configurations have been studied where key angles and internal channel dimensions have been optimized to balance the flow. The non-isothermal steady state flow behavior, including viscous heating and heat transfer between each layer of extruded materials, has been predicted by COMSOL™ using the CFD and the Heat Transfer modules with user specified fluid properties, as determined from experimental measurements.

The viscosities were expressed as a function of temperature and shear rate with a classical power-law model where the shear thinning index "n" is a characteristic property of the fluid. Satisfactory description of the flow geometries...
were obtained with approximately 500,000 tetrahedral elements.

2.1 Governing equations of viscosity:

Power law:

\[ \eta(\dot{\gamma}) = k\dot{\gamma}^{n-1} \]  

(1)

Power law with Arrhenius to express viscosity as a function of temperature:

\[ \eta(T) = \eta_0 \exp \left[ \frac{E}{R \left( \frac{1}{T} - \frac{1}{T_0} \right)} \right] \]  

(2)

2.2 Boundary conditions:

- No-slip boundary condition was considered on every internal surface as determined during the rheological characterization;
- For inlets, laminar flow conditions with constant flow rates and temperature was described for both soft and hard materials;
- Heat exchange was allowed between the fluid and the die as well as between dies and ambient environment.

3. Experimental results

3.1 Mid layer simulations

The first step of the flow optimization was to balance the flow of the mid-layer represented on Figure 1. Figure 2 shows the channel flow pattern for the middle section.

![Figure 2: Flow path of the mid section and element distribution.](image)

The flow balance has been realized using smaller channel sizes near the main feed channel as shown on Figure 3.

![Figure 3: Flow velocity profile (mm/s) pattern in the mid section of the die.](image)

3.2 Isothermal simulations

The second step of flow optimization aimed at stabilizing the geometry to accept the wide range of propellant material properties, while maintaining a balanced flow of the external and internal layer. The flow of the external layer was intentionally faster than the internal layer to maintain the integrity of the extrudate and anticipate the higher viscous heating of the inner section. Figure 5 shows the velocity profile for

![Figure 4: cut section of the optimized flow velocity profile (mm/s) in the top annular distribution and channels.](image)

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various power law index, \( n \) of the highly viscous material while figure 6 shows an example of this profile on a 2D graph:

**Figure 5:** Flow profile of the highly viscous material (mm/s).

![Flow profile of the highly viscous material (mm/s).](image)

**Figure 6:** 2D velocity profile example (mm/s) in the developed region of the outer section of the die as a function of the power law’s ‘\( n \)’ value.

![2D velocity profile example (mm/s).](image)

![Un-optimized die balance: internal (light) vs. external (dark) average velocity at the die exit as a function of the power law’s ‘\( n \)’ value.](image)

**Figure 7:** Un-optimized die balance: internal (light) vs. external (dark) average velocity at the die exit as a function of the power law’s ‘\( n \)’ value.

![Optimized die balance: internal (light) vs. external (dark) average velocity at the die exit as a function of the power law’s ‘\( n \)’ value.](image)

**Figure 8:** Optimized die balance: internal (light) vs. external (dark) average velocity at the die exit as a function of the power law’s ‘\( n \)’ value.

Figure 8 shows the die balance stability for a wider range of power law’s ‘\( n \)’ value covering the majority of propellant dough viscosity types.

### 3.3 Non-isothermal simulations

The last optimization step included the viscous heating effect on the viscosity of the materials and has been conducted with data collected during a rheology study. Results have then been verified experimentally.

The final simulation results are shown in Figure 9 and Figure 10. Figure 9 shows the thermal effects of the extrusion die during the propellant extruding process. This temperature variation had to be considered in the die design optimization.
Figure 9: Thermal profile example in Kelvin of the entire optimized die.

Figure 10: Velocity profile example of the optimized die in m/s.

As shown on Figure 9, the extrusion average velocities of the inner and outer layer are balanced between each other. Since the mid layer comes from another system, it is easily adjustable to match the velocity of the two other layers.

This stability has been verified experimentally as shown on Figure 11.

The model robustness has finally been verified with the non-isothermal simulation of the outer and inner layer only. Initially, the mid layer was replaced by ambient air. The results predicted a less heat transfer from the inner to the outer section which resulted in a higher temperature and velocity of the inner section as shown on Figure 13 and Figure 13:

Figure 11: Cut section of an extrudate showing the straightness of each layer.

Figure 12: Thermal profile in Kelvin of the optimized die, without the heat transfer effect of the mid layer material.
Figure 13: Velocity profile of the optimized die in m/s, without the heat transfer effect of the mid layer material.

The predicted increase in velocity of the model was verified experimentally by extruding only the inner and outer layer as shown on Figure 14 and Figure 15:

Figure 14: Extruded strand with inner section of air.

Figure 15: Extrudate quality without the heat transfer effect of the mid layer material.

A higher velocity of the inner layer has been observed.

4. Discussion

The experimental verifications have established a high confidence level of the robustness of the simulation model realized on COMSOL Multiphysics®.

Isothermal simulations have shown the importance of considering the flow factor ‘n’ or the shear thinning characteristic of the propellant dough when designing an extrusion die of a complex geometry.

However, these isothermal simulations alone are not sufficiently accurate to predict a precise extrusion behavior. Due to the high level of viscous heating and the poor thermal conductivity of the material, heat transfer must be also considered.

5. Conclusions

The balance of the flow velocity between the inner and outer section was the main challenge of this effort. To address this challenge, viscous heating and shear thinning behavior in the die design have been considered.

The simulations conclude with the interaction between the power law index “n” and the viscous heating in the die design. The results obtained by finite elements simulations have been validated experimentally.