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Numerical modelling of solid hydrogen flow through an extruder die

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Abstract. Harnessing energy by nuclear fusion has progressed into technological developments as a result of sufficient progress made in the theoretical investigations. Fueling a tokamak by pellet injection is reported to be most efficient among other fueling techniques. It is thus important to produce a solid hydrogen filament by extrusion process using an extruder-die setup. It is required to arrive at an optimum configuration of the die as the pressure drop in the die decides the load on the extruder. The present analysis focuses on developing a CFD model of a die taking into account the complex rheological behavior of solid hydrogen. A systematic parametric analysis is performed to study the influence of die geometry on the flow behavior. The un-yielded regions are identified from the simulation results. It has been found that the un-yielded region decreases as the contraction ratio and contraction angle is decreased. The un-yielded zone is predominantly present in the region before contraction. However, at lower flow rates, the un-yielded zone appears even after the contraction.

1. Introduction

Nuclear fusion promises to be a viable alternative for the ever rising energy demand. One of the challenges is to meet the reactors stringent fueling requirements. Pellet injection is reported to be an efficient option among various fueling methods[1]. It is thus required to produce a solid hydrogen filament using an extruder-die setup. Development of an extruder die setup involves multiple design iteration processes, which calls for a reliable CFD model taking into account the complex rheological behavior of solid hydrogen. As it is tedious to develop a numerical model for the extruder and the die together due to intricacies involved in meshing the flow geometry, the modelling of the die and extruder are carried out separately and their pressure-flow rate characteristics are superimposed to obtain the operation point[2].



It is important to note that the pressure at the die inlet decides the load on the extruder. Further, the pressure loss in the die attributes to the viscous dissipation occurring in the die. Therefore, it is required to arrive at an optimum configuration for minimum viscous dissipation rate at the given throughput rate. Solid Hydrogen exhibit complex rheological behavior where a minimum critical yield stress is required to sustain the flow and also shear thinning behavior is exhibited as the shear rate increases. Even though some literatures are available on extrusion of similar fluids, no literatures have been reported on solid hydrogen flow through dies.

Mitsoulis and Abdali[3] developed a FEM model to study the flow of visco-plastic fluids through extrusion die to identify the un-yielded zone and its influence on pressure drop. Alexandrou [4] studied the role of Bingham and Reynolds number in formation of un-yielded zones. Mitsoulis[5] provided a comprehensive review of various models to simulate visco-plastic materials. Jay et al. [6] studied the effect of contraction angle and contraction ratio on formation of un-yielded zone and the pressure loss in die. The above mention work reveals the influence of geometry, rheology and flow morphology on the pressure characteristics

This present work intends to develop a robust 3D non-Newtonian CFD model for solid hydrogen flow through die. Another objective of this paper is to arrive at a geometric configuration with minimized viscous dissipation rate for a given flow rate of 500 mm³/s. ANSYS-POLYFLOW a FEM based CFD solver primarily developed to study the viscous flows is used in the present analysis. The rheological behavior of solid hydrogen is incorporated in the Herschel bulkley (H-B) viscosity model. One important assumption made in the present analysis is that solid hydrogen remains at isothermal condition (11 K).

2. Analytical model of the die

In order to get a first-hand perspective, the model from Vinyar and Lukin[7] was adopted in the present analysis. Assuming Newtonian behavior (equation (2)) of solid hydrogen, Vinyar and Lukin[7] related pressure drop and flow rate using the Buckingham formula (equation (1)) for the die with constant cross section.

$$Q = \frac{\pi r^4 \Delta p}{8\mu l} \left[1 - \frac{4}{3} \left(\frac{2\tau_0 l}{r\Delta p} \right) + \frac{1}{3} \left(\frac{2\tau_0 l}{r\Delta p} \right)^4 \right] \quad (1)$$

$$\mu = 0.0027 e^{0.44(T_s - T)} \quad (2)$$

The die characteristics obtained using the above correlations are presented in results and discussions section.

3. CFD modelling

3.1 Rheological behavior

The rheological behavior of solid hydrogen is fitted to Herschel bulkley viscosity model using the empirical correlations arrived by Leachman[8] using a specially developed viscometer. The relationship between shear stress (τ) and strain rate ($\dot{\gamma}$) is given by

$$\tau(\dot{\gamma}, T) = \tau_0 + k\dot{\gamma}^n \quad (3)$$

The flow behaviour index n is equal to 0.5 with τ_0 , k being critical yield stress and flow consistency index respectively given by

$$\tau_0 = a_1 \left(\frac{\vartheta_o + a_5 T_m^{a_6}}{\vartheta_o + a_5 T^{a_6}} \right)^{a_2} \quad (4)$$

$$k = a_3 \left(\frac{\vartheta_o + a_5 T_m^{a_6}}{\vartheta_o + a_5 T^{a_6}} \right)^{a_4} \quad (5)$$

The values for these coefficients are given in Leachman's [8] work.

3.2 Meshing and boundary conditions

The geometric modelling of the die was carried out using SOLIDWORKS. As the solid hydrogen at 11 K behaves as a visco-plastic and visco-elastic fluid, the material does not swell after extrusion. In this view the outlet diameter is fixed to 3 mm as the requirement is to extrude a 3 mm diameter filament. The contraction ratio from the extruder to die ranges from 4:1 to 10:1 with contraction angle ranging from 45° to 90° . Table.1 and figure 1 presents the initial dimensions for the analysis to be carried out.

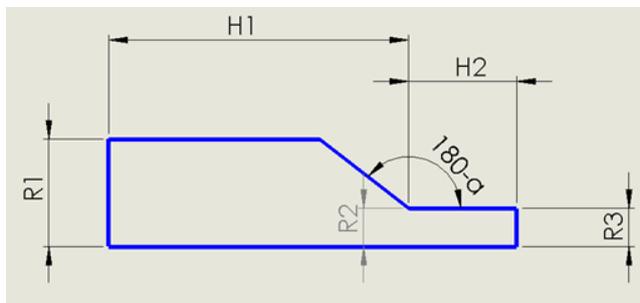


Figure 1. Geometric configuration of die

Table 1. Initial dimensions

Parameter	Dimension
R1	6 mm
R2	1.5 mm
R3	1.5 mm
H1	15 mm
H2	11 mm
α	45°

Figure 2 presents examples of fine hexahedral meshing performed for both sudden and gradual contraction. The meshing was carried out using ICEM CFD employing blocking technique. A systematic grid independency test was performed where the pressure loss and flow structure are independent of mesh size of over 1,50,000 nodes.

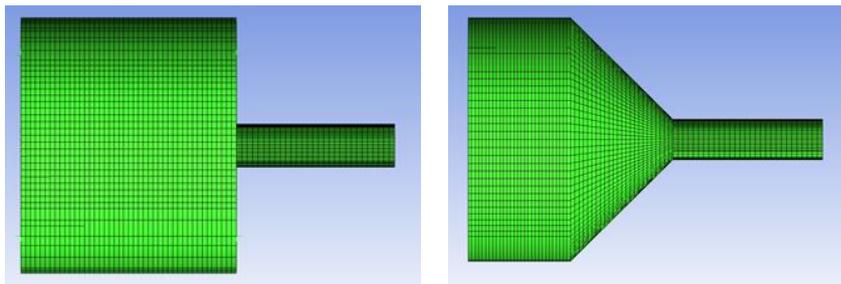


Figure 2. Hexahedral Meshing for sudden and gradual contraction of the computational domain

As it is required to estimate the pressure drop in the die for a given flow rate, the boundary condition at the inlet is imposed with mass flow rate. The normal force i.e. the pressure at the outlet is imposed to be zero and the wall is imposed with no-slip boundary condition. The computational domain and the detailed boundary conditions are presented in figure 3 and table 2 respectively.

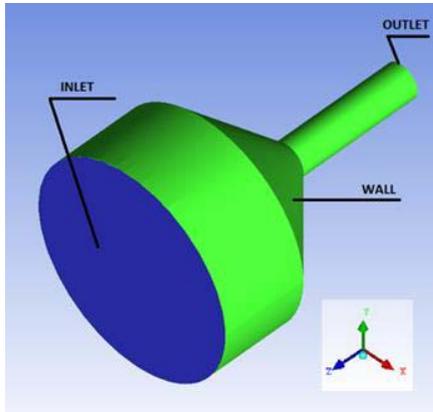


Figure 3. Computational domain

Table 2. Boundary conditions

Surface	Dimension
Inlet	Inflow (mass flow rate)
Wall	Normal and tangential velocity imposed ($v_n=0$ & $v_s=0$)
Outlet	Normal force and tangential velocity imposed ($f_n=0$ & $v_s=0$)

ANSYS POLYFLOW which is specifically built to study complex rheological fluid flows is used in the present analysis. As the viscous force is dominant, the inertia term is neglected in the momentum equation. Picard's iteration is used for viscosity.

4. Results and discussions

To compare the CFD modeling results with that of analytical model, the geometric mean of the inlet and the outlet diameter is taken for the analytical model as it assumes constant diameter for the die. From equation (2), for the Newtonian behavior at isothermal condition (11 K), the viscosity of the fluid boils down to 9420 Pa-s. From figure 4 it can be inferred that the pressure characteristics of CFD modelling results is of same order when compared to that of analytical model which provides first-hand information to confidently proceed to the further analysis.

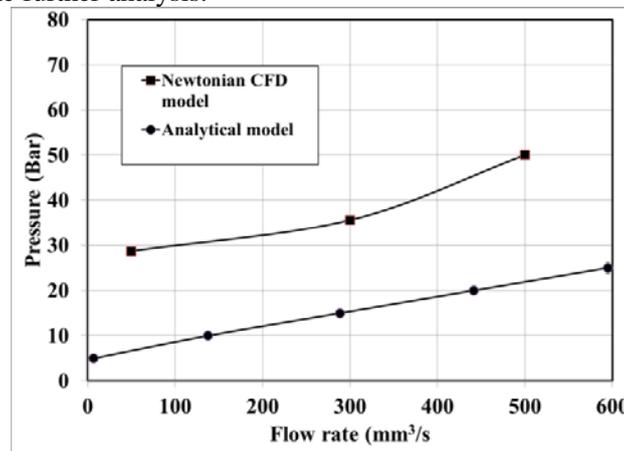


Figure 4. Comparison of the Newtonian CFD model with the analytical model

4.1 Influence of contraction ratio

For the non-Newtonian model, the flow structure as seen in figure 5 is greatly affected at different contraction ratios. It has to be noted that the flow happens in the negative Z direction. Simulations are performed at 500 mm³/s and the un-yielded zones are identified in the corners and as well as in the central region where the local shear rate is less than 1 s⁻¹. The un-yielded zone at the corners is termed as rigid static zone and the un-yielded zone at the central region is termed as rigid moving zone. The rigid static

zone is a stagnant layer where the velocity as well as the local shear rate is close to zero. However the rigid moving zone possesses a finite velocity as it moves along with the flow. This fact is validated from the velocity plot shown in figure 6.

As the contraction ratio is increased from 4:1 to 10:1, the un-yielded zone is predominant throughout the domain where it becomes hard to differentiate between the static and moving un-yielded zone. The rigid static zone accumulates largely at the corners whereas the rigid moving zone grows as we increase the contraction ratio. Interestingly in all the three cases, the pressure loss is the same. This fact can be attributed to the low flow-behavior-index and low Bingham number which is explained in detail by Jay et al.[6] Also, it is important to note that the flow structure after contraction is unaltered in all the three cases.

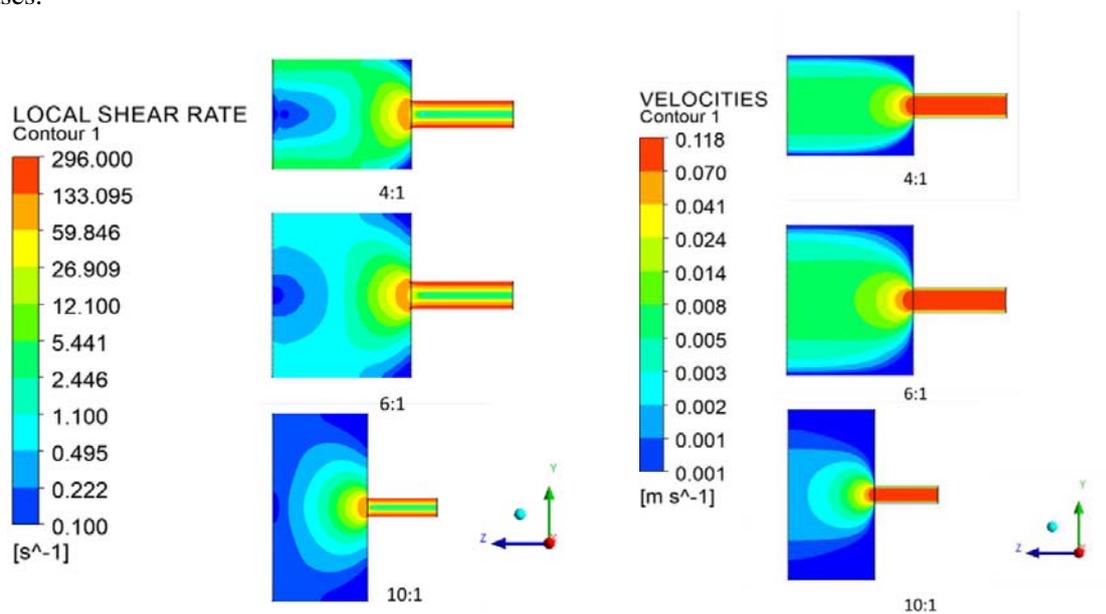


Figure 5. Local shear rate distribution at different contraction ratios

Figure 6. Velocity distribution at different contraction ratios

4.2 Influence of contraction angle

For contraction ratio 4:1, analysis was carried out at contraction angle ranging from 45° to 90° . Figure 7 show that when the contraction angle decreases, the rigid static zone reduces whereas the rigid moving zone is unaltered. In line to that low flow behavior index and low Bingham number, pressure loss even in these three cases happens to be same.

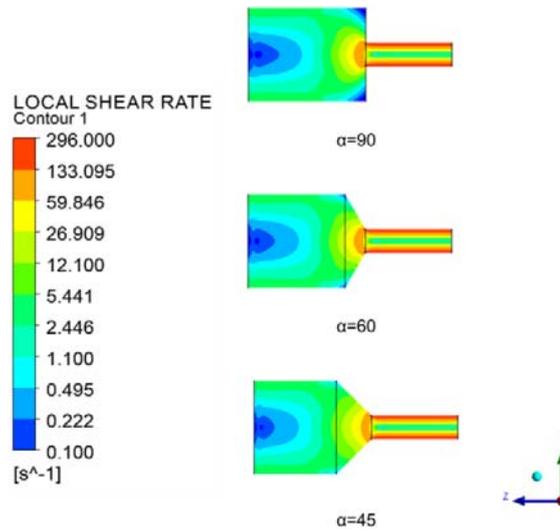


Figure 7. Local shear rate distribution at different contraction angle

4.3 Influence of flow rate

Simulations were carried out at different flow rate with a configuration of 4:1 contraction ratio and 45° contraction angles as shown in figure 8. At very high flow rate of 1500 mm³/s, both the static and moving un-yielded zone vanishes which shows that the viscous stress is predominant than the yield stress. Contrast to that, at lower flow rate of 50 mm³/s the un-yielded zone is found to occupy larger part of the domain. On top of that, the un-yielded zone persists even after contraction. Unlike the results in the previous two sections, the flow structure in the region after contraction varies significantly and it has an influence on the pressure drop in the die (table 3).

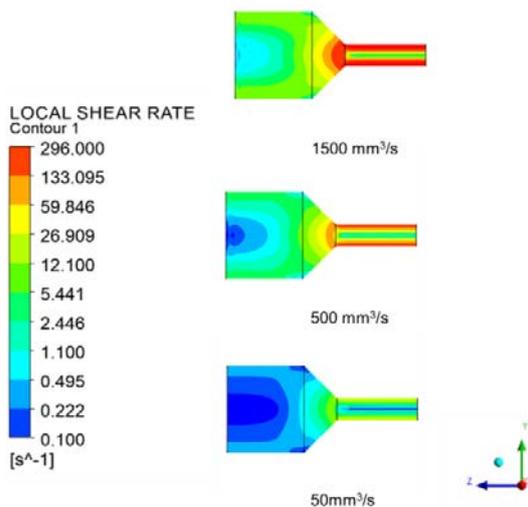


Table 3. Pressure drop at different flow rate

Flow rate (mm ³ /s)	Pressure drop (Bar)
1500	78.56
500	50
50	21

Figure 8. Local shear rate distribution at different flow rate

4.4 Influence of region past contraction

From the analysis carried out so far, it is evident that the pressure drop in the die is largely influenced by the region past contraction. To study the influence of this region, parametric analysis is carried out by decreasing H_2 from 11 mm to 5 mm and by increasing R_2 from 1.5 mm to 3 mm at various flow rates.

For the geometry with 4:1 contraction ratio and 45° contraction angle, when R_2 i.e. the intermediate radius is increased from 1.5 mm to 3 mm, a considerable drop in the viscous dissipation and pressure loss was achieved. For example, at $500 \text{ mm}^3/\text{s}$ the viscous dissipation rate drops from 2.5 W to 1.2 W which corresponds to drop in pressure loss to as much as 25 Bar. At higher flow rate, this effect is even more prominent

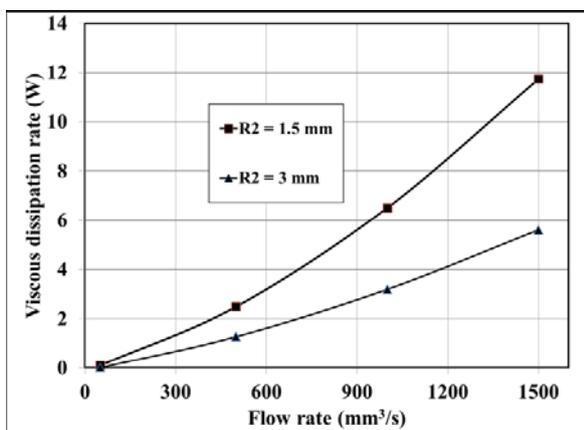


Figure 9. Viscous dissipation rate at different R_2

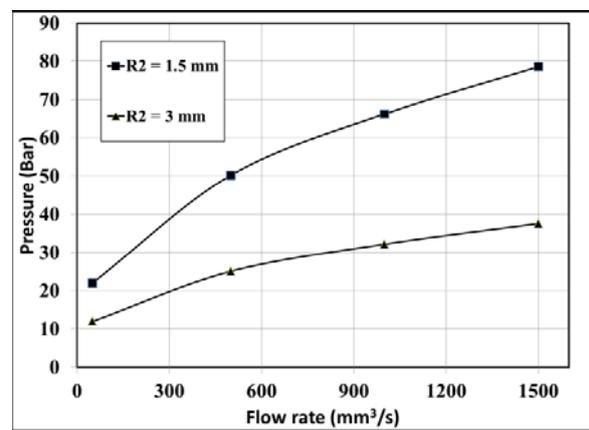


Figure 10. Pressure characteristics at different R_2

When H_2 is decreased from 11 mm to 5 mm, a drop in pressure loss of 22 Bar is achieved at $500 \text{ mm}^3/\text{s}$. From these analyses, it is quite conclusive that the geometry of the region past contraction is sensitive to the pressure drop. A larger intermediate radius R_2 with shorter extrusion length H_2 is an apt option to achieve low pressure loss.

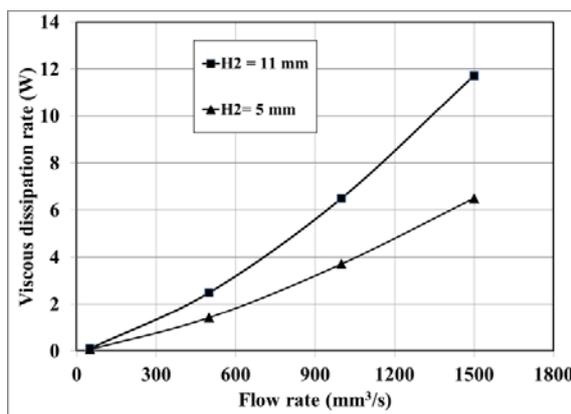


Figure 11. Viscous dissipation rate at different H_2

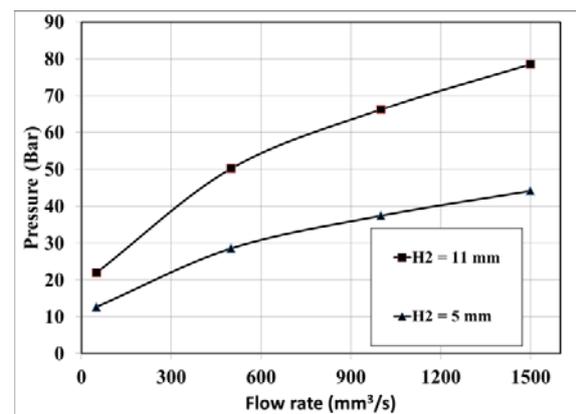


Figure 12. Pressure characteristics at different H_2

5. Conclusions

Numerical model to study the solid hydrogen flow through extruder die is successfully developed. It is found that the un-yielded region decreases with decrease in contraction ratio and contraction angle. The influence of contraction angle and contraction ratio on the pressure drop is not prominent at $500 \text{ mm}^3/\text{s}$ for the present geometric configuration. The flow structure at different flow rate is studied and it is found that un-yielded region appears even after contraction for lower flow rates. The region past the contraction is sensitive to the pressure drop where an increase in intermediate diameter from 3 mm to 6 mm results in drop in pressure loss of about 25 Bar. By shortening the extrusion length from 11 mm to 5 mm, the drop in pressure loss accounts to 22 Bar. Therefore, the die with larger intermediate diameter and shorter extrusion length is prescribed.

Acknowledgments

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