Optimization of bar soap extrusion process parameters through numerical modelling

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Abstract. Mechanical soap plodders refine, homogenize, and compact soap. Processing pressure, screen mesh size, and L/D affect plodder capacity and soap quality. Grittiness, air bubbles, and poor surface finish hinder soap production. This study optimised soap plodder machine screw length, speed, and density to maximise pressure at low-temperature. Soap plodder FEM was made with ANSYS Polyflow software. The rheological and thermal properties of soap paste were measured with a rotational viscometer and transient hot wire. Viscosity, thermal conductivity, and heat capacity were 900 cps, 0.0449 W/m-K, and 17.29 J/Kg-K. A L9 Taguchi DOE was used for three screw speeds (20, 35, and 50 RPM), screw lengths (300, 550, and 800 mm), and soap product densities in FEM simulation. ANOVA and Taguchi optimization modelling were adopted for analysis. The ANOVA showed a positive correlation between extrudate pressure, screw length, speed, and density. Temperature was mostly density-dependent. Ideal conditions were 800 mm screw length, 50 RPM screw speed, and 900 kg/m^3 material density. Response pressure was 4.3604 bar, temperature 315 K. The observed responses would optimize soap plodder pressure, improving refining, homogenization, and soap processing with small mesh screens. The low temperature eliminates the need for a cooling jacket, reducing construction and operating costs

Keywords: Waste cooking oil; Optimization; ANSYS POLYFLOW; Numerical simulation; Soap plodder

1 Introduction

Soap is a salt of fatty acid; it finds application in several industries such as fabric spinning and lubricant production. It is produced by breaking down fat into glycerin and fatty acids in continuous or batch methods [1]. Despite modern technologies like neutralizing fatty acids, most soap manufacturers use batch procedures like cold method saponification, semi-boiled saponification, and the kettle process [2], [3]. Waste cooking oil recovery and use in soap production by endothermic and exothermic techniques have been studied [4]. The soap produced has saponification values appropriate for soapmaking. The use of waste cooking oils in soap production could reduce environmental pollution [4], [5]. This process has worked well for small businesses, who produce soap manually by mold technique. Grittiness, trapped air bubbles, surface fracture, and soap shape issues often result from poor refining and extrusion method necessitating a refining and extrusion machine to process soap into the right shape and quality to increase its value and commercial appeal. Plodders refine, homogenize, and compact soap. A plodder's ability to refine materials depends on the length-to-diameter ratio, processing pressure, and screen mesh size [6].

The quality of bar soap largely depends on the raw material properties and extrusion process variables and selection of the correct variables has a direct influence on the product [7].

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Through design of experiments and numerical modelling, various studies have investigated some of these properties and variables. A study [8] evaluated a screw design through simulation and established that Screw design and production conditions directly affected barrel pressure. Rogowsky [9], analysed and concisely described a screw extrusion machine before submitting a dimensional assessment that produced generalized relationships between pressures, discharge rate, drive power, plastic extruder viscosity, machine speed, and a specific dimension. The velocity distribution of an ideally viscous plastic substance was used to determine discharge and pressure in terms of rectangular screw thread size. To accurately assess extrusion machine capacity, a method was developed [10]. The phrases were used to study the effects of increasing screw starts [9].

Gao et al. [11], simulated single-screw extrusion using the multi-phase flow approach. The study examined how screw speeds affect single-screw extruder extrusion quality and outlet pressure. A detailed study by Lewandowski & Wilczyński [12], examined a single screw extrusion method involving polymer melts and slide effects. The analysis of the pumping properties of die and screw systems is conducted using a thorough three-dimensional non-Newtonian finite element technique. The phenomenon of slipping and its effects on the operation of an extruder was investigated [13]. The study conducted by Zhou et al. [14], investigated the process of propellant single-screw extrusion [8]. The investigation began by examining extrusion viscosity distributions and fluctuations. Extrusion fractures on surfaces of the soap paste compromise their strength and makes the soap unappealing. Domanti and Bridgwater [15], found that increasing die length improves surface properties in pastes with glucose admixtures. It was also reported that increasing extrusion velocity increased fracture depth and tapered dies reduced fracture frequency and depth [16].

Although significant strides have been made in literature in terms of investigation of screw type bar soap extrusion process variables, information on optimization of major process variables in the extrusion process is not clear. This study seeks to address this gap through investigation of the effects of major process variables to pressure and temperature which are the major quality indicators and optimization of these parameters based on Taguchi methodology. Results of this study could provide an insight to bar soap extrusion process designers on suitable screw length and speed design specifications to enhance quality production.

2 Materials and Methods

2.1 Study design

Figure 1 illustrates the procedure adopted for this study. The properties of soap paste material that affect its flow and thermal conditions were determined.

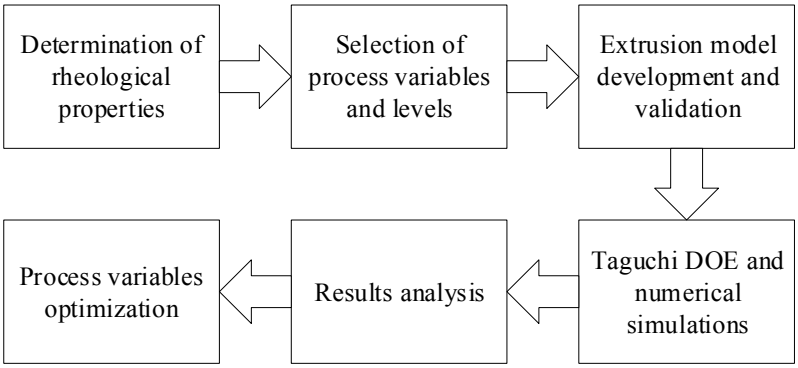

Fig. 1. Study methodology.

ANSYS polyflow was used to model and simulate the extrusion flow to determine the quality responses (pressure and temperature) at the various input combinations (useful screw length, RPM, and density) [12]. The investigation involved the combined problem of non-Newtonian fluid flow and non-isothermal extruder design in a symmetric extruder [17].

2.2 Determination of the Soap Viscosity

The constituent elements were mixed to create a sample of soap paste. First, 375 ml of water and 80 g of caustic soda are mixed then the mixture was added to 500 ml of used cooking oil. The order and rate of mixture were guided by previous studies [5], [18]. The viscosity of the soap paste was determined using a rotational viscometer (NDJ-4) according to ISO 2555. The accuracy of a rotational viscometer (NDJ-4) was ±1% and ±0.2% repeatability The viscometer was set at 6 RPM due to viscometer readability and the expected viscosity range. The viscosity of the soap paste was 900 cps.

2.3 Determination of the Soap Thermal Conductivity

To perform the measurements, an LM35 temperature sensor connected to the nickel-chromium wire passing through the sample and still connected to Arduino, a DC power source, and an Ammeter was used to determine the voltage and current passing through the sample, and the recorded temperature was displayed on the computer through the approach of the hot wire method for measurement of thermal conductivity [19], [20]. The time was recorded in seconds using a timer. The thermal conductivity and specific heat capacity of soap paste found to be 0.0449 W/m-K and 17.2910 J/kg-K, respectively. The experimental results agreed with the known viscosity and thermal conductivity of liquid soap which is in the range of 117.9-340 W/m-K and 0.934-2.532 cps. Since the paste solidifies and becomes more rigid, its viscosity increases. Reduced paste moisture lowers thermal conductivity resulting in higher liquid soap conductivity [21].

2.4 Numerical Simulation

ANSYS polyflow was used to simulate the extrusion flow to determine the quality responses (pressure and temperature) at the various input combinations (useful screw length, RPM, and density). The general non-newtonian solver with finite element method (F.E.M) task and evolution problems was used to solve the inventor-designed geometry model. The model's STEP file was uploaded to ANSYS Polyflow Space Claim, where the material's inlet and outlet were defined. Subsequently, the fluid domain region was extracted and transferred to the next meshing step. The boundary conditions of the material were provided inside the subtask settings, eventually resulting in the generation of the solution and the delivery of the output [12], [22]. The following assumptions were considered during the numerical simulation in this study:

1. There was no chemical reaction or change in density in the extruder
2. The material is completely packed at the area between the hopper and the die end.
3. No heat loss through the barrel.
4. The material properties of the waste oil will be the same irrespective of the brand.

The investigation involved the combined problem of non-Newtonian fluid flow and non-isothermal extruder design in a symmetric extruder. The paste enters the domain at a fixed temperature of 25°C and at a flow rate dictated by the speed of the screw in revolutions per minute. Flow, heat transfer by conduction, and heat creation by viscous dissipation were all involved in the current task. To solve the problem, a sub-task was defined to specify the properties of the paste and a moving part (screw) which was also defined with its material properties namely: density, specific heat capacity, and thermal conductivity. The sub-task had a specific model, a description of the domain, the properties of the materials, and boundary conditions. Viscous heating was considered, and the shear-rate dependence of viscosity follows the Bird-Carreau law. At the exit, it was expected that a uniform velocity profile is obtained. The extruded material experiences no externally applied tension at the exit, so the condition of zero normal and tangential forces was chosen [23]. The flow and

thermal boundary conditions for the paste and the extruder design at the boundaries of the domains are defined below:

(i) Boundary 1: Flow inlet, (298 K, RPM, Q_i)
(ii) Boundary 2: Wall, insulated boundary/symmetry
(iii) Boundary 3: Flow exit, zero normal, and tangential forces imposed.
(iv) Screw surface: Rotational speed and no-slip

Fig. 2 shows the boundary conditions on the fluid domain generated.

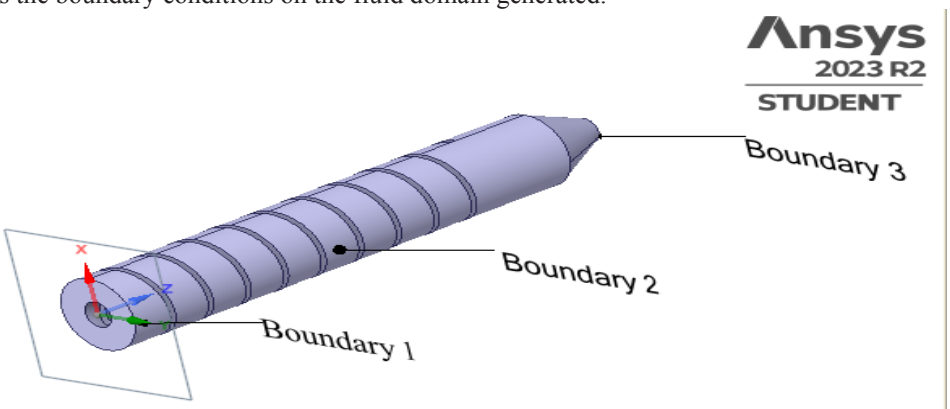

Fig. 2. Fluid domain with the boundary regions.

The mesh utilized in this study was constructed using a tetrahedral mesh with two distinct regions. The first region corresponds to the fluid domain, representing the volume enclosed by the barrel. The second region represents the solid domain, specifically referring to the screws. The integration of these domains took place at the interface of the solid domain, accomplished by establishing the contact zone between the fluid domain and the screw. The configuration of these meshes and grids were designed in a manner that the grids are of higher resolution or a greater number of mesh elements were utilized to accurately represent the material behaviour. The selection of the mesh was determined by prior research undertaken by Konagant and Sobhani et al. [24]. An element size of 0.8mm was chosen, as there was minimal change in the results.

2.5 Governing equations

The numerical model was governed by the following Equations 1-3[12], [25] .

$$Q* = f(\Delta p^*) \tag{1}$$

$$Q* = \frac{2Q}{WH(\pi DN cos\varphi)} \tag{2}$$

$$\Delta p* = \frac{h^{n+1} sin\varphi}{6m(\pi DN cos\varphi)} \frac{\Delta pc}{l_f} \tag{3}$$

Where Q* denotes flow rate, and Δp^* pressure gradient both being dimensionless. The properties were formulated to account for non-Newtonian and non-isothermal flows across a diverse array of screw designs, encompassing single- and twin-screw extrusion with both co-rotating and counter-rotating screws [26]. For result analysis and optimization, ANOVA was carried out at 95% confidence level and Taguchi signal to noise ratios calculated utilizing the larger is better for pressure response and smaller is better for temperature response. Polyflow solves the momentum equations, the incompressibility equation, and the energy equation for

non-isothermal flows for generalized Newtonian flow. The momentum equation has the following form:

$$-\nabla p + \nabla . T + f = \rho a \tag{4}$$

where p denotes pressure, T the extra-stress tensor, f the volume force, ρ the density, and a is the acceleration. The equation for incompressibility is

$$\nabla . v = 0 \tag{5}$$

where v denotes velocity. The energy equation is represented below as Equation (3.17)

$$\rho C_P \frac{DT}{Dt} = r - \nabla q + (\sigma D) \tag{6}$$

where D is the rate-of-deformation tensor, σ is the Cauchy stress tensor, and (σD) is the sum of the diagonal terms of σD. DT/Dt is the material derivative of the temperature:

$$\frac{DT}{Dt} = T : \nabla v + r - \nabla q \tag{7}$$

2.6 Model verification

By substituting Equation 2 and 3 in Equation 1 a resulting equation depicting the change in pressure against change in length was obtained and utilized in expressing the variation in pressure to the change in the length of the screw [12]. The graph depicted in Figure 3 illustrates the comparison between the pressure values derived from the development of equations 2 and 3 along the screw and the pressure data obtained through simulation. The findings demonstrate a favourable link between changes in pressure and changes in length, as observed in both the simulated and predicted outcomes. Hence, verifying the model's predictive capacity. The difference in pressure change observed between the predicted and actual values in the screw extruder can be attributed to various variables, including but not limited to inhomogeneity and non-uniform mixing of the materials involved. Pressure fluctuations can occur in the extruder due to variations in the composition, temperature, or viscosity of the material being processed, as well as the presence of back pressure and material obstructions within the screw, which can interrupt the flow [27].

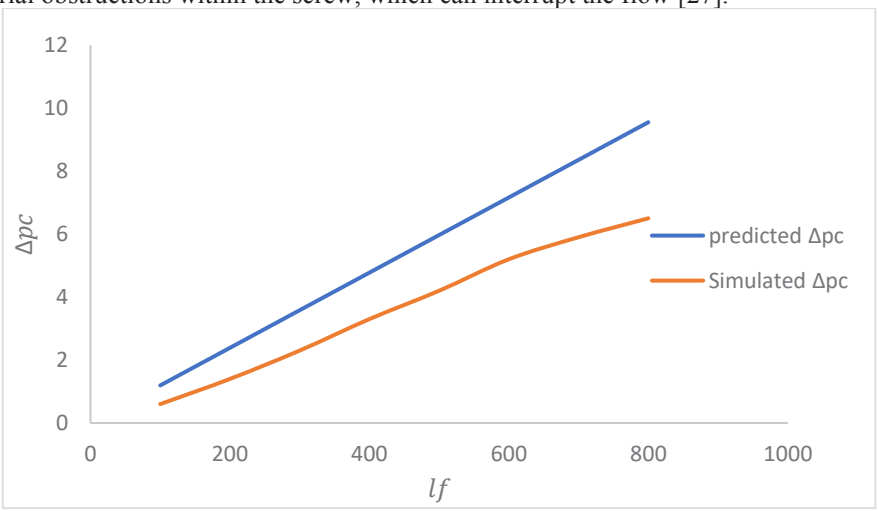

Fig. 3. Plot of change in pressure against change in crew length.

2.7 Taguchi Optimization

After numerical simulations to determine pressure and temperature responses at the given combination of input variables, the signal-to-noise ratios of each output were computed at

each experimental run. With the objective being to maximize screw pressure, a larger screw is better. Equation 4 was used to compute signal-to-noise ratios for pressure. On the other hand, with the objective being to minimize temperature, smaller is better. Equation 5 was used to compute signal-to-noise ratios corresponding to temperature. Inputs with the largest signal-to-noise ratios on the responses were selected as the optimum levels for the particular responses.

$$\mathrm{SN}_L = -10\log\left[\frac{1}{n}\sum_{i=1}^{n}\frac{1}{{y_i}^2}\right] \tag{4}$$

$$\mathrm{SN}_S = -10\log\left[\frac{1}{n}\sum_{i=1}^{n}{y_i}^2\right] \tag{5}$$

Table 1 presents the Taguchi orthogonal array depicting the three input factors over three levels.

Table 1. L9 Taguchi design of experiment (DOE)

Run	Length (mm)	Speed (RPM)	Density (kg/m^3)
L1	300	20	200
L2	300	35	550
L3	300	50	900
L4	550	20	550
L5	550	35	900
L6	550	50	200
L7	800	20	900
L8	800	35	200
L9	800	50	550

3 Results and Discussions

3.1 Effect of Operational and Geometric Parameters

Main effect plots of the signal-to-noise ratios were generated to assess the impact of varying inputs on the outputs. The curve depicted in Fig. 4 illustrates the impact of the key factors on the signal-to-noise ratios of pressure. The pressure of the extrudate increases when there is an increase in all three parameters, namely screw length, screw speed, and density. As depicted in the chart, it can be observed that both the screw length and material density exert a comparable influence on the extrudate pressure. A longer screw increases the available surface area for the compression and compaction of the extrudate, it also increases the distance that the material must travel within the extruder before it exits, allowing for a greater duration during which the screw can exert force upon the material. Thus leading to an increase in pressure [27]. As the density of the material increases, a corresponding increase in force is typically required to facilitate its passage through the extruder. Consequently, this results in an elevation of pressure build-up [28], [29]. The reason for this occurrence is that materials with higher density possess a bigger mass per unit volume, necessitating the screw to apply increased force in order to facilitate their movement during the extrusion process [11]. Materials with lower densities requires a reduced amount of force for the extrusion process which results in low pressure registered [19]. The high rotational speed of the screw results in higher levels of shearing and raised friction between the material and the extruder barrel, hence resulting in an increased screw pressure [11].

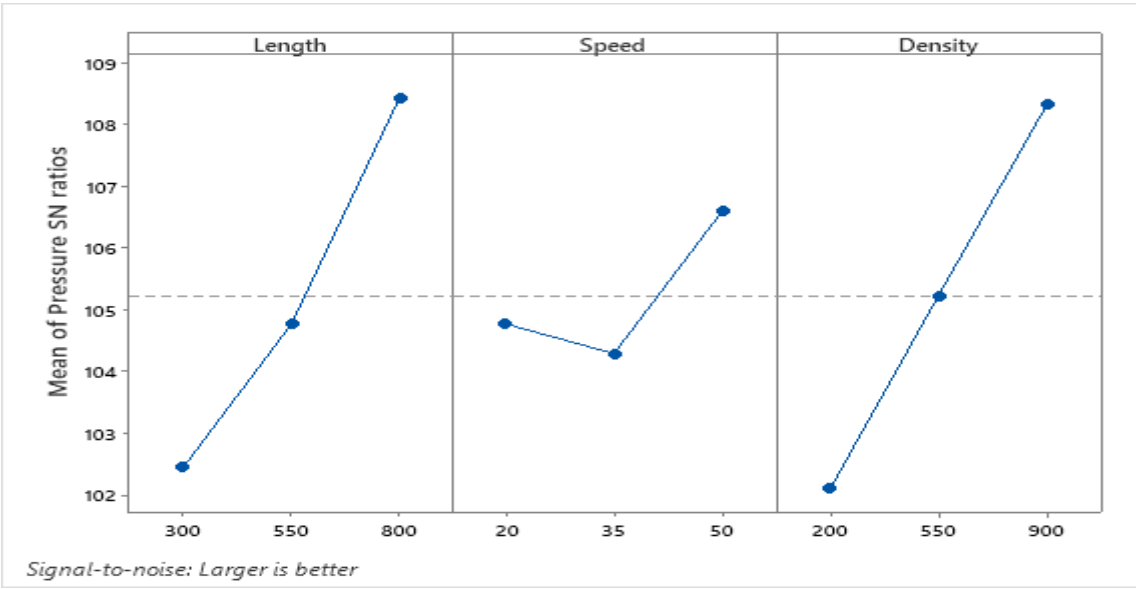

Fig. 4. Mains effect plot of pressure.

Fig. 5 illustrates the main effect plot of temperature signal-to-noise ratios. The signal-to-noise ratio (S/N ratio), an essential measure, is subject to the influence of multiple factors. As the screw length extends, a cascading effect occurs, ushering in a rise in the S/N ratio an indication of temperature reduction. Conversely, when the screw speed is increased or material density is amplified, the S/N ratio descends, suggesting an increase in temperature. The parameter that exerts the most significant influence on temperature is density, with speed being the subsequent factor of importance. An increase in screw speed and density leads to an increased shearing action occurring between the paste material and the surfaces of the screw [30]. The heightened shear experienced can result in elevated heat generation within

the material because of viscous dissipation. As a result, there is a potential increase in the temperature of the material [11], [14].

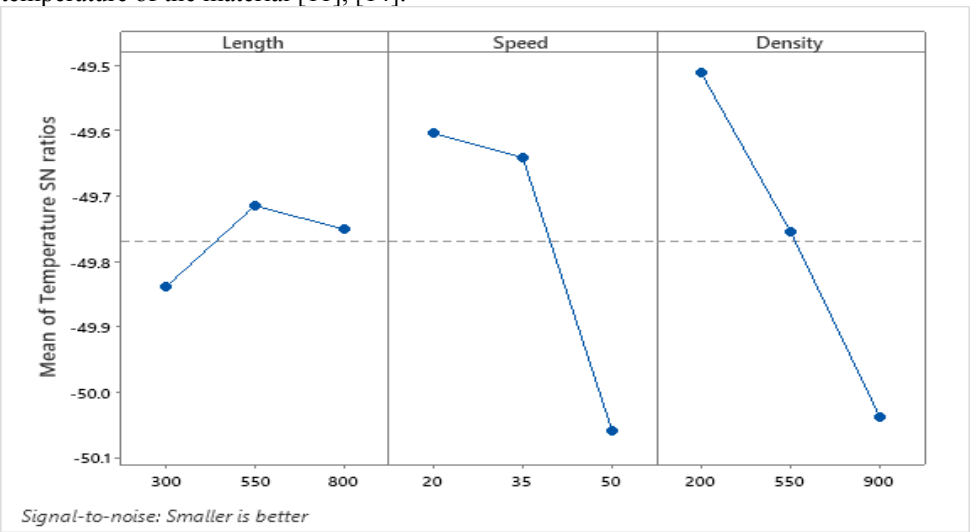

Fig. 5. Mains effect plot of temperature.

Contour plots were generated to evaluate the simultaneous effects of inputs on the outputs. Fig. 6 illustrates the impact of simultaneous variations in density and screw length, which had a higher influence on the extrudate pressure while maintaining a constant screw speed. An increase in density and length leads to a higher pressure as a result of the prolonged residence time of the material in the screw and the material's resistance to flow, which subsequently causes pressure buildup. A variation in screw length at varying densities yields distinct effects on pressure. Specifically, increasing the screw length at lower densities does not result in significant changes in pressure since the screw can penetrate easily due to the lower material density, hence the less force required. When the screw is short and the material density is higher, it is expected that the pressure will be higher. In such a case, the power is concentrated on a smaller contact area [31]. This makes it harder for the screw to go through. hence the high pressure. However, expanding the screw length at higher densities leads to an elevation in pressure. In cases where density remains constant, as is typically observed in numerous applications, an increase in the length of a screw will result in an increase in pressure. Hence, in cases where the material density remains constant, a higher pressure can be attained through an increase in the screw length [32].

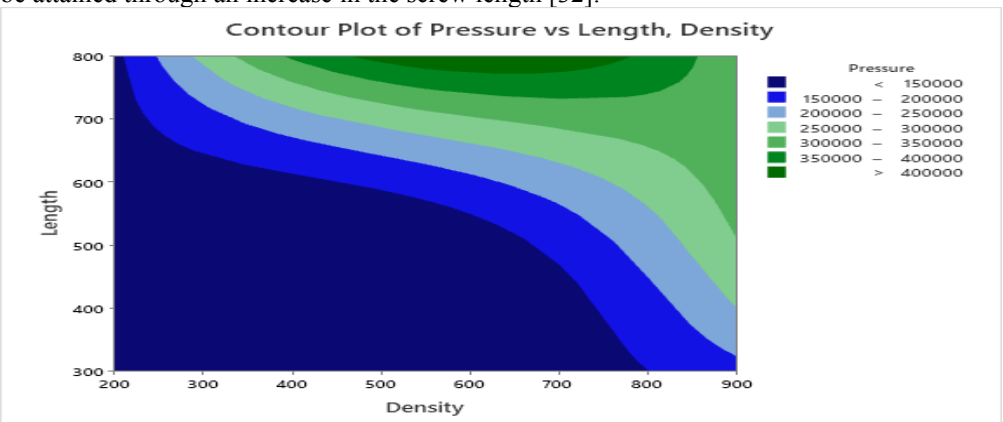

Fig. 6. Contour plot of density and length against pressure.

Figure 7 presents a contour plot that visually represents the impact of simultaneous variations in density and speed on the temperature of the extrudate, with the screw length being held constant. A reduction in extrudate temperature can be achieved by decreasing both the density and screw speeds. The influence of screw speed on temperature is dependent upon the density of the material undergoing processing. When the rotational velocity of the screw is increased at lower densities, the impact on temperature is not shown to be statistically significant. Nevertheless, as the rotational speed of the screw increases under higher densities, it gives rise to an escalated rate of frictional heating, therefore leading to an elevation in temperature [30].

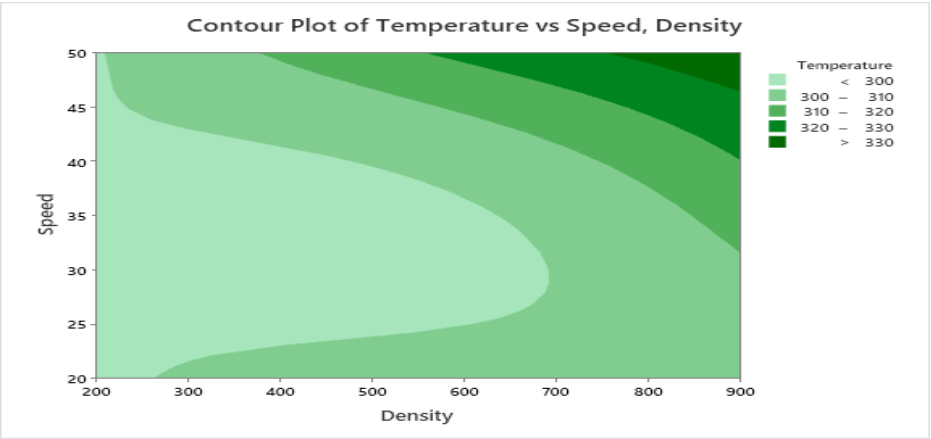

Fig. 7. Contour plot of density and speed against temperature.

To evaluate the significance of the input variables, a meticulous analysis of variance (ANOVA) was executed. This comprehensive evaluation operated at a significance level denoted by α, set at the commonly adopted threshold of $\alpha = 0.05$. The ANOVA findings for pressure are presented in Table 2. The findings of the study demonstrate that both screw length and density have a substantial impact on extrudate pressure, however, screw speed does not exhibit a significant influence.

Table 2. Analysis of Variance for Pressure

Source	DF	Seq SS	Adj SS	Adj MS	F	P
Length	2	38653548109	38653548109	19326774054	2.18	0.045
Speed	2	7294785482	7294785482	3647392741	1.22	0.081
Density	2	31253587203	31253587203	15626793601	1.96	0.050
Residual Error	2	32649543169	32649543169	16324771584		
Total	8	1.09851E+11				

Table 3 presents the ANOVA outcomes about temperature. The ANOVA findings about temperature reveal that both screw speed and material density exert a statistically significant influence on temperature. However, the impact of screw length on temperature is deemed significantly negligible.

Table 3. Analysis of variance for temperature

Source	DF	Seq SS	Adj SS	Adj MS	F	P
Length	2	38.39	38.39	19.19	0.13	0.088
Speed	2	510.45	510.45	255.23	1.68	0.037
Density	2	542.65	542.65	271.32	1.78	0.036

Residual Error	2	304.64	304.64	152.32
Total	8	1396.12		

An increase in screw speed increases throughput and production rate proportionally. The material experiences increased compression and shear stresses as its velocity increases along the screw. As a result, there is an increase in pressure [9], [11]. The increase in screw speeds has the potential to cause excessive shear heating. The thermal effects of shear could cause the material's temperature to rise. Also Increased screw speeds are associated with increased levels of back pressure, particularly when the extruder's output is constrained and material accumulates before the die. Higher density materials require more energy for displacement within the extruder, resulting in increased pressure due to the material's increased resistance to motion. The use of higher density materials causes an increase in back pressure within the extruder [28], [29] The screw's dimensions and intrinsic design have a considerable impact on various aspects of the extrusion process [33]. The use of a longer screw permits the building of increased pressure along the entire length of the extruder barrel. The described phenomena can be due to the extra distance that the material must travel within the extruder before exiting [34]. This longer travel path allows the screw to exert force on the material for a longer period of time. As the screw speed increases, the shearing action between the paste substance and the screw surfaces becomes more intense. The singularities of viscous dissipation can cause an increase in shear forces, resulting in an increase in thermal energy production within the material. Because of their increased viscosity, materials with higher densities exhibit more resistance to flow within an extruder. As a result, these materials have a longer residence period within the extruder. The increased time within the extruder results in enhanced heat transfer from the screw to the material and within the material, resulting in a more noticeable accumulation of thermal energy and resultant temperature rise. The density of materials is important because it has the ability to generate significant heat owing to friction [11], [14].

3.2 Optimum Parameters

The use of signal-to-noise ratio rankings was employed to determine the optimal combination of input factors that would effectively maximize pressure while also minimizing temperature. Upon scrutinising the signal-to-noise ratios (S/N ratios) linked to pressure, a conspicuous pattern emerged. The highest ratios, signifying optimal conditions, align themselves with specific levels of the variables. These include level 3 of length, corresponding to 800 mm, level 3 of speed, clocking in at 50 RPM, and level 3 of density, which is 900 kg/m^3.Therefore, if seeking to maximise pressure, there will be a need to use a screw length measuring 800 mm, a speed of precisely 50 RPM, and a material density pegged at 900 kg/m^3. The data regarding these S/N ratios related to pressure has been presented in Table 4.

Table 4. Response table for signal-to-noise ratios for pressure
Larger is better was used being that the objective was to maximize pressure

Level	Length	Speed	Density
1	102.4	104.8	102.1
2	104.8	104.3	105.2
3	108.4	106.6	108.3
Delta	6.0	2.3	6.2
Rank	2	3	1

The temperature signal-to-noise ratios were analysed to determine the values that corresponded to the largest ratios, which in turn represented the optimum values. The findings are laid out in Table 5, providing a comprehensive overview of the signal-to-noise ratios about temperature. Amidst these vast amounts of data, a few standout observations

come into focus. Specifically, the highest ratios are prominently marked: -49.71 for length at Level 2, -49.60 for speed at Level 1, and -49.51 for density at Level 1. If aiming to achieve a cooler temperature, the optimal conditions call for the utilisation of a screw length measuring 550 mm, a screw speed set at 20 RPM, and a material density measuring 200 kg/m^3.

Table 5. Response Table for signal-to-noise ratios for temperature
Smaller is better was used being that the objective was to minimize temperature

Level	Length	Speed	Density
1	-49.84	-49.60	-49.51
2	-49.71	-49.64	-49.76
3	-49.75	-50.06	-50.04
Delta	0.12	0.46	0.53
Rank	3	2	1

Confirmation runs with the optimal parameters were carried out and provided an average result of pressure 4.3604 bar, and temperature 315 K for the first set of optimal conditions for high pressure. whereas for the second set of optimal conditions, which pertain to low temperature, the average pressure was found to be 1.3541 bar, with a temperature of 299.9 K. These findings demonstrate that the temperature change is minimal, with a difference of 15.1 K. This observation aligns with the data obtained from the previous simulation. Hence, it is deemed justifiable to designate the parameters of an 800 mm length, 50 RPM speed, and 900 kg/m^3 density as the optimal conditions.

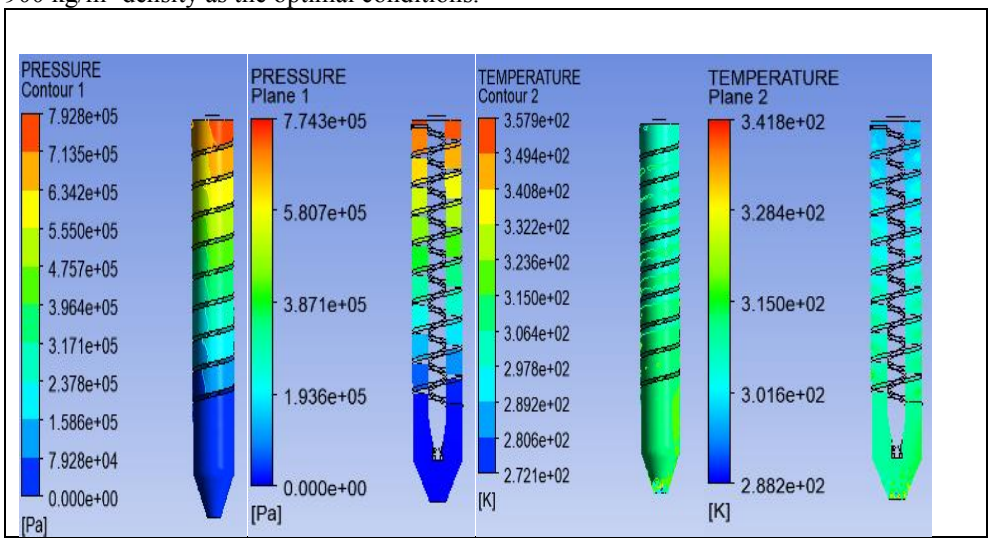

Fig. 8. Pressure and temperature distributions respectively.

Figure 8 shows the distributions of pressure and temperature, the contours show the response distribution on the fluid domain and the plane shows a sliced section of the fluid domain on the xz-plane. This simulation is conducted under optimal conditions for high pressure and low temperature, with a length of 800 mm, speed of 50 RPM, and density of 900 kg/m^3.

4 Conclusions

The objectives of this study were to investigate the effects and optimize major process parameters affecting quality indices in screw-type bar soap extrusion. The following conclusions were made;

1. Material density significantly affects both pressure and temperature whereas screw speed and length significantly affect temperature and pressure respectively.
2. At constant material density, a longer screw length should be used to attain higher pressures
3. Increasing both screw length, speed and material density increases pressure
4. The optimal intended values are achieved with a screw length of 800 mm, screw speed of 50 RPM, and material density of 900 kg/m^3 yielding a high pressure of 4.3604 bar and a low temperature of 315 K.

Nomenclatures

Q rate of flow,
W width of the screw channel,
h depth of the screw channel,
D screw diameter,
N screw speed (RPM),
φ Screw flight angle
Δp_c change in pressure,
l_f screw length of the change in pressure,
m consistency coefficient
n power law exponent.
k thermal conductivity (W/m-K),
t time(s),
a thermal diffusivity (m^2/s) of the test fluid,
γ Euler's constant
q quantity of heat

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