MODELAGEM MATEMÁTICA DE COMPACTAÇÃO DE PÓ DE LIGA METÁLICA

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RESUMO: *A metalurgia do pó é uma área em crescimento que demanda um controle relativamente rigoroso de seus parâmetros de processo com vistas a resultados que justifiquem sua implementação. Nesse contexto, a compactação de pós de ligas metálicas é relevante objetivando prover matéria-prima de características adequadas ao seu pós-processamento. Isso se justifica devido ao grau de compactação do pó influenciar diretamente o processo de densificação, afetando a resistência mecânica do compactado. Diante disto, neste trabalho, a modelagem matemática de compactação de pó de liga metálica em forma de um cilindro chato é apresentada por meio de exemplificação de uma prensagem isostática a frio de punção único. O objetivo é o de mostrar analítica e graficamente (Matlab®) como os principais parâmetros do processo influenciam a plastificação do compactado. Obtêm-se os valores de: (a) carga de prensagem mínima para plastificar todo o pó; (b) carga de extração do compactado; (c) porosidade; (d) tensão radial; (e) distribuição de tensão axial; e (f) recuperação de deformação elástica. Diante dos resultados da modelagem matemática apresentada e exemplificada, é possível obter os parâmetros do processo e implementar melhorias na tomada de decisão dentro do processo de compactação de pós de ligas metálicas.*

PALAVRAS-CHAVE: *Modelagem matemática, Metalurgia do pó, Compactação de pó, Liga metálica.*

MATHEMATICAL MODELING OF METAL ALLOY POWDER COMPACTION

ABSTRACT: *Powder metallurgy is a growing area that demands relatively rigorous control of its process parameters to achieve results that justify its implementation. In this context, the compaction of metal alloy powders is relevant in order to provide raw material with suitable characteristics for post-processing. This is justified because the degree of compaction of the powder directly influences the densification process, affecting the mechanical resistance of the compacted. In view of this, in this work, the mathematical modeling of compaction of metal alloy powder in the shape of a flat cylinder is presented by means of an example of a single punch cold isostatic pressing. The objective is to show analytically and graphically (Matlab®) how the main process parameters influence the plasticization of the compact. The values are obtained for: (a) minimum pressing load to plasticize all the powder; (b) compacted extraction load; (c) porosity; (d) radial stress; (e) axial stress distribution; and (f) spring back effect. Given the results of the mathematical modeling presented and exemplified, it is possible to obtain the process parameters and implement improvements in decision making within the metal alloy powder compaction process.*

KEYWORDS: *Mathematical modeling, Powder metallurgy, Powder compaction, Metal alloy.*

1. INTRODUCTION

Powder metallurgy (PM) is a manufacturing process in which a defined solid shape is obtained from wet raw powder. Occasionally, the product from PM has mechanical properties that avoid post-processing, in which it is denominated green compacted (THÜMMLER and OBERACKER, 1993). However, sometimes the compacted does not have sufficient and adequate properties to perform its designed function. In these cases, post-processing is needed to improve these properties. Post-processing often is composed of heat treatments to improve geometric parameters, powder nature, metallurgical, and mechanical characteristics (UPADHYAYA, 1998). In specific situations, powder conditioning is possible only by mixing additives to powder mass, aiming at connecting, plasticizing, and lubricating the particles.

1.1 Powder reactivity

In what refers to the reactivity of the powder with the environment, one of the most relevant relations is the one between inertial and surface forces, which rises as the particles diminish their sizes. This is evident in the processing of ceramics and hard metals because the involved powders are fine-grained, presenting a high level of surface activity. The specific problems arising from a high activity level addresses: (a) tooling damage; and (b) possible uncontrolled agglomeration (less fluidity). The raw powder mass commonly presents low compressibility (e.g. atomization, in which the particles are cooled quickly), hardening by mechanical comminution work, residual interstitial impurities (oxygen, carbon, nitrogen, oxide layers, etc.). Therefore, powder mass often is subjected to heat treatments for annealing, size enlargement, chemical reduction, degassing, decarburization, etc. (CHIAVERINI, 1992).

1.2 Compaction

Regarding compaction, which is the main process addressed in this work, it provides the needed mechanical strength besides attributing final or almost final geometric characteristics. In addition, the adequate contact between the particles provides densification enough to prepare the compacted to post-processing. Related to the operational method, there are two pressure-assisted compaction methods: (a) cold; and (b) hot. The former can be: (a) axial by punching; and (b) isostatic pressing by hydrostatic pressure from a liquid. The hot method has three main techniques: (a) axial and isostatic pressure; (b) forging; and (c) extrusion (THÜMMLER e OBERACKER, 1993).

Compaction demands rigid tooling when compared to the rigidity of the mass to compact. The die has a cavity inside which the powder mass is pressed by a vertical punch in a top-down movement or there are two moving punches that simultaneously press the powder. The particles are then pressed and their surfaces are cold-welded. The extraction of the compacted mass takes place if the compacted has enough strength. A lubricant may be part of the mixture to minimize the energy spent and improve tooling life (GERMAN, 2005).

The physics of the problem addresses the relation between densification and deformation, i.e. as densification rises, the particles are plastically deformed and become more resistant by deformation (often leveling up the yield strength). In microstructural branch, the largest particles establish bonds around the smallest ones, implying in a larger contact area and, consequently, a decrease in internal shear stress. If the external pressure is constant throughout the process, in the case yield strength reaches a level high enough to surpass the effect of decreasing shear stresses, then densification stops. Moreover, depending on the particle arrangement, they can be elastoplastically deformed and cold or hot work hardened or even more fragmented to rise the compaction efficiency (HÖGÄNAS, 2013).

There are several approaches to describe the powder mass behavior, among which three are here highlighted. The first considers the compacted a homogeneous sample, in which the relations between pressure and density, and between pressure and radial stress are extracted. The second approach applies continuum mechanics and/or computational simulation in order to obtain response stresses, deformations, and density distribution. The last approach, adopted in this work, addresses the compaction micromechanics, in which the individual behavior of the particles under pressure is analyzed.

1.3 Paper scope

Therefore, in this work, the mathematical modelling of metal alloy powder compaction is presented in the context of micromechanics. As an example in Matlab®, metal alloy raw powder turns into a flat cylinder when subjected to cold isostatic pressing by a single punch. The objective is to present the influence of the main parameters of compaction in densification analytically and graphically. This includes presenting the following output data: (a) minimum pressing load to plasticize the powder; (b) extraction load; (c) porosity; (d) radial pressure (stress); (e) axial stress distribution; and (f) spring back effect. Based on these outputs, the compaction process can be adequately planned, configured, and conducted so that the compacted can achieve the required mechanical properties.

2. MATERIALS AND METHODS

In the case of punch and die method, the compaction pressure corresponds to the relation between the applied load and the contact area between the punch and the powder. The pressure to produce compression is equal to the isostatic pressure from the hydraulic fluid. In this paper, the mathematical model derived from the physical phenomena is based on a single-punch cold isostatic pressing of a raw homogeneous powder mass.

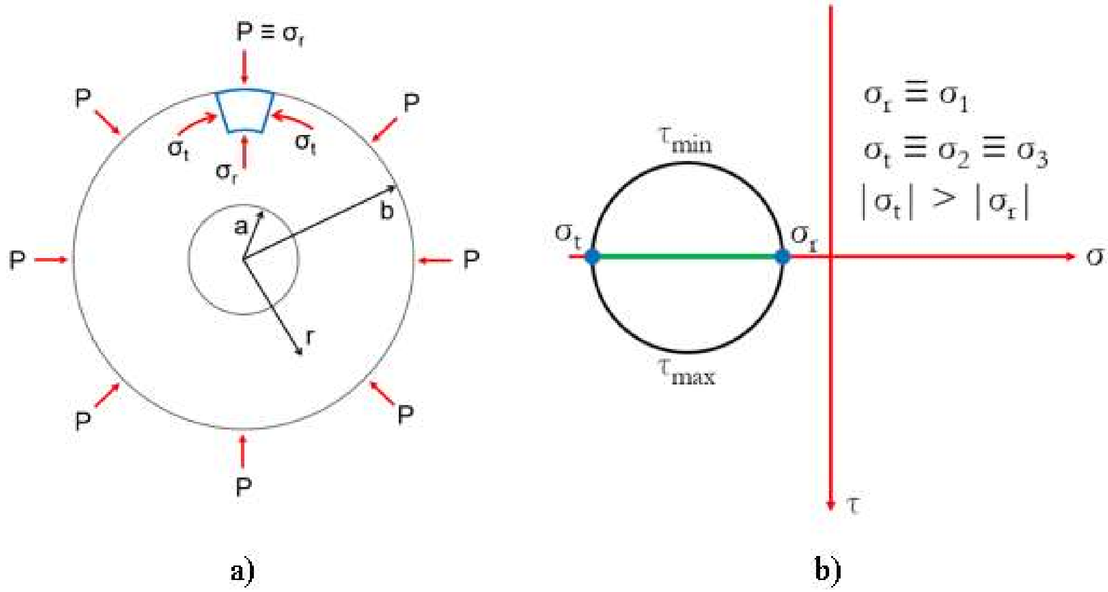
2.1 Mathematical modeling (analytical method)

In what refers to porosity (ϕ), the real and theoretical volumes (V_r , and V_t, respectively) before the compaction process compose the real and theoretical densities ($\rho_r = m / V_r$, and $\rho_t = m / V_t$, respectively), in which m is the mass. These densities compose the mathematical definition of porosity, in Equation 1.

$$\phi(\%) = \left(1 - \frac{\rho_r}{\rho_t}\right)100. \tag{1}$$

As the densification starts, the powder particles are compressed in a magnitude enough to transform the interconnected pores into smaller ones sparsely distributed. This situation is here modeled for each particle and its neighborhood, considering the mathematical model of a hollow sphere under external hydrostatic pressure P (Figure 1(a)), in which σ_r is the radial stress, and σ_t is the tangential stress. The Mohr's circle corresponding to the stress state of the situation described is represented in Figure 1(b), in which σ_1 , σ_2 , and σ_3 are the principal stresses 1, 2, and 3, respectively, and $\tau_{\min}$, and $\tau_{\max}$ are the minimum and maximum shear stresses, respectively.

FIGURE 1. (a) Hollow sphere under external hydrostatic pressure representing a powder particle; (b) Mohr's circle representing a hollow sphere under external hydrostatic pressure.



Source: Authors (2024).

In this work, Tresca's failure criterion is adopted due to its more conservative characteristic. Consequently, plastic deformation occurs when the maximum shear stress at the external surface of the hollow sphere exceeds the shear yield strength, i.e. $\tau(b) = S_Y / 2$, in which S_Y is the material yield strength; a, b, and r are, respectively, the internal, external, and generic radii, such that $a \le r \le b$. By observing the stress state in Figure 1(a), radial and tangential stresses are in the compression direction over the infinitesimal element.

Therefore, Equation 2 corresponds to the yielding function under Tresca's failure criterion for the infinitesimal element shown in Figure 1(a), in which a non-null positive result is not possible due to the material model adopted (elastic-perfectly plastic),

$$f = \sigma_r - \sigma_t - S_y, \tag{2}$$

which addresses that if the yielding function results in a negative value, the point or region under analysis is in the elastic domain. As the external infinitesimal element has the lowest value of radial and tangential stresses, to assure that the entire domain will be in the plastic regime it is enough to calculate the stresses at this element and obtain a null value for the yielding function.

Therefore, radial and tangential stresses (as a function of the radii a, r, and b, and the load P) for this case can be extracted from the theory of elasticity (Sadd, 2021), being expressed by Equation 3 and Equation 4, respectively:

$$\sigma_r = \frac{Pa^3b^3}{\left(b^3 - a^3\right)r^3} - \frac{Pb^3}{\left(b^3 - a^3\right)}, \tag{3}$$

$$\sigma_t = -\frac{Pb^3}{\left(b^3 - a^3\right)} - \frac{Pa^3b^3}{2\left(b^3 - a^3\right)r^3}, \tag{4}$$

In the context of this paper, the most relevant point to obtain the radial and tangential stresses is at radius $r = b$, i.e. at the external surface of the sphere, place where the lowest levels of stresses are present (Equation 5, and Equation 6):

$$\sigma_r\left(a, r, b, P\right)\Big|_{r=b} = -P, \tag{5}$$

$$\sigma_t\left(a, r, b, P\right)\Big|_{r=b} = -P\frac{2b^3 + a^3}{2\left(b^3 - a^3\right)}. \tag{6}$$

Equation 7 results from the substitution of Equation 5 and Equation 6 into Equation 2. Equation 7 corresponds to the minimum requirement for $P_{\min}$ to plasticize the external surface, which includes the entire domain of the hollow sphere because the plastic phenomenon starts at the internal surface and ends at the external one (Kholdi *et al.*, 2020).

$$P_{\min} \geq \left(\frac{2}{3}\frac{b^3 - a^3}{a^3}\right)S_y. \tag{7}$$

Comparing the rigidities of the die with that of the powder mass, the former must present a much greater rigidity in order to maintain its shape and volume. This assumption simplifies the mathematical model because it is not necessary to account for significant deformation contribution from the die.

A first mathematical model relevant to interrelate axial and radial pressures comes from (Long, 1960), which consists of a metal cylindrical plug over which an axial pressure is applied (lower and upper faces). Moreover, the friction is considered negligible because the lubrication is effective enough to provoke considerable losses.

An improved mathematical model was then proposed by (Bockstiegel, 1965), which makes use of Long's model to include the friction phenomenon. The modified model states that the friction load between the powder mass and die is approximately equal to the radial pressure (P_r), which is due to axial pressure (P_a). Therefore, axial stress (σ_a) is a function of radial and axial pressures, where μ is the friction coefficient between die wall and powder mass, and P_r is equal to the radial stress σ_r . Consequently, according to Bockstiegel's model, Equation 8 gives the plastic radial stress during compaction process:

$$P_{rp} = \frac{P_a - S_y}{1+\mu}, \tag{8}$$

In the context of a prismatic solid body under compressive axial load, Saint Venant's principle can be verified in the distribution of axial stresses, where the greatest magnitudes are found in the regions of direct load application. At a sufficient distance from these regions, the effect from the application of load decreases and the stress assumes an almost homogeneous magnitude, the so-called mean stress. An analogous phenomenon occurs with powder mass. As the distance from the analyzed powder mass cross-section to the punch face increases, σ_a decreases. In contact with punch faces, the powder mass is under a high-level axial pressure, resulting in a higher densification. Consequently, in terms of particle distribution, the longer the body, the more heterogeneous it can turn out. To model this phenomenon, a regular cylindrical die with infinite stiffness is the boundary of a powder mass disc of radius r_d (equal to the internal radius of the die), whose longitudinal axis is called y and the infinitesimal length dy . On the upper face of this disc, the axial stress is assumed to be $\sigma_a(y)$. Due to the friction between the inner wall of the die and the lateral surface of the disc, the axial stress acting on the lower face of the disc is $\sigma_a(y+dy)$. Therefore, Equation 9, Equation 10, and Equation 11, respectively, give the forces on the upper surface of the cylinder (F_u), lower (F_l), and friction (F_f) between the cylinder and the die:

$$F_u(r_D, y) = \pi\, r_D^{\,2}\, \sigma_a(y), \tag{9}$$

$$F_l(r_D, y) = \pi\, r_D^{\,2}\, \sigma_a(y + dy), \tag{10}$$

$$F_f(\mu, r_D, y) = \mu\, 2\, \pi\, r_D\, dy\, \sigma_a(y). \tag{11}$$

From equilibrium, Equation 12 can be obtained:

$$F_u - F_l = F_f \Rightarrow \pi\, r_D^{\,2}\left[\sigma_a(y) - \sigma_a(y + dy)\right] = \mu\, 2\, \pi\, r_D\, dy\, \sigma_a(y)\ . \tag{12}$$

The rearrangement of Equation 12 implies in Equation 13, which is the axial stress distribution along the longitudinal axis of a cylinder of powder mass:

$$\sigma_a(y) = \sigma_a(0)\exp\left(-2\,\mu\,\frac{y}{r_D}\right). \tag{13}$$

As mentioned, even after loading stops, there is a remaining radial stress. Consequently, a certain magnitude of force is required to extract the compact from the cylinder. Therefore, Equation 14 expresses the force F_e required to extract the compacted mass from the cylinder:

$$F_e(\mu, r_D, h, \sigma_{rr}) = \mu\, 2\, \pi\, r_D\, h\, \sigma_{rr}\ , \tag{14}$$

where h is the height of the compacted, σ_{rr} is the residual radial stress corresponding to the obtainment of the plastic regime when the powder is under compaction.

After die ejection, the spring back effect (S_b) comes from the natural elastic expansion of the compacted powder, which depends mainly on powder properties, pressure, additives and lubricants used, and die characteristics. Its quantification observes the following formula (Equation 15), which coincides with the definition of deformation:

$$S_b(\%) = \frac{D_f - D_i}{D_i} 100, \tag{15}$$

where D_i and D_f are, respectively, the initial and final diameters of the compacted.

Therefore, the mathematical modeling presented here covers loading and extraction situations. The first step is mainly based on providing the necessary charge to cause the plastic phenomenon in particles approximated by hollow spheres under external pressure. The latter is governed by the remaining radial stress over the contact area between the compacted powder and the die wall, with the aim of finding the load to extract the powder.

2.2 Mathematical modeling (computational method)

The mathematical modeling presented in the previous subsection (2.1) is coded in Matlab® aiming to graphically present the main process parameters that influence the densification of the compacted (already presented in subsection 1.3). The input data in this code are listed in Table 1.

TABLE 1. Input data in mathematical modeling of compaction process.

Input	Symbol	Equations	Example value
Real volume (mm^3)	V_r	1	1873.740
Theoretical volume (mm^3)	V_t	1	1783.440
Mass (g)	m	1	14.000
Compacted powder height (mm)	h	14	12.000
Particle inner radius (mm)	a	3, 4, 7	0.015
Particle outer radius (mm)	b	3, 4, 7	0.020
Material yield strength (MPa)	S_Y	2, 7, 8	250.000
Friction coefficient between powder and die	μ	8, 11, 12, 13, 14	0.150
Die diameter (mm)	$2\,r_D$	9 to 14	14.000
Compacted diameter after extraction (mm)	D_f	15	14.100

Source: Authors (2024).

It is important to note that, due to the most diverse sources of uncertainty inherent to the compression process, it is not possible to guarantee that the real situation will corroborate to what is calculated by the computer program or vice versa, even if all data is entered in a correct manner.

For example, particle size typically refers to an average size and does not encompass the different sizes of all particles in the powder mass. Furthermore, by adopting the mathematical model of a hollow spherical particle, particles of other shapes are no longer taken into account with greater accuracy. Other sources of uncertainty refer to measurement processes, estimates of unknown parameters, etc. In view of this, the output data provided by the code may slightly differ from those of the real situation.

3. RESULTS

Figure 2 shows part of the programming screen in editor’s tab of Matlab®, in which the entire mathematical modeling presented herein was coded.

FIGURE 2. Matlab® screen of the compaction process code in editor’s tab.

```
%POWDER COMPACTION MATHEMATICAL MODELING

%Real volume (mm^3)
V_r = 1873.74;

%Theoretical volume (mm^3)
V_t = 1783.44;

%Powder mass (g)
m = 14;

%Compacted powder height (mm)
h = 12;

%Particle inner radius (mm)
a = 0.015;

%Particle outer radius (mm)
b = 0.020;

%Material yield strength (MPa)
S_y = 250;

%Friction coefficient between powder and die
mu = 0.15;
```

Source: Authors (2024).

The output data are presented in Table 2. The penultimate and the last outputs are, respectively, the results for axial stress (in MPa) at the cylinder height, and at the surface where the load is applied. According to Table 2, the compacted powder has a porosity of 4.819%, a radial stress of 1666.667 MPa during the pressing process, and a spring back effect of 0.714%. In terms of loads, the minimum load to plasticize the entire domain of the flat cylinder is 493.451 kN, and the load to extract the compact powder is 17.210 kN. In other words, the extraction load corresponds to 3.488% of the compaction load.

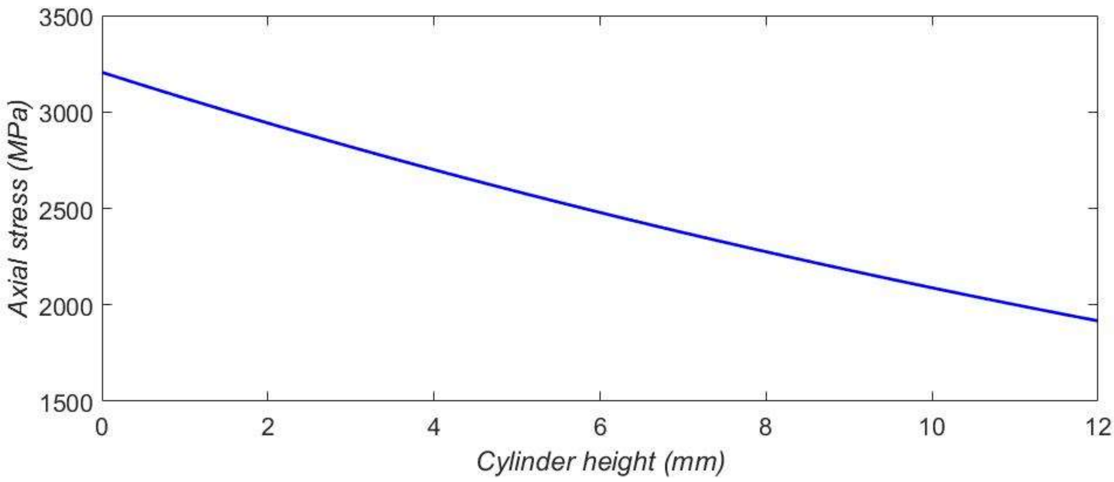
TABLE 2. Output data in mathematical modeling of compaction process.

Output	Symbol	Equations	Value for the example
Porosity ($\%$)	ϕ	1	4.819
Extraction load (kN)	F_e	14	17.210
Applied load (kN)	$P_{\min}$.	7	493.451
Radial stress (MPa)	σ_r	3	1666.667
Spring back ($\%$)	S_b	15	0.714
Minimum of axial stress (MPa)	$\sigma_a(h)$	13	2478.691
Maximum of axial stress (MPa)	$\sigma_a(0)$	13	3205.517

Source: Authors (2024).

Figure 3 presents the graphical exponential behavior of axial stress related to height of the flat cylinder. It can be noted that the upper surface (where the load is applied by the punch) has the highest value of axial stress, while the lower surface has the lowest value of axial stress.

FIGURE 3. Axial stress *vs*. height of the compacted cylinder.

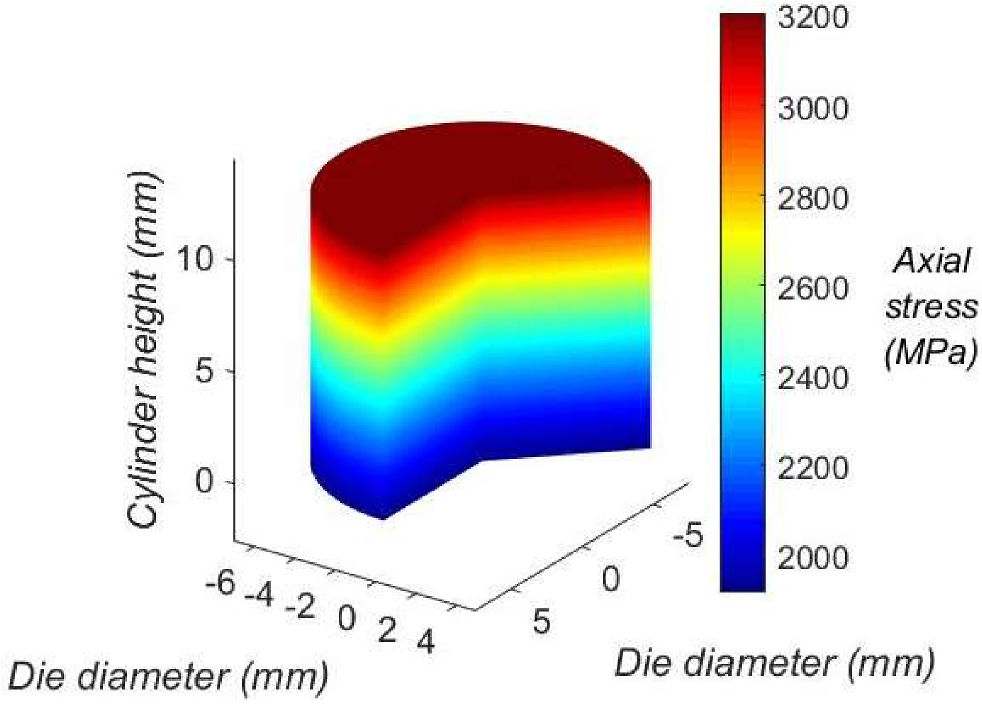


Source: Authors (2024).

Therefore, by observing the graph "Axial stress *vs*. height of compacted powder" (Figure 3), the value of the curve guarantees that at the most distant point, that is, at the lower surface of the compacted powder, the stress state is over the failure criteria limit. In the context of an elastic perfectly-plastic material model, this indicates that the entire compacted powder domain is in the plastic regime.

In a different manner, Figure 4 shows the axial stress distribution throughout the height of the flat cylinder. In Figure 4, the highest value of axial stress occurs at the upper surface of the cylinder, whereas the smallest value can be seen at the lower surface of the cylinder.

FIGURE 4. Distribution of axial stress *vs*. height of the cylinder under compaction *vs*. die diameter.



Source: Authors (2024).

4. CONCLUSIONS

This paper presented the mathematical modeling of the compaction process of metal alloys to assist in the process of pressing metal alloy powders, aiming to ensure that the entire powder mass is in the plastic regime. It was coded in Matlab® and exemplified for a flat cylinder.

Under Tresca's failure criterion, the key output parameters to control in order to theoretically assure that the entire domain of the cylinder is in the plastic regime are the axial and radial stresses. This response in terms of stress varies from the highest value at the face of load application to the lowest value in the lower surface of the flat cylinder. A numerical example of a powder mass was subjected to calculations in this computer code. Specifically with regard to the distribution of axial stresses along the height of the compacted powder, the minimum value mathematically guarantees that the entire volume is in the plastic regime.

The presented mathematical model and applied code aims to: (a) be a helpful tool that encompasses the theoretical basis to more easily conduct the pressing process; (b) provide agility in the preparation and execution of pressing; (c) predict behavior and results related to compacted powder.

Therefore, the program presented here can be used as a tool to assist in the pressing process observing the conditions described in this work, although it can be easily adapted to meet other requirements.

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RESPONSIBILITY DECLARATION

The authors are the only responsible for this work.

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