A SOFTWARE PROGRAM FOR COMPUTER MODELING OF POWDER ELABORATION PROCESS

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INTRODUCTION

Mechanical properties of compacts and sintered parts strongly depend on the physical, chemical, morphological and technological properties of the metallic powders. Due to the complexity of the physical and chemical phenomena that occurs in the atomization process and also due to the numerous influence parameters, makes a difficult task in the mathematical modeling process in order to establish the optimum values for the process variables. It was created a software program that allows recording of all data, parameters and metallic powder properties, obtained by powder metallurgy technology. These data are used for statistical study of powder properties and also for computer modeling of elaboration process.

PROGRAM SOFTWARE DESCRIPTION

MetLab is an application developed in the C++ Builder (vers.3.0) programming language, which utilize the BDE engine (Borland Database Engine), conceived in 32 bits Windows technology. The program allows the recording of all data throw an easy graphical interface in a dBase IV format. Using the relational language SQL does the editing, sorting, filtering and querying data. The window for editing/recording data contain 55 fields corresponding to method of atomization, elaborating parameters - temperature, atomization fluid properties, nozzle geometry and also the properties for metallic powders obtained, as is shown in fig.1.

The statistical characterization of the particles size it was realized on the base of the sieve analysis with the equations presented in table 1, [3]. Equations 4-7 are analogous with to moments of inertia, showing the diameter corresponding to the central point around the distribution can rotate.

Different measurement techniques lead to different means diameters: e.g. a D[1,0] is generated by optical microscopy, a D[2,0] diameter is generated by image software analysis, electro zone sensing technique will measure the volume of each particle and a D[3,0] is generated and by laser diffraction technique we will obtain the D[4,3] diameter, etc. It is possible to do a conversion between different means diameters using the Hatch-Choate transformation equations.

***Table 1**. Mean diameters for metallic powders*

Number-length mean (μm)	Number-surface mean (μm)	Number-volume mean (μm)
$D[1,0]=\frac{\sum_i^N d_i}{\sum_i^N n_i}$ (1)	$D[2,0]=\sqrt{\frac{\sum_i^N d_i^2}{\sum_i^N n_i}}$ (2)	$D[3,0]=\sqrt[3]{\frac{\sum_i^N d_i^3}{\sum_i^N n_i}}$ (3)

Moment Means			
Length-surface mean (μm)	Length-volume mean (μm)	Surface Area Moment Mean (Sauter Mean Diameter)	Volume Moment Mean De Brouckere Mean Diameter
$D[2,1]=\frac{\sum_i^N d_i^2}{\sum_i^N d_i}$ (4)	$D[3,1]=\sqrt{\frac{\sum_i^N d_i^3}{\sum_i^N d_i}}$ (5)	$D[3,2]=\frac{\sum_i^N d_i^3}{\sum_i^N d_i^2}$ (6)	$D[4,3]=\frac{\sum_i^N d_i^4}{\sum_i^N d_i^3}$ (7)

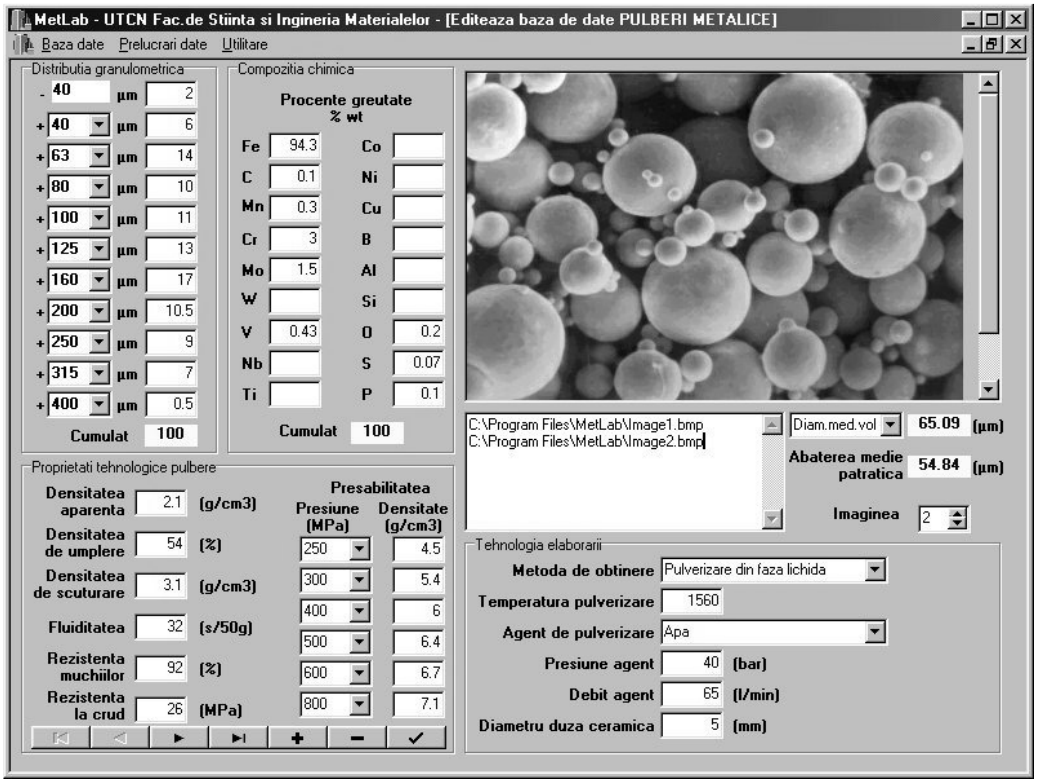


Figure 1. *The window for editing data*

The database can be queried upon to 40 simultaneously conditions, the results obtained being printed under a report form and also compared with the results obtained by mathematics modeling section. The program offers for each recording a graphical representation for the particle size distribution (up to 11 classes) respectively for the compressibility curve (up to 7 points).

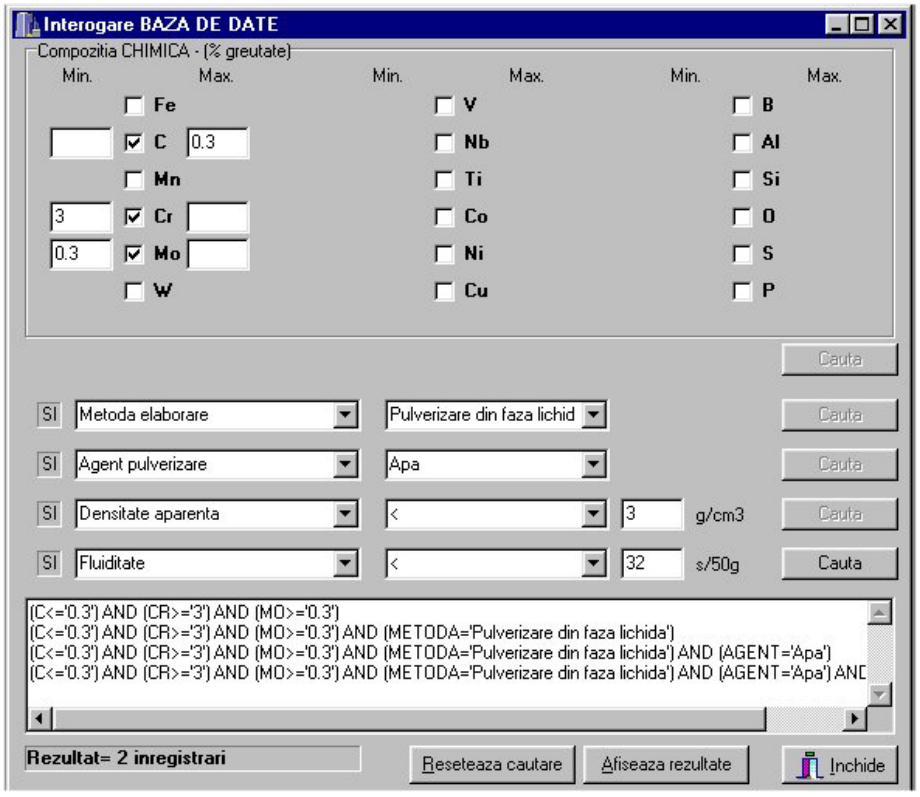


Figure 2. *The window for querying data*

3. ATOMIZATION PROCESS MODELING.

The mainly objective of mathematical modeling of the atomization process is to predict the size of the particle powder, function of the process variables. In the literature are presented two kinds of mathematical modeling methods: analytical and empirical correlation methods. The drawback of the analytical methods is that one mechanism of disintegration is take in consideration at a time since the methods based on the empirical correlation are applicable only for the situations and atomizer designs for which they have been developed. The particle size distribution of metallic powders can be defined by a lognormal curve, (Gauss curve) which is full described by mean diameter and standard deviation.

Analytical methods present a mathematical model based on the molten stream instability (Helmholtz instability). It was identified three stages, functions of the predominant mechanism: primary disintegration, secondary disintegration and solidification. To calculate the ligament diameter was used the Dombrowski and John equation [1]:

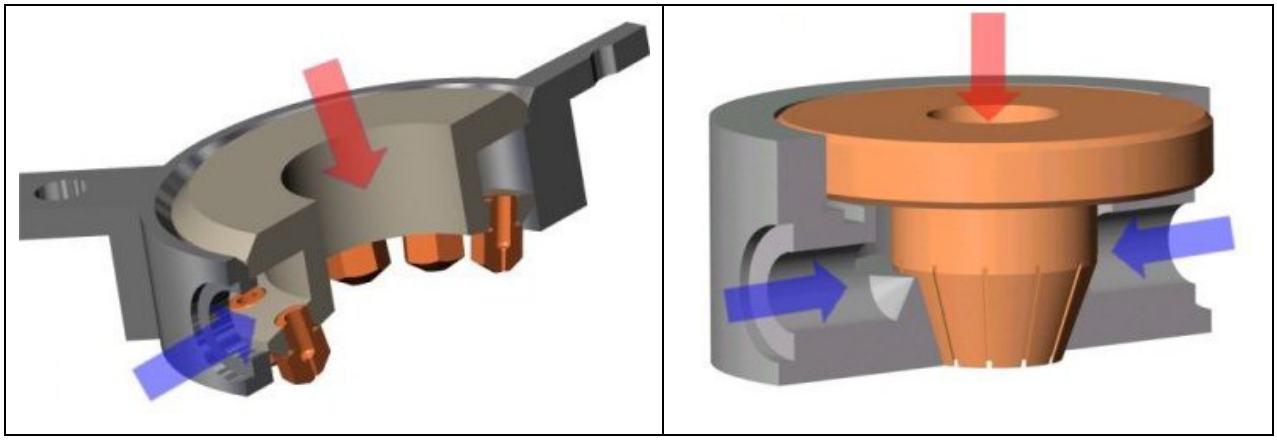
$$d_L = 0.9614 \cdot \left(\frac{k^2 \cdot \sigma^2}{\rho_G \cdot \rho_M \cdot u_r} \right)^{1/6} \cdot \left[1 + 2.6 \cdot \eta_M^2 \cdot \left(\frac{k \cdot \rho_G^4 \cdot u_r^7}{72 \cdot \rho_M^2 \cdot \sigma^5} \right)^{1/3} \right]^{1/5} \quad \text{(m)} \qquad (8)$$

$d_p = \left(\frac{3 \cdot \pi}{\sqrt{2}} \right)^{1/3} \cdot d_L \cdot \left[1 + \frac{3 \cdot \eta_M}{(\rho_M \cdot \sigma \cdot d_L)^{1/2}} \right]$ (9)	Weber has found the diameter of primary drops assuming that at the breakup point the amplitude was equal to the radius of the ligament and only one-drop was produced per wavelength.
$We = \frac{\rho_G \cdot u_r^2 \cdot d_p}{\sigma}$ (10)	The stability of primary drops that moves into gaseous atmosphere depends mainly of the ratio between aerodynamic forces that tend to deform the drops and the surface tension that maintain the spherical shape of drops. This stability it is quantified by the Weber criteria:
$d_{cr} = \frac{16 \cdot \sigma}{\rho_G \cdot u_r^2}$ (11)	Gordon [1] has calculated the critical diameter of drops, which are undergoing to secondary disintegration, the equation being known as the stability criterion.
$\tau_f = \frac{2 \cdot d_p \cdot \rho_M^{1/2}}{\left(\rho_G \cdot u_r^2 - \frac{16 \cdot \sigma}{d_p} \right)^{1/2}} + \frac{32 \cdot \eta_M}{\left(\rho_G \cdot u_r^2 - \frac{16 \cdot \eta_M}{d_p} \right)}$ (12)	Stability criterion with breakup time determines the size and shape of powder particles resulted after the secondary disintegration. The breakup time can be calculated with the equation proposed by Gordon [1]:
$\tau_r = \frac{d_p \cdot \rho_M \cdot C_{pM}}{6 \cdot h_c} \cdot \ln \left[\frac{T_M - T_G}{T_{top} - T_G} \right]$ (13) $\tau_s = \frac{d_p \cdot \rho_M}{6 \cdot h_c} \cdot \left[C_{pM} \cdot \ln \left(\frac{T_M - T_G}{T_{top} - T_G} \right) + \frac{\Delta H}{(T_{top} - T_G)} \right]$ (14) $h_c = \frac{k_G}{d_p} \cdot \left(2 + 0.6 \cdot \mathrm{Re}^{0.5} \cdot \mathrm{Pr}^{0.33} \right)$ (15)	The breakup time must be less than the total solidification time, which is sum of the time required for cooling the droplets to the melting point and the time required for solidification. This condition to ensure secondary disintegration is given by the following equations developed by Naida and Nichiporenko [1]:
$\tau_{sph} = \frac{3}{4} \cdot \frac{\pi^2 \cdot \eta_M}{V_p \cdot \sigma} \cdot \left(r_1^4 - r_2^4 \right)$ (16)	The shape of powder particles it is function of the spherodization time, calculated also by Naida and Nichiporenko.

For **empirical correlations** we have considered a model proposed by Kishidaka and Ternovoj [2], corresponding to water atomization process – equation (17) and for gas atomization we can consider the equation (18) developed by Lubanska and modified by Rao and Mehrotra [1]:

$$d = k \cdot \frac{\eta_M^{0.35} \cdot \dot{M}_M^{1.24}}{\sigma^{0.15} \cdot D_t^{1.03} \cdot \rho_M^{0.56} \cdot \rho_w^{0.25} \cdot \eta_w^{0.07} \cdot u_w^{0.96} \cdot \sin(\alpha)^{0.96} \cdot \dot{M}_w}$$	(17)	water atomization process
$$\frac{D[1,0]}{d_0} = k \cdot \left[\left(1 + \frac{\dot{M}_M}{\dot{M}_G} \right) \cdot \frac{\nu_M}{\nu_G \cdot We} \right]^{m_\alpha}$$	(18)	gas atomization process

Beside the elaboration parameters considerate in modeling process is evaluated also the performance of the atomizing nozzle in order to establish the optimum nozzle geometry, to increase the momentum impact of the fluid atomization on the molten stream.



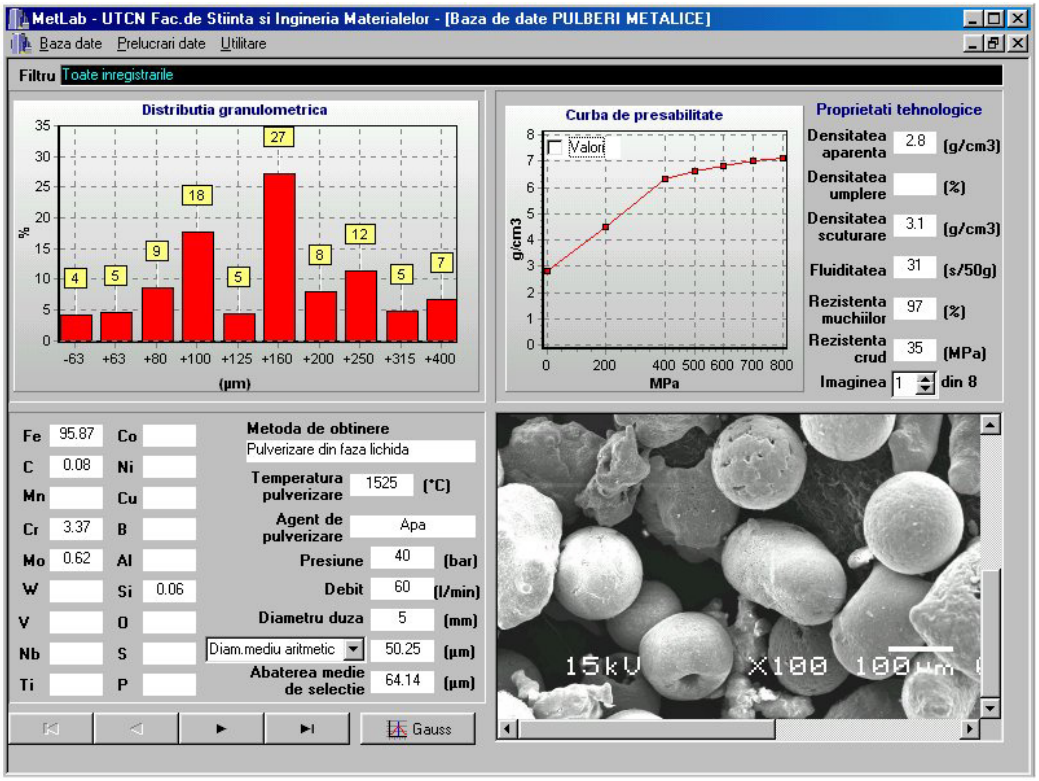


Figure 4. *The window for navigation data*

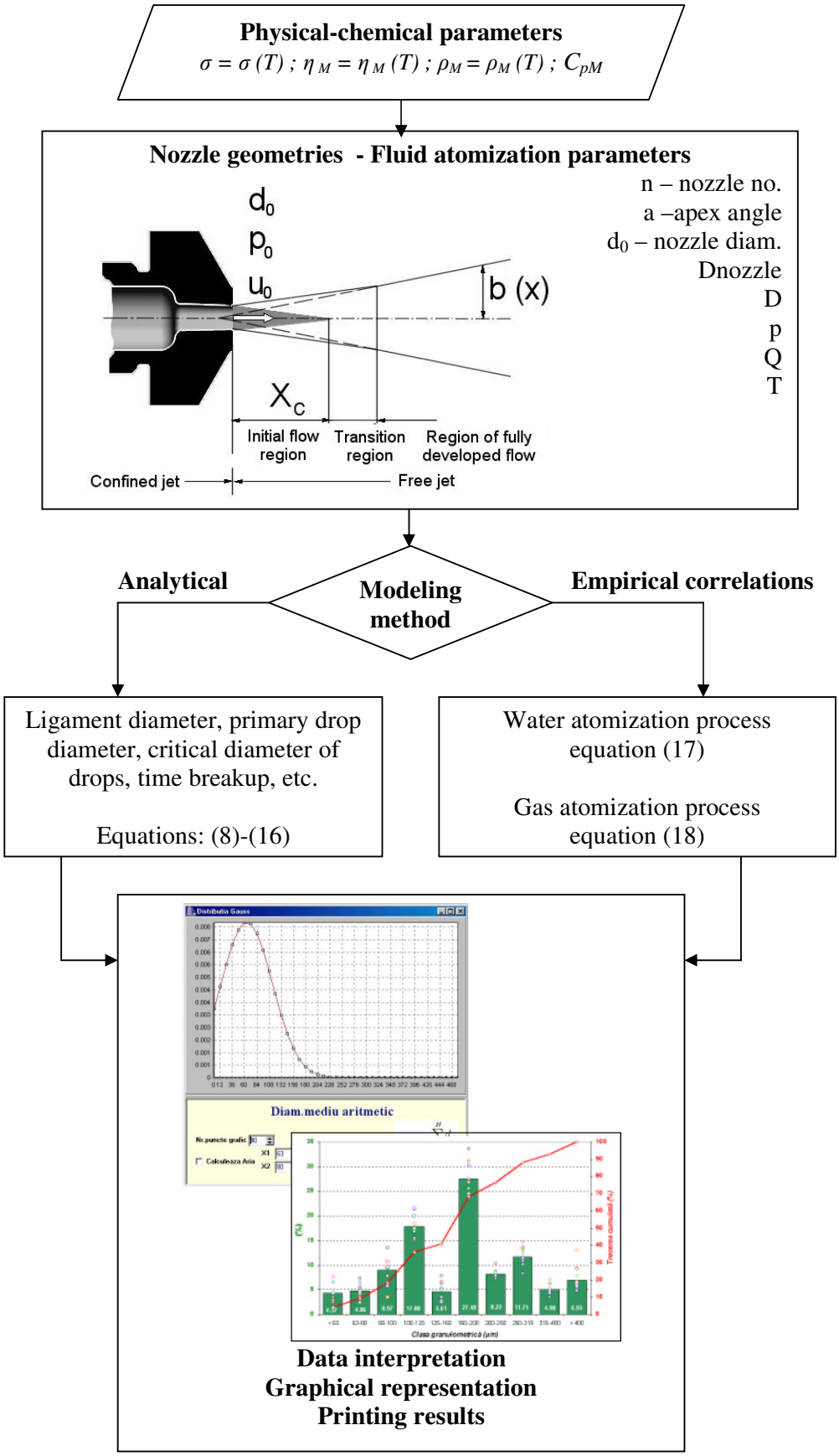


Figure 2. *The logical scheme for MetLab program*

List of Symbols

C_{pM}	Heat capacity of melt
d	Particle size
d_{cr}	Critical diameter – Gordon
d_0	Atomization nozzle diameter
d_i	Particle diameter for class i, where i=$\overline{1...N}$
d_L	Ligament diameter
d_p	Diameter of primary drop
D_t	Tundish nozzle diameter
$D[1,0]$	Number-length mean
$D[2,0]$	Number-surface mean
$D[3,0]$	Number-volume mean
$D[2,1]$	Length-surface mean
$D[3,1]$	Length-volume mean
$D[3,2]$	Surface Area Moment Mean (Sauter Mean Diameter)
$D[4,3]$	Volume Moment Mean (De Brouckere Mean Diameter)
h_c	Heat transfer coefficient
k	Nozzle coefficient – for fluid atomization
k_G	Conductivity of gas
$\dot{M}_M, \dot{M}_G$	Mass flow rate for metal respectively for gas atomization
n_i	Particles number from i class
Pr	Prandtl number
Re	Reynolds number
r_1 , r_2	Radius of drop before/after transformation to spherical shape
T_M , T_G	Temperature of melt , respectively of gas atomization
T_{top}	Melting point of metal
u_r	Relative velocity between drops and fluid atomization
V_p	Volume of a droplet
ΔH	Latent heat of fusion
α	Apex angle
η_M , η_G	Dynamic viscosity of melt, respectively of gas atomization
ν_M, ν_G	Cinematic viscosity of melt, respectively of gas atomization
ρ_M , ρ_G	Density of melt , respectively of gas atomization
σ	Surface tension of melt
τ_f	Disintegration time for primary drops
τ_r	Time required for cooling the droplets to the melting point
τ_s	Time required for solidification at solidus
τ_{sph}	Spherodization time corresponding to action of surface tension σ

4. CONCLUSIONS

The METLAB program is a powerful tool that allows the storing, retrieving large quantities of data needed for computer modeling of atomization process. The program offers the tools for a better characterization of powder particles and can improve the analysis of experimental data by using the advantages offered by SQL relational language.

Due to correlations between the fluid dynamics involved in atomization process and powder properties obtained, is possible to improve the nozzle geometry using the METLAB program capabilities.

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