MATHEMATICAL MODELING OF THE FILTRATION PROCESS OF ALUMINUM MELTS

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In this paper we propose optimizing and modeling with a program of active experimentation (PO2), the main specific parameters of filtering process of Al-Mg-Mn alloys (5xxx series). The parameters taken into consideration were: filtration efficiency (η), temperature (z_1), the melt flow rate (z_2), and the initial concentration of impurities (z_3). It was noted that filtration efficiency (η) increases with lowering flow rate and with increasing of the initial concentration of inclusions and declines as temperature increases. Under the working conditions given, have obtained efficiencies of over 98% and the calculated data are very close to the experimental data, the error being 1.659%.

Keywords: mathematical modeling, optimization, filtration, purification, aluminum alloys, recycling

1. Introduction

To obtain a mathematical model as a polynomial of degree two, composed central programs are used [1]. A mathematical model is a description of a system using mathematical concepts which may help to explain a system and to study the effects of different components [2]. Most experimental studies related to filtration are carried out using water due to the difficulties involved handling the hot metal during experiments.

One of the least understood phenomena related to molten aluminum filtration is inclusion re-entrainment. The process of aluminum filtration is semi-continuous in nature [3]. The importance of understanding the phenomena occurring during long-term filtration is basically to predict the filter performance

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and overall filtration efficiency under specific conditions. During this process, the filter accumulates inclusions decreasing its effective porosity, which may lead to clogging or filter aging.

The models to determine the initial filtration efficiency represent a first approximation to obtain the long-term filtration [4]. Inclusions are typically non metallic phases which includes oxides, carbides, nitrides, borides and can be in the form of a particle or of a thin film; in Al-alloys the most frequent type of inclusion is the aluminum oxide, alumina(Al_2O_3) [5]. The main inclusions that occur during melting of aluminum alloy or holding periods prior to casting are aluminum oxide (Al_2O_3) as dispersed particles or oxide films, aluminum carbide (Al_4C_3), magnesium oxide (Mg0), spinel ($MgAl_2O_4$), titanium diboride (TiB_2), aluminum diboride (AlB_2) and titanium aluminide ($TiAl_3$) [6]. The usual removal element is (CFF) -ceramic foam filters, which have an open pore reticulated structure with very high porosity and very high surface area to trap inclusions.

The open foam structures are composed of ceramic material, such as alumina, mullite or silica. Alumina is the most common filter material [7]. The use and the evaluation of the efficiency of ceramic foam filters (CFFs) in the removal of nonmetallic inclusions from molten aluminum have been studied widely in the literatures [8]. The aluminum industry has developed a number of treatment processes to improve metal cleanliness. CFFs are the most commonly applied filtration process and have been used to filter >50% of the world production of aluminum. The filtration efficiency is defined based on particle counts (either total or grouped into suitable size ranges) [9]:

$$\eta = \frac{Ci - Cf}{Ci} \bullet 100 \qquad (1)$$

Where C_i is the concentration of particles entering into the filter per unit time, and C_f is the count of particles out of the filter per unit time.

2. Experimental

To determine the optimal conditions for filtration efficiency, a program of active experimentation, namely an orthogonal second-order program (PO2) was used [10]. The preliminary studies and researches highlighted the following parameters that have significant influence on process performance: filtration efficiency (η), temperature (z_1), the melt flow rate (z_2), and the initial concentration of impurities (z_3), the other parameters - which have not a significant influence, are maintained at constant values. The experimental data from the filtration of molten AA 5083 alloy and the work matrix are presented in Table 1.

Table 1

The parameters of the filtering process, and the working matrix

Sample	Process parameters (encoded units)			Process parameters (unencoded units)			Filtration efficiency η, %
	Temp. x_1	Flow rate x_2	Initial concentration, C_i x_3	Temp. °C	Flow rate $cm.s^{-1}$	The initial concentration of the inclusions, C_i, ppm	
1	-1	-1	-1	700	0.05	500	87.4
2	+1	-1	-1	780	0.05	500	86.9
3	-1	+1	-1	700	0.29	500	73.2
4	+1	+1	-1	780	0.29	500	66.7
5	-1	-1	+1	700	0.05	700	86.9
6	+1	-1	+1	780	0.05	700	85.5
7	-1	+1	+1	700	0.29	700	62.1
8	+1	+1	+1	780	0.29	700	61.7
9	0	0	0	740	0.17	600	98.1
10	0	0	0	740	0.17	600	97.5
11	0	0	0	740	0.17	600	96.6
12	0	0	0	740	0.17	600	96.2
13	0	0	0	740	0.17	600	95.4
14	-1.471	0	0	681.16	0.17	600	98.1
15	+1.471	0	0	798.84	0.17	600	97.3
16	0	-1.471	0	740	0.00652	600	88.7
17	0	+1.471	0	740	0.34652	600	57.2
18	0	0	-1.471	740	0.17	452.9	89.0
19	0	0	+1.471	740	0.17	747.1	88.2

The AA 5083 alloy (4.65% Mg, 0.49% Mn, 0.28% Fe, 0.15%Si, 0.11%Cr) was melted in an electric resistance furnace at 700-800^{0}C and TiB_2 (as AlTi5B1 master alloy) "synthetic inclusions" [11] was added into the melt. The liquid alloy was stirred and filtered through a ceramic foam filter (50 ppi, 50 mm thick and 50 mm diameter). The filtered alloy was collected over a specific period of time, determining in this way its weight and the flow rate. The concentration of TiB_2 particles was determined by quantitative spectrographic analysis of boron and titanium. The melt rate was 0.05-0.29 $cm.s^{-1}$. The filtration efficiency was calculated with equation (1).

The optimization problem is to find the model parameter values that are consistent with the prior information, and give the smallest misfit or prediction error with the observed data (or, in a statistical). An amazing variety of practical problems involving decision making (or system design, analysis, and operation) can be cast in the form of a mathematical optimization problem, or some variation such as a multi-criterion optimization problem. Indeed, mathematical optimization has become an important tool in many areas. It is widely used in engineering, in electronic design automation, automatic control systems, and optimal design problems arising in civil, chemical, mechanical, and aerospace engineering [12].

A problem of great importance is to find optimal operating conditions for example, the temperature (T) and the concentrations of the various reactants which gave maximum yield (y) [13]. As shown by Box and Wilson since 1951, such a program is obtained by adding a first-order program type *EFC* 2^n (*EFC = complete factorial experiment*) with certain points of the factorial space. In these conditions result:

$$N = N_c + N_\alpha + N_0 \tag{2}$$

Where: N - represents the total number of points in the PO2 program; N_c - number of experiences in a *EFC* 2^n ($N_c = 2^n$) program or a *EFF* 2^{n-p} subprogram if $n > 4$ ($N_c = 2^{n-p}$); N_α - number of so-called "star points" ($N_\alpha = 2n$); N_0 - number of determinations in the core of the program (parallel or repeated measurements) ($N_0 = 5$ was chosen) [13].

Since $n = 3$ are obtained:

$$N_c = 2^3 = 8,\ N_\alpha = 2\cdot 3 = 6,\ N_0 = 5 \text{ and therefore } N = 19 \tag{3}$$

The steps taken in the development of the PO2 program were the following:

a) Based on the results obtained in previous experiments was chosen as the base of experiment the point from factorial coordinates space: $z_1^0 = 740^oC$; $z_2^o = 0.17\frac{cm}{s}$; $z_3^o = 600ppm$, and as variation intervals, the sizes: $\Delta z_1 = 40^oC$, $\Delta z_2 = 0.12\frac{cm}{s}$, $\Delta z_3 = 100ppm$.

b) Using these parameters was determined the values of factors in the 8 points of the program *EFC* 2^3, program that is part of *PO2*, using the relations:

$$z_i^{(-1)} = z_i^0 - \Delta z_i; \qquad z_i^{(+1)} = z_i^0 + \Delta z_i. \tag{4}$$

c) The coordinates of the six "star points" ” ($z_i^{(-\alpha)}, z_i^{(+\alpha)}$) were established using parameter α ("arm star"), whose value was determined by the bipartite equation:

$$\alpha^4 + 2^n\alpha^2 - 2^{n-1}(n + 0{,}5N_0) = 0, \tag{5}$$

respectively

$$\alpha^4 + 8\alpha^2 - 22 = 0. \tag{6}$$

Detailed calculations according to the PO2 program are shown below.

3. Mathematical modeling

3.1. Initial conditions

Mathematical modeling is performed using software MathCAD v.13.

Calculation of α

$N := 19,\ \ i := 0..N-1,\ \ n := 3,\ \ l := 0.5..(n+1)(n+2),\ \ r_0 := 5, \qquad \propto := \sqrt{-4+\sqrt{38}}$

$f(\alpha) := \alpha^4 + 2^n.\alpha^2 - 2^{n-1}(n+0.5r_0)$

$r := root(f(\alpha), \alpha)$

$r = 1.471$

According to the initial data the programming matrix is presented in Table 2.

Table 2

Programming matrix

$x_{i,0} :=$	$x_{i,1} :=$	$x_{i,2} :=$	$x_{i3} :=$	$y_i :=$
1	-1	-1	-1	87.4
1	1	-1	-1	86.9
1	-1	1	-1	73.2
1	1	1	-1	66.7
1	-1	-1	1	86.9
1	1	1	1	85.5
1	-1	-1	1	62.1
1	1	1	1	61.7
1	0	0	0	98.1
1	0	0	0	97.5
1	0	0	0	96.6
1	0	0	0	96.2
1	0	0	0	95.4
1	−α	0	0	98.1
1	α	0	0	97.3
1	0	−α	0	88.7
1	0	α	0	57.2
1	0	0	−α	89.0
1	0	0	α	73.2

Coefficients calculation

$x_{i,4} := x_{i,1}.x_{i,2} \quad x_{i,5} := x_{i,1}.x_{i,3} \quad x_{i,6} := x_{i,2}.x_{i,3}$

$x_{i,7} := x_{i,1}^2 - \frac{\iota[\sum_i (x_{i,1})^2]}{N}$ $x_{i,8} := x_{i,2}^2 - \frac{\iota[\sum_i (x_{i,2})^2]}{N}$ $x_{i,9} := x_{i,3}^2 - \frac{\iota[\sum_i (x_{i,3})^2]}{N}$

$b_{i,j} := \frac{\sum_i (x_{i,j} \cdot y_i)}{\sum_i x_{i,j}^2}$

$b =$

	0
0	84.879
1	-0.809
2	-10.491
3	-1.555
4	-0.625
5	0.6500
6	-1.775
7	-1.402
8	-12.836
9	-5.606

$b^T =$

	0	1	2	3	4	5	6	7	8	9
0	84.879	84.879	84.879	84.879	84.879	84.879	84.879	84.879	84.879	84.879

3.2. Statistical analysis of the model

$Y_i := \sum_j (b_j . x_{i,j})$ $a := \frac{1}{N} \sum_i (x_{i,1})^2$ $a = 0.649$

$v_{\_repetat} := \begin{pmatrix} 88.89 \\ 86.14 \\ 86.88 \\ 87.74 \\ 84.98 \end{pmatrix}$ $D0 := Var(v\_repeatedly)$ $D0 = 2.232$ $Dcon := \frac{\iota.[\sum_i (y_i - Y_i)^2]}{N-1}$

$Dcon = 5.712$

$F_c := \frac{Dcon}{D0}$ $F_c = 2.56$ $FT := qF(0.95, N-1, 4)$ $FT = 5.821$

Fc<FT, therefore the mathematical model is suitable and can be used for optimization purposes.

3.3. Canonical form of regression equation

$B11 := \begin{pmatrix} b_7 & 0.5b_4 & 0.5b_5 \\ 0.5b_4 & b_8 & 0.5b_6 \\ 0.5b_5 & 0.5b_6 & b_9 \end{pmatrix}$ $B11 := \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$ $X_c := -0.5B11^{-1}.B11$

$B11 = \begin{pmatrix} -1.402 & -0.312 & 0.325 \\ -0.312 & -12.836 & -0.888 \\ 0.325 & -0.888 & -5.606 \end{pmatrix}$ $B11 = \begin{pmatrix} -0.809 \\ -10.491 \\ -1.555 \end{pmatrix}$ $X_c = \begin{pmatrix} -0.221 \\ -0.397 \\ 0.089 \end{pmatrix}$

$b0 := b_0 - a(b_7 + b_8 + b_9)$ $b0 = 97.755$

$Ymax := b0 + B1^T X_c + X_c^T B11 X_c$ $Ymax = 99.997$

$a1 := eigenvals(B11)$ $a1 = \begin{pmatrix} -1.364 \\ -5.53 \\ -12.95 \end{pmatrix}$ $z1_0 := 740$ $z2_0 := 0.17$ $z3_0 := 600$

$\Delta z1 := 40$ $\Delta z2 := 0.12$ $\Delta z3 := 100$

$$\eta(x1, x2, x3) := b0 + b_1 x1 + b_2 x2 + b_3 x3 + b_4 x1x2 + b_5 x1x3 + b_6 x2x3 + \\ + b_7(x1^2 - a) + b_8(x2^2 - a) + b_9(x3^2 - a) \quad (7)$$

3.4. Calculation the error of performance (δy)

$Db_j := \frac{D0}{\sum_i (x_{i,j})^2}$ $Db0 := Db_0 + 3aDb_8$ $Db0 = 0.581$

$e := 2^n + 2\alpha^2$ $f := 2^n + 2\alpha^4$ $H := 2\alpha^4[Nf + (n-1)N2^n]$ $E := -2H^{-1}.e\alpha$

$G := H^{-1}[e^2 - N2^n]$ $cov\_b0bii := ED0$ $cov\_biibjj := GD0$

$W_1 := Db0 + Db_2 \sum_{j=1}^{n} (x_{i,j})^2 + Db_8 \sum_{j=1}^{n} (x_{i,j})^4 + Db_5 \sum_{j=1}^{n-1} \sum_{k=j+1}^{n} (x_{i,j})^2 (x_{i,k})^2$

$$Q_i := 2cov\_b0bii \sum_{j=1}^{n} (x_{i,j})^2 + 2cov\_biibjj \sum_{j=1}^{n-1} \sum_{k=j+1}^{n} (x_{i,j})^2 (x_{i,k})^2$$

$$Dy_i := W_i + Q_i$$

$$\eta(x1, x2, x3) := b0 + b_1 x1 + b_2 x2 + b_3 x3 + b_4 x1x2 + b_5 x1x3 + b_6 x2x3 + b_7 x1^2 + b_8 x2^2 + b_9 x3^2$$

$x1op := Xc_0$ $x2op := Xc_1$ $x3op := Xc_2$
$z1op := z1_0 + x1op\Delta z1$ $z2op := z2_0 + x2op\Delta z2$ $z3op := z3_0 + x3op\Delta z3$
$z1op = 731.172$ $z2op = 0.122$ $z3op = 591.134$
$\eta(x1, x2, x3) = 99.997$
$v_1 := Xc_0$ $v_2 := Xc_{01}$ $v_3 := Xc_2$ $j := 1..n$

$$T := Db0 + Db_2 \sum_{j=1}^{n} (v_j)^2 + Db_8 \sum_{j=1}^{n} (v_j)^4 + Db_5 \sum_{j=1}^{n-1} \sum_{k=j+1}^{n} (v_j)^2 (v_k)^2$$

$$R := 2cov\_b0bii\sum_{j=1}^{n}(v_j)^2 + 2cov\_biibjj\sum_{j=1}^{n-1}\sum_{k=j+1}^{n}(v_j)^2(v_k)^2$$

$$Dy := T + R \qquad Dy = 0.623$$

$$tT := qt(0.975\,,\ N-1) \qquad tT = 2.101$$

$$\delta y := tT\sqrt{Dy} \qquad \delta y = 1.659$$

3.5. Practical Efficiency

$$z1op = 731.172 \quad z2op = 0.122 \quad z3op = 591.134$$

$$x1opt := \frac{z1opt - z1_0}{\Delta z1} \qquad x2opt := \frac{z2opt - z2_0}{\Delta z2} \qquad x3opt := \frac{z3opt - z3_0}{\Delta z3}$$

$$\eta(x1opt, x2opt, x3opt) = 99.997$$

$$\eta(x1opt, x2opt, x3opt) - \delta y = 98.338$$

Based on calculations made, in Fig. 1 is shown the response surface of the process performance (filtration efficiency) according to equation (7), for a wide domain (Fig. 1a) and for the studied domain (Fig. 1b), for x1 = 0 which means the temperature of 740^{o}C. Also, are presented the variations of the filtration efficiency for different values of the parameters studied.

Based on the model can be calculated the filtration efficiency depending on the initial concentration of the inclusions, the flow rate of the melt and temperature of the process, and its variation according to any of the parameters at constant values of the other two, is shown in Figs. 2-4.

At 700^{o}C, 740^{o}C and 780^{o}C for flow rates of 0.05 cm/s and 0.17 cm/s and 0.29 cm/s, dependence of filtration efficiency with initial concentration of the inclusions is given in Fig. 2.

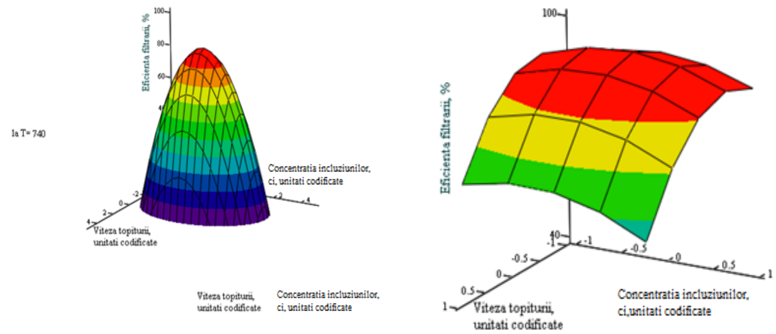

Fig. 1. The efficiency of filtration according to the flow rate and the initial concentration of the inclusions to a temperature of 740°C (The response surface of the objective function (6) for $x1=0$ or t=740°C): for a wide domain a) and for the studied domain b).

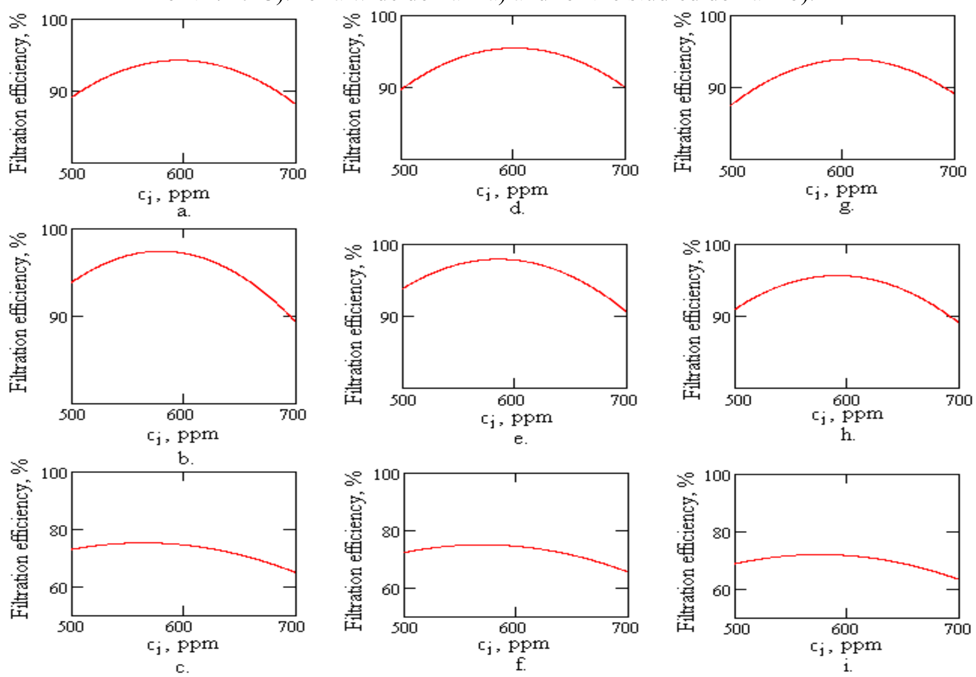

Fig. 2. Filtration efficiency in function of initial concentration of the inclusions at:

a. temperature of 700°C, and flow rate of 0.05cm/s;
b. temperature of 700°C, and flow rate of 0.17 cm/s;
c. temperature of 700°C, and flow rate of 0.29 cm/s;
d. temperature of 740°C, and flow rate of 0.05 cm/s;
e. temperature of 740°C, and flow rate of 0.17 cm/s;
f. temperature of 740°C, and flow rate of 0.29 cm/s;
g. temperature of 780°C, and flow rate of 0.05 cm/s;
h. temperature of 780°C, and flow rate of 0.17 cm/s;
i. temperature of 780°C, and flow rate of 0.29 cm/s;

At 700°C, 740°C and 780°C for initial concentration of the inclusions of 500, 600 and 700 ppm, dependence of filtration efficiency with flow rate is given in Fig. 3.

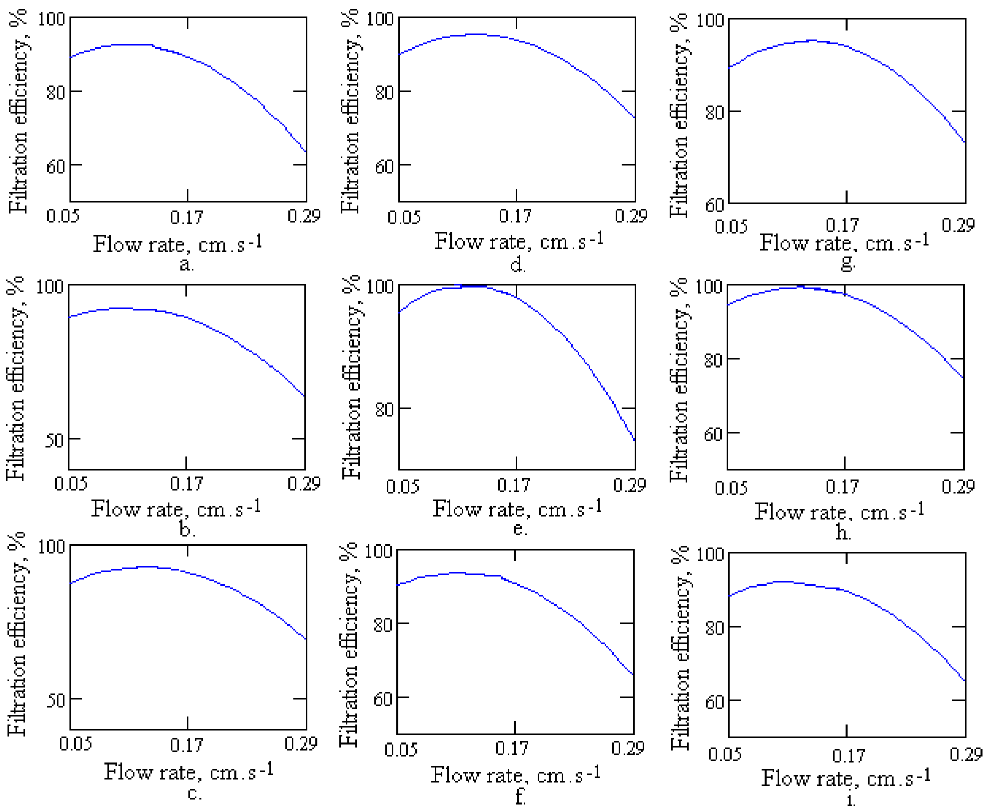

Fig. 3. Filtration efficiency in function of the melt flow rate at:

a. temperature of 780°C, and initial concentration of the inclusions of 700 ppm;
b. temperature of 780°C, and initial concentration of the inclusions of 600 ppm;
c. temperature of 780°C, and initial concentration of the inclusions of 500 ppm;
d. temperature of 740°C, and initial concentration of the inclusions of 500 ppm;
e. temperature of 740°C, and initial concentration of the inclusions of 600 ppm;
f. temperature of 740°C, and initial concentration of the inclusions of 700 ppm;
g. temperature of 700°C, and initial concentration of the inclusions of 500 ppm;
h. temperature of 700°C, and initial concentration of the inclusions of 600 ppm;
i. temperature of 700°C, and initial concentration of the inclusions of 700 ppm;

At 0.05, 0.17 and 0.29 cm/s for initial concentration of the inclusions of 700, 600 and 500 ppm, dependence of filtration efficiency with temperature is given in Fig. 4.

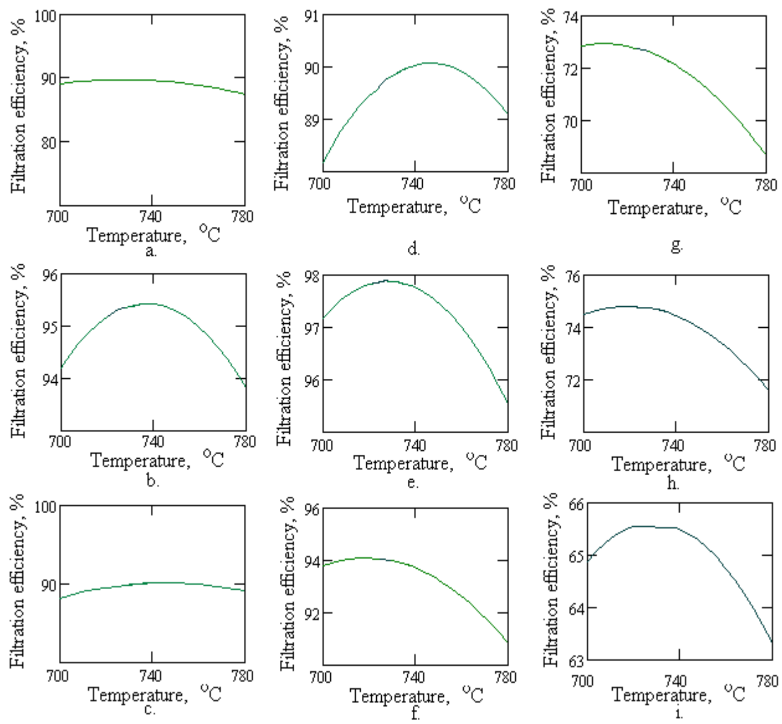

Fig. 4. Filtration efficiency in function of the temperature at:

a. initial concentration of the inclusions of 500 ppm and flow rate of 0.05cm/s; initial concentration of the inclusions of 500 ppm and flow rate of 0.17cm/s; initial concentration of the inclusions of 500 ppm and flow rate of 0.29cm/s; initial concentration of the inclusions of 600 ppm and flow rate of 0.05cm/s; initial concentration of the inclusions of 600 ppm and flow rate of 0.17cm/s; initial concentration of the inclusions of 600 ppm and flow rate of 0.29cm/s; initial concentration of the inclusions of 700 ppm and flow rate of 0.05cm/s; initial concentration of the inclusions of 700 ppm and flow rate of 0.17cm/s; initial concentration of the inclusions of 700 ppm and flow rate of 0.29cm/s;

It was noted that at different concentrations of impurities ranging between 500, 600 and respectively 700 ppm, the optimal flow rates between 0.05 cm/s, 0.17 cm/s and 0.29 cm/s, have different values of the filtration efficiency. To limit the filtering process time - maintaining the metal in liquid state as little time - may be done filtering at higher speeds, but in two or three stages of filtration.

4. Conclusions

Both the studies and preliminary investigations highlighted parameters such as: filtration efficiency (η): temperature (z_1), melt flow rate (z_2) and initial concentration of impurities (z_3) and aimed at achieving their optimization. Thus, filtration efficiency (η) is expected to increase when the flow velocity decreases, will increase with the growth of initial concentration of inclusions and then decreases as temperature is raised. The mathematical model obtained with this program and presented as a polynomial of degree two of three variables, was subjected to statistical analysis, and based on the Fisher criterion was found the correlation between the model and experimental data. The mathematical model being suitable was passed finally to the establishment optimum regimen namely, determining the process parameters that lead to maximum filtration efficiency. The maximum efficiency calculated is 99,997%. Since the calculation error of performance of the process for the considered regime has value 1659, the process efficiency that will be taken into account in the design of industrial plant is 98.338%.

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