OPTIMIZATION OF RAPID PROTOTYPING PROCESS BASED ON SIMULTANEOUS DEPOSITION AND POLYMERIZATION USING ANALYTIC APPROACH

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Abstract: *In function of growth in number both of aditive manufacturing applications and development of new technologies, the optimization of several characteristics of these processes is needed, such as reduction of building time and building cost, increase of building accuracy and mechanical strength of parts. Among those technologies, it is found the process of Simultaneous Deposition and Polymerization (SDP), proposed by Cunico in his Master's thesis. This process consists in deposit photopolymeric material in fluid state and simultaneously polymerized by an non-punctual source of UV light. Whereas this process is still in development, it is highlighted the extreme low deposition velocity, as well as the low accuracy. This work applies methods of programming optimizationand numerical modeling of systems in which are concerned in order to reduce cost of equipment working and to increase the deposition velocity. This study considers the follow variables: a) concentration of initiator; b) power of UV light source; c) length wave of light source; and d) deposition depth; Multiobjective optimization methods were applied in this study. As result, we identified range of feasible solutions in addition to identify criterium of defining equipment lamp. In the study related to cost of equipment, it was found 7.5W as the optimal power of lamp, considering maximization of photopolymerization rate and minimization of cost of investiment and operation. The optimization of material formulation consider resulted in a conversion of 80% in 0.26 seconds, while the initial formulation (recomended by supplier) 2 seconds. Finally, the sensibility of optimization system was analyzed, allowing the identify the range of optimal formulation, according to weight attainment.*

Key words: *Aditive manufacturing, Photopolymerization, Simultaneous Deposition and Polymerization*

1. INTRODUCTION

Besides new necessities of market, as such as the reduction of time of development of new product and the increase of components complexity, additive manufacturing technologies, which are also known as rapid prototyping technologies, have been target of researches in order to tackle these new challenges (VOLPATO, 2007; CUNICO, 2011). Among these technologies, it is found the process of simultaneous deposition and photopolymerization (SDP) (CUNICO, 2011) This process is characterized by the deposition of photopolymeric material in liquid state at the same time that a non-punctual source of UV light cures the deposited material, as shown in Figure 1.

As consequence of his precocity stage, the development of this process faces several restrictions, as such low velocity of deposition and accuracy. However, apart from process parameters, as such accuracy of CNC XYZ equipment and extrusion head, the process can be simply optimized by improving of material formulation. Whereas the increase of polymerization rate directly implies velocity of deposition (CUNICO, 2011).

The purpose of this work is to optimize this process by maximizing the polymerization rate of methyl methacrylate initiated by Benzoin methyl ether, 96%. We apply methods of multi-objective optimization for multivariable problems in addition to considering as variables of this study, concentration of initiator, power of source of UV light, wave length of light source and height of deposition (ODIAN, 2004; RAO, 2009).

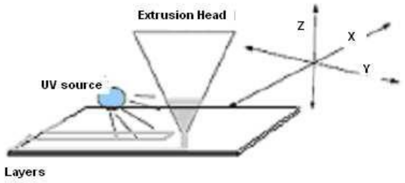

Figure 1 –Illustration of simultaneous deposition and photopolymerization (SDP)

This work was separated in two main stages. The first one is focused on the cost of equipment cost and considers only the power of light source as variable. In this case, both the cost of light source investment and equipment operation are dependent of energy cost, while the second part of study indicates the optimal formulation of material.

On the other hand, the second study emphasizes the optimization of photopolymerization process, considering power of light source, light wave length, and concentration of initiator and height of deposition as variables. The main goal of this study was to identify the point of the maximum value of polymerization rate. However, other secondary objectives are also considered, as such the minimization of concentration of initiator, minimization of power of light source and maximization of light wave length. In function of that, we applied a method of multi-objective optimization for multivariable problems which is know as weighting method (RAO, 2009).

2. Study of cost of equipment

The study of cost of equipment has as main objectives the maximization of polymerization rate and minimization of costs of investment and operation of equipment, being able to be applied as a strong tool for selection of light source of equipment as function of its power.

For proceeding this study, it was considered the same formulation of material, as well as the same light wave length. In the same way, the determination of cost of investment, the price of light source of a family of product has been necessary to find a relationship between power of light source and its price.

The numerical model considers two objective functions: 1) polymerization rate; 2) cost of equipment, which includes the price of light source and the cost of operation of equipment. The constraints of this study were related to the range of power found in the family of lamps used for this work.

With reference to the method of multi*objective optimization, it was applied the weighting method, while for minimization of model, classical methods of optimization, as Modified Newton (RAO, 2009).

2.1. Photopolymerization rate

The process of photopolymerization is the elemental principle of SDP, in which the material in liquid state solidifies at the same time that it is deposited. For regarding the behaviour of material during this process, it can be identify the variation of degree of polymerization along the time. In the Eq. (1), it is possible to see the dependence of polymerization rate on the four variables of our study (D, I_o, α, [A]). Where kp is the constant of polymerization , kt is the constant of termination, [M] is the molar concentration of monomer, [A] is the molar concentration of initiator, D is the height of layer(deposition height), α is the absorption rate, I_o is the luminous intensity, and ϕ is the absorption efficiency, which is considered 1 for non-punctual light source and 2 for laser (ODIAN, 2004).

$$Rp = \frac{kp}{\sqrt{kt}} \cdot [M] \cdot \left(I_o \cdot \alpha \cdot \phi \cdot [A] \cdot e^{-\alpha \cdot [A] \cdot D} \right)^{1/2} \qquad \textbf{(1)}$$

In general, as the luminous intensity is dependent on light wave length and light power. Therefore, it is shown in Eq. (2) an average of values of luminous intensity as function of power of light source and light wave length (ODIAN, 2004).

$$Io = 8{,}36 \cdot 10^9 \cdot P \cdot \lambda \left[mol/cm^2 \right] \qquad \textbf{(2)}$$

2.2. Cost of equipment

In order to determine the relationship of light power and cost related to the investment of equipment, it has been verified the price of lamps of same family of product with the supplier of these products. In other words, all the lamps used in this study provide the same range of light wave length (pick of 295nm) and are fabricated by the same supplier, being supplied in the same base of price. This research is shown in Figure 2, where it is possible to identify the relation between the price and the light power of lamps (PHILIPS, 2006; BULBS, 2011).

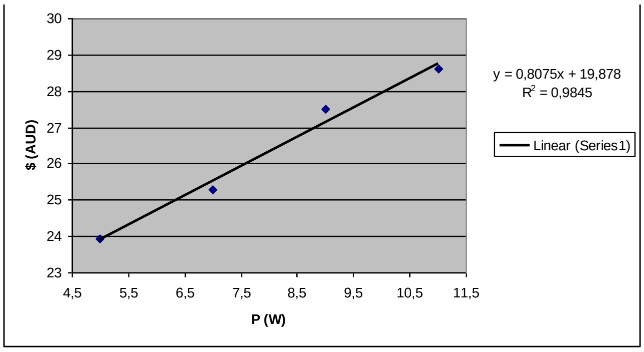

Figure 2 – Analysis of price of lamp as function of light power

As consequence of that, the trend line of this figure shows a linear tendency besides the can be numerically represented in Eq. (3).

$$C_i = 0{,}8075 \cdot P + 19.878 \tag{3}$$

With respect to the cost of operation of equipment, it was directly related to time of operation of equipment. Therefore, it is possible to see that the increase of polymerization rate provide a reduction of time that the equipment is needed in order to polymerize a trajectory of deposition.

It is highlighted by the Eq. (4) that polymerization rate is a variation of molar concentration of monomer as function of time. In that case, the polymerization rate can be used to determine the time that is needed to polymerize a specific quantity of material (ODIAN, 2004).

$$Rp = \frac{-d[M]}{dt} \tag{4}$$

Additionally, defining that the filament deposited must target a specific degree of polymerization in a distance from the centre of nozzle, the time per mm of deposition can be determined and presented in Eq. (5). Where T is the time of polymerization per millimetre (s/mm), Pd is the expected degree of polymerization, and L is the distance from centre of nozzle (mm) that the material is expected to be polymerized (CUNICO, 2011).

$$T = \frac{P_d}{Rp \cdot L} \tag{5}$$

In that way, we could identify the dependency of energy consumption of equipment as function of polymerization rate and light power. Therefore, finding the power of the main components of equipment and the cost of electrical energy per hour, it was possible to define the cost of operation of equipment per millimetre worked.

In Table 1, it is presented the relation of the main components of equipment and their respective power consumption. Nevertheless, the power of light source remain as variable.

Table 1 - Relation of main components of equipment

Main Components	P(W)
Axes motors	33,75
Extruder	11,25
Computer	100
Light source	P
Total	145+P

In addition to that, Equation (6) provides the cost of operation of equipment, finishing the composition of cost of equipment. Where, C_e is the cost of operation (R\$), P is the power of light source (W) and R_e is the service tax of energetic company ($\frac{R\$}{W \cdot s}$) (COPEL, 2011).

$$C_e = \frac{R_e \cdot P_d \cdot (P + 145)}{R_p \cdot L} \tag{6}$$

Finally, the total cost of equipment is presented in Eq. (7), relating the cost of investment and operation of equipment with the power of light source.

$$C_t = C_e + C_i \tag{7}$$

2.3. Optimization

As this study has multiple objectives, it was applied weighting method in order to characterize the optimization problem. The objectives of this problem are the maximization of Rp and minimization of Ct through the variation of power of light source, as described bellow:

Maximize Rp (P) **(8)**

Minimize Ct **(9)**

Subject to:

$$w_1 + w_2 = 1 \tag{10}$$

$$5 \leq P \leq 13 \tag{11}$$

Where w1 is the weight attained for Rp and w2 for Ct.

As consequence of that, the optimization problem is defined in Eq. (12) and (13). In that case, the values of both weights of Eq. (10) were replaced by one single variable, *w*.

$$\min\ f = \frac{w}{R_p} + (1 - w) \cdot C_t \tag{12}$$

Subject to:

$$5 \leq P \leq 13 \tag{13}$$

The values of constants that were applied in this study are represented in Table 2, where is also presented the source of value, as such bibliography.

Table 2 - Values of constants of study

Constants	Values	Value Source
Pd (%)	0,75	Study determination
Kp/Kt^0.5	7,14	(BRANDUP *et al.*, 1975)
M(wt %)	96	Study determination
M (mol/l)	9,38873352	(ALDRICH, 2010)
A(wt %)	4	(JASTY, 1999)
A(mol/l)	0,146703082	(JASTY, 1999)
D (mm)	0,12	(JASTY, 1999)
L (mm)	1	Study determination
Re(R$/kW*h)	0,22	(COPEL, 2011)

The initial value of power of light source was 9 W, while the method for solving the optimization problem was Modified Newton. For a weight of 0.5, which implies the same weight for both of objective functions, we found 7,75W as result. Nevertheless, for analyzing the variation of optimization results as function of weight of objective functions, it was applied an optimal Pareto, which is shown in Figure 3 (RAO, 2009). In that picture, it was presented the relation between costs of equipment, the optimized value of light power and the time that light source need to polymerize 80 % of material, in addition to the variation of weighting was found between 0.3 and 0.75.

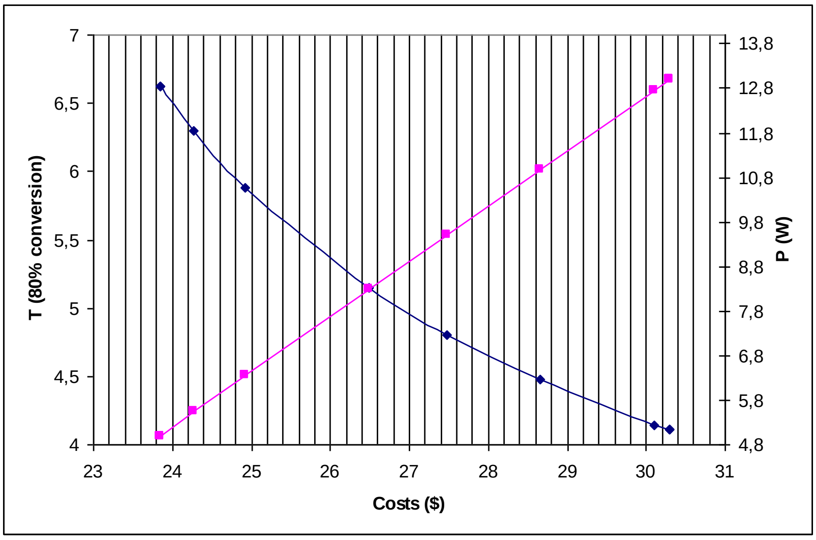

Figure 3 – Curves of optimal Pareto of multi-objective optimization, which highlight the contour edge of feasible solutions (optimum results)

Therefore, this picture allows us to identify criteria for selecting a particular optimized solution, taking in consideration the cost of equipment. Certainly, this resource is shown to be an interesting tool due to the fact that a range of optimum values of power of light source is allowed to be selected by either restriction of cost, time of polymerization or importance over an objective. For example, if the project of product considered a cost of product 2.3 times more important than the velocity of fabrication of parts, the suitable power of light source would be 5 W. Otherwise, the suitable power of light power would be 12,5 W.

Certainly, in this case, it would also be necessary to use another parameter for determining how much a reduction of 2.5 seconds is worthwhile against $6.00. However, a reduction of 50% of time would lead to increase of 50% of deposition velocity.

3. Study of photopolymerization process

The second study approached by this work emphasizes the determination of the best condition of process through the variation of initiator concentration, power of light source, light wave length and height of layer (deposition height). This study is separated in two stages. The first one considers an optimization problem with a single objective while the second, with multiple objectives.

The main objective of the first stage of this study is only maximization of polymerization rate, which is represented in Eq. (1). In addition to that, the second stage has also undergone the maximization of light wave length, as well as the minimization of concentration of initiator and the power of light source.

The values of constants that were used in this study can be seeing in Table 3, which are the same used in the first study. For the first stage, it was applied the method of optimization Modified Newton, while for the second stage, weighting method allied to Modified Newton (RAO, 2009).

In both of cases, it was considered the variation of light absorption as a function of light wave length, whereas this is an intrinsic characteristic of photoinitiator (BRANDUP *et al.*, 1975; JASTY, 1999).

Table 3 - Values of constants of study of photopolymerization process

Parameters	Value
$Kp / Kt^{1/2}$	7,14
M(wt %)	1
M (mol/l)	9,38873352

The absorption rate is a variable that is directly related to light wave length, being possible to be identified by the determination of absorbance of spectroscopic curve of photoinitiator. Therefore, it is possible to determine the absorption rate due to Equation (14) (BRANDUP *et al.*, 1975; JASTY, 1999).

$$absorption = 2{,}3 \cdot \alpha \cdot \left[A\right] \tag{14}$$

The photoinitiator used in this study is Benzoin methyl ether, 96%, whose spectroscopic curve is shown in Figure 4. Therefore, by applying the Eq. (14) and restrict the curve between 250 and 350 nm, we have been able to estimate a numerical equation based on trend line. This equation, which is exposed in Eq. (15), was applied in the model of this study.

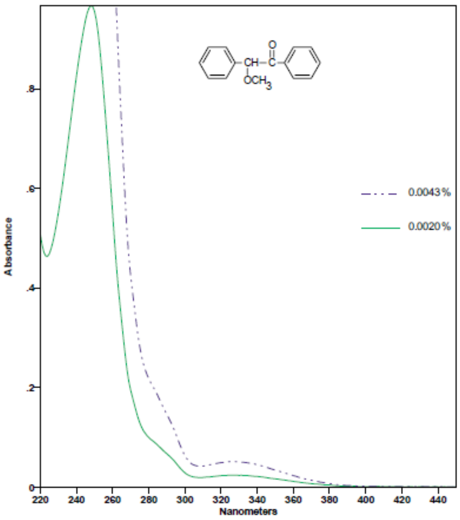

Figure 4 - Spectroscopic curve of photoinitiator Benzoin methyl ether, 96% (JASTY, 1999)

$$absorption = 1{,}08 \cdot 10^{-6} \cdot \lambda^{6} - 1{,}81 \cdot 10^{-3} \cdot \lambda^{5} + 1{,}26 \cdot \lambda^{4} - 465{,}95 \cdot \lambda^{3} + 96966{,}84 \cdot \lambda^{2} - 1{,}07 \cdot 10^{7} \cdot \lambda + 4{,}95 \cdot 10^{8} \qquad \textbf{(15)}$$

3.1. Single objective Optimization

In this stage of study, the optimization problem considered only a single objective, which was the maximization of polymerization rate. The variables of this study are concentration of initiator, height of layer (deposition layer), power of light source and light wave length. The methods of solving the problem was Modified Newton, which considered as initial values of variables, A=0.04, P = 9W, d= 0.12mm, λ = 300nm. Additionally, the error resolution applied in this case was 0.001. The description of optimization problem is shown in Equations {(16), (17), (18), (19) and (20)}

Maximize Rp **(16)**

Subject to:

$$250 \le \lambda \le 300 \qquad \textbf{(17)}$$

$$5 \le P \le 13 \qquad \textbf{(18)}$$

$$1 \le A \le 10\% wt \qquad \textbf{(19)}$$

$$0{,}05 \le d \le 0{,}5 mm \qquad \textbf{(20)}$$

With respect to the results of optimization, the maximum value of instant polymerization rate was 1,816 ml/s. For such value, the time which is needed to polymerize 80% of material is 0.26 seconds. About the values of variables of optimization, it was found A=10%, P=13W, λ=250nm and D=0,05mm, showing that the variables target the limit of each constraints.

Consequently, if the constrains were extended, there is a tendency that the polymerization rate would be increased by the increase of concentration of initiator and power of light source. Additionally, it would also be susceptive to reduction of height of layer. However, the decrease of light wave length would not present such behaviour, whereas the absorbance of initiator is shown to have its maximum value in 250nm. Therefore, the reduction of light wave length would imply the reduction of absorbance, instead of its gain.

In generally, this part of study pointed to better rates of polymerization for thin layers and big quantities of initiator, in addition to source of light more powerful and maximum value of absorbance.

3.2. Optimization of multi-objective optimization

As the second stage of this study considered parameters that interfere on cost, in addition to maximization of polymerization rate, the optimization regard to other objectives, as such the maximization of light wave length, whereas the value of lamps is cheaper when closer of visible range. The other objectives that were applied in this optimization in order to reduce the cost of lamp and material are: minimization of light power and concentration of initiator.

As method for determining the multi-objective optimization problem, it was applied weighting method, while for solving, Modified Newton (RAO, 2009). Considering a resolution error of 0.001, the initial values applied for the variable were, A= 4%, P = 9W, d= 0.12mm, λ = 300nm. Additionally, the description of optimization problem can be seen in equations bellow.

Maximize Rp, λ **(21)**

Minimize A, P **(22)**

Subject to:

$$250 \leq \lambda \leq 300 \tag{23}$$

$$5 \leq P \leq 13 \tag{24}$$

$$1 \leq A \leq 10\%wt \tag{25}$$

$$0.05 \leq d \leq 0{,}5mm \tag{26}$$

$$w_1 + w_2 + w_3 + w_4 = 1 \tag{27}$$

In that case, the cost function were defined and shown in Eq. (28).

$$f(A, \lambda, P, d) = w_1 \cdot \frac{1}{Rp} + w_2 \cdot \frac{1}{\lambda} + w_3 \cdot A + w_4 \cdot P \tag{28}$$

Initially, considering an equal distribution of weighting for all objective function, it was found 1,32ml/s as the result of polymerization rate. This value is provide a polymerization of 80% in 0.35 seconds. As consequence of that, the equivalent values of variable are A = 7.3%; P= 5W; λ= 250nm and D=0.05mm.

In the other side, analyzing the variation of weighting for each objective function, as presented in Table 4, it is possible to identify the effect of weighting of each objective function over the optimum of process. Therefore, this analysis can be used to determine criteria of decision along the development and improvement of process.

Table 4- Relation of optimization results for variation of weighting

Rp	A	P	nm	Minimize f=1/RP+A+P+1/λ				
w1	w2	w3	w4	Rp	P	λ	A	d
0,9	0,03	0,03	0,03	2,882626	13	250	0,1	0,00005
0,03	0,9	0,03	0,03	0,684404	7,3	250	0,01	0,00005
0,03	0,03	0,9	0,03	1,632096	5	250	0,083299	0,00005
0,03	0,03	0,03	0,9	1,841238	6,15	275	0,1	0,00005
0,47	0,47	0,03	0,03	2,245356	13	250	0,060591	0,00005
0,47	0,03	0,47	0,03	1,787729	5	250	0,1	0,00005
0,47	0,03	0,03	0,47	1,787729	5	250	0,1	0,00005
0,03	0,47	0,47	0,03	0,653284	5	250	0,013314	0,00005
0,03	0,47	0,03	0,47	0,726661	6,88	250	0,01197	0,00005
0,03	0,03	0,47	0,47	1,632428	5	250	0,083333	0,00005
0,25	0,25	0,25	0,25	1,632079	5	250	0,07385	0,00005

With reference to the case of heavier weight for minimization of photoinitiator, it was found A = 1 %; P= 7,3W; Λ= 250nm e d=0,05mm as values of variables. Otherwise, in the case of heavier weight for minimize of light power, these values are A = 8.33 %; P= 5W; λ= 250nm and D=0.05mm. In contrast with that, considering the heavier weight for maximization of light wave length, it is found A = 10%; P= 6.15W; λ= 275nm e d=0.05mm

It is important to highlight that the height of layer remain the same independent of weighting of objective functions. It shows that all the optimized solutions of this problem are found by using inferior limit of height of layer provides.

The worst value of polymerization rate was found when the weight was heavier for minimization of initiator. For this case, the time which is needed to polymerize 80% of material was 0.75s.

In comparison with the current status of development of equipment, whose velocity of deposition is 120 mm/min, the new velocity of deposition provided by the best optimized condition of this study would be 230 mm/min. This condition is almost 50% better than the current material, which uses oligomer in formulation.

4. Conclusions

This work allows seeing the optimization of photopolymerization process, and consequently, their contribution for optimization of the SDP. It was possible to identify values of variables that provide optimum responses.

In the first study, it was analyzed the influence of power of light source over the cost of equipment, as well as the polymerization rate. Additionally, it was possible to find 7.75 W as result for a homogenous distribution of weight among the objective functions. In that case, the time needed to polymerize 80 % of material is 5 seconds, in addition to the price of investment is $25.00.

It was also found an optimal Pareto which relates the optimum values of optimization and variable as function of distribution of weights. It makes possible to select the best option in accordance with the importance attained to each objective.

With respect to the first stage of second study, it was identified the maximization of polymerization rate for attaining the maximum values of constraints to light power and concentration of initiator, besides the minimum values to light wave length and height of layer (A=1%; λ=250nm; P=13W, d=0.05mm). In that case, the time which is needed to polymerize 80% of material was 0,26s.

On the other hand, the second stage, which considers an optimization with multiple objectives, allows us to identify the influence of the weight of each objective function over response. When the distribution of weights is homogeneous, the time needed for polymerization of 80 % of material is 0.35 seconds. However, when the heavier weight is found over maximization of polymerization rate, the result is the same of the first stage of this study, 0.26 seconds.

It was also highlighted the influence of height of layer into the photopolymerization process, whereas all results of optimization were obtained at the minimum value of height.

In conclusion, it was possible to determinate sceneries which provide the optimized result as function of polymerization rate and cost of equipment and material, being a strong tool for selection of light source and definition of concentration of initiator.

5. References

ALDRICH. SAFETY DATA SHEET - Methyl Methacrylate. Sigma Aldrich. 2010. Disponível em: <www.sigmaaldrich.com/>. Acesso em: 01/02/2011.

BRANDUP, J., E. IMMERGUT, *et al.* Polymer handbook. **Interscience, New York**. 1975.

BULBS. Germicidal Single. 2011. Disponível em: <www.bulbs.com/>. Acesso em: 01/02/2011.

COPEL. Taxas e Tarifas. 2011. Disponível em: <www.copel.com/>. Acesso em: 01/02/2011.

CUNICO, M. M. W. M. Development of New Rapid Prototyping Process. **Rapid Prototyping Journal**, v.17, n.2, p.6-6. 2011.

JASTY, S. Aldrich Polymer Products Application and Reference Information. Sigma-Aldrich. 1999. Disponível em: <www.sigmaaldrich.com/aldrich/brochure/al_pp_applications.pdf>. Acesso em: 10 jul. 2008.

ODIAN, G. G. **Principles of polymerization**: John Wiley and Sons. 2004

PHILIPS. Ultraviolet Purification Application Information. 2006. Disponível em: <www.lighting.philips.com/>. Acesso em: 01/02/2011.

RAO, S. S. **Engineering optimization: theory and practice**: Wiley. 2009

VOLPATO, N., Ed. **Prototipagem rápida: tecnologias e aplicações**: Edgard Blücher ed. 2007.