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Logistic regression and response surface design for statistical modeling of investment casting process in metal foam production

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Abstract

A metal foam represents a promising material since it keeps the high mechanical properties of the metal while reducing the weight up to 90%. Among several manufacturing processes, the investment casting is a foundry process flexible enough to be suitable both for stochastic and for regular foams. This paper presents an experimental determination of the manufacturing process of metal regular foams by investment casting. The goal is to derive experimentally an actual "formability map". The use of logistic regression and response surface design is proposed as an effective tool for determining a statistical model of the metal foam casting process.

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Keywords: Metal foams; Logistic regression; Generalized linear models; Design of Experiments (DoE)

1. Introduction

The terms cellular metals, or porous metals, are general expressions referring to metals having large volume of porosities, i.e., with pores deliberately integrated in their structure. These materials have low densities and novel physical, mechanical and thermal properties. They are potential materials for lightweight structures, for energy absorption and thermal management applications. They can be divided into closed and open cell structures.

In this paper, the open cell structures are treated. The typical applications of this material are catalytic supports, heat exchangers, filter elements, acoustic absorbers, crash absorbers, etc., because they have special properties, such as the permeability of the open cell structure, high porosity and high ratio of surface area to volume.

When the porosity cannot be subdivided into well-defined cells, the material is usually referred to as *metal sponge*. On the other hand, the terms foamed metal or *metal foam* apply to porous structures whose solid matrix has a large fraction of interconnected, homogenous and *regular* open cells [1].

The open cell metal sponges and foams can usually be made by a foundry process (e.g., sand-casting). The process relies on the casting of the metal around a preform of particles that defines the shape of the porosity in the final material [2]. After cooling, the preform can be removed by solvent leaching. A popular use of this technique utilizes salt (NaCl) as a space holder to produce aluminum sponges and foams [3]. NaCl has several advantages such as being readily accessible, non-toxic and can be removed from the foam by dissolution in water. By having a melting point of 801 °C, it can be used with metals that have a melting point lower than this value.

Substitution of NaCl with higher melting point materials also permits the production of foams from higher melting point metals [4]. This may include other water-soluble materials, or insoluble ones including different types of sand. In this form, the process becomes more like conventional sand-casting processes.

The pore size and porosity of the foam can be varied through selecting appropriate geometry of particles. For example, the Kelvin's structure is considered as a model metal foam with homogenous and regular open cells [5]. To produce this kind of metal foams by sand-casting process, a preform is build by stacking of shaped plates, each containing several polyhedrons. These plates are made of agglomerated sand.

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In general, the infiltration/sand-casting process is simple and with low cost because of the relatively cheap raw materials and simple processing equipment. However, the metal foams produced by this process have a low porosity, only from 50% to 80%.

Metal foams can also be fabricated without directly foaming the metal. The investment casting (a.k.a. lost-wax casting), in which the material is poured into a ceramic cavity designed to create an exact duplicate of the desired part by means of soluble preforms (wax patterns), can also be used as manufacturing process for metallic foams. The ceramic cavity is obtained by investing (surrounding) the wax patterns of a refractory material. The fragile wax patterns must withstand forces encountered during the mould making.

Aluminum alloys are usually used in investment casting mainly due to their high fluidity, but other metals can also be processed. The densities and foam morphologies are of course determined by the preforms. Porosities typically range from 80 to 97%. The investment casting is a foundry process flexible enough to be suitable both for metal sponges (stochastic foams) of sub-millimetric pore size and for periodic (regular) foams with pore sizes of several millimeters.

In the research activity carried out at the University of Salento, an investment casting process was considered in order to produce aluminum alloys foams with homogeneous and regular open cells. Examples of metal foams obtained by in the research are depicted in Fig. 1.

The present paper presents an experimental determination of the investment casting process of metal foams with homogeneous and regular open cells, which are employed as catalytic supports. Basically, catalytic metal foams have to offer low resistance to thermal transport [6], low resistance to mass transfer [7] and needs to be easily coated with a catalytic layer on their surface via dip coating or other loading methods [8]. In this kind of applications, the geometrical characterization of produced metal foam assumes a primary importance. The goal of our research is to derive an actual "formability map" of the investment casting process based on the geometric characteristics of the produced metal foam.

The remainder of the paper is organized as follows. In section 2, the investment casting process is detailed. Section 3 describes the experimental procedure implemented. In section 4, a statistical model of experimental data is presented, while in section 5 the actual results are discussed. Finally, conclusions are provided in section 6.

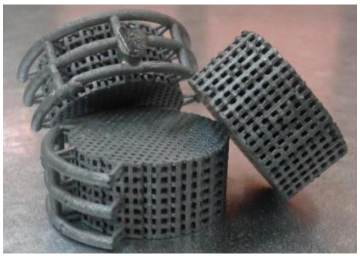


Fig. 1. Example of cylindrical metal foams obtained by investment casting.

2. The investment casting process

In this section, a technique to manufacture metal foams by investment casting is discussed. The starting point is a polymer foam used as prototype (a.k.a. wax patterns). In our work, the polymer foam was processed into a structure with open pores by an additive process (3D printing).

The next step consists of embedding the resulting foam with a special slurry of heat resistant (refractory) material, e.g., a mixture of mullite, phenolic resin and calcium carbonate (plaster). This material is water-soluble and capable of withstanding the temperature of the molten metal under vibrating and tapping.

After embedding, the mould is dried and then baked to harden the embedded material and to decompose (and evaporate) the polymer foam, leaving behind a negative image of the foam. This mould is subsequently filled with molten metal in hot state under a moderate pressure. After solidification and cooling, the mould materials are removed (e.g., by water under high pressure), leaving the metal foam which is an exact image of the original polymer prototype.

A detailed description of the process is presented in the following subsections.

2.1. Polymer foam preparing

A polymer prototype with the desired cell size, and relative density was selected first (Fig. 2). It will be soaked in some organic liquids for minutes before using it as a template, which is helpful to infiltrate the mould obtained from pouring plaster slurry into this foam hereafter by molten metal.

Once a prototype is produced, it is assembled with other components: the runners and sprue gating, to form a casting cluster or assembly (see Fig. 3). The sprue gating is provided by a gate, i.e., the location at which the liquid metal enters the mould cavity.

2.2. Plaster slurry

The entire assembly is then dipped in a plaster slurry (Fig. 4). Since there are some reactions shrinkage and phase transition shrinkage the plaster while it is being dried and baked, cracking and corresponding strength decreasing of the plaster mould will be induced.

Also, it is difficult for plaster to be dissolved in water because the solubility of calcium carbonate in water is limited. So, in order to obtain strong and soluble mould, it is necessary to add some kinds of other materials into the plaster. Mullite and phenolic resin are typically used to increase the strength and solubility. In addition, the agitation during the preparation of plaster slurry is necessary for homogenization.

The speed should be appropriate, because very high speed will induce the slurry spray and gas dissolution to decrease its strength. On the contrary, very slow speed will make it inhomogeneous.

2.3. Plaster drying and baking

The dipping process is repeated until a shell of about 6-8 mm is applied, then the composite is maintained for about 2-3 hours to harden it and finally it is being dried and baked in a steam autoclave to remove most of the polymer foam and the remaining amount of polymer that soaked into the shell is burned out in a furnace.

Fig. 2. Example of polymer foam used as wax pattern in the investment casting and of runners.

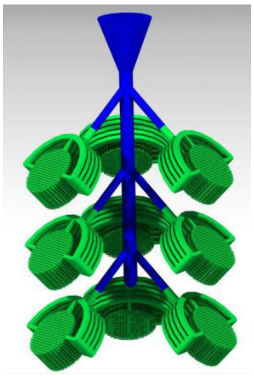


Fig. 3. Example of a sprue gating and runners to form a casting cluster of polymer foams.

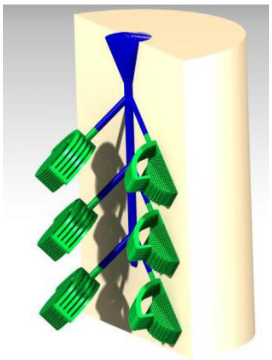


Fig. 4. Example of wax assembly is dipped plaster slurry.

Since heating the plaster mold at high speed will induce cracks, the process of temperature ascending step by step is carried out. The composite is kept at 90 °C for a certain time to remove the water in it slowly. The polymer begins to burn out and evaporates at about 240 °C and this process will continue until the temperature reached at about 500 °C because some of its component are difficult to be evaporated.

2.4. Infiltration process

The plaster mould is infiltrated by molten metal under moderate pressure, with plaster mould preheating temperature of about 500 °C. The pressure applied by combination of compressed air and vacuum suction during infiltration is to overcome the molten aluminum flowing resistance in the mould. After solidification and cooling, the composite of metal and plaster is machined to the desired shape and size. Then the plaster is removed by leaching, leaving the open-cell metallic structures (Fig. 5).

Once the casting has cooled sufficiently, the mold shell is chipped away from the casting. Next, the sprue gating and runners are cut from the casting. After minor final machining post-processing, the castings (identical to the original wax patterns) are complete and ready for use.

3. Experimental determination of the casting process

One of the results of our research activity, is a library of 3D CAD macros implemented in order to support the design process of foamed structures with a large fraction of interconnected, homogenous and regular open cells. The design process is guided by quality specifications of the metallic foam such density and material volume/wettable surface ratio. As a result of the 3D CAD macros implemented, the structure of the foam, its homogeneity and its effective properties can be rigorously controlled.

An example of cylindrical foamed structure is given in following Fig. 6. From Fig. 6, it can be observed that three geometrical parameters are characterizing the cylindrical foamed structure: (i) the size of the external shell bounding the foam (*S*), (ii) the height of the cylinder (*H*) and (iii) the thickness of the open cell (*tk*).

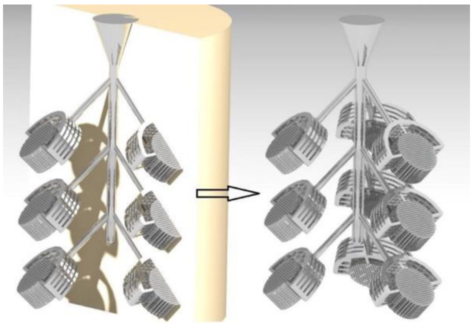


Fig. 5. the plaster is removed by leaching, leaving the open-cell metallic structures.

The aim of the research was to carry out an experimental determination of the investment casting process consisting in performing a set of metal foam casting tests, where the geometric characteristics of the foam (*S*, *H* and *tk*) were changed. After each test, the observed quality of the metal foam was labeled to as 'failed' or as 'safe' point in the set of process parameter combinations (some examples of 'failed' products are depicted in Fig. 7). The goal is to derive experimentally an actual "formability map" of the metal foam casting process.

Starting from a set of experimental tests, the formability map was empirically built using a statistical analysis of collected tests. Statistical approaches are required to properly account for the unavoidable randomness of the failure phenomenon. Linear regression is a very common tool for experimental analysis of data, when the response variable is continuous. If the response variable can assume only a small number of values (i.e., is dichotomous or ordinal), linear regression is unfit to correctly model the data and alternative techniques, such as logistic regression, should be used.

In this work, logistic regression is used as an effective tool for determining a statistical model of the metal foam casting process. Logistic regression, like linear regression, allows estimating the relationship between some predictor variable (the foam geometric parameters *S*, *H* and *tk*) and a discrete outcome. In the case of metal foam casting process, the dependent or response variable is dichotomous, such as failed/safe. In practice, logistic regression allows to directly estimate the probability of failure (or 'risk'), by considering both the failed and safe experimental points in the analysis.

The use of logistic regression for statistical modeling of experimental data should also be combined to appropriate Designs of Experiments (DoE).

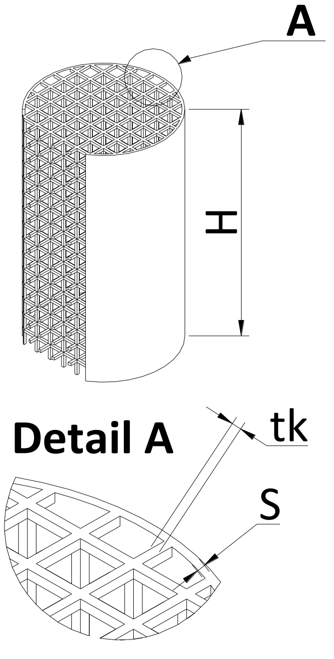


Fig. 6. A cylindrical foamed structure designed with a CAD macro.

Fig. 7. Example of cylindrical metal foams obtained by investment casting.

The Response Surface Methodology (RSM) is widely used for process development and optimization, product design, and as part of the modern framework for robust parameter design. For normally distributed responses, the standard second-order RMS designs have relatively high efficiencies. When the response variable is dichotomous or ordinal (as in the logistic regression) standard RSM is inappropriate and different approaches should be used to construct experimental designs. A widely-used approach to handing a non-normal response as in the logistic regression is fit an appropriate generalized linear model (GLM) to the response data.

4. Optimal designs for generalized linear models

A GLM is an extension of ordinary normal-theory linear regression that encompasses both linear and non-linear models, and admits any response distribution that is a member of the exponential family, which includes the familiar normal distribution, as well as the binomial and the Poisson distributions.

A generalized linear model contains three elements: (i) a response distribution, (ii) a linear predictor that involves the design variables, (iii) a link function that relates the natural mean of the response distribution to the linear predictor. The reader is referred to [9] for a comprehensive presentation on generalized linear models. In this work, we are focusing on: (i) a response distribution which is a binomial in order to model the dichotomous variable (failed/safe), (ii) a linear predictor which is a complete second-order response surface model as follows (where *k* is the number of design variables):

$$\mathbf{x}'\boldsymbol{\beta} = \beta_0 + \sum_{i=1}^{k}\beta_i x_i + \sum_{i=1}^{k}\beta_{ii} x_i^2 + \sum_{i=1}^{k}\sum_{j>i}^{k}\beta_{ij} x_i x_j \tag{1}$$

and a logistic link so that the model the experimenter fits is the familiar logistic regression model as follows:

$$E(y) = \frac{e^{\mathbf{x}'\boldsymbol{\beta}}}{1+e^{\mathbf{x}'\boldsymbol{\beta}}} \tag{2}$$

Now consider finding a DoE for these models, i.e., finding the the *n* experimental points. For the familiar case of a linear model, finding a design involves using one of the standard second-order RSM designs, including the central composite design (CCD) and its variations (the rotatable CCD and the spherical CCD), the Box-Behnken design etc. However, GLMs are non-linear models and the standard designs are not always appropriate. For these scenarios, optimal designs have been suggested and are frequently used in practice. The so called D-optimal design is usually chosen in order to maximize the determinant of the information matrix. Because the information matrix contains the unknown model parameters $\boldsymbol{\beta}$, the problem of finding a D-optimal design for a GLM might be difficult for the process engineer. One approach to the D-optimal design problem for a GLM is to guess or estimate values of the unknown parameters $\boldsymbol{\beta}$. An alternative is to employ a Bayesian approach, which uses a prior distribution to specify the uncertainty in the parameter values $\boldsymbol{\beta}$. Until recently, the construction of a D-optimal design for a GLM with a Bayesian approach was computationally prohibitive.

Gotwalt et al. [10] have recently developed a method that greatly reduces the computing time to implement such an approach and that exhibits excellent numerical accuracy. This procedure is implemented in the nonlinear design routine of SAS JMP commercial software and allows computationally efficient construction of D-optimal designs for nonlinear models. Gotwalt et al. [10] presented examples on this technique. The reader is also referred to [11] for further details on D-optimal designs for GLMs.

5. Second-order response surface design

The nonlinear design routine of SAS JMP was used to construct a D-optimal design for a complete second-order response surface for the logistic regression models of $k=2$ design factors: (i) x_1 the size of the external shell bounding the foam (S) and (ii) x_2 the height of the cylinder (H).

In particular, a value of S ranging between *0.25mm* and *1.00mm* was considered combined to values of H ranging between *15mm* and *60mm*. This design was replicated for two different values of the open cell thickness: *tk=0.4mm* and *tk=0.5mm*. These factor levels are of interest in manufacturing of metal foams used as catalytic supports.

The prior information used on the model parameters was a normal distribution with zero mean and ±3 limits. The fitted model has six unknown parameters (β_0, β_1, β_2, β_{11}, β_{22}, β_{12}), i.e., it is a second-order model in two factors. This model contains an intercept (β_0), two linear terms (β_1 and β_2), two pure quadratic terms (β_{11} and β_{22},), and one cross-product (two-factor interaction) term (β_{12}).

We used a 15-run design. The SAS JMP 15-run Bayesian D-optimal design is shown in Table 1. All the 15 runs are distinct (no replication). Table 1 also reports the coded value for both S and H ranging in [-1,1]. Note that the design was first obtained by the design routine of SAS JMP in coded variables. The actual values of S and H were determined by a linear transformation and approximation to the actual factor level of the real investment casting process.

The column y is related to the actual experimental observation on the cylindrical metal foam obtained by using the design parameters S and H. The value $y=1$ represents a safe product and $y=0$ a failed one.

The same design was replicated for *tk=0.4mm* and *tk=0.5mm*. The only difference observed in the experimental results is related to the case *S=0.35mm H=30mm* where the foam process failed for *tk=0.4mm*, not for *tk=0.5mm*.

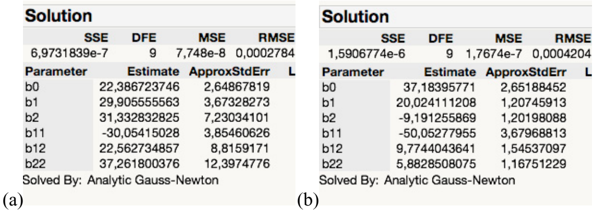
Table 1. 15-run Bayesian D-optimal design for *tk=0.4mm* [*tk=0.5mm*]

S (mm)	*S coded*	*H (mm)*	*H coded*	*y*
1.00	1.000	45	0.309	1
0.25	-1.000	55	0.747	0
0.45	-0.492	60	1.000	1
0.50	-0.290	25	-0.516	1
1.00	1.000	55	0.890	1
0.80	0.428	15	-0.965	1
0.30	-0.874	35	-0.008	0
0.60	-0.127	45	0.282	1
0.80	0.373	35	-0.074	1
1.00	1.000	30	-0.365	1
0.25	-1.000	15	-0.990	0
0.80	0.439	60	1.000	1
0.45	-0.471	45	0.238	1
0.35	-0.723	45	0.288	0
0.35	-0.687	30	-0.426	0[1]

5.1. Discussion

The model parameters fitted on the experimental results are showed in Fig. 8. In both cases (*tk=0.4mm* and *0.5mm*), the most important factors are the linear term and the pure quadratic term related to the S factor (b_1 and b_{11} estimators of β_1 and β_{11} respectively). Fig. 9 and Fig. 10 present the formability maps of the process obtained by SAS JMP on the fitted second-order model. In these figures, the red area represents the failure zone, i.e., the zone where the predicted probability to obtain a safe result is lesser than 90%. It is apparent that operating the process in the vicinity of high value of S presents the best opportunity for safe results.

Fig. 10 (*tk=0.5mm*) shows that values of the coded variable S greater than *-0.5* (i.e., an actual size of S greater than *0.44mm*) allow to obtain a safe result in the process, regardless of the value of the height of the cylinder (H). In order to obtain safe results by using slight lesser values of S, small values of H should also be used. Similar conclusions can be drawn for *tk=0.4mm* (Fig. 9) where coded values of S greater than -0.3 (i.e., an actual size of S greater than *0.5mm*) should be used in order to obtain safe results (feasibility of the process for S closer to *0.25mm* combined to values H closer to *60mm* should be better investigated in the future research).



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Solution
         SSE    DFE       MSE      RMSE
 6,9731839e-7     9  7,748e-8 0,0002784
Parameter         Estimate  ApproxStdErr   L
b0             22,386723746   2,64867819
b1             29,905555563   3,67328273
b2             31,332832825   7,23034101
b11            -30,05415028   3,85460626
b12            22,562734857    8,8159171
b22            37,261800376   12,3974776
Solved By: Analytic Gauss-Newton
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(a)

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Solution
          SSE    DFE       MSE      RMSE
 1,5906774e-6      9  1,7674e-7 0,0004204
Parameter         Estimate  ApproxStdErr   L
b0              37,18395771   2,65188452
b1             20,024111208   1,20745913
b2             -9,191255869   1,20198088
b11            -50,05277955   3,67968813
b12            9,7744043641   1,54537097
b22            5,8828508075   1,16751229
Solved By: Analytic Gauss-Newton
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(b)

Fig. 8. Model fitting parameters for a complete second-order response surface for the logistic regression models for (a) *tk=0.4mm* and (b) *tk=0.5mm*.

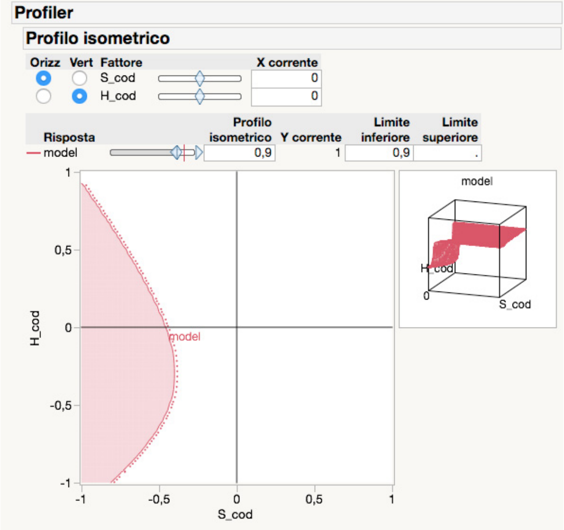

Fig. 9. Prediction profiler and contour plot from SAS JMP: *tk=0.4mm*. The red area represents the failure zone of the process.

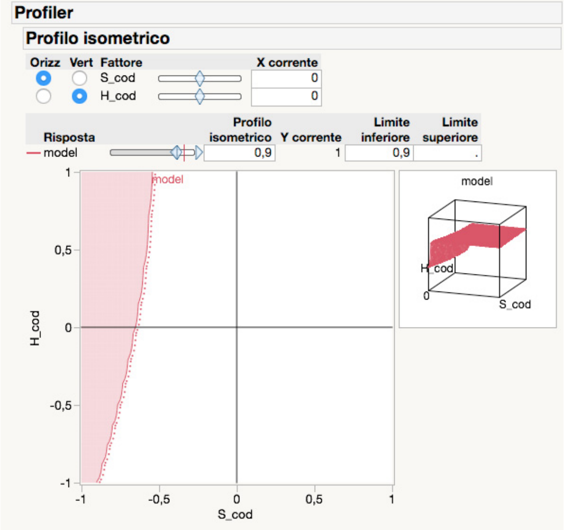

Fig. 10. Prediction profiler and contour plot from SAS JMP: *tk=0.5mm*. The red area represents the failure zone of the process.

6. Conclusions

Investment casting is a foundry process suitable for production of metal foams. In this process, the geometric characteristics of the foam (*S*, *H* and *tk*) are important parameters that may have an influence on the successful production.

The present paper presented an experimental determination of the manufacturing process of metal foams by investment casting. The research goal was to derive experimentally a "formability map". The use of logistic regression and RSM design was proposed as an effective tool for determining a statistical model of the metal foam casting process. In order to handing the non-normal response in the logistic regression an appropriate GLM was fitted to the response data. In this paper, we also demonstrated that modern computer software implementation of the Bayesian criterion makes it relatively straightforward to generate a D-optimal design for the GLM.

From the experimental results, it appears that operating the investment casting process for values of the size of the external shell bounding the foam (*S*) greater than *0.5mm* presents the best opportunity for defect reduction, for any values of the thickness of the open cell (*tk=0.4mm* and *tk=0.5mm*), as well as for any value of the foam height (*H*) ranging between *15mm* and *60 mm*.

However, in the case of an open cell thickness equal to *tk=0.4mm*, feasibility of the process for *S* closer to the minimum value (*0.25mm*) combined to values *H* closer to the maximum (*60mm*) should be better investigated in the future research.

Acknowledgements

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