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Research Article

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Application of the Cell Automata Method to the Brittle Material Thermal Fatigue Fracture Simulation

A.V. Zabolotsky*, L.M. Axelrod

Magnezit Group ltd., 194342, St. Petersburg, Beloostrovskaya str., 17-2-504, Russia

Abstract T An approach to mathematical modeling of cracks appearance and growth in brittle structural materials, used in conditions of thermal load is proposed. For example, technical ceramics and refractory materials. The proposed algorithm is based on a combination of finite element and cell automata methods. An element (automat) inner structure influence on the result of material destruction simulation is considered. The fracture pattern predicted by this method generally coincides with actual damage of the model object (RH-degasser snorkel) under operating conditions.

Keywords Mathematics modeling, finite element method, cell automata method, metallurgy, RH- degasser, brittle material, ceramics, crack growth

1. Introduction

Strength characteristics of refractory materials are measured by standard methods [1, 2], which results are of statistical nature, due to the heterogeneous microstructure of material, which in turn is result of manufacturing method. Typically, a ceramic or refractory material is a combination of filler grains and voids (hexagons and ovals respectively at fig. 1) more or less evenly distributed in relatively uniform matrix (fig. 1.2). The matrix, in turn, is represented by small crystals that have grown together during heat treatment of material at high temperature and voids - micro-level pores. Grains and pores at all levels of material structure, on one hand, are concentrators of thermo-mechanical stresses and, accordingly, sources of crack growth, on the other hand - they are obstacles to the growing crack which can stop its growth.

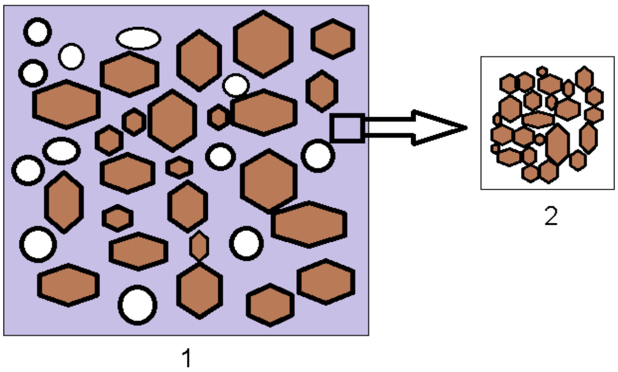

Figure 1: Typical structure of refractory. 1 - macro-level, 2 - micro-level

Thus, refractories strength can vary significantly from product to product, as well as in different areas of the same product. This leads to the knowledge that destruction of refractory materials is also of statistical nature. A technique for behavior analyzing of refractories under service conditions is necessary, linking the arising loads with structure and properties of material, which makes it possible to evaluate probability of destruction and to predict its character.

Thermal destruction of material is a consequence of solid phases thermal expansion. A sudden change in ambient temperature, which leads to mechanical damage of the object, is named "thermal shock". Technical ceramics and refractories are most prone to thermal shock, due to conditions of their service. The operation of such materials occurs at high temperature and is accompanied by rapid cooling and heating.

The nature of thermal shock is uneven temperature change of material different zones with a sudden change of ambient temperature. This leads to an uneven and rapid local change of material geometry, occurrence of mechanical stresses of various directions, and, as a consequence, the appearance or growth of material structure defects (cracks). The ratio of temperature change rate for outer and inner zones of material can be determined using the Bio criterion [3]:

$$\beta = \frac{r_m \cdot \alpha_{he}}{2 \cdot \lambda} \tag{1}$$

where r_m – the characteristic size of material sample (thickness or diameter), α_{he} – heat exchange coefficient for sample surface, λ – sample heat conductivity. At high values of the Bio criterion (more than 20), when the rate of surface heat exchange significantly exceeds intensity of heat removal inside material, the probability of thermal shock and object destruction is high. Also, possibility of thermal destruction of material is determined by the criteria of heat resistance - calculated surface temperature "jumps", leading to appearance of cracks:

$$\Delta T_d = \frac{\sigma_d \cdot (1-\mu)}{\psi \cdot E \cdot \alpha} \cdot S \tag{2}$$

where ΔT_d - the destructive temperature "jump", σ_d – material strength, μ – Poisson's ratio, ψ - a coefficient, characterizing the rate of sample heating (is a function of the Bio criterion and takes values from 0 to 1), E – material elasticity, α – thermal expansion coefficient, S – form factor [4, 5].

The possibility of material destruction under thermal load can also be determined by direct numerical stress modeling [6, 7, 8], or using analytical evaluation [9], which is a development of equation (2):

$$\tau_{ts} = \frac{\sigma_d \cdot \rho_{wl} \cdot c_{wl} \cdot \lambda_{wl}}{\alpha \cdot \Delta T_{mp} \cdot \alpha_{he}^2 \cdot E} \tag{3}$$

where τ_{ts} – a time, needed for stress growth up to the crack-initiation level, ρ_{wl} – dencity of material, c_{wl} – material specific heat, λ_{wl} – sample heat conductivity, ΔT_{mp} – difference between ambient and surface temperature at the process beginning. Crack growth possibility is inversely proportional τ_{ts}, if $\tau_{ts} > 100$ seconds, crack growth possibility becomes << 1.

At the present time engineers have a sufficiently powerful mathematical apparatus that makes it possible to evaluate possibility of materials destruction under certain conditions of thermal loading. It should be noted that one of the most common causes of high-temperature ceramics (refractory) failure, along with chemical and abrasive wear, is thermal shock, capable of disabling equipment at the very beginning of its operation.

At the present time, due to the progress of computer technology, methods of materials high-temperature behavior modeling, requiring numerous computations become important and allow us to determine not only fundamental possibility of material destruction, but also to predict scale and geometric shape of destruction. Such methods include finite element (FEM) [10] and cell automata (CA) methods [11].

FEM is actually the basis of professional software packages for modeling temperature fields and mechanical stresses in structures (ANSYS, Abaqus, etc.). The CA method is currently introducing into engineering calculations, but is already widely used in scientific research.

2. Problem Formulation

2.1. Mathematics Method

The first stage of ceramic or refractory materials thermal destruction modeling is calculation of a dynamic temperature field. In ordinary cases, for samples of a simple geometric shape or a wall of constant thickness [12], iterative methods can be used to calculate it. In the case of stationary heat exchange regimes and complex shape of the object, the relaxation method demonstrates good results [13, 14].

A sufficiently reliable tool for constructing dynamic temperature fields is FEM, which allows transient modeling for bodies of complex shape under influence of multiple sources (sinks) of heat [15]. Within the same method, an algorithm for mechanical stress fields calculating can be implemented. However, cracks appearance forecast is difficult, using FEM.

In this case, the CA method can be chosen, allowing to consider each element of the system, called an automat, as an array, containing information for the state describing of sample corresponding area. The state of this region (automat) is understood as the aggregate of any numerical characteristics (physical parameters: temperature, density, etc., and also degree of destruction). This method variant, called the method of moving cell automata (MCA), allows elements independent movement modeling, in addition, in other words, processes of motion in a solid under mechanical load [7, 16, 17], including complex load (bending, torsion, tearing). In this case, automat compulsory contains data on its motion vector.

One of the main terms of the CA method is concept of "neighbors" which are elements, able to influence changes in the state of an arbitrary cell automat [18]. The degree of influence can be a function of relative location of "neighbors" (for example, influence of neighbors with a common face is different from those that have only a common edge or vertex). An important feature is that in the CA method, "neighbors" can be not only elements that directly border this element, but also separated from it by algorithm specified distance (such model will be considered below). This feature gives an advantage to the method due to the possibility of calculating of mechanical loads at some point on the basis of corresponding vast neighborhood parameters.

The CA method may contain a procedure for temperature field determining, or it can use temperature field, obtained by any other method as initial data for mechanical stresses calculating and material destruction modeling.

2.2. Mathematical model

In this paper, we propose an approach to modeling of the refractory material damage during service process, based on usage of relatively large areas of a heterogeneous body as cell automata, in such a way that each automat has some average characteristics. In the used formulation of the problem, each automat is a porous body (its porosity corresponds to the experimentally determined porosity of a real refractory) with pores evenly distributed in a solid matrix. Models used by authors of [7, 17], does not allow different phases presence inside the same automat (that is why solid and voids were modeled, using different automata). At the present entry FEM was used for temperature field determination, and the CA method was used for mechanical stresses calculation and identification of the structure damaged zones. The problem was solved, using the example of RH-degasser snorkel (the apparatus, widely used in ferrous metallurgy to clean steel from dissolved gases). Two-dimensional case of the problem was considered (Fig. 2).

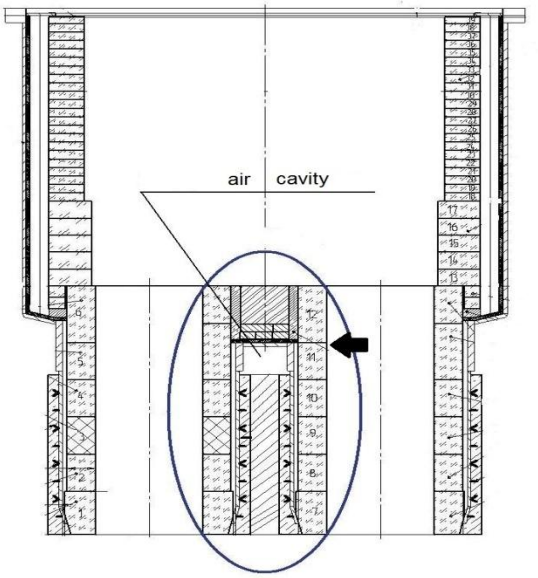

Figure 2: The scheme of the modeled object - RH-degasser snorkels. The calculated area is highlighted by oval. An arrow indicates the location of defects, which photo is shown in Fig. 5.

A dynamic temperature field was calculated, for the system heating from initial stationary state (ambient temperature) to the readiness for metal receive (temperature of the lining working surface - 1100 °C). The heating was carried out in several stages, which were stages of heating and holding at a constant temperature to remove the accumulating thermal stresses, following one after another.

Heat exchange conditions at each surface of the object were taken into account, including an intensive heat exchange in the inner zone of the structure (cooled air cavity, Fig. 2), while dynamic temperature field calculating. Thus, a boundary condition of the first kind was applied for surfaces of the aggregate, contacting heating agent in the inner space - temperature of surfaces was set in accordance with the heating schedule. The third-kind boundary condition was applied for surfaces in thermal exchange with atmospheric air - a law was specified to determine heat transfer rate as a function of installation surface temperature.

The calculation of thermo-mechanical compressive and tensile stresses was carried out in accordance with Hooke's law:

$$\sigma_0 = \Delta T \cdot \alpha \cdot E \tag{4}$$

where σ_0 – thermo-mechanical stress of material, ΔT–temperature change of the calculating element. Calculations take into account stresses in perpendicular directions, the effect of uneven expansion (compression) of adjacent layers of the structure and presence of joints between bricks that are closed during heating due to thermal expansion of refractory.

The process of thermal stress reducing during isothermal exposures is known as stress relaxation. The following relationship is used for fixing resultant stresses [19]:

$$\sigma = \sigma_0 \cdot \exp\left(-\frac{\tau \cdot E}{K_1}\right) \tag{5}$$

Where, σ - real material stress, σ_0 – stress without relaxation consideration (calculated, using equation (4)), τ – time, passed after relaxation begin, K_1 – a variable characterizing the rate of stress relaxation, depending on viscous properties of material. Variable K_1 for ceramic and refractory materials varies from 10^{15} at room temperature down to 10^7 - 10^9 at service temperature (1550 - 1700 °C) [20]. Possible methods of K_1 calculating and experimental determination are considered in [8].

Thus, each cell automat in the developed algorithm is characterized by the following set of values:

$$X \quad Y \quad Z \quad T \quad [\sigma] \qquad E(T) \quad N(\tau) \quad K_1(T) \quad \alpha(T) \tag{6}$$

In addition to geometric coordinates (X, Y, Z), temperature (T), mechanical stress tensor ([σ]), elastic characteristics (E(T)) and expansion coefficient (α(T)), this mathematics matrix contains value of K_1(T) and characteristic of the accumulated stresses N(τ).

For fracture modeling, it was necessary to develop an "averaged" model of material structure on the basis of data on its porosity. The "averaged" model assumes presence of same size pores, evenly distributed in homogeneous solid matrix. The crack penetration through an arbitrary automat is equivalent to breaking walls between pores in thinnest sections at a length equal to the geometric dimension of the automat. This mechanism of crack formation is presented at Fig. 3.

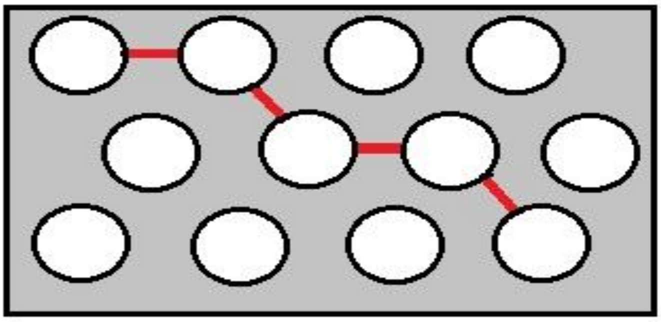

Figure 3: Crack growth scheme, used for modeling

Several models of crack propagation have been considered, for example, such as simultaneous destruction of all walls when one of mechanical stress components in the automat reaches the value of material strength, measured experimentally. However, this and similar schemes led to total destruction of the object, which have no experimental confirmation. For example, modeling with the described criterion resulted in a simulation of the destruction of more than 20 % of automata only while the preheating stage. Such a degree of destruction for ceramics, makes is unfitness to further use and is considered to be complete destruction [21]. Undoubtedly, such patterns of destruction are not observed at the stage of preheating of metallurgical equipment.

As a result, the fatigue thermal destruction model of material was chosen as the working one. Its essence lies in the following: thermal stresses arising in the automat due to its own expansion or contraction, calculated according to von Mises, as well as the influence of "immediate neighbors" [18], are concentrated in one of the walls between pores until they reach a value, sufficient for it destruction (it is expected that there are no structural defects in these walls). A thermodynamic approach was used (the thermal displacement method [22]) for calculating of the stress magnitude, required to break a single wall. Tables [23] were used as an initial data for theoretical strength of refractory calculating. At the moment of one wall destruction inside the automat, stress magnitude is reset in it and in automata, considered to be "neighbors from the area of influence", including not only immediate neighbors (it means the Moore's neighborhood, the order of which was determined at the stage of model validation). According to [24, 25], automat region of influence has the same order of geometric size as the automat itself.

Complete destruction of the automat occurs after destruction of all walls between pores at the maximum geometric size of it. In case of rectangular elements, maximum size is diagonal of the figure. The choice of maximum geometric dimension as a characteristic is dictated by the fact that direction of crack growth before calculation begins is unknown. Thus, when the maximum geometric dimensions are used, the crack growth rate is obtained underestimated, except if direction of its growth coincides with the automat diagonal, and when automat side length is used as a characteristic dimension, fracture rate is higher than actual, if the crack is not perpendicular to one of cell sides. The parameter $N(\tau)$ is the counter of broken walls inside automat. When $N(\tau)$ reaches the critical value - destruction of all walls, automat is excluded from calculation and marked as completely destroyed.

This model is a kind of models of fatigue failure [26]. In other words, mechanical stress in automat increases cyclically up to a certain critical value, after which it decreases down to zero. The complete destruction of material (automat) is observed after a certain number of such cycles.

3. Problem Solution

The verification of this fracture model was carried out by a computational experiment that simulated preheating of RH-degasser snorkel. $MgO-Cr_2O_3$ system products have been used as the working (internal) lining of snorkels (these material is widely used for service in thermal shock conditions, including working lining of metallurgical degassers). High-alumina, heat-resistant concrete is commonly used at the outer layer of the lining. Thermal properties of lining materials were determined in accordance with [27], and their elastic characteristics with tables [28].

Standard preheating of degasser lining is carried out for 44 hours with several isothermal exposures to remove thermo-mechanical stresses. As a result of this heating, temperature of the lining working surface becomes 1100 °C.

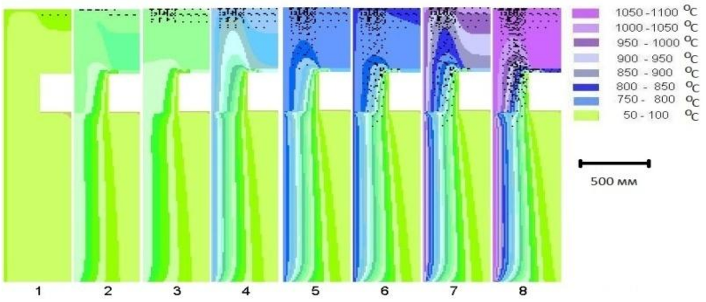

Figure 4: Results of CA method usage - a combination of temperature field with destruction map

The dynamic temperature field was calculated by FEM. Further, the obtained temperature fields were used as an initial data for modeling of thermal cracks formation and growth with the CA method. Pores size for "averaged" structure model was chosen based on material porosity, so that total porosity of model corresponded to the experimentally measured value, and number of stress accumulation cycles before automat was completely destroyed was 100. The size of zone inside which stresses were zeroed upon the destruction of one wall, was equal to 4 linear dimensions of the automat (Moore's neighborhood of the 4th order). Automata themselves were of square shape with side of 10 mm.

Results of calculations were presented graphically - diagrams of temperature field with zones of destruction applied to it. Damaged and completely destroyed automata were distinguished by contrasting points. The successive development of fractures is shown in Fig. 4. Color temperature field is graduated in Celsius.

At the first stage, approximately during the first three hours of heating at a rate of about 15 °C/h, the greatest increase in stress is observed at a distance of 230-400 mm from the vertical working surface and about 30-40 mm from the horizontal surface (Fig. 4.1). Further, 16 hours after the heating start, when temperature rise rate becomes 100 °C/h, the layer, close to horizontal lining surface, is damaged (Fig. 4.2). At the end of this heating stage (19-20 hours), penetration of the damaged zone into interior of the object is observed up to 200 mm (Fig. 4.3), Temperature of the lining working surface is about 300 °C at the moment. Formation of an extensive horizontal damage zone is completed at 25 - 28 hours of heat treatment with surface temperature of 600-700 °C (Fig. 4.4). Later, a vertical damage zone with a high defect density near the upper corner of the inner cavity is formed (Fig. 4.5 - 36 hours, 4.6 - 39 hours, 4.7 - 42 hours, 4.8 - 44 hours).

Complete destruction (as a result of preheating) is observed only in 4 automata, located in the object's upper layer, near the junction of vertical and horizontal working surfaces. In addition, a high density of damages is observed along the internal bisector of angle between these surfaces and in the upper corner of inner cavity vicinity. In fact, real object in the process of operation also demonstrates chipped corners, cracking of the upper corner bricks along the bisector and horizontal cracking of the snorkel working lining at the inner cavity upper edge level (Fig. 5).

Figure 5: Appearance of the snorkel damage. The arrow indicates place of crack exit to the lining surface (after slag and metal erosion).

The effect of material pores size distribution on character and scale of failure was investigated by a computational experiment, during which destruction of a sample with the same total porosity as in the control, but with substantially larger pores was considered. The ratio of pore volumes in these variants of calculation was 10. The effect of this fact on calculation algorithm was expressed in increase of mechanical stress, required to break the wall between pores and corresponding decrease of cycles amount before automat was completely destroyed.

A comparison of calculation results for two pore size distribution variants showed that the number of fully destroyed automata does not differ in these two cases. However, the number of partially damaged automata is higher in the case of a sample with larger pores, and also the destruction zone for this sample is much wider. In Fig. 6 diagrams of damaged automata location for 28 hours after the start of preheating are given for a sample with small pores (Fig. 6.1) and a sample with larger pores (Fig. 6.2). The temperature of the lining working surface at this moment is 690 °C.

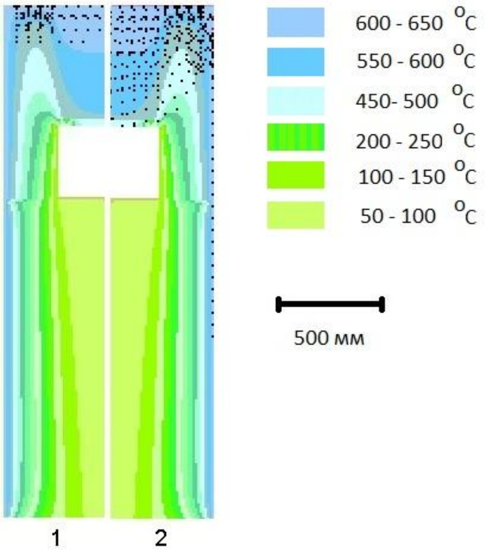

Figure 6: A comparison of damage modeling for samples with different pore sizes

The simplest explanation of this fact can be the accumulation of potential energy before the material destruction. In case of thick walls (corresponding to a large pores sizes), the accumulated energy is substantially higher, so, the residual energy after isothermal exposures is also higher. Because of the higher actual strength of the walls, the energy release during their destruction is less frequent, it leads to accumulation of stresses in adjacent zones. Thus, amount of partially damaged automata increases with pore size growth.

The change in general picture of failure with geometric pore size increasing indicates an uneven increase of mechanical stresses in different object zones. Therefore, changing the time interval between successive "dumps" of energy leads to the destruction of the wall inside another automat, which was not damaged during simulation for a sample with a different porosity character.

Earlier, damage of snorkel was simulated using ANSYS software [29]. At the same time, results of calculations in ANSYS generally correspond to results obtained with self-developed CA software. When modeling in ANSYS, maximum stresses were detected in the same zone of the unit as at the present study (Fig. 7).

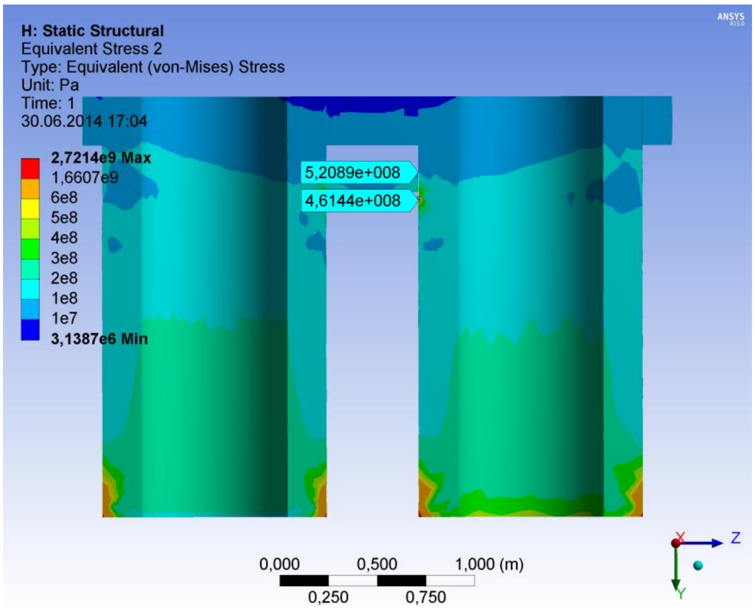

Figure 7: Mechanical stress of the object, calculated with ANSYS usage

A three-dimensional model was prepared for modeling with ANSYS usage, this model allowed considering the stresses in the volume of the lining, but not allowed predicting the geometric shape of the emerging crack.

4. Conclusion

An approach to fracture modeling of brittle refractory material under the action of thermal loading, based on mathematical methods of finite elements and cell automata is proposed.

The proposed fatigue failure algorithm allows taking into account both: structural features of material and their effect on crack geometry and rate of failure. Influence of material pore size distribution on sample damage location is demonstrated and the assumption of the object destruction pattern formation mechanism is put forward.

Comparison of damaged zones location, revealed by computational experiment with actual data on the destruction of working lining of RH-degasser snorkel, shows a satisfactory correlation - the location of the greatest damage zones obtained by numerical simulation coincides with cracks localization of the real lining.

Comparison of results, obtained with solution of a similar problem in ANSYS environment, showed that both approaches equally determine the location of arising lining defects. However, each model has certain advantages and disadvantages compared to the other. The proposed model allows to predict the geometry of the emerging crack, however, at this stage it does not allow to solve three-dimensional problem.

The applied method makes it possible to fix the necessary initial data for the calculation of stresses (dynamic temperature fields), both with help of built-in procedures, and use object's temperature fields generated by other methods. For example, temperature field of RH-degasser snorkel was previously calculated using FEM.

It is obvious, that the proposed algorithm can be used both in the case of a sharp temperature drop (thermal shock) and a gradual accumulation of thermal stresses with a relatively slow change of temperature field.

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