Determination of softening curves by backward analyses of experiments and optimization using an evolutionary algorithm

Beate Villmann
Leipzig University of Applied Sciences, Leipzig, Germany

Thomas Villmann
University of Leipzig, Leipzig, Germany

Volker Slowik
Leipzig University of Applied Sciences, Leipzig, Germany

ABSTRACT: A method for determining softening curves of cementitious materials is presented. Whereas the fracture energy of concrete or related materials may be obtained directly in bending or wedge splitting tests by measuring the fracture work, the determination of the complete softening curve requires backward analyses of the experiments. In these analyses, the experimentally determined load-displacement curves are approximated by repeated numerical simulations of the experiments and correcting the softening curves assumed in the individual simulations. The best fit gives the resulting softening curve for the tested material. For this data fitting process, a new optimization method based on an evolutionary algorithm is proposed. It includes local neighborhood attraction for convergence improvement. The method has been tested on the basis of experimental data from wedge splitting tests in order to check the plausibility of the results and to evaluate the performance of the algorithm.

Keywords: softening, wedge splitting test, simulation, evolutionary algorithm, computational intelligence

1 INTRODUCTION

The application of discrete or smeared crack models in numerical analyses of concrete structures requires the usage of the appropriate fracture mechanics material parameters, as are the tensile strength, the fracture energy and the shape of the strain softening curve. Following the discrete crack approach, the softening curve describes the strength degradation as a function of the local crack opening. While the fracture energy may be easily obtained from fracture mechanics experiments by measuring the total work done by the test loads and dividing it by the ligament area, the determination of tensile strength and softening curve appears to be technically difficult.

In uniaxial tension tests, tensile strength and softening parameters may be determined directly on the basis of the experimental results. However, these tests are expensive and time consuming. The problem of strain gradients in the ligament due to non-uniform cracking causes additional problems. Therefore, uniaxial tension tests are not an appropriate method for practical materials testing and may be performed for research purposes in specialized laboratories only.

Wedge splitting tests (Brühwiler & Wittmann 1990) and under certain conditions bending tests (RILEM 1985) have proved to be suitable technical means for determining the fracture energy of concrete. Especially the wedge splitting test is a very efficient and reliable experimental method. It is characterized by a relatively large ligament length to concrete volume ratio and a comparably small influence of the specimen self weight on the test results. In Figure 1 the experimental setup is shown. Wedges are pressed between roller bearings imposing a splitting force on the notched specimen. The crack mouth opening displacement in the loading line and the applied vertical load are measured. The latter allows to calculate the applied splitting force for the given wedge angle. Usually, the test is run under crack mouth opening control.

On the basis of the experimental results from wedge splitting or bending tests, only the fracture energy may be determined in a direct way. Tensile strength and softening parameters need to be obtained by backward analyses (Roelfstra & Wittmann 1986). In these analyses, finite element simulations of the experiments are undertaken by using the discrete or smeared crack approach of non-linear fracture mechanics. In the beginning, a softening curve is assumed and the load-displacement curve obtained by the numerical simulation is compared to the one determined experimentally in a fracture test. Subsequently, the numerical results are fitted to the experimental ones by updating the assumed softening curve and re-analyzing in several iterations. When the best fit of the numerical and the experimental results is obtained, the assumed softening curve is considered to be the one characterizing the behavior of the material investigated in this particular test.

The iterative fitting process described above may be undertaken manually. This kind of fitting is certainly more work intensive than using an automatic algorithm. Nevertheless, using appropriate software tools, even in this way an acceptable result for one individual experiment may be obtained within a few minutes. It can be shown that from the mathematical point of view several possible solutions for the softening curve exist. However, on the basis of experimental observations made in direct tension tests and by considering analogies between related materials, the physically sound and realistic solution may be identified.

In the past, optimization methods have been proposed for an automatic softening curve fitting. Roelfstra & Wittmann (1986) were the first to present a corresponding algorithm and the software tool SOFTFIT. The algorithm is based on the discrete crack approach and a bilinear softening curve. Experience has shown that the performance of SOFTFIT does not allow a considerably more efficient determination of the softening curve as compared to the method of manual fitting, although the program has been successfully used in numerous investigations (Slowik 1995). The algorithm requires a "first guess" of the input parameters which is quite close to the iteration results.

The Japan Concrete Institute (2001) proposes an algorithm for the determination of the softening behavior based on a completely different concept. A poly-linear softening curve is assumed and the individual slopes are determined successively by adjusting a corresponding increment of the calculated load-displacement curve to the experimental one. In this way, the softening curve is formed step by step while the crack is propagating in the simulated experiment. This poly-linear approximation allows a high performance of the optimization procedure. The algorithm, however, should be comparably sensitive to variations in the fracture properties

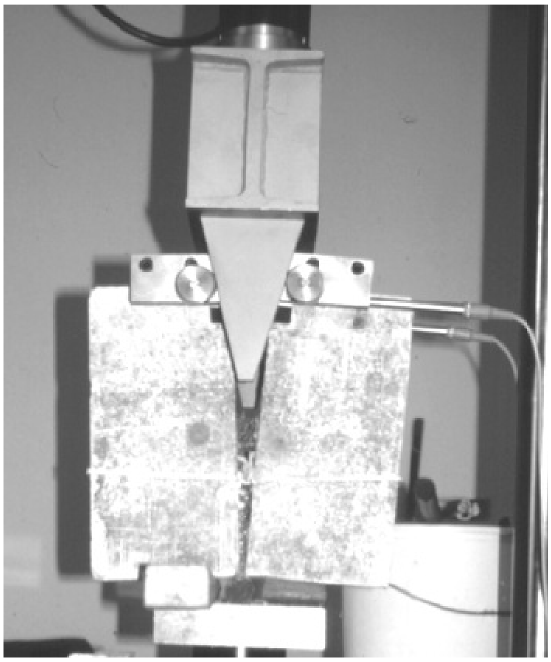

Figure 1. Wedge splitting test.

along the crack path. The individual slopes of the poly-linear softening curve depend only on certain limited regions of the experimentally determined load-displacement curve. For that reason and because of the problems related to the required assumption of the initial cohesive stress as the starting point for the poly-linear approximation, the algorithm presented here is not based on this concept.

The intention was to find an appropriate optimization method for performing an automatic approximation of the softening curve. In each of the individual iterations of the optimization process, the complete experiment is numerically simulated using a certain softening curve. Hence, the error estimation is based on a pair of complete load-displacement curves determined experimentally and numerically.

2 PROPOSED ALGORITHM

2.1 *Numerical simulation of the experiments*

The mechanical analysis is based on the Finite Element method. Since the optimization algorithm outlined below might require a comparably large number of individual iterations, possibly several thousand, a major precondition was the high speed of the numerical fracture simulation. Special attention had to be given to this aspect of the mechanical modeling. The high speed has been achieved by using a pre-analyzed elastic "macro-element" representing one half of the structure, for instance a wedge splitting specimen (Fig. 2). In this way, the number of degrees of freedom is reduced significantly as compared to a two-dimensional "full" model. The material non-linearity resulting from the softening is limited to the axis of symmetry. Unfortunately, the increase in efficiency is accompanied by a major limitation of the algorithm. The specimen geometry has to be known before and the corresponding stiffness relations for this particular geometry need to be calculated in an elastic pre-analysis. However, since the dimensions of actual test samples exhibit the same regularity because of existing formwork, this limitation of the algorithm is acceptable. Figure 2 also shows a Finite Element mesh used for determining the elastic behavior of an undamaged half-model. Since this pre-analysis has to be performed only once for the corresponding geometry it was suitable to use a comparably fine mesh along the crack path and at the loading point. Bending tests may be simulated by applying a similar procedure.

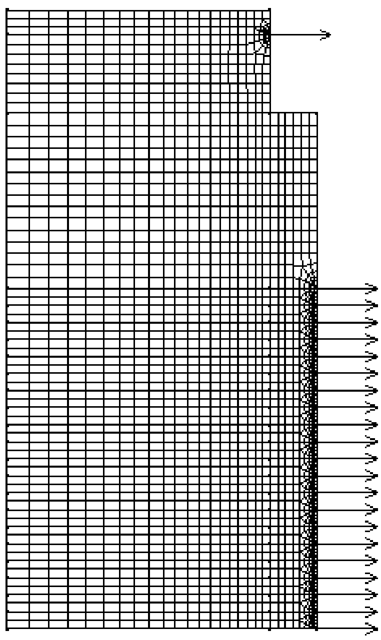

Figure 2. Finite Element model of a wedge splitting specimen with degrees of freedom used for the simulation of crack propagation.

The simulation of the crack propagation is based on a discrete crack approach. Starting from the notch, the crack tip is moved incrementally along the crack path and the corresponding external load and displacement values are determined. In each analysis step, the stress at the crack tip is equal to the tensile strength. The specimen self weight may be taken into account.

The algorithm works for any type of softening function. But so far, the optimization method has been tested for functions having up to six independent parameters only. In addition to strain softening, the hardening behavior of new high-performance fiber reinforced materials may be considered.

2.2 *Optimization method*

The parameter optimization of the softening function for a given data set is highly non-trivial. In fact, the manual optimization requires a lot of fine tuning and experience. Therefore, a more adequate procedure is requested. Unfortunately, the underlying model does not allow a gradient descent on a cost function due to mathematical reasons and difficulties.

Evolutionary algorithms (EAs) provide a general alternative to these problems (Schwefel 1981). EAs are biologically motivated iterative stochastic optimization methods, the roots of which point to biological genetics as described by Mendel's laws of heredity and Darwin's evolution model by natural selection. (We summarize by the concept of "evolutionary algorithms" both genetic algorithms (GA) as well as evolutionary strategies which are sometimes handled in a more separate way in the literature.) The key idea in EAs is to separate the variation of the object to be optimized from its evaluation as we find it in nature (geno-/phenotype).

In the following, the basics of EAs are shortly summarized and a special version to be applied here is described. For a more general overview we refer to Bäck (1996) and Michalewicz (2002).

2.2.1 *Basic EA scheme*

Let M be a model to be optimized and $\boldsymbol{c} = [c_1,\ldots,c_m]$ a string or vector of model parameters of potential problem solutions. Let f be a semi-positive evaluation function (a map from m dimensional space onto the positive real axis) of the model, called *fitness function*. For a given parameter vector $\boldsymbol{c}$, the fitness of the model is $f(\boldsymbol{c})$ and we further assume without loss of generality that minimizing $f(\boldsymbol{c})$ is equivalent to optimizing the model. An instance of $\boldsymbol{c}$ is called individual. Hence, the task is to find an individual $\boldsymbol{c}^*$ which minimizes the fitness function.

In EAs, in each time step t, called generation t, a set $C(t)=\{c^1(t),\ldots,c^\mu(t)\}$ of possible parameter configurations is considered. The fittest individual of a generation $C(t)$ is the currently found solution of the EA. Thereby, the initial generation $C(0)$ is randomly given. In each time step, from the current generation $C(t)$ an intermediate generation (offspring) of $\lambda > \mu$ new individuals is created by certain genetic operations applied to the individuals of $C(t)$. Genetic operations are formal manipulations of the strings (individuals) $\boldsymbol{c}$ closely related to the biological origin. The main types are mutations (random variation of string position values) and crossovers by randomly cutting two strings and "gluing" them together in a crossed way (combination of strings). There exists a broad variety of such operations, we refer to Bäck (1996), Michalewicz (2002), Beyer & Schwefel (2002) for an overview. After application of the genetic operations, all offspring individuals are evaluated according to the given fitness function. In this way the manipulation of the objects is separated from their evaluation.

After the evaluation follows a selection procedure in order to obtain μ individuals for the new generation $C(t+1)$. Two basic selection schemes are known: the $[\mu , \lambda]$-strategy replaces the μ individuals of $C(t)$ by the μ best individuals of the offspring. In case of the $[\mu + \lambda]$-strategy the μ best individuals of both $C(t)$ and offspring are selected to survive in $C(t+1)$. The $[\mu , \lambda]$-strategy exhibits a higher diversity within a generation and is therefore preferred during the convergence phase (fine tuning) whereas the $[\mu + \lambda]$-strategy has advantages in the initial generations of the adaptation process (Bäck 1996). We prefer a combination of both approaches, called $[\mu * \lambda]$-strategy, which allows a smoothed transition between both strategies combining their advantages (Villmann 2002).

2.2.2 *Extension of the basic EA scheme – the neighborhood attraction approach*

There exist several extensions of the basic EA scheme to improve the convergence or/and to adapt it for special problems. Thereby, hybrid approaches which also incorporate other optimization strategies play an important role (Villmann 2001). Here we extend the EAs by local search mechanisms. The resulting approach is called memetic algorithm (Moscato 1989). In particular, a special local search procedure is applied which takes the similarity of parameter vectors into account and is named *neighborhood attraction* according to a neural network learning strategy (Huhse et al. 2002). In general, neighborhood attraction improves the convergence rate. Moreover, the neighborhood attraction reduces the risk of getting caught by non-attractive local minima of the fitness landscape (Huhse et al. 2003, Villmann et al. 2004).

Neighborhood attraction is applied after the offspring generation but before the selection. For a given individual $\boldsymbol{c}$, taken now as an usual vector, the geometric neighbors according to the vector distance are identified by comparing their fitness. If one or more of the fitness values are better than the fitness of the selected individual, it is shifted by a small increment towards the fittest neighbor (vector shift). Otherwise, if all neighbors of an individual have a weaker fitness, these individuals are shifted towards the considered one, i.e. the individuals swarm around the (local) best. Therefore, we may regard this type of local search as a special kind of particle swarm optimization (PSO) (Krink & Løvbjerg 2002). As outlined above, the neighborhood attraction is a special type of neighborhood cooperativeness which also plays a fundamental role in nature (Hyvärinen 2002).

3 APPLICATION OF THE ALGORITHM

3.1 *Real experiments*

For testing the proposed algorithm the softening behavior of five different cement mortar compositions has been evaluated. The actual samples, the mix design and the results of strength testing have been kindly provided by Ma, Schneider & Wu (2003). The intention of the test series was to investigate the fracture behavior of high-strength mortar. Mix design and strength values are given in Table 1. The splitting strength results from Brazilian tests.

For determining the fracture mechanics material properties wedge splitting tests were carried out under crack mouth opening displacement (CMOD) control by means of a hydraulic testing machine. The specimens had the dimensions of 300 x 300 x 100 mm³ and a notch length of 142 mm.

Although three wedge splitting tests were performed for each of the five mortars, the following determination of the softening behavior is based on five characteristic load-displacement curves (Fig. 3) which were chosen from the available tests. This procedure of selecting representative curves for further processing is more suitable than averaging the results which would lead to curves with wider peaks and, consequently, to misleading results of backward analyses.

As expected, the maximum splitting force increases with the compressive strength, i.e. from mixture M20 to M180. Whereas the difference between normal-strength mortar, M20, and the high-strength mortars is significant, only small

Table 1. Mix design and strength properties of the tested materials (Ma, Schneider & Wu 2003).

	M20	M60	M100	M140	M180
CEM I 42.5R	1.0	1.0	1.0	1.0	
Silica fume (dry), sf	---	---	0.08	0.30	
Low calcium fly ash, fa	0.25	0.2	0.15	---	
Quartz powder	---	---	---	0.428	
Water	0.695	0.374	0.327	0.268	
Superplasticizer (dry), related to cement mass	1.3%	1.5%	1.5%	1.7%	
Sand (0-2 mm)	3.555	2.279	2.107	---	
Sand (0.3-0.8 mm)	---	---	---	1.532	
Water-binder ratio w/(c+0.4fa+sf)	0.632	0.346	0.287	0.206	
Density of hardened concrete [kg/m³]	2235	2305	2383	2320	2415
Compressive strength [N/mm²]	40.0	81.2	106.6	149.1	196.3
Splitting strength [N/mm²]	3.5	6.8	8.9	10.5	13.2
Modulus of elasticity [GPa]	25.5	35.0	43.0	45.9	52.0

Component ratios given per mass. For M20, M60 and M100 a viscosity agent was used in order to prevent bleeding and segmentation.

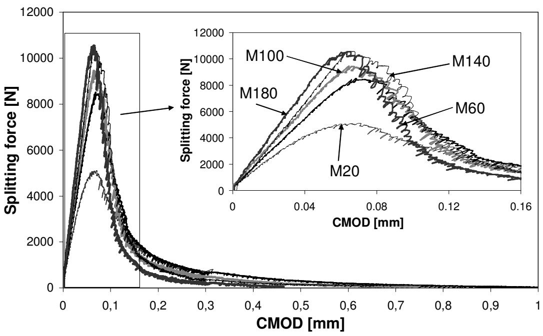

Figure 3. Load-displacement curves determined in wedge splitting tests.

variations among the different high-strength mortars could be observed.

Before the algorithm for determining the softening curves was applied, the experimentally determined splitting force-CMOD curves were smoothed in order to reduce the number of data points and to allow more efficient error detection during the optimization.

3.2 *Numerical Approximation*

For the automatic fitting process, the following error criteria have so far been proved to be suitable. The first criterion is the relative error:

$$E_1 = \frac{1}{n}\sum_n \left| \frac{x_n - a_n}{x_n} \right| \tag{1}$$

where x_n = experimental splitting force at the calculated CMOD value; a_n = corresponding calculated splitting force; n = number of calculated data points. For curves with a narrow peak, this criterion does not always lead to satisfying results. For such cases a different criterion, a weighted error, appeared to be more suitable:

$$E_2 = \frac{1}{n}\sum_n \left(\frac{w \cdot x_n}{x_{\max}} + 1 \right) \cdot \left| \frac{x_n - a_n}{x_n} \right| \tag{2}$$

where w = weighting factor; x_{max} = maximum splitting force of the experimental load-displacement curve. Additionally, a criterion based on the fracture energy G_F was applied in order to obtain a good fit also at the tail of the load-displacement curve:

$$E_3 = \frac{1}{2}\left(\left| \frac{G_{F\exp} - G_{Fnum}}{G_{F\exp}} \right| + \left| \frac{G_{F\exp} - G_{Fnum}}{G_{Fnum}} \right| \right) \tag{3}$$

The multi-parametric error function appears to be cliffy and during the optimization local minima might prevent the finding of the optimum. Therefore, the parameter optimization does not necessarily lead to an unique solution. In order to avoid misleading results, the variation range for each of the parameters needs to be predefined on the basis of background information and experience (see section 1).

Because of the stochastic character of the optimization method, the choice of the starting parameters has no significant influence on the results. It was found however, that the influence of the Finite Element size in the mesh used for the elastic pre-analysis (see section 2.1) might be significant especially in the case of very brittle high-strength cementitious materials. In further investigations, this effect will be quantified and recommendations for an appropriate elastic pre-analyses will be formulated in order to provide objectivity of the results.

As far as the performance of the proposed algorithm is concerned, obtaining the softening curve on the basis of a single load-displacement curve takes about 30 min by using a personal computer.

3.3 *Results*

In the following, the results of a first application of the algorithm are presented. Because of the limited number of individual wedge splitting tests, the analyses were intended to prove the applicability of the algorithm but not to draw final conclusions concerning the fracture properties of the investigated materials.

Before the optimization was carried out the influence of the specimen self-weight on the simulation results was evaluated. This effect appeared to be insignificant for the specimen dimensions used here and was neglected in the following analyses.

An exponential softening function proposed by Hordijk (1991) has been adopted:

$$\sigma = c_1 \left\{ \begin{array}{l} \left(1 + \left(c_3 \dfrac{w}{c_2}\right)^3\right) \exp\left(-c_4 \dfrac{w}{c_2}\right) - \\ - \dfrac{w}{c_2}\left(1 + c_3^{\,3}\right)\exp\left(-c_4\right) \end{array} \right\} \quad (4)$$

where σ = softening stress and w = crack opening. The four parameters c_1 to c_4 need to be determined in the optimization.

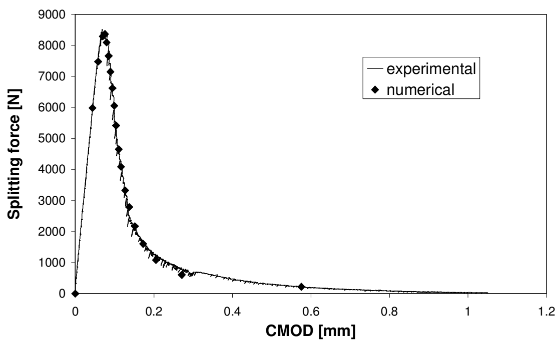

Figure 4. Comparison of the experimental and the calculated load-displacement-curves for the mortar M60.

Figure 4 shows an example for the best fit obtained in the approximation of the experimentally determined load-displacement curve. A nearly perfect match was achieved which would have been almost impossible by manual approximation.

In Figure 5 the obtained softening curves for the investigated high-strength mortar samples are shown. A significant increase of tensile strength and initial slope of the softening curve with increasing compressive strength (Table 1) was observed. The directly measured fracture energy and the one calculated from the softening parameters are in good accordance. The values vary from about 50 N/m for M20 to about 60 N/m for all the other mortar batches.

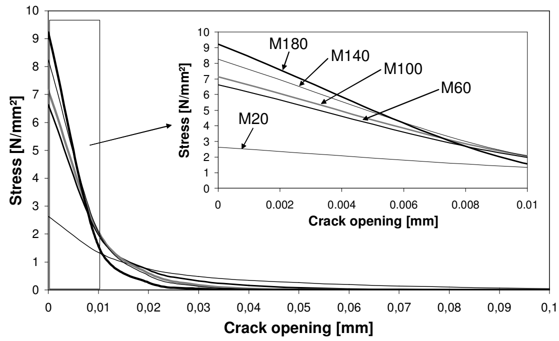

Figure 5. Calculated softening curves for the different mortar compositions.

For evaluating the deviations between the three wedge splitting tests performed for one mortar composition, the proposed algorithm was applied to all of the three corresponding curves for M60. Figure 6 shows load-displacement curves determined experimentally and Figure 7 the obtained softening curves. Only minor deviations may be observed.

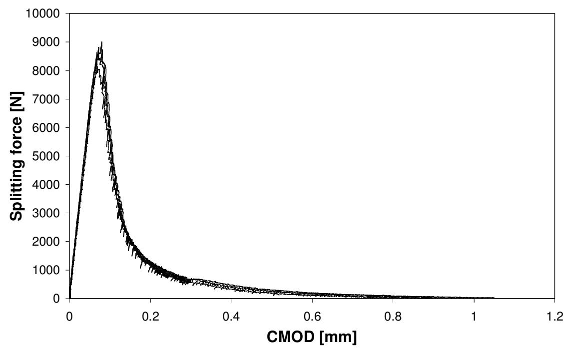

Figure 6. Load-displacement-curves for three samples of the mortar M60.

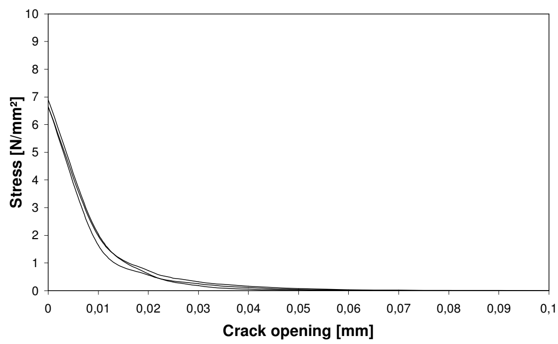

Figure 7: Obtained softening curves for three samples of the mortar M60 (Fig. 6).

Finally, four different shapes for softening functions were applied for approximating an experimental load-displacement curve. Figure 8 shows the obtained results. The optimization yielded softening parameters resulting in approximately the same fracture energy of about 60 N/m. With the exception of the linear function, the shapes of the different curves appear to be quite similar.

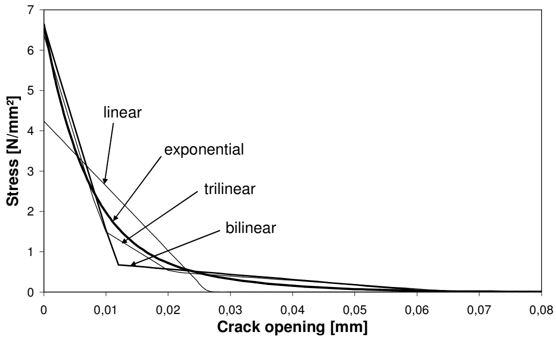

Figure 8. Comparison of various types of functions used for determining the softening curves for the mortar M60.

4 CONCLUSION

A new method for determining softening curves of cementitious materials based on an evolutionary algorithm has been proposed and tested. The algorithm and the corresponding software tool proved to be applicable in practical materials research and evaluation. However, in order to identify physically sound solutions, the application of the method requires some experience as far as the fracture behavior of cementitious or related materials is concerned. Further investigations into the mesh dependency of the simulation results as well as into the reliability of the optimization algorithm are under way.

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