UNCERTAINTY ON THE STRENGTH DURABILITY PREDICTIONS OF GRCs

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ABSTRACT

The durability of glass fibre reinforced concrete remains a widely study topic. Within literature several models for strength durability predictions have been made available. However when one wants to perform strength predictions it is not clear which model is the best approximating model for the data set at hand. Therefore in this paper an objective and effective method for the selection of the best approximating model based on a sound statistical background is presented and illustrated. This method is based on Akaike's Information Criterion and not only takes into consideration the vertical distances between the modeled and the experimental values but also the number of parameters which need to be determined and number of data points in the data series.

1. INTRODUCTION

Concrete and mortar are inherently brittle materials. However, by reinforcing cement pastes with glass fibres, composites with improved ductility can be obtained. When using textile glass reinforcement in cements, the mechanical properties of the composite can be improved in such a manner that it becomes a very suitable material for the production of load-bearing thin elements with variable shapes in which the steel reinforcement can be omitted ([1], [4]-[6]). However these concrete composites are subject to degradation of their mechanical properties with ageing, especially in wet environments. The most important manifestation of this ageing is the loss of tensile strength. Many researchers have tried to determine the mechanisms which govern this ageing in order to further improve the strength durability. Three main mechanisms are generally recognized: (1) chemical attack of the fibres [1], (2) growth of hydration products [2] and (3) static fatigue [3]. The development of Alkali Resistant (AR) glass fibres with a high Zirconium content has already improved the durability of GRCs but has however not completely resolved the durability issues. Several strength durability models were developed over the years to model the recorded strength loss. Within this paper only some of these strength durability models ([3], [4], [5], [6]) - based on a similar physical background - will be closely studied. The basic assumption is that flaws (nano-defects) inherently present on the surface of the glass fibres will grow with time - due to chemical attack and/or growth of hydration products and/or static fatigue - resulting in a decrease in failure strength. In this paper four models based on this physical background will be presented. The essential difference between these models is the general expression assumed for the rate of flaw growth. These models need to be calibrated before they can be used for strength predictions and this is usually done through accelerated ageing testing. For these accelerated ageing tests, specimens are immersed in hot water for various periods of time and their strength loss due to this exposure is then determined. Through an inverse method the model parameters can then be determined. These - in the previous step determined - model parameters can then be used for a strength prediction over the life span of the material. The strength loss occurring over an established period in a certain climate can be defined by for instance assuming that over the life span of the material an average temperature of the climate will occur in combination with a relative humidity of 100%. This assumption however leads to an overestimate of the strength loss. A more accurate strength prediction can be achieved by including the fluctuations in climatic conditions (temperature and humidity) [7]. This provides the user with a certain absolute value for residual strength for the material combination under study.

When confronted with strength durability predictions one thus first needs to perform accelerated ageing tests. Then in a second step a strength durability model needs to be chosen and fitted on the results. With these model parameters, obtained in the previous step, in the final step the strength prediction can be made. For the second step (the model selection) no real guidelines can be found in literature. Each researcher generally praises his own strength durability model. Therefore within this paper a sound statistical method will be presented which enables the selection/determination of the best approximating model for the experimental data at hand. This method not only takes into account the Sum-of-Squares but also the number of data points and number of parameters which need to be determined for each strength prediction model. Not only the Sum-of-Squares method for fitting will be presented but also a method which uses cost functions. With these cost functions the scatter on the individual test results, which lead to the averaged data points, will be taken into account as thus weighing the individual data points. With the help of this method within this paper for a wide variety of accelerated ageing tests out of literature the best approximating strength durability model will be determined and the results will be discussed. For the fitting of the results the Sum-of-Squares approach as well as the cost function approach will be used

2. STRENGTH DURABILITY MODELS

Some recent durability studies ([1], [3], [4], [8]) state that the strength losses recorded for GRCs are directly related to the strength loss of the glass fibres. For Textile Reinforced Concrete (TRC) elements where large voids are present within the fibre bundles and we thus assume that embrittlement due to the growth of hydration products will play a minor role. The growth of flaws (nano-defects) inherently present on the surface of the glass fibres is assumed to result in the decrease in failure stress with time. These flaws can grow as a result of chemical attack and/or growth of hydration products and/or static fatigue. As basis of these strength durability models, the classical Griffith relationship between the free energy of a cracked body under stress and the crack size is assumed. For the bulk tensile strength of the fibre the following expression can then be constructed:

$$\sigma_t = \frac{K_{IC}}{A \cdot \sqrt{\pi \cdot a}} \qquad (1)$$

Where: σ_t is the bulk tensile strength of the fibre at time t (MPa)
K_{IC} is the critical stress intensity factor (Mode I) (MPa$\sqrt{nm}$)
A is a shape factor (-)
a is the flaw size at time t (nm)

If one assumes that the critical stress intensity factor and the shape factor remain invariable with time, a general expression for the residual strength (S) can be derived with the help of equation 1:

$$S = \frac{\sigma_t}{\sigma_{t=0}} = \frac{1}{\sqrt{1 + \frac{X}{a_0}}} \quad (2)$$

With:

$$a = a_0 + X \quad (3)$$

Where: a_0 is the initial flaw size (nm)
X is the flaw growth over a time span t (nm)
σ_t is the failure strength at time t (MPa)
$\sigma_{t=0}$ is the initial failure strength (MPa)
S is the residual strength (-)

This flaw growth phenomenon is function of moisture, temperature and pH.

Durability model	Rate of flaw growth	Residual strength
Kinetic model	$\frac{dX}{dt} = k_{1*}$ (4) k_1^* [nm/day] k_1 [day^{-1}]	$S = \frac{1}{\sqrt{1 + k_1 \cdot t}}$ (5) With: $k_1 = \frac{k_{1*}}{a_0}$ (6)
Diffusion model	$\frac{dX}{dt} = \frac{k_{2*}}{X}$ (7) k_2^* [nm²/day] k_2 [day^{-1}]	$S = \frac{1}{\sqrt{1 + \sqrt{k_2 \cdot t}}}$ (8) With: $k_2 = \frac{k_{2*}}{a_0^2}$ (9)
Non linear model	$\frac{dX}{dt} = \frac{k_{3*}}{X^m}$ (10) k_3^* [nm$^{(m+1)}$/day] k_3 [day^{-1}] m (n) is **not** function of the temp.	$S = \frac{1}{\sqrt{1 + (k_3 \cdot t)^n}}$ (11) With: $k_3 = \frac{(m+1) \cdot k_{3*}}{a_0^{m+1}}$ (12) and $n = \frac{1}{m+1}$ (13)
Combined model	$\frac{dX}{dt} = \frac{1}{\frac{1}{k_4} + \frac{X}{k_5}}$ (14) k_4 [nm/day] k_5 [nm²/day]	$S = \sqrt{\frac{1}{1 - p + \sqrt{p^2 + q \cdot t}}}$ (15) With: $p = \frac{k_5}{k_4 \cdot a_0}$ (16) and $q = \frac{2 \cdot k_5}{a_0^2}$ (17)

Table 1: All strength durability models under study in this work, with their flaw growth rate and residual strength expressions.

Over the years several models were constructed based on these assumptions. Within this paper four of these models will be discussed in further detail and they will be respectively referred to as: (1) the kinetic model, (2) the diffusion model, (3) the non-linear model and (4) the combined model. The main difference between these models is the general expression assumed for the rate of flaw growth (dX/dt) (see table 1). Some researchers [3] state that the recorded decrease in failure stress can be attributed to a constant flaw growth rate. This philosophy gave rise to the Kinetic model of which the expressions can be found in Table 1. Other scientists [4] are however of the opinion that the rate of strength loss gradually decreases with time, this due to reaction products covering the surface of the fibres with time and/or a bottle neck effects (the confined space within the growing flaw could - in combination with a deposition of reaction products within this flaw - also limit the reaction possibilities). With these premises the Diffusion model was constructed (for expressions see Table1). Other research groups ([4], [8]) suggested a Non linear model (see Table 1) with a non linear progression of the flaw depth. This might for instance be the result of a varying Zr content across the section of the fibres or a varying flaw shape with time due to ageing. In literature certain researchers ([1], [6]) are convinced that the rate of degradation is initially determined by kinetics and becomes diffusion controlled in a later stage of the degradation which resulted in the Combined model (for the expressions see Table 1).

Several durability studies, available in literature ([1], [3], [4], [6], [9]), indicated that an Arrhenius type relationship (see Equation 18) exists between the rate of the chemical reaction and the temperature at which the test is carried out (at all temperatures ranging from 20-80°C, except for certain specialised matrices, e.g. those modified with meta-kaolin [10]).

$$k_i = k_{0,i} \cdot e^{-\frac{E_{A,i}}{R \cdot T}} \qquad (18)$$

Where: k_i rate coefficient of the chemical reaction i
$k_{0,i}$ reference rate coefficient of the chemical reaction i
$E_{A,i}$ Activation energy of the chemical reaction i
T temperature (in Kelvin) at which the test is performed
R Gas constant

This implies that each of the temperature dependant rate coefficients within Table 1 (k_1, k_2, k_3, k_4, k_5, k_1^*, k_2^* and k_3^*) should show an Arrhenius type relationship in function of the temperature. Each of these temperature dependant rate coefficients can thus be written as a function of two model parameters (an activation energy $E_{A,i}$ and a reference rate coefficient $k_{0,i}$) which are solely function of the material combination under study. When faced with GRC durability research instead of testing specimens in real climatic conditions, specimens are thus stored in well controlled lab conditions. Specimens are immersed in hot water at temperatures ranging from 20°C-80°C for various periods of time and the Arrhenius relationship is derived.

3. DETERMINATION OF THE BEST APPROXIMATING MODEL

Many models have been developed over the years for the strength durability of GRCs. The question however remains which of these models will be the best approximating model for a given data set. Therefore it is the aim of this paper to provide the reader with an effective and objective means for the selection of the “best approximating model”. Within statistics literature different model comparison methods can be readily found. Two main groups of methods are generally recognised: (1) model selection methods based on null hypothesis testing *and* (2) model selection methods based on information theory. Methods within the first group generally assume that the simpler model (the one with fewer parameters) is correct and provides the null hypothesis. The potential improvement of the fit of the more complicated model is then evaluated and the null hypothesis is then, at a certain chosen P-value, concluded to be either significantly better or the null hypothesis is rejected. The second group of model selection methods is on the other hand based on a combination of information theory and mathematical statistics and is a relative new approach within the biological and statistical world to model selection. Within literature several authors [11] encourage the use of the second group of methods for the analyses of biological data. One such approach is Akaike's Information Criterion (AIC) which combines maximum likelihood theory, information theory and the concept of the entropy of information. The method allows the user to calculate which model is more likely to be correct and even quantifies how much more likely the model is. The theoretical basis of the method is very complicated but the method on itself is however easy to compute and the results are easy to analyse. The theoretical background of the AIC method goes beyond the scope of this present paper. For further information the reader is encouraged to read references [11] and [12] which provide a deeper insight in the theories underlying this model comparison method.

3.1 Approach

When confronted with an accelerated ageing data set and different candidate strength durability models one first needs to determine all parameters relative to each model. This fitting issue can be resolved in many ways. When confronted with the comparison of the different models a difficulty however rises: the estimated parameters need to be determined on exactly the same data and thus on the complete data set. As a result one can not simply determine the rate coefficients at each individual temperature and construct the Arrhenius relationship (which is generally done in literature) but one needs to fit the Arrhenius relationship on the whole data set (over all the temperatures simultaneously) and thus determine the activation energy $E_{A,i}$ and reference rate coefficient $k_{0,i}$ for each occurring chemical reaction. This implies that for the Kinetic and the Diffusion model each time 2 parameters need to be determined while for the Combined model 4 parameters need to be determined (2 for the Kinetic part and 2 for the Diffusion part of the reaction). For the Non linear model 3 parameters need to be fitted: the activation energy $E_{A,3}$, reference rate coefficient $k_{0,3}$ and the n parameter. For the fitting of the different models we use the Sum-of-Squares method. The approach is quite straight forward, the parameters which need to be determined for each individual model are altered until the sum of the squares of the vertical distances (ε_i) between the modelled values and the experimental data is minimized. The model parameters corresponding with this optimum are retained.

The best approximating model can not be determined on the sole basis of the Sum-of-Squares values. One needs to take into consideration the amount of parameters which need to be estimated and the amount of data on which the results are fitted. First of all, the improvement in Sum-of-Squares needs to justify adding parameters to the strength durability equation. Secondly, if the data set is not sufficient enough one can also not easily justify adding parameters to the equation. To resolve this issue within this paper we will use Akaike's Information Criterion (AIC) which was developed in the mid 1970's. Akaike's Information Criterion (AIC) can be written in the form presented in

Equation 19 this in the assumption of normally distributed errors with a constant variance for all the models in the set.

$$AIC = N \cdot \ln\left(\frac{SS}{N}\right) + 2 \cdot K \qquad (19)$$

Where: N is the number of data points
SS is the Sum of Squares of the vertical distances
K is the number of parameters +1 (since the SS is also estimated)

In literature a correction of this AIC can be found (AICc) taking into account small values of N compared to K. When using large data sets the correction on AICc will be trivial and AICc will approximate AIC.

$$AICc = AIC + \frac{2 \cdot K \cdot (K+1)}{N - K - 1} \qquad (20)$$

The model corresponding with the smallest AICc (or AIC) value is more likely to be correct but it doesn't quantify how much more likely. To quantifying this relative likelihood of a model one needs to determine Akaike's weights.

$$w_i = \frac{\exp\left(-\frac{1}{2}\Delta_i\right)}{\sum_{r=1}^{R} \exp\left(-\frac{1}{2}\Delta_r\right)} \qquad (21)$$

With: $\Delta_i = AICc_i - AICc_{\min}$ (22)

ω_i provides the weight of evidence in favour of model i being the best approximating model for the particular data set under study, given that one of the R models is the best approximating model.

3.2 Results and discussion

To illustrate the method elaborated above different results - resulting from a wide variety of test methods (full composite, SIC and single filament tests) - were taken from literature. A listing of the results can be found in Table 2 with all the necessary references and essential information (number of data points within the data series, specimen type and material combination).

Code used	# of data points	Specimen type	Material	Ref.
O-SF-OPCII	25	Single Filament	OPC + 2^{nd} gen. AR fibres	[1]
O-SIC-OPCII	23	SIC	OPC + 2^{nd} gen. AR fibres	[1]
O-TSP-OPCII	30	Dog bone specimen	OPC + 2^{nd} gen. AR fibres	[1]
P-Comp-OPCI	24	Composites spec.	OPC + 1^{st} gen. AR fibres	[13]
P-Comp-OPCII	16	Composites spec.	OPC + 2^{nd} gen. AR fibres	[13]
L-SIC-OPCI	148	SIC	OPC + 1^{st} gen. AR fibres	[8]

Table 2: Test results from literature used within this paper.

The method, presented in the previous section, will now be adapted on these results to determine the best approximating strength durability model for each of the individual results. In Figure 1 a scheme summarizes all the necessary steps which need to be taken in order to achieve this goal. For all the models under consideration the model parameters are first determined by optimizing the fit with the experimental results. Within a next step, with the help of Akaike's Information Criterion (AIC) the best approximating model is determined taking into consideration the Sum-of-Squares (SS) value (or the Cost functions), the number of data points and the number of model parameters within each strength durability model.

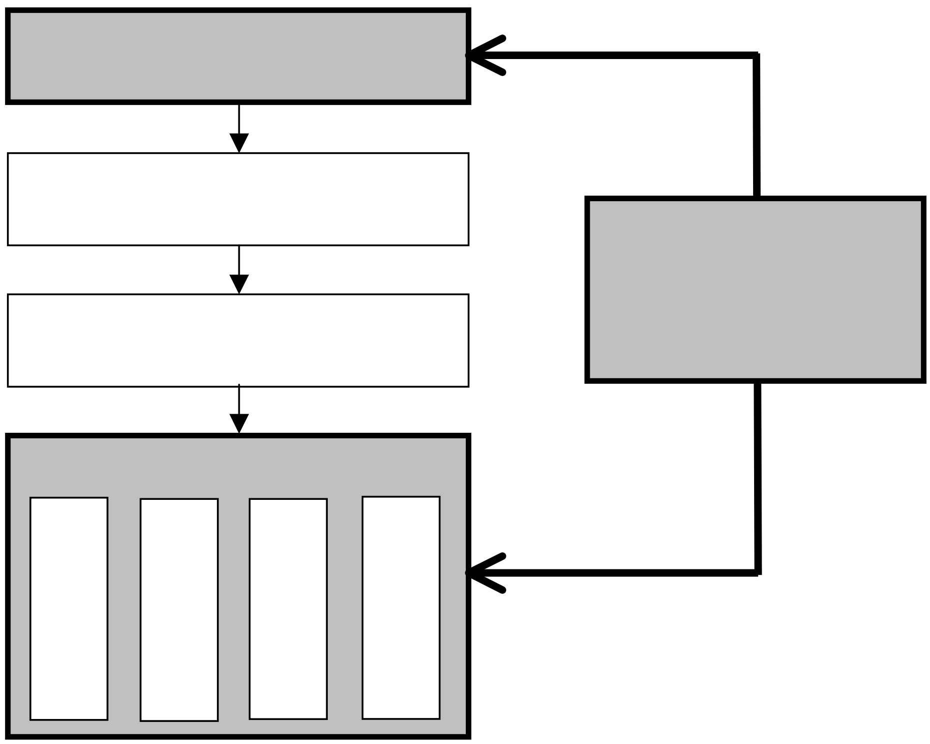

Figure 1: Scheme used for the selection of the best approximating model

Within Table 3 a list of the Sum-of-Squares and related AIC values can be found corresponding with the best fit of the individual strength durability models (K= Kinetic model, D= Diffusion model, N= Non linear model and C= Combined model) and this for each of the accelerated ageing data sets given in Table 2. The AIC value gives the weights of evidence (ω_i) in favour of the model being the best approximating model (for example if D=70% it means that there is a 70% chance that the Diffusion model is the best approximating model for the data at hand). The grey areas within Table 3 indicate the best approximating model (with the highest weight of evidence (ω_i)) and best fitting model (with the lowest Sum-of-Squares) for the data set which is under study.

If the selection of the best approximating model is solely base on the individual Sum-of-Squares values the higher degree models seem to fit the data best. The Combined model (C) is almost always the best fitting model (in +/-80% of the cases) and in the other case it is the Non linear model. However, if we check whether the improvement in Sum-of-Squares justifies the introduction of more parameters the effectiveness of the lower degree models however becomes better. The best fitting models are only in +/- 20% of cases also the best approximating models. When analysing the best approximating models for the data sets at hand, a high diversity is observed. The material combination used, the matrix formulation, the type of AR glass fibres, the type of coating on the fibres etc… might all influence the degradation rate. This becomes very clear when observing the weights of evidence (ω_i). One can certainly not state that a specific model will be the best approximating model for all standard GRC applications, independent of the specific material combination under study. The weight of evidence in favour of the best approximating is generally around 70%. The attention of the reader is however directed to 2 specific results within Table 3: (1) L-SIC-OPCII and (2) P-Comp-OPCI. Both of these results show a relative high weight of evidence in favour of the combined model. The results denoted as L-SIC-OPCII are the most elaborated data set available in literature up till now and the evidence in favour of the combined model is significant (C=100%) indicating that this model seems to nicely catch the occurring degradation. For the results P-Comp-OPCI the evidence in favour of the combined model is also convincing (C=92,1%) and certainly taking into account that the data set only consists out of a limited number of data points (24, see Table2).

	Sum-of-Squares				**AIC** (ω_i)			
	K	D	N	C	K	D	N	C
O-SF-OPCII	*0,1961*	*0,0335*	***0,0333***	*0,0334*	*0,0%*	***76,3%***	*19,7%*	*4,0%*
O-SIC-OPCII	*0,1311*	*0,0349*	*0,0349*	***0,0298***	*0,0%*	***66,9%***	*15,2%*	*17,9%*
O-TSP-OPCII	*0,1446*	*0,1008*	*0,0845*	***0,0830***	*0,1%*	*17,1%*	***63,3%***	*19,4%*
P-Comp-OPCI	*0,0333*	*0,1041*	*0,0237*	***0,0168***	*0,6%*	*0,0%*	*7,4%*	***92,1%***
P-Comp-OPCII	*0,0855*	*0,1314*	*0,0831*	***0,0796***	***78,8%***	*2,5%*	*16,1%*	*2,6%*
L-SIC-OPCII	*0,9028*	*0,6752*	*0,3796*	***0,2681***	*0,0%*	*0,0%*	*0,0%*	***100%***

(K= Kinetic model, D= Diffusion model, N= Non linear model and C= Combined model)

Table 3: Listing of the Sum-of-Squares and AIC values for all models under study and this for each result from literature (see Table 2).

Since for GRCs, coefficients of variation of 10-15% on experimental results are quite common and often only a very small amount of specimens are used, scatter might have a considerable influence on accelerated ageing tests. This sometimes high scatter on the results might also influence the determination of the best approximating model. To overcome this problem we could work with cost functions (V) instead of the Sum-of-Squares method. This approach can take into consideration the scatter of the individual test results and the number of test results which lead to each individual average data point.

$$V = \sum_{i=1}^{N} \frac{\varepsilon_i^2}{\frac{1}{n}\hat{\sigma}_i^2} \qquad (23)$$

With: $$\hat{\sigma}_i^2 = \frac{1}{n-1}\sum_{k=1}^{n}\left(S_k^i - \bar{S}_i\right)^2 \qquad (24)$$

Where: n is the number of experimental results which give the average data point ($\bar{S}$)

To obtain Table 4 the cost function given in equation 23 was utilized and this on the first 3 results from Table 2, this since for the other results the values of the individual results were not available. For the second and the third data set (O-SIC-OPCII and O-TSP-OPCII) only minor differences are recorded. However for the first result (O-SF-OPCII) when cost functions are used instead of the Sum-of-Squares method the weight of evidence in favour of the Diffusion model drops from 76,3% to 47,4% and the evidence in favour of the Non linear model increases from 19,7% to 50,3%. The results within Table 4 thus clearly indicate the necessity of using cost functions for the analyses of GRC accelerated ageing tests.

	Cost function				**AIC** (ω_i)			
	K	D	N	C	K	D	N	C
O-SF-OPCII	*282,29*	*37,65*	***33,42***	*37,65*	*0,0%*	***47,4%***	***50,3%***	*2,3%*
O-SIC-OPCII	*315,02*	*102,13*	*101,49*	***90,13***	*0,0%*	***70,0%***	*17,1%*	*12,8%*
O-TSP-OPCII	*133,59*	*77,23*	*64,36*	***61,41***	*0,0%*	*14,4%*	***58,1%***	*27,5%*

Table 4: Listing of the Cost function and AIC values for all models under study and this for each result from literature (see Table 2).

4. CONCLUSIONS

Within this paper a method was presented which enables the selection of the best approximating strength durability model for a given accelerated ageing test. The application of this method on several results taken from literature illustrated that it is not obvious to state that 1 specific strength durability model presented within the scope of this paper will always be the best approximating model for GRCs with a standard OPC matrix independent from the material combination used. The literature results analysed within this paper clearly indicated that the material combination used, the matrix formulation, the type of AR glass fibres, the type of coating on the fibres etc… all influence the degradation rate and thus also the best approximating model. The importance of the scatter of the individual results on the selection of the best approximating model was also clearly shown; as a result the AIC method should always be combined with the cost function approach for the determination of the model parameters for an accurate estimation of the best approximating model.

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