Probability for probabilistic criteria - Design with brittle materials

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Designing with ceramic materials is nowadays a very good solution for specific technical problems, but it has also several great handicaps. First problem is the necessity to use numerical methods for a good application of resistance theory to brittle materials. Second one one is to achieve a correct interpretation and use of their characterisation parameters. The KERB program, a FEM subprocessor developed at the IMW, offers a solution to both of them

Heute bieten keramische Werkstoffe in Konstruktionen sehr gute Lösungsmöglichkeiten für spezifische technische Anwendungen. Es gibt aber auch einige wesentliche Nachteile. Erstens müssen numerische Methoden für die Anwendung der Festigkeitstheorie spröder Werkstoffe verwendet werden. Zweitens muß eine korrekte Interpretation und Verwendung der charakteristischen Parameter erreicht werden. Das KERB-Programm ist ein FEM-Subprozessor und wurde am Institut für Maschinenwesen der TU Clausthal entwickelt und bietet Lösungen für beide Probleme.

1 Design with ceramic materials

Ceramics offer nowadays different advantages in relation with metals and organic materials. This causes that this kind of materials are everyday more important for technology applications in multiple fields /1/ due to their multiple advantages as low thermal expansion, resistance to high temperatures, lower density, higher corrosion and erosion resistance, higher toughness and lower thermal conductivity.

Despite the numerous advantageous properties of engineering ceramics, designers still hesitate to use them for load bearing applications. The main subjective reason seems to lie in the different methodology, based on probabilistic fracture mechanics, which is required for designing with brittle as opposed to conventional, ductile materials.

Ceramics are prone to brittle failure due to their intrinsically high yield strength and low fracture toughness. Their inability to relax stress concentrations at the tips of microscopic surface or volume flaws can result in any one of these flaws propagating catastrophically in an uniform tensile stress filed.

Failure of ceramic components is caused by unstable extension of natural crack-like defects, which are always present due to manufacturing and surface treatment. These defects are responsible of the brittle behaviour of ceramics. A crack behaves as a stress concentrator that creates a stress state in the material much more higher that it would suffer as a ductile one.

Assuming that a component fails if any one flaw initiates fracture (the weakest link hypothesis), and that there is no interaction between flaws, the probability of failure P_f , equals to the probability of encountering at least one destructive flaw in the component. If the component is divided in N subvolumes or surfaces, the probability of survival would be:

$$\mathsf{P}_{\mathsf{S}} = \left(1 - \mathsf{P}_{\mathsf{f}}\right)^{\mathsf{N}} \cong \prod^{\mathsf{N}} \exp(-\mathsf{P}_{\mathsf{f}}) = \exp\left(-\sum^{\mathsf{N}} \mathsf{P}_{\mathsf{f}}\right)$$

or what would be equivalent

 $= \exp(R_{f})$

$$P_{f} = 1 - \exp\left(-\frac{1}{V_{0}}\int_{v}\left(\frac{\sigma - \sigma_{u}}{\sigma_{0}}\right)^{m}dV\right)$$
(2)

Where R_f (risk of failure) is the most probable number of destructive flaws, that means, their mean number in a large set of identical components. This is obtained by integrating the local density of destructive flaws over the volume assuming that flaws of different length are uniformly distributed over the volume.

It can be shown /2/ that any distribution of flaw lengths which for a $\longrightarrow \infty$ converges towards zero as fast as a^{-k}, where k is any constant, leads to the Weilbull distribution of strength

(1)

$$P_{f} = 1 - \exp\left(-\frac{1}{V_{0}}\int_{v}\left(\frac{\sigma - \sigma_{u}}{\sigma_{0}}\right)^{m}dV\right)$$
(3)

with the Weibull modulus m, σ_0 the characteristic stress, σ_u the minimum stress where no failure component occurs (usually set to zero in the experimental characterisation) and V₀ a certain reference or unit volume. The integration should be made only in those regions of the component under tension, but it has been proved thea compression can also generate a local risk of failure.



Figure 1: Ceramic ventilator calculated with KERB



Figure 2: Ceramic ventilator calculated with KERB

2 Use of the subroutine KERB

Nowadays to calculate the resistence of ductile components it is necessary its calculation through FEM programmes, due to the complex multiaxial stress state which suffer when loaded, it is even more necessary to apply its potential to brittle materials. Commercial powerful FEM programmes offer the user the possibility to run his own private calculations in each integration point, with the data calculated by the programme as tensions, deformations, temperature.... This possibility was used in the IMW to develop a subprocessor programme which enables the user to calculate the Risk of failure associated to each integration point, according to the material data provided by the user. These calculations are run at the same time as the FEM job with a special subroutine (KERB)

The different fracture criteria could be resumed in two main groups, first of all, phenomenological criteria, based in experimental results, and second one, Fracture Mechanic's criteria based, as its own name says in the Fracture Mechanic theory. Both types are implemented in this subprocessor.

Both of them need the stress state in each point of the component, to calculate with it the resultant risk of failure associated to each integration point. Obtained the complete risk of failure of the piece the calculation of the Probability of failure is a direct result of it.

Those criteria can be applied not only to static load cases (contact, mechanical, thermal or coupled jobs) but also to cases where loads act over the piece during different time intervals and even to fatigue cases.

Apart from the Risk of failure fields for different criteria, the programme allows the user to calculate another important variable, the intensity of failure, variable which minimise the meshing size influence which could distort local results, and as said before, offers also global data as the probability of failure for the whole component, and a security design factor, taking as reference a desired P_f given by the user.

The use of subroutine KERB assures a high degree of confidence for the resultsas it has been thouroughly checked.

3 Data scattering

The aim of this stay was to find a way to reflect in a numerical method the experimental characterisation of this kind of materials and also its usual parameter scattering.

The first goal was to find a way to calculate uniaxial parameters used in the characterisation of ceramics (eq. 3), usually, the characterisation of these is done using the experimental data obtained for three or four-point-bending tests /3/ with a quite diverse geometry and stress state from what a uniaxial case would be, these data are translated into uniaxial data using geometrical integrals quite difficult and most times impossible to calculate in a theoretical way /4/.



Figure 3: Equivalence of experimental characterisation



Figure 4: 3-point testing bar equivalent tension, calculated with KERB

The programme KERB has been modified along this stay to calculate the uniaxial equivalent data, running under a experimental card, based in the experimental data given by the user. Now the user can indicate in the input card that he wants to run his FEM model as an experimental case (that indicates the programme that the user is given experimental data <m_{exp}, σ_{θ} > and not characteristic values <m, σ_0 >) and the programme will return, based in the geometry, stress state and experimental data of the FEM job, the uniaxial equivalent characterising values needed to work with the material for general purposes design. To calculate them, the programme uses basically a normalised integral of the FEM model and bases its theoretical background in the equations:

$$\mathbf{m} = \mathbf{m}_{\rm exp} \tag{4}$$

$$V_{ef} = \frac{1}{\sigma_{max}^{m}} \int_{V} \sigma^{m} dV$$
 (5)

$$\sigma_0 = \sigma_0 \sqrt[n]{\frac{1}{m}} \frac{V_{ef}}{V}$$
(6)

Being V the unit volume considered as representative for the material (V_0) and V_{ef} the equivalent uniaxial volume for the experimental run as flexure one.

Another well known problem is the scattering of the experimental data due to the material production. To resume it in a simple way, although the characterisation of ceramics is done with a certain number of tests, this set of tests is run usually with a kind of material produced in a short period of time. Their properties vary depending strongly on the production process, so if the experimental characterisation is run with a set of probes all produced in a short term of time, it could be assumed that they are produced in the same way with almost the same properties (m_{exp1} , $\sigma_{\theta 1}$), but perhaps the same characterisation run a coupled of weeks later would offer as result a complete different pair of experimental characterising data (m_{exp2} , $\sigma_{\theta 2}$).

That should drive to calculate ceramic characteristic properties not only like a simple pair of experimental data (m_{exp} , σ_{θ}) but to consider them as probabilistic data themselves (although they have been calculated through a proper statistical process) given by its media and variance. They would follow a normal distribution quite common for the material characterisation data depending on production variables, and could be supposed as independent ones, although this will be checked with a future experimental procedure.

It should be possible to obtain the estimated media and variance for each of them (supposing they followed a normal distribution) equalling them to their estimators (to accept the estimator of the variance as correct it will be necessary to have a number of data relatively high as it has a deviation of $-\sigma^2/N$) /5/:

$$\mu = \overline{x} = \frac{\sum x_i}{N}$$
(7)

$$\sigma^{2} = s^{2} = \frac{\sum \left(x_{i} - \overline{x}\right)^{2}}{N}$$
(8)

With this data uniaxial characterisation (m, σ_0) of the population is found and also two normal distributions with their media and variance for (m, σ_0). The programme KERB has been modified to enable the user to introduce, as external data, couples of values (m_i, σ_{0i}) (that could be calculated with (m_{expi}, $\sigma_{\theta i}$) through the simple geometrical integral mentioned before with a previous run). With them it calculates their media and variance, considering them as independent variables (fact that should be checked in future experimental studies as it was mentioned before).

The supposed distribution followed by each of them, would be a normal distribution quite usual for experimental results depending on scattering variables as production ones, and those distributions can be easily normalised as:

$$\alpha_{\rm m} = \frac{{\rm m} - {\rm \overline{m}}}{\sigma_{\rm n}}$$

$$\alpha_{\sigma 0} = \frac{\sigma_0 - \sigma_0}{\sigma_{\sigma 0}} \tag{9}$$

Or what would be equivalent:

$$\mathbf{m} = \mathbf{s}_{m} \boldsymbol{\alpha}_{m} + \mathbf{m}$$
$$\mathbf{s}_{0} = \mathbf{s}_{s0} \boldsymbol{\alpha}_{s0} + \overline{\mathbf{\sigma}}_{0}$$
(10)

With this data it will be possible to calculate for any ceramic material not only the P_f of the FEM job but its media and variance depending on the media and variance of their material properties.

Based in a Taylor's approximation of any function:

$$\mathbf{f}(\mathbf{x}) \cong \mathbf{f}(\mathbf{x}_0) + \frac{\partial \mathbf{f}}{\partial \mathbf{x}}\Big|_{\mathbf{x}_0} (\mathbf{x} - \mathbf{x}_0) +$$

$$\frac{1}{2} \frac{\partial^2 f}{\partial x^2} \bigg|_{x0} (x - x_0)^2 + \dots$$
 (11)

This expression could be applied to a general function, depending on several independent variables considered them normalised as done through eq. 9 /6/:

$$F(x_i) \cong F(x_{0i}) + \sum F_i^{I} \alpha_i + \sum \sum \frac{1}{2} F_{ij}^{II} \alpha_i \alpha_j \qquad (12)$$

In this case all this mathematical process was applied to the P_f depending on the characteristic properties of ceramics (m, σ_0), and could be used to calculate through it the media and variance of the function.

Taking the complete expression of the P_f:

$$P_{f}(m, \sigma_{0}) = 1 - \exp(-R_{f}(m, \sigma_{0})) =$$

$$P_{f}(\alpha_{m}, \alpha_{\sigma 0})$$
(13)

and the Taylor expression (eq. 7), it is possible to express the media and variance of P_f, with the previous normalisation of the variables (m, σ_0). The value of the media is, as it would be expected:

$$\mathsf{P}_{\mathsf{f}}^{\mathsf{0}}(\mathsf{m}, \sigma_{\mathsf{0}}) = \mathsf{P}_{\mathsf{f}}(\overline{\mathsf{m}}, \overline{\sigma}_{\mathsf{0}}) \tag{14}$$

To calculate the covariance of the P_f it was used an approximation till the first derivative term, due to the complexity of the operation and to be this work a first display of the problem

$$Var(P_{f}) = E\left[\left(P_{f} - P_{f}^{0}\right)\left(P_{f} - P_{f}^{0}\right)^{T}\right] = \sum \sum P_{\alpha i}^{I} P_{\alpha j}^{I} E\left(\alpha_{i} \cdot \alpha_{j}\right)$$
(15)

Taking the two possible normalised variables (α_m, α_{o0}) the expression would result as:

$$Var(P_{f}) = (P_{\alpha m}^{I})^{2} E(\alpha_{m} \cdot \alpha_{m}) + P_{\alpha m}^{I} P_{\alpha s0}^{I} E(\alpha_{m} \cdot \alpha_{s0}) + (P_{\alpha s0}^{I})^{2} E(\alpha_{s0} \cdot \alpha_{s0})$$
(16)

to evaluate the value of :

$$\mathsf{E}(\alpha_{\mathsf{m}} \cdot \alpha_{\mathsf{s0}}) = \mathsf{E}(\alpha_{\mathsf{m}})\mathsf{E}(\alpha_{\mathsf{s0}}) + \mathsf{Cov}(\alpha_{\mathsf{m}}, \alpha_{\mathsf{s0}}) \ (17)$$

it was supposed that α_m and $\alpha_{\sigma 0}$ act as independent variables, thing that will have to be checked in a experimental way. That means that the term $Cov(\alpha_m, \alpha_{\sigma 0})$ was supposed as null.

So the implemented expression was:

$$Var(P_{f}) = (P_{\alpha m}^{I})^{2} E(\alpha_{m})^{2} +$$
$$P_{\alpha m}^{I} P_{\alpha s0}^{I} E(\alpha_{m}) E(\alpha_{s0}) + (P_{\alpha s0}^{I})^{2} E(\alpha_{s0})^{2}$$
(18)

With this expression the programme was able to calculate the variance and media of the global probability of failure of any component run with a FEM programme, depending on the media and variance of (m, σ_0).

Being the different terms in the previous expression:

$$\mathsf{P}^{\mathsf{I}}_{\alpha\mathsf{m}}=\sigma_{\mathsf{m}}\mathsf{P}^{\mathsf{I}}_{\mathsf{m}}$$

$$\mathsf{P}_{\alpha\sigma0}^{\mathsf{I}} = \sigma_{\sigma0} \mathsf{P}_{s0}^{\mathsf{I}} \tag{19}$$

and

$$P_{s0}^{I} = -m \cdot R_{f} \cdot exp(-R_{f})$$
⁽²⁰⁾

$$P_{m}^{I} = \exp(-R_{f}) \cdot \left(\frac{1}{V_{0}4\pi}\right) \iint_{V\Omega} \left(\frac{\sigma_{eq}}{\sigma}\right)^{m} \ln\left(\frac{\sigma_{eq}}{\sigma_{0}}\right) d\Omega dV \quad (21)$$

4 Conclusions and Resume

The first part of the changes introduced during this stay, the calculation of the characteristic properties <m, σ_0 > taking as basis <m_{exp}, σ_{θ} >, offers a power-

ful way to calculate characteristic variables of ceramics through a simple implementation of the geometry and load case for any experimental geometry case. The integrals run by the programme will be quite handy for experimental characterisation and enables a quite fast and powerful way to translate experimental results to theoretical ones, thing that can be very useful for people working in this field.

The calculation not only of the P_f of a component but its variance, depending on the scattering of the variables (m, σ_0), will make possible to calculate ceramic components taking into account the different production circumstances given usually during the production of a set of components, this seems really important when the actual experimental characterisation of ceramics, produced supposedly with the same material, shows a wide scattering depending on slight changes in the production variables.

Initial checks show quite possible the concordance between experimental and numeric results, but it will be necessary to run experimental results to get a thorough stochastic comparison of the model.

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