NUMERICAL MODELLING AND DETERMINATION OF FRACTURE MECHANICS PARAMETERS FOR CONCRETE AND ROCK: PROBABILISTIC ASPECTS

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Abstract
Damage evolution in quasi-brittle materials is a complex process in which heterogeneity plays an important role. The best way to introduce the effect of heterogeneity in fracture models is still a matter of discussion. This paper focuses on stochastic approaches to non-standard damage models. Central to the stochastic approach is concept of random field modelling of the governing parameters of the gradient damage model. The problem of parameter identification is addressed.

1 Introduction

Failure in quasi-brittle disordered materials, such as concrete, involves a progressive concentration of deformation in narrow zones. This phenomenon is referred to as strain localisation. The heterogeneity of concrete may play an important role in the localisation process in quasi-brittle materials. Therefore, the use of stochastic approaches to the damage process seems essential.

A first approach is based upon the mapping of the random particle structure onto a discrete representation and then use the finite element method to perform numerical simulations, see for example Schlangen (1993). These discrete models are computationally intensive and require complete finite element calculations for each simulation. Regarding the trends toward probability-based limit states design for engineering structures, these approaches have a limited applicability.

For engineering purposes, continuum fracture models are usually preferred. In this area, homogenisation techniques are intensively used, which can be seen as a intelligent filter of the material discreteness at a lower level toward a continuum description at a higher level. When a good separation exists between the lower scale of the discrete medium and the higher scale of the equivalent continuum material, we can arrive at formulating a deterministic constitutive law. However, experimental data for concrete show that the localisation region is in the order of a few times the grain size. Hence, there exists no sufficient separation between the scales. Due to the bad separation of the scales, two important consequences have to be considered. First of all, one is forced to deal with spatial random fluctuations of the continuous material properties. Secondly, a certain internal length scale l for the equivalent continuum material will exist, which measures the distance over which a strong micro-structural interaction will exist. This concept is also introduced by nonlocal and gradient models. Thus, a stochastic nonlocal continuum model rather than a deterministic local model has to be used.

The best way to derive a stochastic nonlocal continuum damage model is still a matter of discussion. One way is to derive the constitutive equations from micro-mechanics using extended homogenisation methods (Ostoja-Starzewski, 1994, Mirfendereski and Der Kiureghian 1994). A more phenomenological approach, which is used in this paper, is based on a stochastic formulation of deterministic non-standard fracture models (Carmeliet and Hens 1994, Carmeliet and de Borst 1995). The non-standard damage models properly describe the localisation process of strain softening materials. However, the deterministic character of these formulations has to be contrasted with the probabilistic nature of fracture and damage phenomena. In the stochastic approach, we model the governing continuum properties of the fracture model as random variables. In modelling the spatial distribution of the material properties, different levels of sophistication can be used:

(a) Each material property is specified by a single random variable.
(b) Each material property is specified by a vector of independent random variables. Each entry of this random vector corresponds to a sort of local homogenisation neglecting any spatial correlation.
(c) Each material property is specified as a random field, describing the distribution and spatial interdependency of the material properties.

The last case also forms the basis for stochastic finite elements and advanced reliability methods. The stochastic finite elements can be regarded either as a perturbated version of deterministic schemes or as repeated analyses of the basic problem with data which are realizations of random fields. The reliability finite element methods offer a framework for efficiently analyzing the failure probability or reliability of mechanical structures.

2 Gradient damage model

In this section, we present the gradient formulation of the nonlocal damage model as developed by Peerlings et al. (1995). The nonlocal damage model as well as the gradient damage model start from the classical isotropic elasticity-based damage theory:

$$\boldsymbol{\sigma} = (1 - D)\, \mathbf{C}\, \boldsymbol{\epsilon} \tag{1}$$

where $\mathbf{C}$ is the initial elasticity tensor of the virgin material, $\boldsymbol{\sigma}$ and $\boldsymbol{\epsilon}$ are the stress and strain tensors and D the damage variable, which grows from zero to one (complete loss of integrity). Damage growth is determined by an evolution law $D = F(\epsilon^{eq})$, in which ϵ^{eq} is an equivalent strain measure defined by Mazars and Pijaudier-Cabot (1989). Damage growth is possible if the damage loading function $f = \epsilon^{eq} - K$ vanishes. The damage parameter K initially equals the damage threshold K_0 and during damage evolution equals the maximum value of ϵ^{eq} ever reached during the loading history. The damage loading function f and the rate of damage growth $\dot{D}$ have to satisfy the discrete Kuhn-Tucker conditions: $f \leq 0$, $\dot{D} \geq 0$, $f\dot{D} = 0$.

In the original nonlocal model (Pijaudier-Cabot and Bazant 1987) the equivalent strain ϵ^{eq} is replaced by a spatially averaged or non-local equivalent strain value $\bar{\epsilon}$, such that:

$$\bar{\epsilon}(\mathbf{x}) = \frac{1}{V_r} \int_V \epsilon^{eq}(\mathbf{x}+\tau)\,\alpha(\tau)\,dV$$
$$\alpha(\tau) = \exp\left(-|\tau|^2/2\,l^2\right) \tag{2}$$

with τ the separation vector, V_r a normalising factor, α a squared exponential weight function and l the so-called internal length scale.

In the gradient damage formulation of the nonlocal concept, the integral equation of eq. 2 is replaced by the partial differential equation:

$$\bar{\epsilon} - c\,\nabla^2\bar{\epsilon} = \epsilon^{eq} \tag{3}$$

with $c=l^2/4$. Introducing C^0-continuous quadratic interpolation functions N for the displacement field and the C^0-continuous linear interpolation functions H for the nonlocal equivalent strain field, the coupled incremental finite element formulation of the equilibrium equation and differential equation (3) reads (Peerlings et al. 1995):

$$\begin{bmatrix} \mathbf{K}_{uu} & \mathbf{K}_{ue} \\ \mathbf{K}_{eu} & \mathbf{K}_{ee} \end{bmatrix} \begin{bmatrix} \mathbf{du} \\ \mathbf{d\bar{e}} \end{bmatrix} = \begin{bmatrix} \mathbf{F}_{ext} + \mathbf{F}_u \\ \mathbf{F}_{\bar{e}} \end{bmatrix} \tag{4}$$

with $\mathbf{du}$ and $\mathbf{d\bar{e}}$ the incremental nodal displacements and nodal nonlocal equivalent strains, $\mathbf{F}_u$ the internal forces, $\mathbf{F}_{\bar{e}}$ the internal nonlocal forces and $\mathbf{F}_{ext}$ the external forces. The partial matrices $\mathbf{K}_{uu}$, $\mathbf{K}_{ue}$, $\mathbf{K}_{eu}$ and $\mathbf{K}_{ee}$ are given by Peerlings et al. 1995.

2.1 Identification of the model parameters Sensitivity analysis

In the classical damage model the following parameters are used: the elastic modulus E, the initial damage threshold $K_0 = f_t/E$, with f_t the tensile strength and the damage function D. An additional parameter that emerges in the gradient damage model is the length parameter c, which is connected to the internal length scale l. For the damage function we adopt an exponential function:
$D = 1 - (K_0/\bar{\epsilon})\,[\,(1 - a_D) + a_D \exp(-b_D(\bar{\epsilon} - K_0))\,]$, with a_D and b_D model parameters. The elastic modulus E can be determined from

elementary tests. However, the tensile strength, the damage function and the internal length scale are not directly derivable from elementary tests. One must proceed in an inverse manner, whereby the parameters are estimated by minimizing the differences between the experimental and numerical results of different types of tests. Optimisation methods can be used to solve the parameter estimation problem. These methods are generally based on the calculation of the partial derivatives of the structural response **S** to the model parameters **X**.

In this paper a first attempt to the parameter estimation is made by studying the sensitivity of the structural response **S** to the different parameters. First, a reasonable estimate of the parameters $\mathbf{X}_0$ is made based on the experimental results: the load-elongation curve of a double notched direct tensile test and the load-deflection curve of four point bending tests with three different notch depths (Hordijk 1991). Figure 1 compares the measured and calculated results. Table 1 gives the estimated parameters $\mathbf{X}_0$.

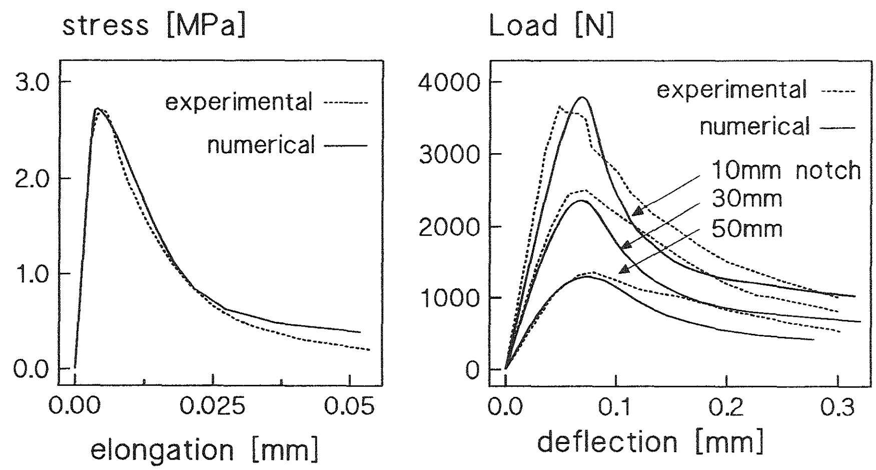

Fig. 1. Load-displacement curve for tensile test. Load-deflection curve for bending test for three notch depths.

Then, the sensitivity β_i, which expresses the relative influence of the parameters X_i on the structural response S_i is calculated as:

$$\beta_i = \frac{\partial S_i}{\partial X_i} \frac{X_{0i}}{S_{0i}} \tag{5}$$

Table 1. Estimated model parameters $\mathbf{X}_0$

	X_0
f_t (MPa)	3.1
E (MPa)	32860
c (mm^2)	1.5
a_D (-)	0.9
b_D (-)	600

Table 2. Sensitivity index β of the structural response to the model parameters

sensitivity	P_t	U_t	P_b	U_b
f_t	0.98	0.97	0.76	0.95
E	0.03	0.17	0.26	0.06
c	0.02	0.37	0.12	0.23
b_D	0.03	0.75	0.26	0.42

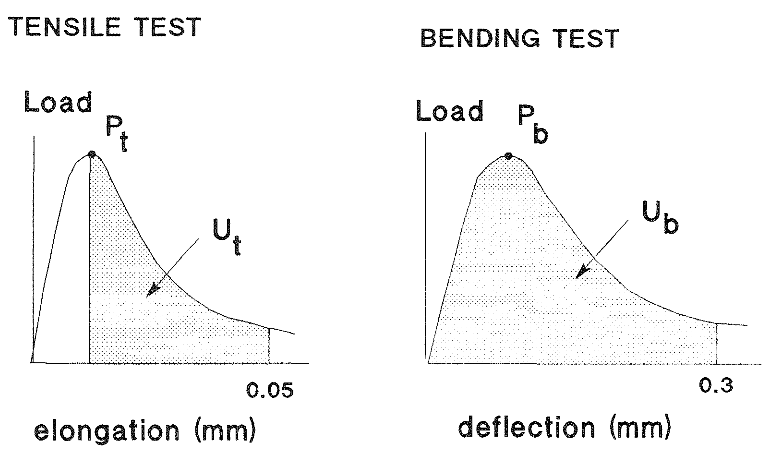

Fig. 2 Definition of structural response variables P_t and U_t for tensile test, P_b and U_b for bending test.

with S_{0i} the calculated response using the parameters $\mathbf{X}_0$. A value of β close to one means a high sensitivity, a values near zero means a low sensitivity. The gradients are evaluated using a finite difference technique.

The structural response **S** is characterized by different variables: the maximum forces P_t and P_b and the energies U_t and U_b for respectively the tensile and bending test (figure 2). The energies U_t and U_b are used as measures for the post peak damage behaviour. Table 2 summarizes the results. We observe that the tensile strength f_t highly influences all the response variables. This indicates the need for an accurate determination of the tensile strength. The response variable P_t is only influenced by the tensile strength. This indicates that the tensile strength can be accurately obtained from the maximum force P_t. The other response variables P_b, U_t and U_b are influenced to a greater or less extent by the different parameters. This means that only indirect techniques can be used for the parameter identification. It is also noted that the response variables **S** are less sensitive to the length parameter c. This means that a very accurate determination of the length parameter on the basis of these tests is not possible. Similar sensitivity studies on different geometries and loading conditions should elucidate which combination of experiments is most suitable for a proper parameter determination.

3 Stochastic approach to gradient damage model

In the stochastic approach, the governing parameters of the gradient damage model are modelled as random fields. An important issue is the selective modelling of certain parameters as random fields in order to ensure computational efficiency and sufficient accuracy. It appears logical to consider only those parameters as random variables, which have a significant influence on the structural response. The other variables can be considered deterministic. Therefore, we will only model the parameter which showed the highest sensitivity, namely the tensile strength as a random field. The tensile strength f_t or equivalently the initial damage threshold $K_0=f_t/E$ is represented by a non-Gaussian correlated random field. For the non-Gaussian field a three-parameter extreme value distribution type III function is assumed:

$$f_{K_0}(K_0) = \lambda \mu (K_0 - K_0^{min})^{\mu-1} \exp \left[- \lambda \left(K_0 - K_0^{min}\right)^{\mu} \right] \tag{6}$$

with K_0^{min} the lower bound of the initial damage threshold. The choice of this distribution function is based on the following physical considerations: (i) the initial damage threshold K_0 will show a finite lower bound rather than an infinite lower tail; (ii) the initial damage will very likely be asymmetrically distributed; (iii) the initial damage in a macroscopic sense is strongly influenced by the largest microstructural flaw and will therefore follow an extreme value distribution. Furthermore, we assume the field to be homogeneous and isotropic, which implies that the autocorrelation coefficient function $\rho(\tau)$ can be expressed in terms of the separation vector $\tau=[\tau_x,\tau_y,\tau_z]^T$ between the points $\mathbf{x}$ and $\mathbf{x}+\tau$. The autocorrelation coefficient function is assumed to be of the same form as the weight function of the nonlocal damage model:

$$\rho(\tau) = e^{-\left(\frac{|\tau|^2}{2d^2}\right)} \tag{7}$$

with d a length parameter, which is a measure for the rate of fluctuations of the random field. For finite element analysis involving random field properties, it is necessary to discretise the continuous random field into random vector representations. In this paper, we will use the midpoint method.

3.1 Identification of the random field parameters.

The following additional parameters are introduced in the stochastic approach: the length parameter d of the correlation function, the parameters K_0min, λ and μ describing the distribution function. It has been shown in (de Borst and Carmeliet 1994) that the length parameter d has only a minor influence on the results. Therefore, we can assume as reasonable estimate for the length parameter d a value equal to the internal length scale l. The distribution parameters are estimated from statistical test data. A large number of direct tensile tests were performed on polymer modified cement mortar specimens. Figure 3a shows the cumulative distribution of the tensile strength. The numerical cumulative distributions are calculated from the responses of several samples using the Monte Carlo technique. Comparing the numerical responses to the experimental distribution of tensile strength, the following values for the parameters were obtained: $\lambda=6.56\ 10^5$, $\mu=1.6$, $K_0^{min}=0.66\ 10^{-4}$.

To validate the stochastic damage model, we study the tensile behaviour of a cement composite material. The composite material consists of the polymer modified cement mortar and a glass fibre fabric. In the numerical modelling, the interaction between mortar and fibres is determined by a shear traction-slip relation, which is the constitutive equation for the interface elements. The glass fibre reinforcement has been modelled with bar elements and behaves as a linear elastic material. The material data are given in Carmeliet and Hens (1992). Figure 3b compares the experimental and numerical cumulative distributions for specimens with different fibre volume fractions. The calculations agree well with the experimental results. Also the deterministic results are shown. For high volume fractions, we see that the deterministic model only slightly underestimates the mean tensile strength. The small difference may be explained by the advantageous role of the fibres in the load-sharing mechanism, avoiding the progressive collapse once the weakest part in the specimen fails. This mechanism is not considered in the deterministic model.

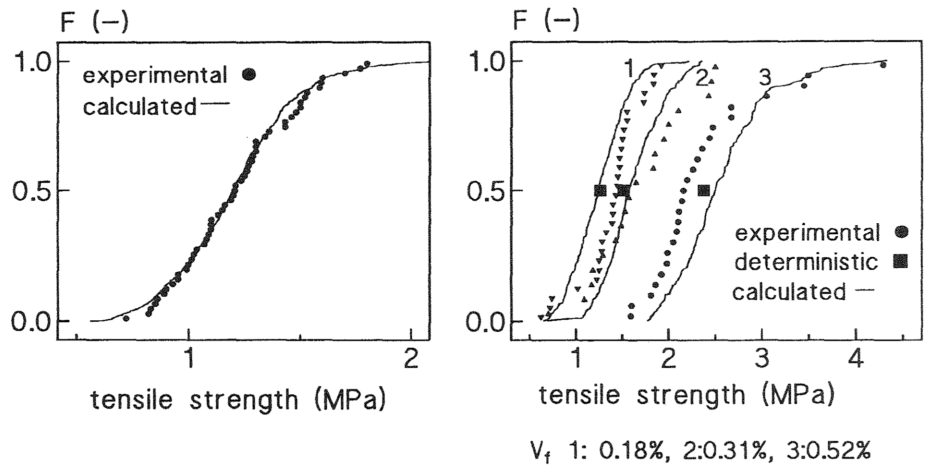

Fig. 3 (a) Cumulative distribution of tensile strength of polymer modified cement mortar.
(b) Comparison of experimental and calculated cumulative distribution of tensile strength for glass fibre reinforced mortar with different fibre volume fractions V_f.

3.2 Three point bending test

To more clearly illustrate the difference between the deterministic and stochastic model, three point bending beams with different widths are analyzed. The beam has a length of 160 mm and a height of 30 mm. Two widths are considered: 10 and 30 mm. Fig. 4 shows the calculated cumulative distribution of the maximum load per unit width. The distributions for the two widths differ markedly. For the beams with a larger width, due to load-sharing and damage redistribution the development of the critical damage zone will be slowed down, resulting in higher maximum loads. For the beams with smaller width, the sharing mechanism is less effective resulting in a shift of the distribution to lower maximum loads. It is interesting to note that the deterministic prediction of the maximum load fully coincides with the median value of the maximum load distribution for the small beams. This is logical because the improvement of the structural response due to the sharing mechanisms for very small widths will be negligible.

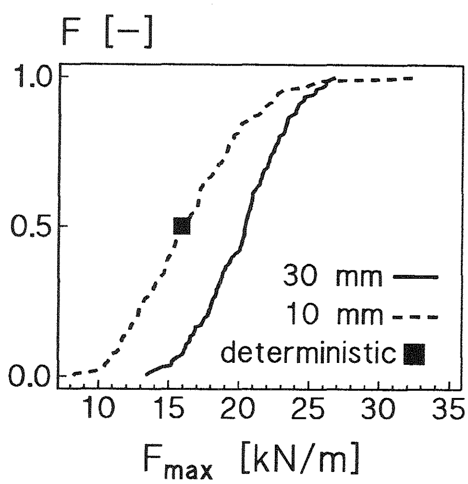

Fig. 4 Cumulative distribution of maximum load for two widths of beam in three point bending. Deterministic versus stochastic results.

3.3 Pull-out of an anchor bolt

To show the importance of a stochastic approach for damage processes in quasi-brittle heterogeneous materials, the example of a pull-out of a steel anchor bolt embedded in concrete is selected. The pull-out analysis of an anchor bolt has been proposed by RILEM-committee TC90-FMA as a round-robin analysis in order to compare different methods. The geometry and material properties of the second proposal have been used in this study (Vervuurt et al. 1993). Because of the stochastic nature of the material, symmetry does not exist. Nevertheless, for the sake of simplicity, symmetry is assumed and only the half of the specimen has been discretised with 3327 four noded plane stress square elements with a four-point integration. The finite element discretisation is given in figure 5a. Only the upper part of the specimen, where the damage will develop has been modeled as a random field. For the lower part of the specimen the mean value of the initial damage threshold is assumed.

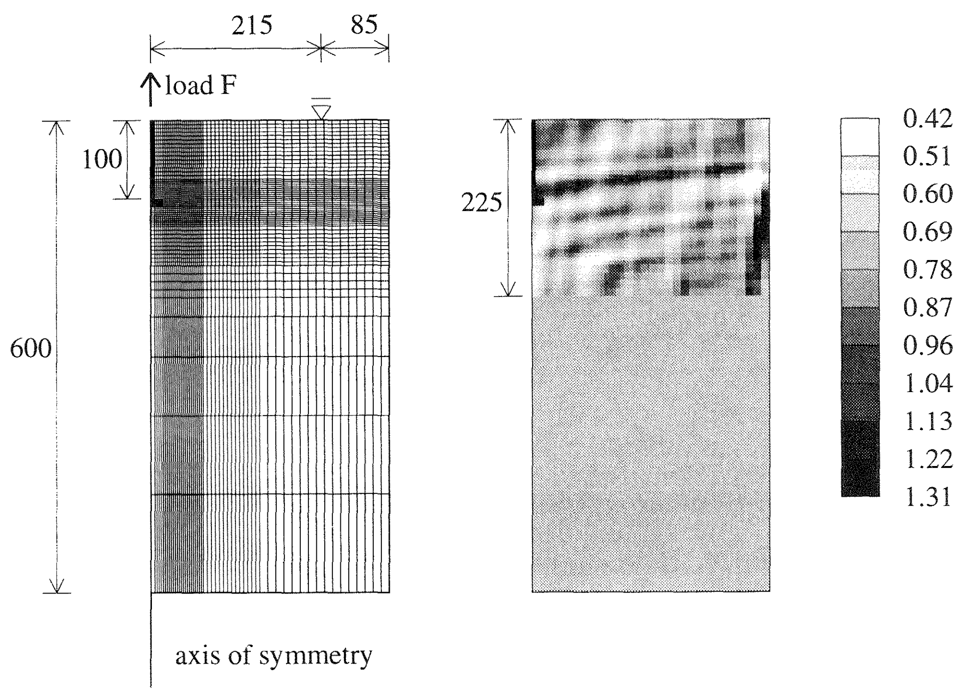

Fig. 5 Pull-out of an anchor bolt. Finite element and stochastic element model.

The material properties are given in de Borst and Carmeliet (1995). The results are given as the load versus displacement of the upper-outer edge of the anchor head (fig. 6a) and the crack patterns at different stages of the damage process (fig. 7). Figure 6b shows the cumulative distributions for the maximum load calculated from the responses of 50 samples using the Monte Carlo technique An important scatter in maximum load F_{max} is observed. This can be explained by the fact that the maximum load is highly dependent on the presence of initial defects in a small zone surrounding the anchor bolt. The different crack patterns for the three different specimen show that the exact failure

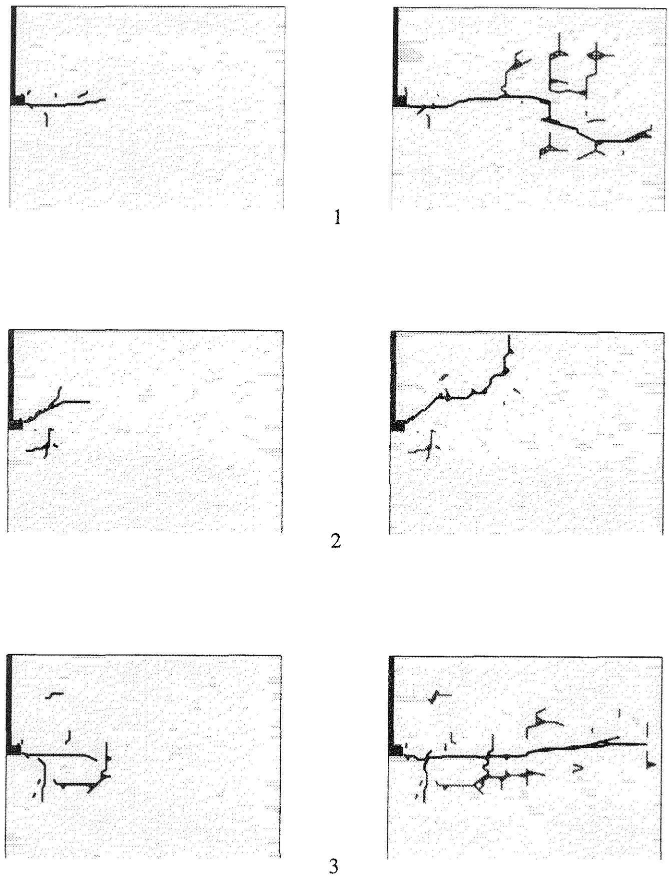

Fig. 7 Crack pattern at maximum load (a) and at final loading (b).

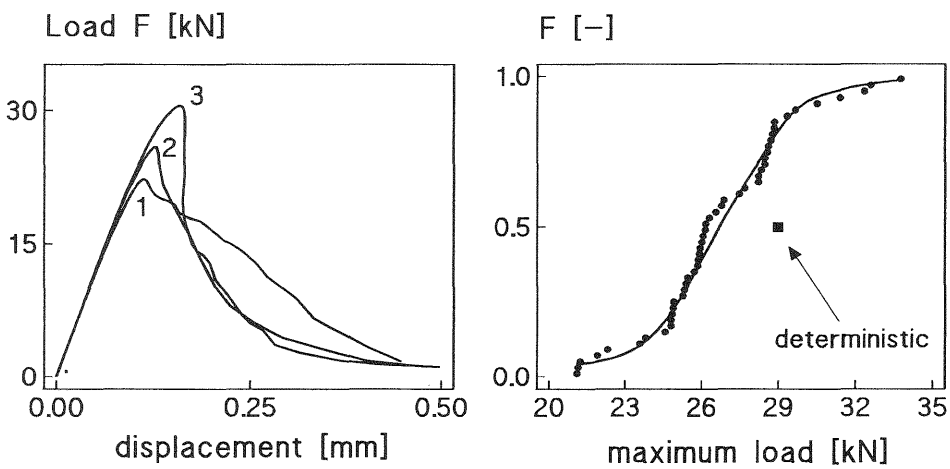

Fig. 6 (a) Load-displacement diagram. (b) Cumulative distribution of maximum load.

mode can be highly dependent upon the precise initial flaw distribution. Also the deterministic result is shown. Apparently, the maximum load for the deterministic analysis is higher than the mean value of the stochastic results.

4 Conclusions

1 A stochastic approach to damage processes in quasi-brittle materials is presented. The approach is based on the random field modelling of the governing parameters of the gradient damage model.

2 The parameters can only inversely be identified by minimizing the differences between the experimental and numerical results of different types of tests. Optimisation methods can be used to solve the parameter estimation problem.

3 Sensitivity studies can elucidate which combination of experiments is most suitable for a proper parameter determination.

4 Deterministic models fail or are inefficient when material heterogeneity governs the structural response.

5 References

Carmeliet, J., and Hens, H. (1992). Fracture of a fabric reinforced mortar based on a stochastic approach to initial damage. **Proc., Conf. on Localized Damage II: Fatigue and Fracture Mechanics**, (eds M.H. Aliabadi et al.), Computational Mechanics Publications, Southampton, 283-298.

Carmeliet, J. and Hens, H. (1994) Probabilistic nonlocal damage model for continua with random field properties. **ASCE J. Engng. Mech.**, 120, 2013-2027.

Carmeliet, J., and de Borst, R. (1995) Stochastic approaches for damage evolution in standard and non-standard continua. **Int. J. Solid Structures.**, 32, 1149-1160.

de Borst, R. and Carmeliet, J. (1994) Stochastic approaches for damage evolution in standard and non-standard continua. **Iutam Symp.on Size-scale effects in the failure mechanisms of materials and structures**, to appear.

Hordijk, D. (1991) Local approach to fatigue of concrete. PhD Thesis, Delft University of Technology, Delft, The Netherlands.

Mazars, J. and Pijaudier-Cabot, G. (1989) Continuum damage theory - Application to concrete. **J. Engrg. Mech., ASCE**, 115(2), 345-365.

Mirfendereski, D. and Der Kiureghian A. (1994) Probabilistic analysis of micro-fabricated multicrystalline beams, **Proc. Int. Conf. Structural Safety & Reliability** (eds G.I.Schuëller, M.Shinozuka and J.T.P.Yao), Balkema, Rotterdam, 361-368.

Ostoja-Starzewski, M. (1994) Micromechanically based random fields, **Proc. Int. Conf. Structural Safety & Reliability** (eds G.I.Schuëller, M.Shinozuka and J.T.P.Yao), Balkema, Rotterdam, 629-636.

Peerlings, R.H.J., de Borst, R., Brekelmans, W.A.M., and de Vree,J.H.P. (1995) Computational modelling of gradient-enhanced damage for fracture and fatigue problems, in **Computational Plasticity: Theory and Applications** (eds D.R.J. Owen, E. Oñate and E.Hinton), Pineridge Press, Swansea, 975-986.

Pijaudier-Cabot, G. and Bažant, Z.P. (1987) Nonlocal damage theory.**ASCE J. Engng. Mech.**, 113, 1512-1533.

Schlangen, E. (1993) Experimental and numerical analysis of fracture processes in concrete, PhD. thesis, Delft University of Technology, Delft, The Netherlands.

Vervuurt, a., Schlangen, E. and Van Mier, J. (1993) A numerical and experimental analysis of the pull-out behavior of steel anchors embedded in concrete. Report 25.5-93-1, Delft University of Technology, The Netherlands.