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MODELING THE QUASI-BRITTLE FRACTURE OF STRUCTURAL MATERIALS USING A MIXED STABILIZED TWO-FIELD FINITE ELEMENT FORMULATION

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Abstract. The *fracture process zone* (FPZ) is typically characterized as a small region around a crack where non-linear phenomena occur, such as plasticity. In brittle materials, this zone is small and can be safely neglected. However, in quasi-brittle materials, which exhibit a combination of brittle and ductile behavior rather than a clear manifestation of either, the material within the FPZ tends to damage and displays a softening curve after reaching peak load. This behavior is frequently observed in structural materials like concrete and timber, and it can be challenging to model. Traditionally, displacement-based irreducible finite element (FE) formulations have been widely used for simulating structural materials. However, this approach comes with significant drawbacks, such as mesh dependence and convergence problems, when applied to certain phenomena like softening, localization, and fracture. To address these challenges, various techniques have been employed, including extended FE methods and phase-field modeling. In this work, the utilization of a mixed FE formulation in which both displacement and strain serve as primary unknowns within the system, is proposed. To ensure satisfaction of the *inf-sup* condition, which is associated with saddle point stability in mixed formulations, we employ the *variational multiscale method* to introduce stabilizing terms into the system. The implementation is conducted using FEniCS, an open-source FE software that offers a high-level programming interface written in Python. The implementation is validated by comparing the obtained results with those reported in the literature for bending test in notched specimens. The results demonstrate remarkably good performance in terms of maximum load, softening curve, and structural size effect in various specimens, exhibiting minimal mesh dependence even when using low-order interpolation elements.

1 INTRODUCTION

A wide variety of quasi-brittle materials are in demand due to their structural value, such as timber or concrete. As a result, the study of fracture in this type of material becomes relevant not only for the safety and reliability of structures, but also for their durability, which also has environmental implications [1].

In general, fracture processes exhibit a non-linear softening zone around the crack called the *fracture process zone* (FPZ), in which stresses decrease as deformations increase. This zone, in turn, is surrounded by another non-linear hardening zone, characterized by inelastic behavior. On some occasions, the size of the FPZ can be neglected, in which case the tools of linear elastic fracture mechanics can be used. In the case of quasi-brittle fracture, this zone has a considerable size and is characterized by damage, due to complex micro and mesoscale mechanisms, leading to the progressive softening of the material.

Traditionally, the quasi-brittle fracture problem is addressed using phase-field models (PFM) and the extended finite element method (XFEM). PFM are based on obtaining a continuous representation of the crack with a smooth transition between the intact material and the damaged material, ensuring irreversibility in the process and crack propagation independent of the mesh. However, to achieve mesh objectivity, PFM require the use of very fine meshes, which leads to a high computational cost [2]. On the other hand, XFEM proposes to enrich the finite element, representing the crack as a discontinuity in the displacement field without altering its conformity [3]. By increasing the degrees of freedom exclusively at the nodes where the crack passes, XFEM presents itself as a low computational cost alternative. However, it is a mesh-dependent method, so crack tracking algorithms are required that require the use of a propagation criterion [2].

An alternative to the aforementioned methods are the mixed FE formulations, which, through the selection of appropriate unknowns, allow us to address problems such as strain localization and crack propagation. However, the solution of the variational problem associated with the unknowns requires the satisfaction of the *inf-sup* condition, also known as Ladyzhenskaya–Babuŝka–Brezzi (LBB) condition, associated with *saddle point* stability. One way to address this difficulty is to use the variational multiscale method (VMS), in which the classical Galerkin solution is complemented with a solution at the fine scale. One of the relevant aspects of mixed formulations is that it addresses the quasi-brittle fracture problem from the variational formulation, also obtaining results with low mesh dependency and without the need for crack tracking techniques [3].

In addition to the above, quasi-brittle behavior materials exhibit a noticeable structural size effect, which varies depending on the size of the FPZ. In structures with a size that does not exceed by much the size of the FPZ of the material, the failure presents a quasi-ductile behavior, while in structures with a size several orders of magnitude greater than the size of the FPZ, the failure of the structure is almost brittle [1]. Therefore, it becomes necessary to have a numerical tool capable of correctly capturing the localization of simulation fields, with low mesh dependence and in reasonable calculation times.

In this work, the use of a mixed formulation based on deformation and displacement fields, stabilized by VMS, is proposed for the simulation of quasi-brittle fracture of concrete. This paper presents the mixed formulation, its stabilization and the constitutive modeling, including the simulation of the structural size effect. The model is validated with reference numerical and experimental results from bending tests in notched specimens obtained from the literature.

2 FINITE ELEMENT MODEL

In a mixed formulation, the system of equations derived from the weak form involves multiple unknowns. The weak formulation of the problem can be expressed in a matrix form, that usually holds as follows:

$$\begin{bmatrix} \boldsymbol{A} & \boldsymbol{B}^T \\ \boldsymbol{B} & \boldsymbol{0} \end{bmatrix} \begin{Bmatrix} \boldsymbol{x} \\ \boldsymbol{y} \end{Bmatrix} = \begin{Bmatrix} \boldsymbol{f} \\ \boldsymbol{g} \end{Bmatrix} \tag{1}$$

where $\boldsymbol{A}$ and $\boldsymbol{B}$ are $n \times n$ and $m \times n$ matrices respectively; $\boldsymbol{x}$ and $\boldsymbol{y}$ are the study fields; and $\boldsymbol{f}$ and $\boldsymbol{g}$ are vectors associated with the study fields. An important drawback of these formulations is the stability of the solution, expressed in the *inf-sup* condition of the first variable, leading to unstable solutions if the interpolation is not suitable. In order to obtain a stable formulation, this work employs the VMS framework.

2.1 Mixed finite element formulation

A suitable mixed formulation for quasi-fragile fracture simulation can be derived in terms of strains and displacements ($\boldsymbol{\varepsilon}/\boldsymbol{u}$) [3, 4]. The strong form of the continuous problem for a body occupying a convex, open, and bounded region $\Omega \in R^3$, with a boundary $\partial\Omega$, can be expressed in terms of the study fields ($\boldsymbol{\varepsilon}/\boldsymbol{u}$) as follows:

$$-\mathbb{C} : \boldsymbol{\varepsilon} + \mathbb{C} : \nabla^s \boldsymbol{u} = \boldsymbol{0} \tag{2a}$$

$$\mathrm{div}(\mathbb{C} : \boldsymbol{\varepsilon}) + \boldsymbol{f} = \boldsymbol{0} \tag{2b}$$

where Eq. 2a corresponds to the kinematic and constitutive equations, while Eq. 2b represents the equilibrium of the linear momentum equation. Both equations are subject to their respective Neumann and Dirichlet boundary conditions. The corresponding weak formulation is obtained by introducing the test functions $\boldsymbol{\gamma}$ for strains and $\boldsymbol{v}$ for displacements, which are associated with the functional spaces $\mathbb{G} \subset \mathcal{L}^2(\Omega)^{\dim}$ and $\mathbb{V} \subset \mathcal{H}^1(\Omega)^{\dim}$, respectively. Applying the divergence theorem:

$$-(\boldsymbol{\gamma}, \mathbb{C} : \boldsymbol{\varepsilon}) + (\boldsymbol{\gamma}, \mathbb{C} : \nabla^s \boldsymbol{u}) = 0 \qquad \forall\, \boldsymbol{\gamma} \in \mathbb{G} \tag{3a}$$

$$(\nabla^s \boldsymbol{v}, \mathbb{C} : \boldsymbol{\varepsilon}) = \boldsymbol{F}(\boldsymbol{v}) \qquad \forall\, \boldsymbol{v} \in \mathbb{V} \tag{3b}$$

where $F(\boldsymbol{v}) = (\boldsymbol{v}, \boldsymbol{t})_{\partial\Omega} + (\boldsymbol{v}, \boldsymbol{f})$ represents the tractions on $\partial\Omega$ ($\boldsymbol{t}$) and the body forces in Ω ($\boldsymbol{f}$).

2.2 Stabilization

To overcome the compatibility challenges of the mixed finite element method and the stringent requirements of the *inf-sup* condition, stabilization can be achieved using the VMS method [5], where it is assumed that the continuous variables can be separated into coarse and fine components. The coarse scale can be approximated by the finite element; however, it cannot be applied to solve the fine scale (subscale). The effect of the subscale is locally included, contributing to the stability of the study fields in the mixed formulation. Following the methodology outlined by Cervera et al. [6], by introducing the separation proposed by the method, the study fields can be approximated as follows:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_h + \tilde{\boldsymbol{\varepsilon}} \tag{4a}$$

$$\boldsymbol{u} = \boldsymbol{u}_h + \tilde{\boldsymbol{u}} \tag{4b}$$

where $\boldsymbol{\varepsilon}_h \in \mathbb{G}$ and $\boldsymbol{u}_h \in \mathbb{V}$ correspond to the coarse scale, while $\tilde{\boldsymbol{\varepsilon}} \in \tilde{\mathbb{G}}$ and $\tilde{\boldsymbol{u}} \in \tilde{\mathbb{V}}$ correspond to the subscale. The corresponding test functions for the subscale, $\tilde{\boldsymbol{\gamma}} \in \tilde{\mathbb{G}}$ and $\tilde{\boldsymbol{v}} \in \tilde{\mathbb{V}}$, are also considered, and it is assumed that the subscale vanishes at the edges of each element. Including the sub-scales leads to the decomposition of the initial problem into four equations that are linearly independent of each other. The stabilized form can be derived as follows:

$$-(\boldsymbol{\gamma}, \mathbb{C} : \boldsymbol{\varepsilon}) + \tau_\varepsilon(\boldsymbol{\gamma}, \mathbb{C} : \tilde{\mathcal{P}}_\varepsilon(\boldsymbol{\varepsilon} - \nabla^s \boldsymbol{u})) + (\boldsymbol{\gamma}, \mathbb{C} : \nabla^s \boldsymbol{u}) \dots$$
$$\dots - \tau_u(\mathrm{div}(\mathbb{C} : \boldsymbol{\gamma}), \tilde{\mathcal{P}}_u(\mathrm{div}(\mathbb{C} : \boldsymbol{\varepsilon}) + \boldsymbol{f})) = 0 \tag{5a}$$

$$(\nabla^s \boldsymbol{v}, \mathbb{C} : \boldsymbol{\varepsilon}) - \tau_\varepsilon(\nabla^s \boldsymbol{v}, \mathbb{C} : \tilde{\mathcal{P}}_\varepsilon(\boldsymbol{\varepsilon} - \nabla^s \boldsymbol{u})) = \boldsymbol{F}(\boldsymbol{v}) \tag{5b}$$

where $\tilde{\mathcal{P}}_\varepsilon$ and $\tilde{\mathcal{P}}_u$ are projection operators that incorporate the effect of fine sub-scales into the finite element solution. Additionally, τ_ε and τ_u are stabilizing parameters given by:

$$\tau_\varepsilon = c_\varepsilon \frac{h}{L_0} \quad ; \quad \tau_u = c_u \frac{L_0 h}{\mathbb{C}_{\text{min}}} \tag{6}$$

where c_ε and c_u are algorithmic constants, L_0 is a characteristic length of the computational domain (geometry), h is the characteristic length of the finite element, and $\mathbb{C}_{\text{min}} > 0$ is the smallest eigenvalue of $\mathbb{C}$. Moreover, the stabilizing term $-\tau_\varepsilon(\nabla^s \boldsymbol{v}, \tilde{\mathcal{P}}_\varepsilon(\mathbb{C} : \nabla^s \boldsymbol{u}))$ generates a coefficient matrix $\boldsymbol{K}_{uv}$ leading to the form:

$$\begin{bmatrix} \boldsymbol{K}_{\varepsilon\gamma} & \boldsymbol{K}_{u\gamma} \\ \boldsymbol{K}_{\varepsilon v} & \boldsymbol{K}_{uv} \end{bmatrix} \begin{bmatrix} \boldsymbol{\varepsilon} \\ \boldsymbol{u} \end{bmatrix} = \begin{bmatrix} \boldsymbol{0} \\ \boldsymbol{F} \end{bmatrix} \tag{7}$$

that solves the compatibility issues associated with the initial mixed formulation.

2.3 Constitutive modeling

Classical fracture mechanics models failure in materials using an energy criterion, which can be complemented by a strength (or yield) criterion. Furthermore, it assumes that failure does not occur simultaneously along the entire failure zone but rather propagates through the structure. Despite this, due to the nature of quasi-brittle fracture, it is consistent to model it using damage mechanics in continuous media. For simplicity, an isotropic damage model is considered, relating stresses to strains as shown in the equation 8.

$$\boldsymbol{\sigma} = (1 - d)\mathbb{C}^e : \boldsymbol{\varepsilon} \tag{8}$$

where $\mathbb{C}^e$ is the elastic constitutive tensor and $d \in [0, 1]$ is an internal damage variable. This model considers a transition region between the intact material and the fractured material, characterizing a progressive reduction in stiffness. Additionally, the concept of effective stress $\boldsymbol{\sigma} = \mathbb{C}^e : \boldsymbol{\varepsilon}$ can be introduced, based on the hypothesis of evolution as a function of total strains. Thus:

$$\boldsymbol{\sigma} = (1 - d)\overline{\boldsymbol{\sigma}} \tag{9}$$

The damage criteria ϕ is defined as:

$$\phi(\tau, r) = \tau - r \leq 0 \tag{10}$$

where τ is a scalar, non-negative, and continuous function associated with the undamaged part of the stresses, referred to as the equivalent stress; and r is a scalar internal variable called the damage threshold, which defines the scalar damage function $d = d(r)$. It is assumed that the solid has an initial value $r(0) = r_0$ in an undamaged state. To model material degradation, the Rankine damage criterion is used, which considers only the material's tensile strength. Thus, an equivalent stress τ is defined by the effective principal stress $\overline{\sigma}_1$ as:

$$\tau = \langle \overline{\sigma}_1 \rangle \tag{11}$$

From the Kuhn-Tucker consistency conditions, the evolution of the damage threshold is explicitly obtained, so that r increases monotonically according to Ec. 12.

$$r = \max\{r_0, \max\, \tau\} \tag{12}$$

On the other hand, a relationship between d and r can be established through a softening law. In this case, it is assumed that softening occurs exponentially [7], where $d(r)$ is expressed as:

$$d(r) = 1 - \frac{r_0}{r}\exp\left[2H_s\left(\frac{r_0 - r}{r_0}\right)\right] \tag{13}$$

where H_s is a positive defined softening parameter that regulates the rate of material degradation, derived from the crack band theory [8]. Moreover, the softening parameter is linked to the material's fracture energy (G_f) and and tensile strength (f_t) [4], and can be computed as follows:

$$H_s = \frac{\overline{H}_s\, b}{1 - \overline{H}_s\, b} \tag{14}$$

where b is the crack band width and $\overline{H}_s$ is the reciprocal of the characteristic length of Irwin given by:

$$\overline{H}_s = l_{ch}^{-1} = \frac{f_t^2}{2\,E\,G_f} \tag{15}$$

Furthermore, this formulation considers that the localized crack band width b can be computed as:

$$b = (1 - \tau_{\boldsymbol{\varepsilon}})\,2h + \tau_{\boldsymbol{\varepsilon}} h = (2 - \tau_{\varepsilon})\,h \tag{16}$$

where h is the size of the finite element and τ_{ε} is the stabilization parameter of the mixed formulation.

3 SIMULATIONS AND RESULTS

The following section shows the numerical predictions of the quasi-fragile fracture modeling in structural elements. Numerical simulations are conducted based on experimental tests proposed by Grégoire et al. [9] and Hoover et al. [10]. The mixed $\boldsymbol{\varepsilon}/\boldsymbol{u}$ stabilized finite element formulation is implemented in the open-source software FEniCS [11]. The FEniCS environment is characterized by a high-level programming interface written in Python, which allows the introduction of the mathematical formulation expressed in its variational form in a symbolic manner [12].

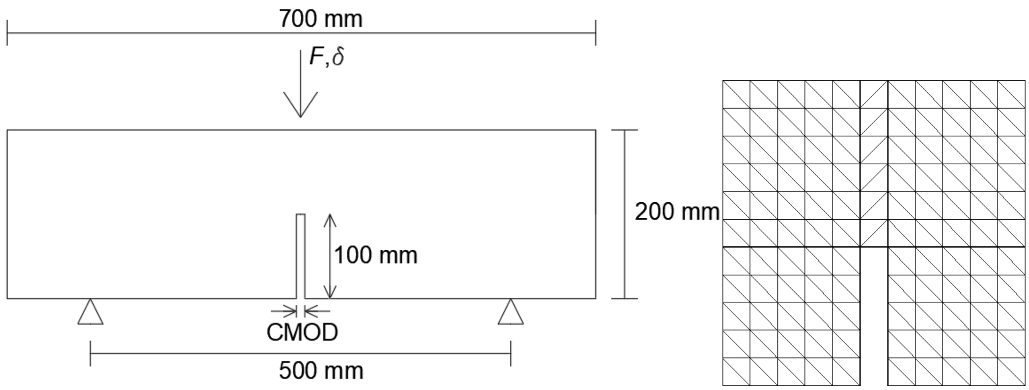
3.1 Grégoire test

The tests performed by Grégoire et al. [9] consist of three-point bending tests using specimens with a notch at the center, which allows the study of mode I fracture. For this purpose, both crack propagation and applied load vs crack mouth opening displacement (CMOD) curves are studied [9]. In this work, the simulation of this test has been performed to study if the stabilized mixed finite element formulation exhibits a dependence with respect to the orientation of the mesh. For this purpose, a $700\,\mathrm{mm} \times 200\,\mathrm{mm} \times 50\,\mathrm{mm}$ beam with a $2\,\mathrm{mm}$ wide and $100\,\mathrm{mm}$ high notch in the center of the beam is simulated. The details of the mode are shown in Figure 1. The mesh used has $12\,377$ nodes and $25\,196$ triangular elements arranged in a structured manner in a band of width equal to the height of the beam around the notch. The material parameters used in the simulations are consistent with concrete characterized by the mechanical properties shown in Table 1. The simulations consider linear interpolations for the deformations and displacements, and a plane stress hypothesis.

The Force vs. CMOD results obtained from the FEniCS implementation is shown in Figure 2 together with the numerical results obtained by Barbat et al. [13] and the experimental range obtained by Grégoire et al. [9]. Overall, the results shows a remarkable good agreement with the experimental results range, both from the maximum load and softening curve prediction.

3.2 Hoover tests

Similar to the Grigoire test, the Hoover test [10] is a bending test performed on beams of different heights and notch sizes, intended to capture the size effect on a mode I fracture. In this



(a) Geometry. (b) FE mesh.

Figure 1: Model of the Grégoire test.

Table 1: Grégoire test material parameters.

Parameter	Value
Young's Modulus	37×10^3 MPa
Poisson's Ratio	0.21
Tensile Strength	3.9 MPa
Fracture Energy	0.09 N mm^{-1}

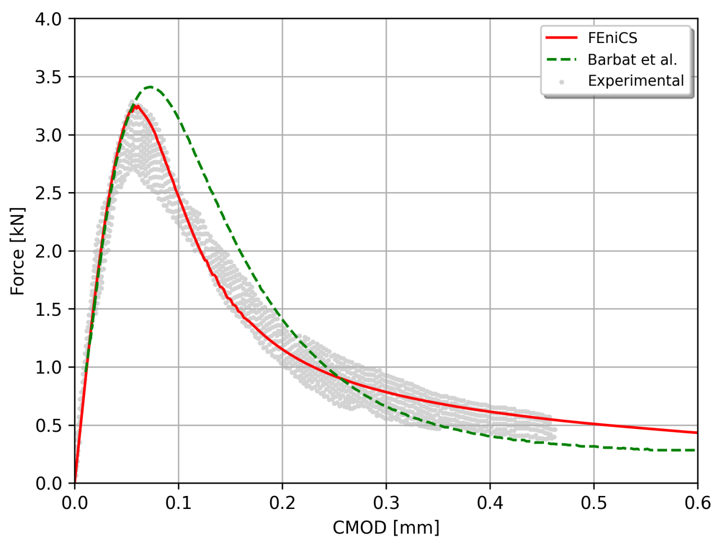


Figure 2: Grégoire et al. test force-diplacement results.

case, 7 geometries are simulated as a function of beam height D and notch/beam ratio α. Details of the simulated geometries are shown in Figure 3. The simulations considers the mechanical

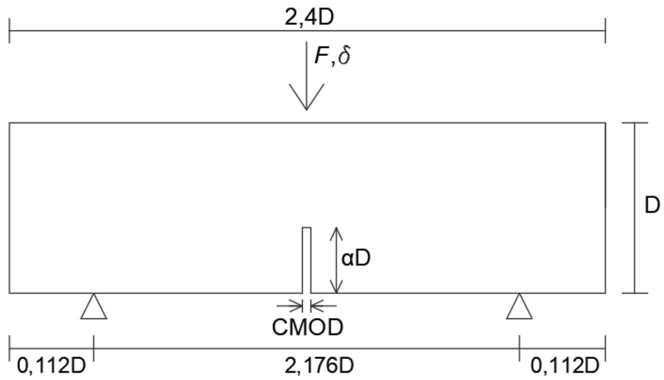


Figure 3: Hoover test geometry [10].

properties shown in Table 2, as well as linear interpolations and a plane stress hypothesis.

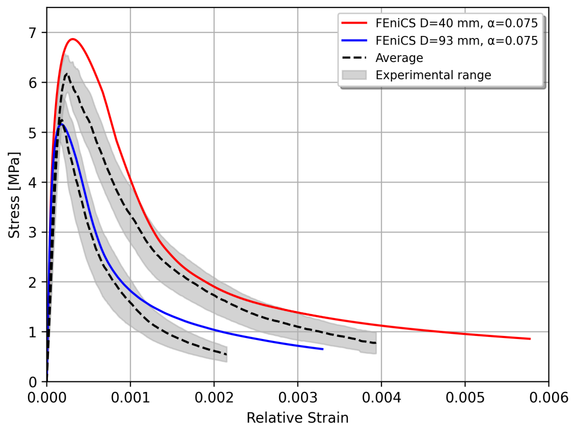
Parameter	Value
Young's Modulus	$34.38 \times 10^3\,\mathrm{MPa}$
Poisson's Ratio	0.172
Tensile Strength	$5.1\,\mathrm{MPa}$
Fracture Energy	$0.096\,94\,\mathrm{N\,mm^{-1}}$

Table 2: Hoover test material parameters.

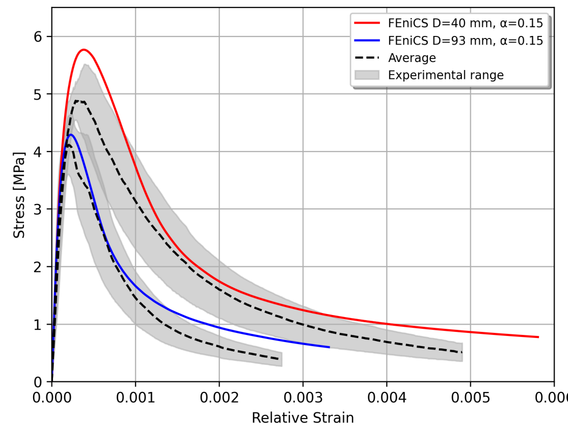
Stress vs. Relative Strain results obtained from Hoover test simulations are shown in Figure 4 and compared to experimental results from Wendner et al. [14]. The results show a behavior that fits well with the experimental range, which changes depending on the size of the beam. Smaller beams exhibit more ductile behavior than larger beams, and the latter reach smaller relative strains before failure. Despite the fact that the curves of the smaller beams do not effectively capture the experimental peaks, they fit within the experimental range better than the larger beams after the change in concavity of the softening curve. On the other hand, larger beams manage to better capture the average experimental peaks.

4 CONCLUSIONS

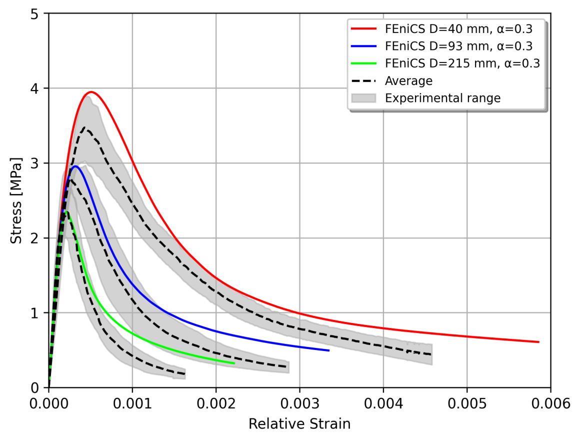
In this work, quasi-brittle fracture and the structural size effect of concrete are modeled using a mixed displacement-deformation formulation stabilized by VMS. Bending tests on notched specimens are simulated, accurately capturing the maximum load, material softening, and the structural size effect phenomenon. This is achieved with minimal mesh dependency and in reasonable calculation times, demonstrating the suitability of the formulation used. Future work



(a) $\alpha = 0.075$.



(b) $\alpha = 0.15$.



(c) $\alpha = 0.30$.

Figure 4: Nominal stress vs. relative strain curves.

will focus on a constitutive modeling that allows describing other types of failure modes, as well as studying the effect of stabilization on stress distribution and damage.

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