Phase-field models for ductile fracture: a comparative study

Lívia Ramos Santos Pereira[1], Samuel Silva Penna[2]

[1,2]*Dept. of Structural Engineering at the Federal University of Minas Gerais*
Av. Antônio Carlos, 6627, Pampulha, Belo Horizonte, 31270-901, MG, Brazil
[1]*lrsp@ufmg.br,* [2]*spenna@dees.ufmg.br*

Abstract. Fracture is a usual failure mode of engineering structures. Thus, the prediction and prevention of cracking-induced failure is a crucial point in engineering projects. Many formulations have been proposed for modeling this phenomenon. The Phase-Field (PF) theory has become popular because it couples Continuum Damage Mechanics and Fracture Mechanics principles. Initially proposed for brittle fracture, the PF theory has been extended for ductile materials. A possible strategy is introducing a yield surface degradation function that depends on the PF variable. Besides this consideration, the stored energy must also be changed, including a plastic work contribution. A different option is to couple the yield surface degradation function with a fracture toughness depending on the accumulated plastic strain. In this case, the phase-field driving force remains defined only by the elastic strain. From this context, this paper presents both PF models' formulations applied to an elastoplastic constitutive model and their implementation. These two approaches are compared. The material parameters are also evaluated to identify how they influence the models' behavior. Finally, numerical simulations via the Finite Element Method are presented to highlight the ductile phase-field models' main characteristics.

Keywords: Phase-field, constitutive models, ductile fracture.

1 Introduction

The prediction of material failure is a central subject in engineering. In plain and reinforced structures, the fracture is a critical mode of deformation and degradation. To handle the presence of discontinuities, researchers and engineers have studied this phenomenon since the 19th century. Although the numerous theories and computational methods available to represent fracture, most of them are focus on crack propagation, neglecting the occurrence of nucleation, branching, and coalescence. The variational approach has emerged with Francfort and Marigo [1] to overcome such gaps, culminating in the Phase Field Models (PFM) formulation.

Originally proposed for brittle fracture, the phase-field theory has been extended to ductile materials. In this paper the models of Borden et al. [2] and Yin and Kaliske [3] are highlighted. The first work is based on the decomposition of the stored energy functional into an elastic and a plastic part, besides introducing a yield surface degradation function. On the other hand, the second study operates on the fracture toughness, that it is not a constant anymore, but depending on the accumulated plastic strain. From this context, the current paper presents both PF models' formulation and implementation, confronting these two approaches. The material parameters are evaluated to identify how they influence the models' behaviors. Finally, numerical simulations via the Finite Element Method are presented to highlight the ductile phase-field models' main characteristics.

2 Phase-Field Models (PFM) for ductile fracture

The variational approach proposed by Francfort and Marigo [1] generalizes Griffith's theory [4] of the brittle fracture using the potential energy minimization. Such an approach was the basis of the Phase-Field Model presented by Bourdin et al. [5]. A limitation of this standard PFM is the insensibility to differentiate tensile and compressive behavior. To improve it, Lancioni and Royer-Carfagni [6] and Amor et al. [7] proposed the volumetric-deviatoric energy slipt. Although, the complete suppression of cracks in compression areas was reached with the spectral decomposition of Miehe et al. [8].

The initial attempts to extend the variational theory to ductile fracture have been documented in Ambati et al. [9, 10] and Miehe et al. [11, 12]. In this works, the differences between brittle and ductile formulations are the term in the degradation function related to the plastic strain and the historical parameter, also modified by the plastic strain. The plastic response, however, remains the same. Neither the yield surface nor the hardening modulus considers the phase-field influence. The experimental results obtained by Ghahremaninezhad and Ravi-Chandar [13] put these hypotheses on questioning since the ductile PFM could not reproduce the real material behavior. This contradiction motivated later studies, as the models developed by Borden et al. [2] and Yin and Kaliske [3].

2.1 Ductile PFM by Borden et al. [2]

The original paper by Borden et al. [2] proposes a PFM of fracture in ductile material, including five main contributions: (1) a cubic degradation function that provides a stress-strain response in the ascending branch closer to the linear elastic behavior: $g(\phi) = m(\phi^3-\phi^2)+3\phi^2-2\phi^3$, where ϕ is the PF variable and $m > 0$. (2) Governing equations for finite deformation problems. (3) A yield surface degradation function to correct the material behavior after the crack initiation. (4) A measure of stress triaxiality into the driving force. (5) An adapted return mapping algorithm as a strategy to calculate stress.

Some adjustments and reformulations were required to make this model available for infinitesimal strain. The first adaptation replaces the finite strain for small strain. Then, the strain tensor ($\boldsymbol{\varepsilon}$) is split into an elastic ($\boldsymbol{\varepsilon}^e$) and a plastic parcels ($\boldsymbol{\varepsilon}^p$),

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p. \tag{1}$$

Consequently, the energy function is given by

$$\psi_{pot}(\boldsymbol{\varepsilon}, \Gamma) = \int_\Omega (g(\phi)\psi_e^+(\boldsymbol{\varepsilon}^e) + \psi_e^-(\boldsymbol{\varepsilon}^e))d\Omega - \int_\Omega \boldsymbol{b}\cdot\boldsymbol{u}d\Omega + \\ + G_c\int_\Omega\left(\frac{\phi^2}{2l_0} + \frac{l_0}{2}\left|\nabla\phi\right|^2\right)d\Omega + \int_\Omega \psi_p(\alpha)d\Omega, \tag{2}$$

where the first term is the elastic strain energy, the second term is the external work, the third term is the fracture energy, and the last term is the plastic potential. Since the PFM by Miehe et al. [8] is adopted, only the positive elastic strain portion is subject to the degradation function. The external force is $\boldsymbol{b}$ and $\boldsymbol{u}$ is the displacement vector. The characteristic length is l_0 and the hardening internal variable α is given by the effective plastic strain $\bar{\varepsilon}^p$.

The historical parameter is also modified

$$\mathcal{H}_{ep} = \beta_e \max_{\tau\in[0,t]} \psi_e^+(\boldsymbol{\varepsilon}(\boldsymbol{x},\boldsymbol{\tau})) + \beta_p\left\langle\psi_p(\alpha) - W_0\right\rangle, \tag{3}$$

where β_e and β_p are weighting coefficients that control the contribution of the elastic and the plastic work, respectively. The initial plastic work limit is given by W_0, and $\langle x\rangle$ represents Macaulay's brackets.

About the yield criterion, the classic von Mises criterion is adopted, which is a function of the second deviatoric stress invariant (J_2). Furthermore, the degradation function effect is now included. Considering the linear hardening (H), the yield surface is written as

$$f_y = \sqrt{3J_2} - g(\phi)\sigma_y(\bar{\varepsilon}^p) = \sqrt{3J_2} - g(\phi)\sigma_{y0} - g(\phi)H(\bar{\varepsilon}^p), \tag{4}$$

where

$$J_2 = \frac{1}{2}s_{ij}s_{ij}. \tag{5}$$

Based on the Prandtl-Reuss' Law, it is possible to calculate the flow rule

$$\dot{\boldsymbol{\varepsilon}}^p = \dot{\gamma}\boldsymbol{N} = \dot{\gamma}\frac{\partial\Phi}{\partial\boldsymbol{\sigma}} = \dot{\gamma}\sqrt{\frac{3}{2}}\frac{\boldsymbol{s}}{\|\boldsymbol{s}\|}, \tag{6}$$

and the evolution rate of the equivalent plastic strain, which is equal to the plastic multiplier ($\dot{\gamma}$)

$$\dot{\alpha} = \dot{\bar{\varepsilon}}^p = \sqrt{\frac{2}{3}\dot{\boldsymbol{\varepsilon}}^p : \dot{\boldsymbol{\varepsilon}}^p} = \sqrt{\frac{2}{3}}\left\|\dot{\boldsymbol{\varepsilon}}^p\right\| = \dot{\gamma}. \tag{7}$$

The plastic multiplier is calculated via the return mapping algorithm. Although [2] use a general algorithm to incremental finite plasticity problems [14], the closest point projection is adopted in the current work.

The hardening law evolution can be obtained by

$$H = -\frac{\partial f_y}{\partial H}\frac{\partial H}{\partial\bar{\varepsilon}^p} = -(-g(\phi))\mathscr{H} = g(\phi)\mathscr{H}. \tag{8}$$

It is highlighted that the Kuhn-Tucker's conditions ($f_y \leq 0$; $\dot{\gamma} \geq 0$; $f_y\dot{\gamma} = 0$) must be fulfil.
Table 1 summarizes the main equations of PFM adapted from Borden et al. [2].

2.2 Ductile PFM by Yin and Kaliske [3]

Yin and Kaliske [3] propose an alternative approach for ductile PFM, where the fracture toughness G_c varies with the accumulated plastic strain. Then, the ductile fracture evolution is simultaneously governed by the historical parameter and G_c. Such an approach was formulated for small strain and the classic von Mises plasticity. The strain tensor split was based on the model by Amor et al. [7].

The idea of establishing a dependence between the fracture toughness degradation and the plastification evolution comes from the PFM for fatigue. A function f operates in the initial fracture energy G_c^0, reducing it. This function is called the hardening degradation function, and its parameter is the internal variable ζ. The described relation is given by

$$G_c = f(\zeta(t))G_c^0. \tag{9}$$

The function f is characterized by the properties

$$0 < f \leq 1, \quad f(\zeta \leq \zeta^{cr}) = 1 \quad \text{e} \quad \frac{\partial f(\zeta \geq \zeta^{cr})}{\partial \zeta} \leq 0. \tag{10}$$

The first condition in eq. (10) represents the physical limits of f, the second condition defines an internal variable threshold (ζ^{cr}) to control the degradation start, and the third condition indicates a monotonic decrease of G_c. The hardening degradation function is defined as

$$f(\zeta) = \begin{cases} 1, & \zeta < \zeta^{cr}, \\ \dfrac{1-b}{a^2}(\zeta - \zeta^{cr} - a)^2 + b, & \zeta^{cr} \leq \zeta < a + \zeta^{cr}, \\ b, & \zeta \geq a + \zeta^{cr}, \end{cases} \tag{11}$$

where a and b are parameters that control the degradation profile of f. The parameter b controls the minimum value f can assume, an infinitesimal $0 < b << 1$. The factor a is responsible for the plastic yield.

Adopting the von Mises criterion, the internal variables is given by

$$\zeta = \sqrt{\frac{2}{3}} \int_0^t \sqrt{\dot{\boldsymbol{\varepsilon}}^{\boldsymbol{p}} : \dot{\boldsymbol{\varepsilon}}^{\boldsymbol{p}}}\, dt. \tag{12}$$

Finally, the governing equation for ductile phase-field is written as

$$g'\mathcal{H}_{ep} + G_c^0 \left(f(\zeta) l_0 \Delta\phi + l_0 \nabla f(\zeta) \cdot \nabla\phi - f(\zeta)\frac{\phi}{l_0} \right) = 0, \tag{13}$$

$\mathcal{H}_{ep}$ is the historical parameter, which is the maximum elastic driving force related to the tension energy ψ_e^+.
Table 1 lists the main definitions of the ductile PFM proposed by Yin and Kaliske [3].

Table 1. PFM for ductile fracture: main relations.

Formulation	Borden et al. [2]	Yin and Kaliske [3]
Strain tensor split	$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p$	$\boldsymbol{\varepsilon}_{dev} = \boldsymbol{\varepsilon}^e_{dev} + \boldsymbol{\varepsilon}^p_{dev}$
Stress tensor split	$\boldsymbol{\sigma} = g(\phi)\boldsymbol{\sigma}^+ + \boldsymbol{\sigma}^-$	$\boldsymbol{\sigma} = \boldsymbol{\sigma}_{dev} + \boldsymbol{\sigma}_{vol}$
Yield criterion	$f_y = \sqrt{3J_2(\boldsymbol{s}(\boldsymbol{\sigma}))} - g(\phi)\sigma_y(\bar{\varepsilon}^p)$	$f_y = \Vert\boldsymbol{\sigma}_{dev}\Vert - \sqrt{\frac{2}{3}}\sigma_y(\bar{\varepsilon}^p)$
Hardening law	$\dot{\bar{\varepsilon}}^p = \dot{\gamma}H = \dot{\gamma}g(\phi)\mathscr{H}$	$\dot{\bar{\varepsilon}}^p = \dot{\gamma}\frac{\partial f_y}{\partial \sigma_y(\bar{\varepsilon}^p)} = \sqrt{\frac{2}{3}}$
Flow rule	$\dot{\boldsymbol{\varepsilon}}^p = \dot{\gamma}\frac{\partial f_y}{\partial \boldsymbol{\sigma}}$	$\dot{\boldsymbol{\varepsilon}}^p = \dot{\gamma}\sqrt{\frac{3}{2}}\frac{\boldsymbol{s}}{\Vert\boldsymbol{s}\Vert}$
Kuhn-Tucker's conditions	$f_y \leq 0;\ \dot{\gamma} \geq 0;\ f_y\dot{\gamma} = 0$	$f_y \leq 0;\ \dot{\gamma} \geq 0;\ f_y\dot{\gamma} = 0$
Degradation function[1]	$g(\phi) = m(\phi^3 - \phi^2) + 3\phi^2 - 2\phi^3$	$g(\phi) = (1-\phi)^2$
Geometric crack function	$\alpha(\phi) = \phi^2$	$\alpha(\phi) = \phi^2$

[1] Although [2] adopt a cubic $g(\phi)$, we use the quadratic function for both models to a straight comparison between the formulations.

Based on this model, this paper presents a modified version. The only differences between the classic von Mises elastoplastic model and the ductile PFM are the historical parameter and the phase-field tangential matrix $\boldsymbol{C^t_{PF}}$, where $\alpha(\phi) = \phi^2$ is the geometric function.

$$\boldsymbol{C^t_{PF}} = \begin{bmatrix} \left(g''(\phi)\mathcal{H}_{ep} + \frac{f(\zeta)G^0_c\alpha''(\phi)}{C_0 l_0} \right) & 0 & 0 \\ 0 & \frac{2.0 f(\zeta) G^0_c l_0}{C_0} & 0 \\ 0 & 0 & \frac{2.0 f(\zeta) G^0_c l_0}{C_0} \end{bmatrix}, \tag{14}$$

3 Numerical simulations

The described models have been implemented in the INteractive Structural ANalysis Environment (INSANE). The INSANE is an open-source code developed at the Department of Structural Engineering of the Federal University of Minas Gerais (`https://www.insane.dees.ufmg.br/en/home/`). Three numerical examples were performed to analyze its response: a uniaxial tension test, a bending bar with a V-notched (Fig. 1), and a parametric study. Such examples permit the comparison between the PFM for ductile fracture by Borden et al. [2] and Yin and Kaliske [3], highlighting the simplifications required to adapt this model to the INSANE platform. The parametric analysis shows the models' sensitivity to the input parameters.

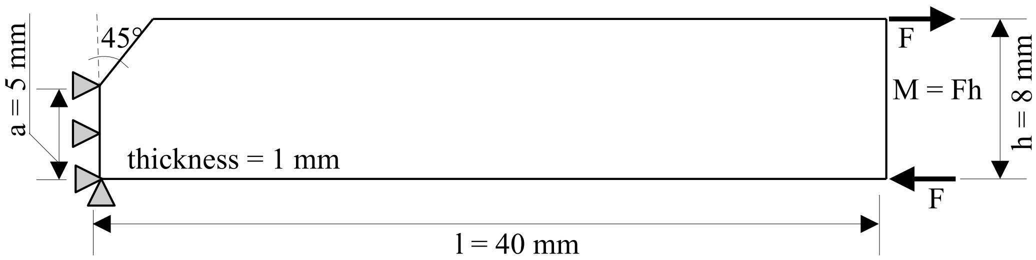


Figure 1. Bending of a V-notched bar.

3.1 Uniaxial response

This example presents a uniaxial tension test to validate the capability of the discussed models to reproduce the phase-field phenomenon. A single four-node element with unit dimension sides is subject to unit load. The parameters adopted are given in Table 2. The reference curve is a no fracture case with isotropic linear hardening and von Mises criterion. The quadratic degradation function was adopted (Table 1). The results are shown in Fig. 2a.

Table 2. Model parameters for uniaxial stresses

E	68.8 GPa	ν	0.33	σ_y	320 MPa	H	655 MPa	a	1000000
l_0	2 m	G^0_c	138 MN/m	ζ_{cr}	0.0	W_0	0.0	b	0.00000001

The curves in Fig. 2a show that the model adapted from Borden et al. [2] reproduced a fragile behavior since the yield is not present. Otherwise, the modified version of the model by Yin and Kaliske [3] represents both the yield and the phase-field decay. Even for non-zero values of W_0, the model by Borden et al. [2] still showing a fragile fracture. This phenomenon must be related to using this model for infinitesimal strain, while it was originally developed for finite deformations. On the other hand, the model by Yin and Kaliske [3] considers an infinitesimal regime. The PF variable also acts as reducing the stress associated with the yield strength.

3.2 Bending of a V-notched bar

The bending of a V-notched bar studied by Souza Neto et al. [14] and Monteiro [15] is analyzed here. Because of the symmetry, only half of the bar is simulated (Fig. 1). A mesh of 150 four-node elements is adopted. Table 3 lists the model parameters adopted in the current analysis.

Table 3. Model parameters for the bending of a V-notched bar

E	210 GPa	ν	0.30	σ_y	240 MPa	H	0 MPa	a	1000000
l_0	1 mm	G_c^0	15 N/m	ζ_{cr}	0.0	W_0	0.0	b	0.00000001

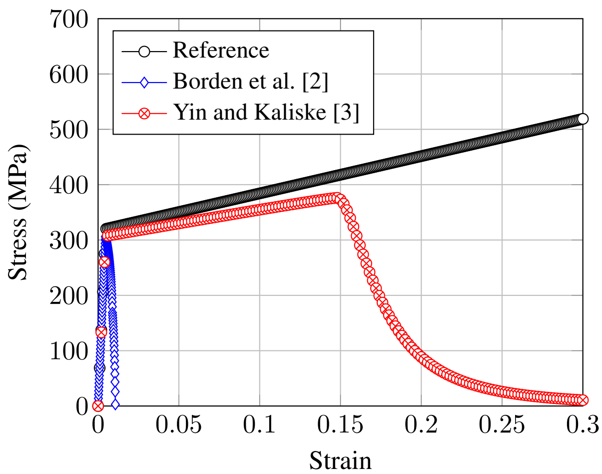
For a notch angle of 90°, the upper bound moment per unit is

$$M_u = 0.623\ ca^2 = 0.623 \times 120,000,000\ N/m^2 \times \left(5 \times 10^{-3}\right)^2\ m^2 = 1869\ N.m, \quad (15)$$

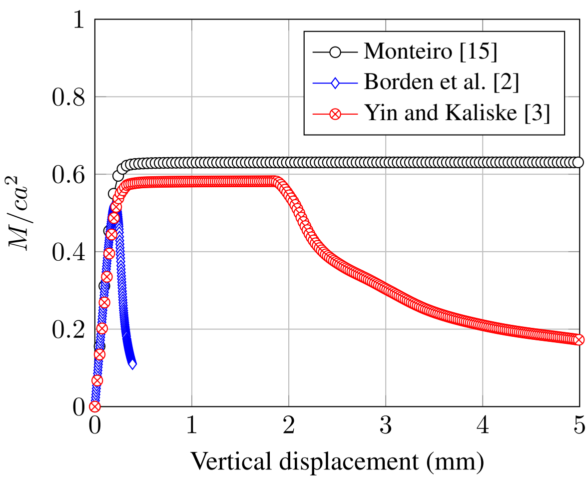
where a is the height of the bar in the neck, and c is the shear strength, given as $c = \sigma_y/2$. Such moment is applied using two opposite nodal forces with equal intensity F

$$F = \frac{M_u}{h} = \frac{1869}{0.008} = 233625\ N. \quad (16)$$

The relation *vertical displacement* × *normalised bending moment per unit* (M/ca^2) is illustrated in Fig. 2b.



(a) Uniaxial response.



(b) Bending of a V-notched bar.

Figure 2. PFM for ductile fracture.

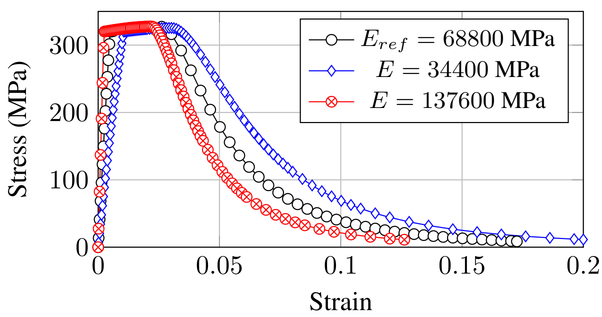
As in the tension test, the model adapted from Borden et al. [2] was not able to reproduce the yield, being restricted to a fragile behavior. The model by Yin and Kaliske [3] proves to be a better approach to ductile fracture using PFM coupled to small strain.

3.3 Parametric analyses

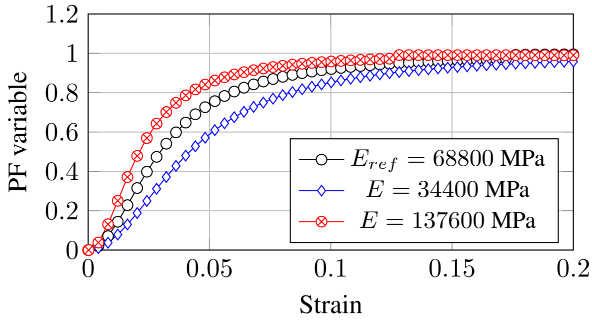
Based on section 3.1 and section 3.2 results, the modified model of Yin and Kaliske [3] performed better the ductile fracture. Then, the parametric study adopts this model to show how the structure response varies with the input parameters. The simulation present in section 3.1 is taking as reference. The analyzed parameters are: Young modulus E (Fig. 3), hardening modulus H (Fig. 4), yield stress σ_y (Fig. 5), and fracture toughness G_c (Fig. 6).

The results show that the Young modulus and the fracture toughness affect both the stress-strain behavior and the evolution of the PF variable. While the Young modulus controls the elastic branch of the *stress*×*strain* response, the fracture toughness interferes in the post-peak branch, regulating the plastic yield and the softening. A large value of E accelerates the PF evolution. On the other hand, an increase of G_c induces a slower PF growth.

The yield stress and the hardening modulus variation do not lead to changes in the PF evolution. The stress-strain behavior, however, presents alteration. A large value of σ_y raises the stress associated with plastification, while a smaller plastic yield is observed. The hardening modulus impact is restricted to the plastic yield slope, and its effects are subtle.

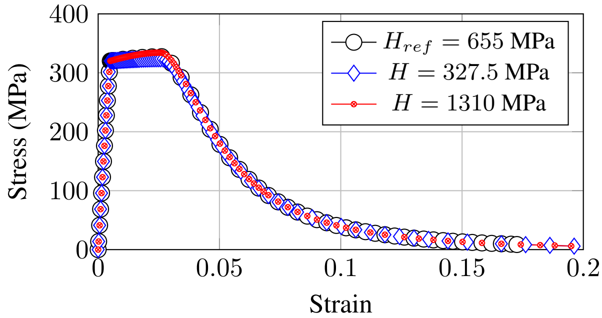


(a) *Stress* × *strain* response.

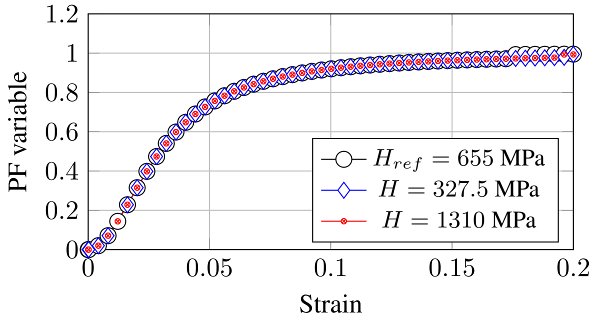


(b) Phase-field evolution.

Figure 3. Parameter: Young modulus E.

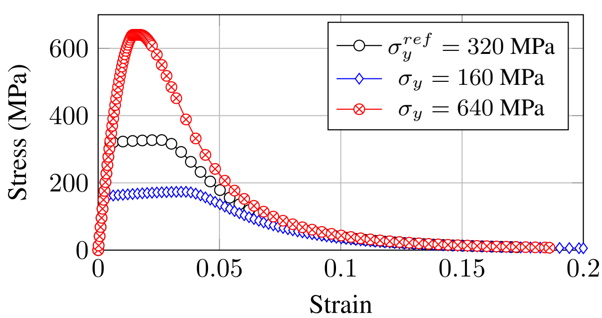


(a) *Stress* × *strain* response.

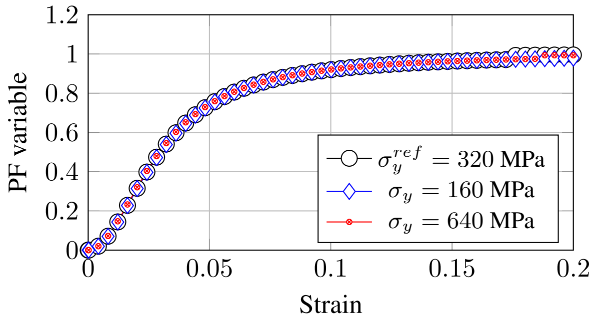


(b) Phase-field evolution.

Figure 4. Parameter: hardening modulus H.

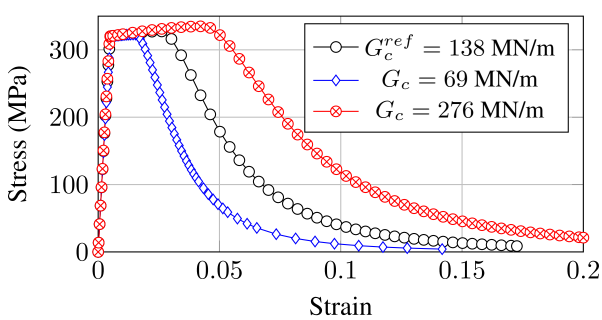


(a) *Stress* × *strain* response.

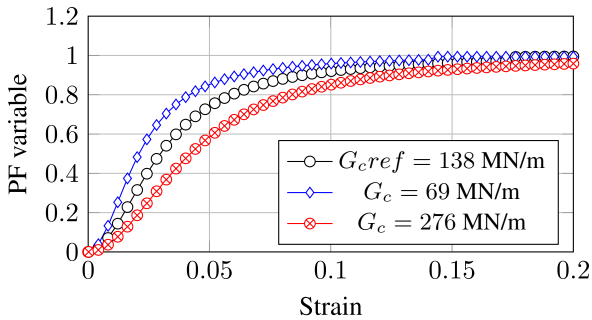


(b) Phase-field evolution.

Figure 5. Parameter: yield stress σ_y.



(a) *Stress* × *strain* response.



(b) Phase-field evolution.

Figure 6. Parameter: fracture toughness G_c.

4 Final considerations

This study presented two phase-field models for ductile fracture. The results permit the following conclusions:

- The ductile fracture is characterized for two main phenomena: the plastic yield (plastification) and the stress decay after the crack opens (fracture propagation);
- The model by Yin and Kaliske [3] proves to be a better approach for ductile fracture using PFM coupled to small strain;
- The model by Borden et al. [2] must be associated with finite deformations to analyze its true potential;
- The parameter E changes the slope of the *stress* $\times$ *strain* curve, and the evolution of the PF variable is faster for larger values of E;
- The parameter H only interferes with the plastic yield slope of the curve.
- The higher is the parameter σ_y, the higher is the yield strength, and the lower is the plastic yield;
- The increase of G_c conducts to a larger plastic yield and a slower PF evolution.

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