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Phase-field modeling of hydraulic fracturing in RVEs of heterogeneous materials

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Abstract. Modeling hydraulic fracturing is a complex task, involving the occurrence of various physical phenomena, with the emergence of complex crack patterns, increased by the interaction between the fluid, the medium and the crack. It is, however, an indispensable subject for achieving efficiency and safety in various processes in the geotechnical sectors, the oil and gas extraction industry and structural engineering. Furthermore, most hydraulic fracturing applications deal with materials that are heterogeneous at a certain scale. At the microscopic level these materials, especially composite and natural materials, can be interpreted as a heterogeneous media formed by a series of components with different mechanical properties. Given that material damage begins with the appearance of microcracks at the microscale, and that these degraded regions can have their behavior affected by the presence of pressure load, the study of hydraulic fracture propagation in heterogeneous materials is a topic to be explored. In this sense, the aim of this work is to model the behavior of multiphase materials in pressure-driven fracture propagation scenarios. The phase-field model will be used, as it is an advantageous approach, capable of representing complex trajectories of numerous cracks directly without restricting their propagation directions and not demanding the use of additional techniques. Furthermore, this model allows the discretization of the different constituents of the material without the appearance of strain concentration problems. Numerical results will be presented showing the influence of the pressure load on different random distributions of components in representative volume elements (RVEs) of quasi-brittle materials. The entire implementation was carried out using INSANE software, developed and made available by the Department of Structural Engineering at the Federal University of Minas Gerais (UFMG).

Keywords: Phase-field, Hydraulic fracturing, Heterogeneous materials

1 Introduction

Hydraulic fracturing occurs when the crack environment is under the influence of hydraulic loads, commonly referred to as hydraulic pressure, which affects the onset and propagation of the crack. Adachi et al. [1] highlights the challenges in modeling such problems, which require accounting for interactions between the medium and the fluid; crack propagation; and, in more complex models, fluid flow within both the medium and the fracture. The applications of hydraulic fracturing encompass different sectors such as the gas and oil extraction industry, structural engineering dealing with structures in hydraulic environments, geological material and geothermal reservoir studies, mining, among others, which justifies the increasing interest in this field of study.

Most applications of hydraulic fracturing concern industrial, engineering, and natural materials, which are heterogeneous at a certain scale. Addressing these heterogeneities remains a key issue for many researchers, since the presence of heterogeneities affects the mechanical response of the medium. Therefore, the study of hydraulic fracturing from a multiscale approach is an interesting topic to explore. In this context, at least one of the scales must be able to represent the different material phases, typically referred to as the microscale, which is modeled through representative volume elements (RVEs). According to Khan et al. [2], in general, the fracture process begins at this microscale, affecting the stiffness and strength characteristics at the macroscale.

At the microscopic level, most materials can be interpreted as a heterogeneous media comprising a variety of components with different mechanical properties. Numerical modeling of fractures in heterogeneous media faces several challenges, mainly related to fractures of complex topology with the presence of phenomena such as bifurcation and sudden changes in direction [3]. In this sense, the adoption of a robust model that does not limit the crack propagation path is essential, as is the case with the phase-field model. Wheeler et al. [4] also highlight that

the application of this model to heterogeneous media is straightforward, without the need for additional deductions.

The phase-field model has already been used in several applications involving pressurized cracks in homogeneous and heterogeneous media, with the pioneering formulation by Bourdin et al. [5] being adopted in this paper. Accordingly, this study proposes the investigation of different samples of heterogeneous materials under traction tests to assess the influence of pressure load on material response and crack development. The importance of considering the interfacial transition zone (ITZ), identified by Wriggers and Moftah [6] as having a major influence on the onset of microcracking, is also evaluated.

All implementation and numerical simulation was performed using INSANE software, an opensource program developed at the Department of Structural Engineering at the Federal University of Minas Gerais. Finite element meshes with different particle distributions were also generated in INSANE with the help of GMSH software features. The phase-field contour plots were generated using Paraview.

2 Theoretical foundation

This work is based on the use of the variational phase-field approach in modeling pressurized cracks in heterogeneous media. These topics will be briefly discussed below.

2.1 Phase-field modeling of hydraulic fracture

The phase-field model is a diffuse fracture model in which the level of degradation of the medium is quantified by using an additional continuous field variable to the classical elasticity problem, the phase-field variable, here denoted by ϕ. The damaged material is represented by $\phi = 1$, while the intact material is represented by $\phi = 0$, extreme values separated by a smooth variation of $0 \leq \phi \leq 1$, whose width depends on the material parameter called length scale (l_0). Given that it is a model capable of representing complex cracking patterns without any prior knowledge of their trajectory, its use is widespread in the study of hydraulic fracturing, as reviewed by Heider [7]. Here, the formulation proposed by Bourdin et al. [5], pioneers in the study of pressurized fractures based on the phase-field model, was employed. Their simplified approach considers a constant pressure load in a quasi-static setting, an impermeable medium with no porosity, and incompressible fluid.

The formulation of the model is based on minimizing the total energy functional, given by eq. (1), which presents an additional term in relation to the classical problem, referring to the work of the pressure load p_f in the crack domain.

$$E_t(\boldsymbol{u}, \phi) = \int_\Omega \psi(\boldsymbol{\varepsilon}(\boldsymbol{u}), \phi) dV + \int_\mathcal{B} G_c \gamma(\phi, \nabla\phi) dV - \int_\Omega \boldsymbol{b} \cdot \boldsymbol{u} dV - \int_{\partial\Omega_N} \boldsymbol{t} \cdot \boldsymbol{u} dA + \int_\Omega p_f \boldsymbol{u} \cdot \nabla\phi dV, \quad (1)$$

where $\boldsymbol{u}$ is the cinematically admissible displacement field, ψ is the strain energy density, G_c is the critical energy release rate, γ is crack surface density, $\boldsymbol{b}$ is the vector of body forces, $\boldsymbol{t}$ is the vector of surface forces and p_f is the fluid pressure load.

In the phase-field model, the strain energy ψ depends on ϕ through the energy degradation function $g(\phi)$, responsible for connecting the mechanical field and the crack field. In this paper, the function $g(\phi) = (1 - \phi)^2$ will be used. The crack surface density function γ depends on the geometric crack function $\alpha(\phi)$ that defines the phase-field distribution along the degradation band. Here, the quadratic function $\alpha(\phi) = \phi^2$ was adopted. In addition, the isotropic constitutive model will be used, in which cracks arise due to both tension and compression, without distinction. The use of this model does not lead to the appearance of non-physical cracks in the study proposed here, since only plain tensile tests are simulated. Both the $g(\phi)$ and $\alpha(\phi)$ functions and the constitutive model were proposed by Bourdin et al. [8].

The solution $(\boldsymbol{u}, \phi)$ that minimizes the energy functional presented in eq. (1) can be obtained using staggered solvers that seek convergence of each field independently until global convergence is achieved. Here, the staggered bound-constrained solver ([9]) will be used, which reinforces the crack irreversibility condition and the constraint of $0 \leq \phi \leq 1$, criteria that are of concern to some researchers due to the fracture pressure term ([10]).

2.2 Phase-field modeling of heterogeneous media

A major advantage of using phase-field modeling in heterogeneous media, in addition to the absence of strain concentration with the use of refined meshes, which allows the discretization of small phases, is its direct

application to materials with different properties without any modification to the original model framework, as highlighted by Wheeler et al. [4].

This paper will address the modeling of materials such as concrete, which have constituents with markedly different properties that are seen discretely at small scales of observation (i.e., microscale). The microscale will be defined by a representative volume element (RVE) where the constitutive behavior of each constituent is modeled. Here, the heterogeneous medium will be represented by a cementitious matrix into which particles representing the aggregates are inserted. The interfacial transition zone (ITZ) can also be considered in order to more accurately represent the behavior of the material.The domain is generated based on the definition of the volume percentage of aggregate and composition of the particle size distribution curve that follows the limits presented in ABNT NBR 7211:2022 [11]. The arrangement of aggregates, taken as circular particles, in the matrix is performed using the take-and-place method described by Wang et al. [12] and Wriggers and Moftah [6].

3 Numerical results

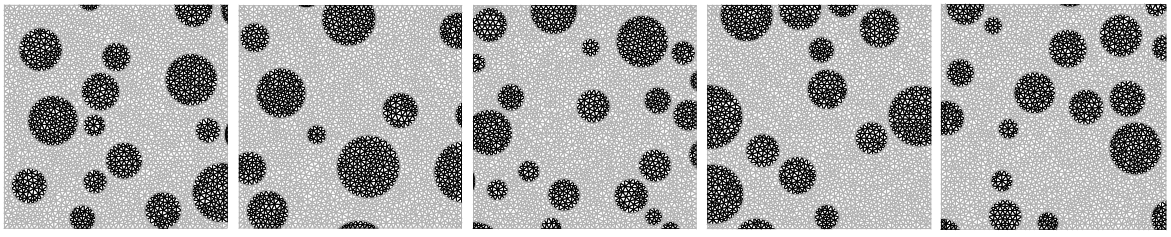
This section will present a series of numerical results obtained from simple tensile tests on RVEs of heterogeneous media. In section 3.1, the RVEs have two distinct phases, namely aggregates and mortar, while in section 3.2, the RVEs also present an interface between the materials. All simulations consider the left edge of the model with zero horizontal displacement, and the horizontal displacement of the right edge is incremented by 1.625×10^{-4} mm per analysis step. The phase-field model was used for the three constituents of the material with the properties shown in Table 1. Square RVEs measuring 65 x 65 mm were used, with a particle size distribution curve with a minimum aggregate size of 9.5 mm and a maximum aggregate size of 25 mm.

Table 1. Properties of RVE constituents

Material	E (MPa)	ν	l_0 (mm)	G_c (N/mm)
Aggregate	100000	0.2	5.61	0.128
Mortar	32000	0.2	5.65	0.0181
ITZ	17000	0.2	0.525	0.0011

3.1 Specimen with aggregates and mortar

For tests with RVEs containing a cementitious matrix with aggregates, three aggregate fractions were considered: 30%, 35%, and 40%, each analyzed with five different random particle distributions. Figure 1 shows the finite element meshes for each of the distributions for RVEs with 30% aggregates, considering triangular elements with a mean nodal distance of 1.5 mm.



(a) (b) (c) (d) (e)

Figure 1. Finite element meshes for RVEs with aggregate volume fraction of 30% and different particle distributions: (a) Distribution 1. (b) Distribution 2. (c) Distribution 3. (d) Distribution 4. (e) Distribution 5.

Each of the five samples of three particle fractions were evaluated in the tensile test considering the pressure load in the fracture region, with $p_f = 0.05$ MPa, and without considering the presence of this load. The equilibrium curves are shown in Fig. 2. It can be seen that the characteristic behavior of RVEs is maintained with the presence of pressure load, making it possible to define a representative envelope of the material's behavior for all cases

analyzed. As expected, higher peak loads are achieved in samples with a higher percentage of aggregate, and a decrease in the load factor is observed when the pressure load is considered, since, in this case, there is more load affecting the model for the same displacement increment.

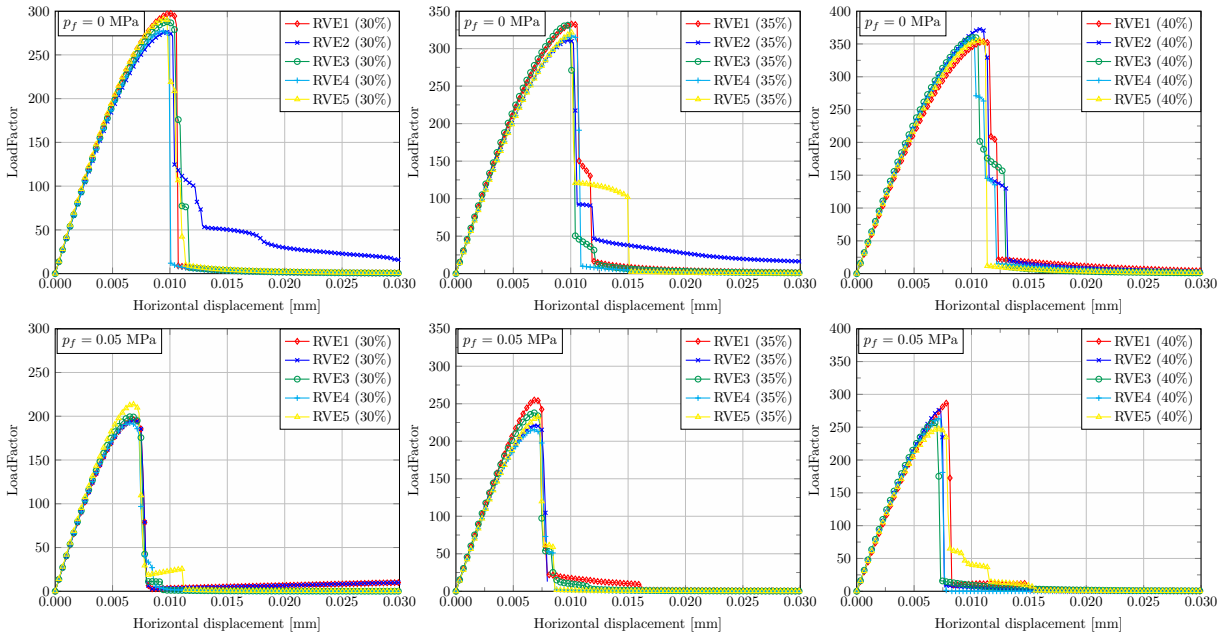
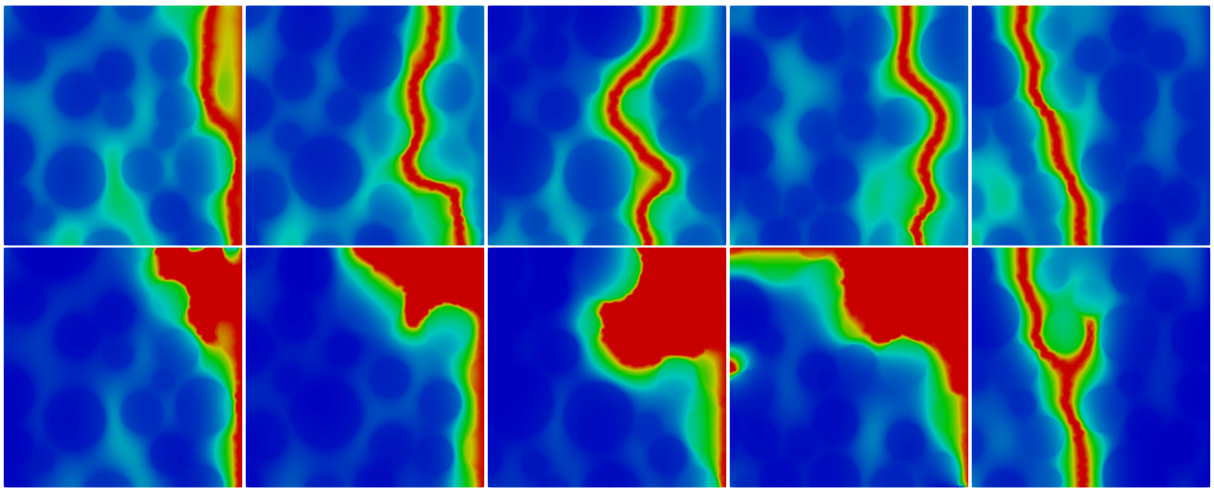


Figure 2. Equilibrium trajectory for RVEs with different particle distributions without pressure load (first row) and with pressure load $p_f = 0.05$ MPa (second row).

Figure 3 shows the phase-field contour plot for the final step of the analysis considering different distributions for a 40% aggregate fraction. It can be seen that the matrix forms a preferential path for the crack, which seeks to deviate from the aggregates. The pressure load caused instability in the crack propagation for almost all RVEs. The phase-field model was efficient in tracking the crack trajectory in all cases.

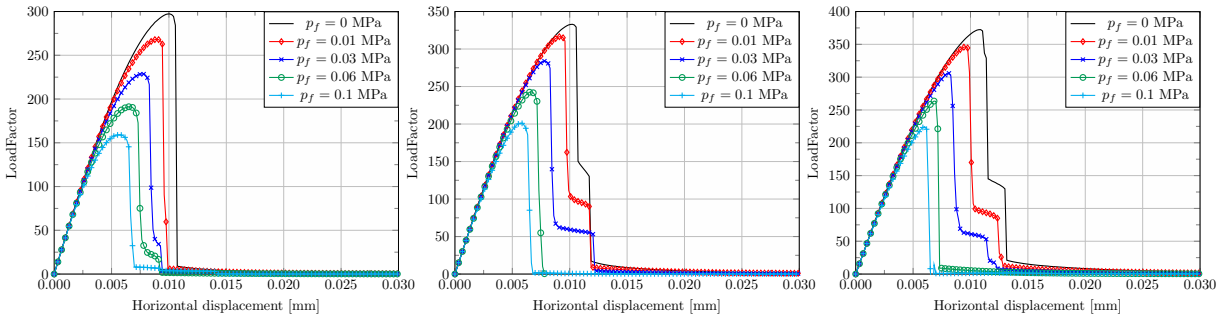


(a) (b) (c) (d) (e)

Figure 3. Phase-field contour plot for aggregate volume fraction of 40%: without pressure load (first row) and with pressure load $p_f = 0.05$ MPa (second row): (a) RVE 1; (b) RVE 2; (c) RVE 3; (d) RVE 4; (e) RVE 5.

A second study sought to evaluate the influence of pressure load magnitude. To this end, a particle distribution

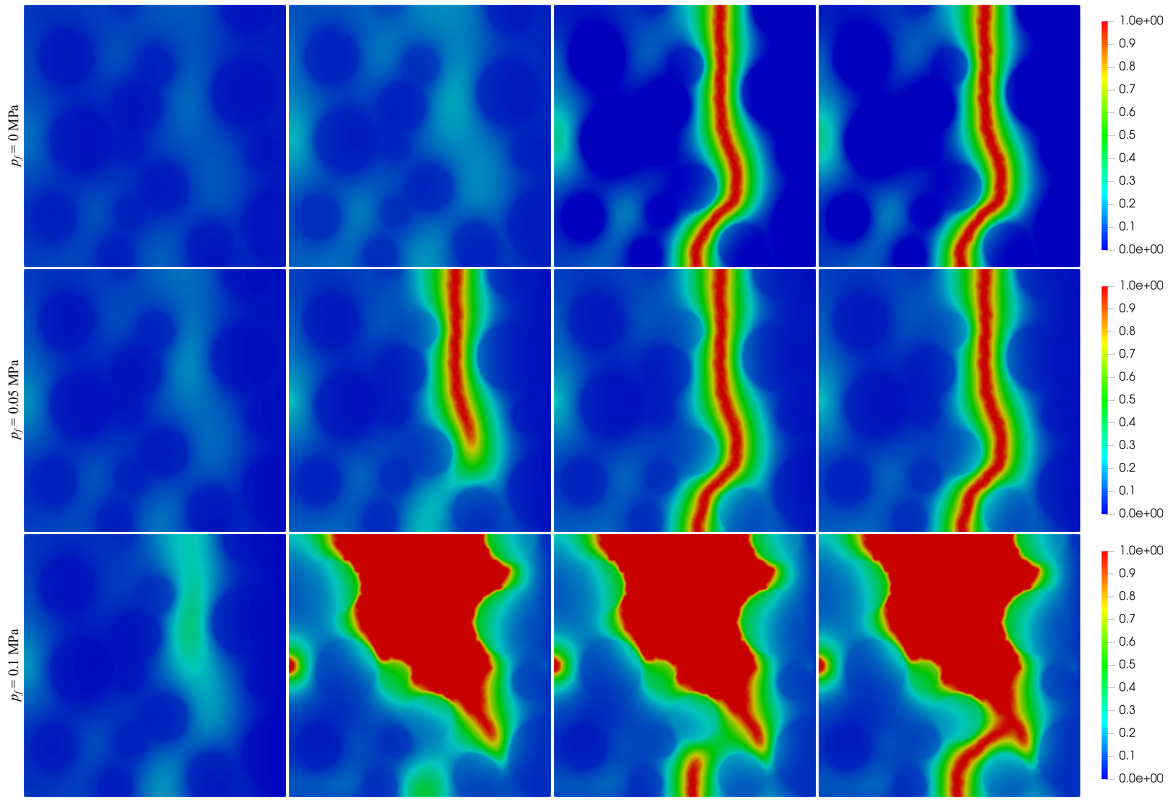
was selected for each of the fractions under study, and pressure values between 0.01 and 0.1 MPa were considered. The results of the load versus horizontal displacement curves of the right side of the RVE are presented in Fig. 4. A standard behavior of a decrease in the load factor with increasing pressure can be observed.



(a) (b) (c)

Figure 4. Equilibrium trajectory for different pressure load values: (a) Aggregate volume fraction of 30%. (b) Aggregate volume fraction of 35%. (c) Aggregate volume fraction of 40%.

Figure 5 shows the phase-field contour plot for different pressure load values at different times during the analysis for aggregate volume fraction of 30%. For lower pressure magnitudes, its presence only accelerated the propagation of the crack, without altering its trajectory. Whereas for a higher pressure load, the crack propagates in a more unstable manner, abruptly occupying a large part of the domain.

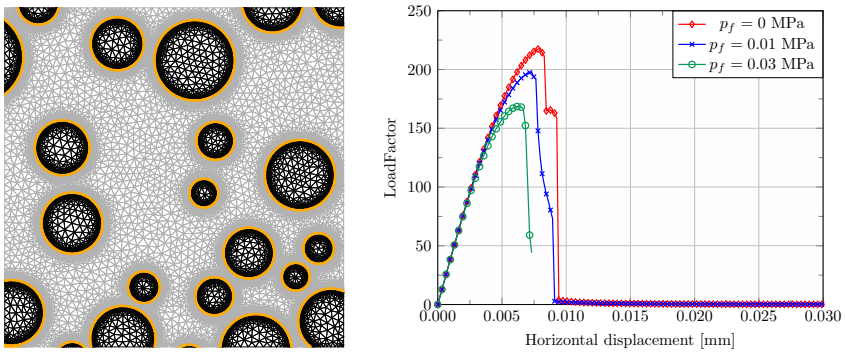


(a) (b) (c) (d)

Figure 5. Phase-field contour plot for aggregate volume fraction of 30%: (a) Step 40; (b) Step 50; (c) Step 75; (d) Step 100.

3.2 Specimen with aggregates, mortar and ITZ

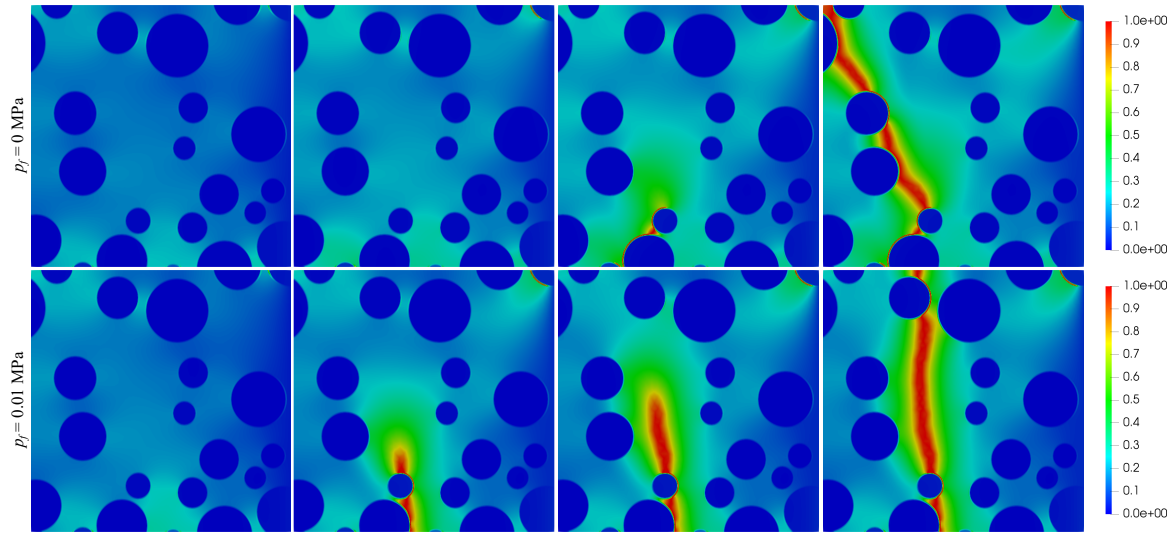
Tensile tests on RVE containing matrix, aggregates, and ITZ between materials were performed for only one particle distribution considering an aggregate volume fraction of 35%, as shown in Fig. 6(a). In this study, the model was analyzed only with the external tensile load and in combination with pressure loads of 0.01 MPa and 0.03 MPa. The equilibrium trajectories are shown in Fig. 6(b). Due to the presence of the interface, which has lower stiffness, the analysis became unstable and stopped converging in the softening regime for $p_f = 0.03$ MPa. The interface was defined with a thickness of 0.55 mm, and in this region, the triangular elements have a mean nodal distance of 0.1375 mm, keeping the dimension of 1.5 mm in the rest of the mesh.



(a) (b)

Figure 6. RVE with mortar, 0.35 aggregate fraction, and ITZ: (a) Finite element mesh; (b) Equilibrium trajectory for different pressure load values

Figure 7 illustrates the phase-field distribution in the analyses with and without pressure loading for different horizontal displacement increments. It can be observed that the presence of pressure caused a deviation in the crack trajectory. However, in both cases, the crack propagated preferentially along the ITZs, around the aggregates, crossing the matrix to pass from interface to interface.



(a) (b) (c) (d)

Figure 7. Phase-field contour plot for aggregate volume fraction of 35% with ITZ: (a) Step 45; (b) Step 50; (c) Step 55; (d) Step 60.

4 Conclusions

This paper presented the application of a phase-field model for pressurized fractures in quasi-brittle heterogeneous samples. The model was able to accurately represent traction tests considering two- and three-phase media, namely matrix and aggregates, and matrix, aggregates, and interface, respectively. It was possible to observe complex crack trajectories that deviate from the aggregates, resulting in phenomena such as bifurcation. The pressure load significantly affects crack propagation and equilibrium trajectories, while the characteristic behavior of the RVE responses across different particle distributions is preserved. In general, low pressure load magnitudes only accelerate crack propagation, whereas higher pressures may alter the crack trajectory, often resulting in unstable behavior. Thus, it was possible to verify the ability of the phase-field model to simulate complex crack patterns, even with the presence of hydraulic stimulation within the crack domain, and its application to material samples with constituents of different properties. The applications presented highlight the potential of the model as an efficient approach for multiscale studies of hydraulic fractures, a topic of considerable scientific and practical importance. Future work could apply this model to microscale analysis of complex structural systems, including dams and geological massifs, where material-scale damage and its macroscale effects can be better captured in a multiscale framework.

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