MODELING OF DAMAGE PROPAGATION IN COHESIVE-FRICTIONAL MATERIALS
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TITLE: Modeling of Damage Propagation in Cohesive Frictional Materials

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Abstract

The primary focus in this research is on proposing a methodology for modeling of discrete crack propagation in geomaterials such as soil, rock, and concrete. Structures made of such materials may undergo damage due to several reasons. Here, mechanical loading and chemo-mechanical interactions that result in degradation of strength parameters are considered as the sources of damage initiation. Both tensile and compressive cracks are investigated.

For analysis of crack propagation, two different methodologies are employed; the Constitutive Law with Embedded Discontinuity (CLED) and the Extended Finite Element Method (XFEM). The CLED approach is enhanced here to describe the discrete nature of crack propagation. This is done by coupling the CLED with explicit modeling of crack path using the Level-Set method. The XFEM is used as a verification tool to check the results from CLED analysis. An algorithm is proposed for crack initiation and propagation that results in stable and a mesh-independent solution. The CLED approach is further improved by developing the return-mapping and closest-point projection algorithms. Extensive numerical investigations are conducted that include mode I cracking in a three point bending test, mode I cracking in notched cantilever beam, mixed cracking mode in a plate subjected to shear and tension, and a mixed mode cracking in a notched beam under four point loading. For frictional interfaces, the shear band formation in a sample subjected to bi-axial compression and the shear band formation in a geo-slope are studied.
The thesis also addresses the topic of the response of unsaturated cohesive soils undergoing an infiltration process. The problem is approached within the framework of Chemo-Plasticity. It is assumed that the complex chemo-mechanical interactions are the controlling factors for degradation of strength parameters during this process. A return mapping integration scheme is developed and the approach is employed to investigate the stability of a geoslope subjected to a heavy rainfall.

Analysis of shear band formation is further investigated in the context of sedimentary rocks. The microstructure tensor approach is used to describe the inherent anisotropy in this class of materials. The orientation of the shear band is defined by invoking the Critical Plane approach and the closest-point projection algorithm is developed for numerical integration of the governing constitutive relations. The model is used along with CLED for analysis of the mechanical response of Tournemire argillite. It is shown that the friction between loading platens and sample can play an important role in the process of shear band formation and the associated assessment of the ultimate load. A mesh-sensitivity analysis employing the CLED framework is also conducted here.

The research clearly demonstrates that the discrete representation of crack path propagation is essential for an accurate analysis of failure in various engineering structures. It is shown that if the classical smeared Constitutive Law with Embedded Discontinuity is enhanced to simulate the discrete nature of the damage process, it can yield very accurate results that are virtually identical to those obtained from discrete approaches such as XFEM.
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Ehsan Haghighat
McMaster University
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List of Publications

This dissertation consists of following papers:

Paper I

Paper II

Paper III

Paper IV

Paper V
Pietruszczak, S, & Haghighat, E. Modeling of delayed failure of embankments due to water infiltration. Accepted in *Journal of Architecture Civil Engineering Environment*. 
Co-Authorship:
This dissertation has been prepared in accordance with the regulations for a “sandwich” thesis format and the papers have been co-authored with my supervisor.

Chapter 2: Assessment of slope stability in cohesive soils due to a rainfall
by: S. Pietruszczak and E. Haghighat
The chemo-plasticity framework has been proposed by Dr. S. Pietruszczak. The displacement formulation and the numerical integration scheme have been developed and implemented in the FEM code by E. Haghighat. The simulations have been conducted by E. Haghighat in consultation with Dr. S. Pietruszczak. Chapter 2 was prepared by E. Haghighat and then revised/finalized by Dr. S. Pietruszczak.

Chapter 3: Discrete modeling of cohesive crack propagation via an enhanced continuum approach
by: E. Haghighat and S. Pietruszczak
The development of the discrete representation of CLED and its implementation was done by E. Haghighat in consultation with Dr. S. Pietruszczak. The XFEM code was developed by E. Haghighat. The numerical simulations have been conducted by E. Haghighat in consultation with Dr. S. Pietruszczak. Chapter 3 was written by E. Haghighat and revised by Dr. S. Pietruszczak.

Chapter 4: On modeling of discrete propagation of localized damage in cohesive-frictional materials
by: E. Haghighat and S. Pietruszczak
The development of an enhanced numerical procedure for simulating the shear band localization in frictional materials was done by E. Haghighat in collaboration with Dr. S. Pietruszczak. The numerical simulations were conducted by E. Haghighat in consultation with Dr. S. Pietruszczak. Chapter 4 was prepared by E. Haghighat and revised by Dr. S. Pietruszczak.

Chapter 5: On the modeling of shear band formation in anisotropic rocks
by: S. Pietruszczak and E. Haghighat
The coupling of the micro-structure tensor approach with shear band formation has been proposed by Dr. Pietruszczak. The numerical model for simulating the localized failure has been developed and programed by E. Haghighat in consultation with Dr. S. Pietruszczak. The numerical simulations have been conducted by E. Haghighat in consultation with Dr. S. Pietruszczak. Chapter 5 was written by E. Haghighat and revised by Dr. S. Pietruszczak.

Chapter 6: Modeling of delayed failure of embankments due to water infiltration
by: S. Pietruszczak and E. Haghighat
This is an extension of the work reported in Chapter 2. The constitutive model has been proposed by Dr. S. Pietruszczak, while the numerical integration scheme incorporating the effect of localization was developed and implemented in FEM code by E. Haghighat. The simulations have been conducted by E. Haghighat in consultation with Dr. S. Pietruszczak. Chapter 6 was written by E. Haghighat and subsequently revised by Dr. S. Pietruszczak.
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Chapter 1- Thesis summary

In this chapter, a summary of the research conducted in this study is provided. The thesis is framed around the topic of modeling of damage propagation in geomaterials such as soils, rocks and concrete. Two approaches are addressed here. The main focus is on the Constitutive Law with Embedded Discontinuity (CLED) approach, while the Extended Finite Element Method (XFEM) is used as a verification tool. Contributions made in this research are provided in the form of journal papers as separate chapters. In the overview presented below, a brief summary of each paper is given. The chapter starts by pointing out the motivation and objectives behind this thesis. Subsequently, a short background on the numerical modeling of damage propagation in engineering structures is provided. The methodologies and tools that have been developed and applied in this dissertation are then reviewed, followed by a summary of contributions made in each paper. This chapter closes with conclusions and provides some guidelines for future studies.

1.1 Goals and motivations

During the last few decades, an intensive amount of research has been conducted in the area of modeling of the onset and propagation of damage. Over the years a number of different methodologies have been developed which include Node Separation (Ngo & Scordelis, 1967; Nilson, 1968), Smeared Cracking (Bažant & Cedolin, 1979; Nayak & Zienkiewicz, 1972; Pietruszczak & Mroz, 1981; Rashid, 1968), Boundary Integral (Blandford & Ingraffea, 1981), Element-Free (Belytschko et al., 1995; Liu et al., 1997),
and Extended Finite Element (Belytschko & Black, 1999; Moës et al., 1999) approaches. Among those, the Extended Finite Element Method that was introduced in 1999 appears to be the most commonly used approach for analysis of crack propagation. The primary reason is that the analysis is mesh independent and there is no need for adaptive mesh refinement, which results in a faster solution. Although XFEM is similar to standard FEM, there are certain disadvantages associated with its implementation, so that most software companies have still not incorporated it into their packages. The main difficulty is dealing with additional degrees of freedom and the associated enrichment functions. In addition, a special integration scheme must be incorporated and also a special treatment of data structures is required. Finally, the numerical problems arise due to stress singularities in locations where the interface is close to a node. The main motivation in this study is to develop a methodology that does not have the issues associated with XFEM, yet is still able to properly model the damage propagation process for a broad range of cohesive-frictional materials. The methodology pursued here incorporates an enhanced form of the Constitutive Law with Embedded Discontinuity approach that is capable of modeling the discrete nature of crack propagation very efficiently within the standard FEM mesh. A comprehensive investigation is conducted to verify the accuracy of the proposed approach in relation to XFEM and its applicability to various class of problems. Two main sources of damage in structures are investigated here, i.e. damage due to mechanical loading and damage due to degradation of material properties triggered by chemo-mechanical interactions.
The starting point of this research is the incorporation of the effect of chemical interaction between water and clay particles in cohesive frictional soils using the chemo-plasticity framework. A scalar parameter is defined that monitors the degradation of material properties due to an increase of saturation associated with a heavy rainfall. The research is then continued into modeling of localized failure associated with CLED and XFEM analysis of cracking under various loading scenarios.

1.2 Background

Modeling of damage in geomaterials such as soil, rock, and concrete is one of the most challenging problems, as it involves very complex computations due to the highly nonlinear response of these materials. Analysis of damage propagation, which is usually associated with localized deformation, is very important specifically for the assessment of the loss of stability. The latter is one of the main sources of loss of life in such natural disasters as earthquakes and landslides. In this thesis, the problem of damage initiation and propagation due to mechanical loading and chemo-mechanical interactions is addressed. The main focus is on the development of models which are not only capable of accurately describing these phenomena but can also be easily incorporated into any commercial package.

The research reported here was initiated with the formulation of a chemo-plasticity framework for the modeling of loss of cohesion in clayey soils after an intense rainfall. It is well known that a period of heavy rainfall can trigger a loss of stability of cohesive/cementitious slopes, where the water infiltration leads to a chemical interaction resulting in degradation of the mechanical properties of the material. This is addressed
classically using the notion of suction pressure as a state parameter (Alonso et al., 1990). However, the suction depends on microstructure of saturation and at very low degrees of saturation its measurement is not possible for clayey soils due to complex chemical interactions between particles of clay and the water. Recognizing this limitation, the approach implemented here is based on a phenomenological framework of chemo-plasticity (cf. Hueckel, 1997; Pietruszczak et al., 2006). A scalar variable is defined that monitors the evolution of strength parameters. The proposed methodology is believed to be a pragmatic alternative to both the micro-mechanical approach and the classical notions of unsaturated soil mechanics. Within the proposed framework, the injection of water is said to trigger a volume change (swelling/collapse) that is coupled with reduction in suction pressures that, in turn, results in degradation of strength and deformation properties. It needs to be emphasized that this approach is used only in the range of very low degrees of saturation when the water phase is discontinuous, i.e. water is present only near the interparticle contacts.

The study of stability of clayey soils is followed by the introduction of an enhanced form of the constitutive law with embedded discontinuity capable of modeling damage initiation and propagation in a discrete manner. This is in contrast to the original studies (Pietruszczak, 1995; Pietruszczak & Mroz, 1981) which were focused on smeared modeling of shear band localization in geomaterials.

As mentioned earlier, modeling of damage initiation and propagation has been one of the most intensely researched topics over the last few decades. Existing analytical solutions are restricted to an elastic material and involve simple geometries and boundary conditions.
Therefore, they are not directly relevant to practical engineering problems. The latter require, in general, a numerical simulation that typically involves the use of the Finite Element Method (FEM). The early methodologies for capturing the progressive damage were based on tracing the crack propagation on the element boundaries (Schellekens & de Borst, 1993). In addition, some smeared techniques have also been proposed that incorporated plasticity-based strain-softening relations (Lubliner et al., 1989; Parks, 1977; Rots & Blaauwendraad, 1989). Later, in order to avoid remeshing in the context of FEM, the mesh-free Galerkin method was introduced (Belytschko et al., 1996; Fleming et al., 1997). More recently, after introduction of the partition of unity approach (Melenk & Babuška, 1996), the Extended Finite Element Method (XFEM) was developed (Belytschko & Black, 1999; Dolbow et al., 2000; Moës et al., 1999; Moës et al., 2003), which enables the incorporation of discontinuous displacement fields as well as tip enrichments into the approximation space.

The XFEM has shown good predictive abilities in modeling discrete cracking problems; however, it is still not a practical approach in engineering applications although a great amount of research has been conducted on that. The primary difficulty arises from its implementation. Although the approach is based on FEM, special elements and integration schemes along with special algorithms for dealing with the increased number of degrees of freedom of the system are required. The solution shows artificial singularities for the cases where an interface passes through the proximity of an FEM node, which is unavoidable in general engineering applications. In contrast to this methodology, the smeared approaches have been widely used in engineering applications due to their simplicity in
implementation. The main problem with the early formulations was the sensitivity of the solution to discretization. The issue has been addressed by incorporating a length scale into the formulation, resulting in a mesh-independent framework (Pietruszczak & Mroz, 1981). This approach was later revised (Pietruszczak, 1999) and applied to a broad range of practical engineering problems (e.g., Pietruszczak & Gdela, 2010; Shieh-Beygi & Pietruszczak, 2008; Xu & Pietruszczak, 1997). The main difficulty, nonetheless, with smeared approaches is the lack of stability in numerical simulations that in turn causes convergence issues. It is believed here that a discrete representation of crack propagation can resolve the convergence issue and provide a stable algorithm capable of advancing the analysis beyond the peak load to model the post failure response.

As most geomaterials show anisotropic behaviour that is mainly related to their microstructure, the next part of this research is focused on the modeling of shear band formation in sedimentary rocks. As an example, Tournemire argillite has closely spaced bedding planes and exhibits a strong anisotropic response, so that its strength as well as deformation properties are directionally dependent. A comprehensive review on this topic, examining different approaches, is provided in the articles by Duveau and Henry (1998) and Kwasniewski (1993). One of the first attempts to describe the conditions at failure in anisotropic rocks was the work reported by Pariseau (1968), which was an extension of Hill’s criterion (Hill, 1967). This was followed by more complex tensorial representations (Amadei, 1983; Boehler & Sawczuk, 1977; Nova, 1980). A simple and pragmatic approach, which incorporates a scalar anisotropy parameter that is a function of a mixed invariant of the stress and the structure orientation tensor, was next developed by Pietruszczak (2002)
and Pietruszczak and Mroz (2000). This approach was later applied to the modeling of sedimentary rocks (Lade, 2007; Lydzba et al., 2003). Here, the microstructure tensor approach is combined with the CLED for modeling of shear band formation under axial compression. The effect of boundary conditions on crack formation and peak load is also investigated.

1.3 Methodologies and developed tools

As discussed earlier, two approaches are investigated here, standard FEM with CLED and XFEM. For this purpose, a two-dimensional nonlinear finite element program is developed. The program is designed in a robust way so that it can be easily implemented in ABAQUS as a user element library. The computer program can also be run separately for conducting quasi-static analysis. Thus, the problem can be completely defined in the ABAQUS environment, and an ABAQUS “inp” input file can be used to perform the analysis.

1.4 Contributions

In this section a summary of the papers that comprise this dissertation is presented.

**Paper I: Assessment of the slope stability in cohesive soils due to a rainfall**

The loss of stability of geoslopes after a heavy rainfall is still a source of major natural disasters. An example here is the recent slope failure in Oso, Washington, that resulted in 43 deaths and a significant damage to the surrounding area. In this paper, a methodology is
proposed for the assessment of stability of natural/engineered slopes in clayey soils subjected to water infiltration. In natural deposits of fine-grained soils, the presence of water in the vicinity of minerals results in an interparticle bonding. This effect cannot be easily quantified as it involves complex chemical interactions at the micromechanical level. Here, the framework of chemo-plasticity is employed to address the evolution of material properties. The degradation of strength, including the apparent cohesion resulting from initial suction at the irreducible fluid saturation, is taken into account by incorporating a scalar parameter that monitors the progress of chemical interaction. It should be stressed again that the proposed chemo-plasticity framework addresses the mechanical response of cohesive soil only at very low degrees of saturation when water does not exist in a free state. At the stage when the water phase becomes continuous, the soil properties are commonly described by considering suction pressure as a state variable. In general, however, the behaviour strongly depends on the microstructure of saturation. Therefore, it seems more appropriate to employ some averaging procedures whereby the compressibility of the mixture is expressed as a function of properties of constituents (free water and air) and the microstructure of saturation itself. The paper provides first the governing constitutive relation, followed by the development of a return mapping integration scheme. Subsequently, the coupled transient formulation is presented. The framework is applied to examine the stability of a slope subjected to a prolonged period of intensive rainfall. It is shown that the formulation can adequately describe the water infiltration problems, including the assessment of the stability of geo-structures.
**Paper II: Modeling of cohesive crack propagation: a constitutive law with embedded discontinuity vs XFEM**

(Submitted to International Journal for Numerical Methods in Engineering, May 2014)

The research reported here is focused on the problem of damage propagation in *brittle* materials. The approach incorporates a constitutive law with embedded discontinuity (CLED). As mentioned earlier, this methodology has been previously used within the context of smeared modeling of localization problems. The primary novelty here is an extension of this framework to model the *discrete* nature of fracture propagation process. This has been achieved by coupling the original approach with the Level-set method to capture the path of the crack propagation and to enable an accurate assessment of the characteristic length parameter. Thus, within the proposed framework the discontinuity is defined at the element level rather than at an integration point, which is in contrast to the classical smeared approaches. The paper provides a new analytical representation of the governing equations. In addition, a new implicit integration scheme is developed to impose the condition of continuity of traction along the interface. The efficiency and the accuracy of the proposed approach are verified using the framework of XFEM. The numerical simulations include a simple tension test, a three-point bending test, and a mixed mode cracking test in which a specimen is subjected to both shear and tension. It is shown that the approach can provide very accurate results for modeling discrete cracking with a very simple implementation through a user material subroutine, which can be done within almost all FEM packages. It is also concluded that the new approach is computationally more efficient as there is no need to incorporate additional degrees of freedom associated with discontinuous motion.
Paper III: On modeling of discrete propagation of localized damage in cohesive-frictional materials
(Submitted to International Journal for Numerical and Analytical Methods in Geomechanics, August 2014)

Here, the study initiated in the previous paper is extended to model the localized deformation associated with shear band formation in frictional media. Again, the research is focused on discrete tracing of the path of crack/shear band propagation. The CLED approach is extended here to deal with elasto-plastic materials. Some new numerical simulations are conducted and the results are compared again with XFEM to show further applications of the approach. The simulations include a mode I cohesive crack propagation in a cantilever beam, a mixed mode cracking problem in a four-point beam test, a problem of shear band formation in a biaxial compression test conducted on dense sand, and the evolution of localized damage in a cohesive slope. It is demonstrated that the CLED approach can be applied to a broad range of problems in the same way as XFEM, without the need for changing the main subroutines of the program as required in XFEM implementation.

Paper IV: Modeling of deformation and localized failure in anisotropic rocks
(Submitted to International Journal of Solids and Structures, November 2014)

The introduced methodology for modeling of damage propagation, i.e. CLED, is further investigated in the context of materials exhibiting a strong inherent anisotropy. The main focus here is on shear band formation and propagation in sedimentary rocks. In order to consider the material's anisotropy, the microstructure tensor approach is employed and a simple criterion is defined for the inception of shear band. The critical plane approach is
then applied in order to find the orientation of the crack. The closest-point projection algorithm is developed for both the anisotropic constitutive model and the constitutive law with embedded discontinuity for accurate integration of the constitutive relations. The problem of shear band formation in biaxial plane strain compression tests is studied for samples at different orientations of the bedding planes relative to the loading direction. It is demonstrated that the model can accurately reproduce a mesh-independent response. The effect of friction between loading plates and sample is also studied here. It is shown that it plays an important role in the damage evolution process and may affect the peak load significantly.

**Paper V: Modeling of delayed failure of embankments due to water infiltration**  
(Journal of Architecture Civil Engineering Environment, in print)

The problem that was initiated in Paper I is further investigated taking into account the localized failure mechanism associated with the shear band formation triggered by water infiltration. The framework incorporating CLED is extended here to deal with a coupled hydro-mechanical loading conditions.

Note that in this article some passages from paper I, in relation to the numerical example provided, have been quoted verbatim. This, however, is consistent with publisher policy on reusing author’s own article.

**1.5 Concluding remarks**

In paper I, a methodology for modeling a coupled hydro-mechanical response of clayey soils has been presented. The following main conclusions emerge from this work
Within the proposed framework, as long as the water phase is discontinuous, the material is treated as a single phase medium undergoing evolution of mechanical properties as a result of chemo-mechanical interactions. At this level of saturation, the approach does not require a specification of suction-saturation relationship as the suction pressure is said to be the product of interaction of a complex system of mineralogical and chemical factors. The developed return mapping combined with the subincrementation approach significantly improves the convergence of the global solution for unsaturated flow in porous media. The analysis of a geoslope subjected to an intense rainfall revealed that the water infiltration may trigger a loss of stability resulting from degradation of strength properties. It is also concluded that for an accurate assessment of stability, a methodology that is capable of modeling the localized failure associated with a shear band formation is required, which is the main study in following papers.

The research reported in paper II that dealt with the discrete modeling of crack propagation using the constitutive law with embedded discontinuity and the extended finite element method, led to the following major conclusions:

- The work clearly demonstrated that the constitutive law with embedded discontinuity can be successfully employed for modeling of discrete damage propagation. This has been accomplished by coupling the approach with the level-set method for tracing the crack path. It was demonstrated that a discrete representation of crack propagation process results in a stable, mesh-independent methodology that reproduces almost identical results to those obtained from XFEM. The developed
implicit integration scheme extends the range of applicability of this approach to any interfacial description, including traction free and cohesive models. The other significant conclusion is that the CLED methodology is computationally more efficient than the XFEM, since there are no additional degrees of freedom/enriched interpolations involved in the calculations. The CLED framework can be easily incorporated into any FEM package through the constitutive model subroutine. This is in contrast to XFEM, which requires development of special elements and algorithms for dealing with additional DOFs. Finally, a simple procedure was developed for tracing the crack initiation and propagation that is based on the averaging of the values of the failure function and the crack orientation in the domain adjacent to the crack tip. The result is a smooth cracking pattern that is mesh-insensitive.

The work reported in paper II was further extended in paper III to deal with more complex problems that involved frictional interfaces leading to localization into a shear band. The final remarks emerging from this study are as follows:

- It was shown that the approach incorporating CLED can be applied to problems in which the localization is associated with the onset and discrete propagation of a shear band. In contrast to XFEM, where artificial singularities (when interface passes through the vicinity of a node) may cause difficulties in the numerical analysis, the CLED approach proved very efficient in the context of elasto-plastic simulations. The return mapping scheme that was developed for both the intact material and the one
with embedded discontinuity showed a stable response and proved to be capable of accurately modeling the post-failure behaviour of the structure.

In paper IV, the problem of description of the deformation process in argillaceous rocks that display a strong inherent anisotropy was investigated. The scope of the work and the primary conclusions are summarized below:

- The mechanical characteristics of Tournemire shale were examined and the effect of boundary condition on the shear band formation was investigated for a series of plane strain biaxial compression tests. It was shown that in the case of a frictionless interface between loading platens and the sample, the deformation field remains homogeneous and the failure mode is diffused. With a presence of friction, however, the stress state is significantly perturbed which results in formation of a shear band/macrocrack. In this case, the ultimate strength of the sample is noticeably less than the one attained under frictionless conditions. A series of simulations for samples with different orientations of bedding planes was also conducted. It was shown that in samples with horizontal and vertical bedding planes, the failure mode is diffused for both frictionless and fully constrained cases; however the peak strength is still noticeably different for both these cases. The results of simulations clearly demonstrated that the kinematic constraints can play an important role in the process of evolution of damage and may significantly affect the strength characteristics that are commonly perceived as a material property. This is particularly the case for inclined samples. The mesh-dependency of the solution was also examined here. It was concluded that by invoking the constitutive law with embedded discontinuity,
which incorporates a characteristic dimension, the solution is virtually mesh independent.

In paper V, which was an extension to the study conducted in paper I, the problem of shear band propagation in materials undergoing a chemo-mechanical degradation was investigated and following conclusion was arrived at

- Comparison of the results with those presented in paper I shows that incorporation of the localized deformation mode significantly affects the displacement field as well as the stress distribution and thereby impacts the assessment of the safety factor of the slope. The solution incorporating the localized failure mode is, in general, more accurate and consistent with the field observations.

1.6 Suggestions for future work

- In the next step, the research should focus on the application of CLED approach to three dimensional problems. In this case, XFEM simulations are expensive and computationally inefficient.
- Further detailed analysis on the mesh-sensitivity and the rate of convergence of the proposed approach should be conducted.
- The accuracy of the CLED approach for can be further investigated within the context of more accurate meshfree methods and the recently developed isogeometric approach.
- Further applications of the proposed methodology to a broad class of problems involving hydro-thermo-mechanical interaction could be undertaken. The simplicity
of this approach, while retaining the accuracy, can be an asset in terms of analysis of these complex coupled problems.

- The random-based simulations of cracking and shear banding can also be effectively investigated using this approach, due to its simplicity of implementation.

### 1.7 References


ASSESSMENT OF THE SLOPE STABILITY IN COHESIVE SOILS DUE TO A RAINFALL

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ABSTRACT: The primary focus in this work is on proposing a methodology for the assessment of stability of natural/engineered slopes in clayey soils subjected to water infiltration. In natural deposits of fine grained soils, the presence of water in the vicinity of minerals results in an interparticle bonding. This effect cannot be easily quantified as it involves complex chemical interactions at the micromechanical level. Here, the evolution of strength properties, including the apparent cohesion resulting from initial suction at the irreducible fluid saturation, is described by employing the framework of chemo-plasticity. The paper provides first the formulation of the problem; this involves specification of the constitutive relation, development of an implicit return mapping scheme as well as the outline of a coupled transient formulation. The framework is then applied to examine the stability of a slope subjected to a prolonged period of intensive rainfall. It is shown that the water infiltration may trigger the loss of stability resulting from the degradation of material properties.

KEYWORDS: chemo-plasticity, rainfall infiltration, slope stability, unsaturated flow

1. INTRODUCTION

It is well known that a period of heavy rainfall can trigger a loss of stability of slopes. This is particularly the case for slopes constructed in cohesive soils, such as clay or a cemented soil, where the water infiltration leads to a chemical interaction resulting in degradation of mechanical properties of the material.

The problem of stability of natural and engineered slopes has been a subject of research for a number of decades. In particular, the notion of influence of suction pressure on the stability has become an important issue. In recent years, several case histories have been documented (e.g., in Hong Kong, Korea, Malaysia, Singapore) whereby the loss of stability was related to the loss of suction triggered by the local weather conditions [1-3].

The primary difficulty in modeling the loss of stability due to a heavy rainfall lies in assessing the in-situ conditions and in describing the coupling between the time-dependent process of water infiltration and the evolution of stress field. The problem is typically analyzed by integrated software in which the transient seepage analysis is coupled with traditional limit

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equilibrium slope stability analysis [4-6]. Alternatively, the frameworks for unsaturated soil are implemented in which the suction pressure is considered as a state parameter and an optimization technique is used to search for a critical slip surface (e.g., [4]). In general, the conventional methods for assessing the stability of unsaturated soils, based on limit equilibrium approach, significantly underestimate the safety factors. Therefore, more accurate techniques are required.

Specification of properties of clays is difficult as it involves a very complex system of mineralogical and chemical factors. There are significant variations in composition, size and relative orientation of the mineral phase, as well as composition and the amount of aqueous phase. Therefore, a micro-mechanically based description of physical properties of clays represents an overwhelming task.

In clays, the bond strength increases rapidly with decreasing water content. It is rather apparent that free water in clays has low compressibility and virtually no viscosity. The water in the vicinity of minerals, however, has quite different properties which cannot, in fact, be quantified due to complex chemical interactions. Therefore, the measurement and/or control of suction pressures are difficult. Recognizing the above limitations, a different methodology is proposed here as an alternative to a micro-mechanical approach. At the range of irreducible saturation (cf. [7]), when the water phase is discontinuous, the behavior of the material is described based on a phenomenological framework of chemo-plasticity (cf. [8-10]). Within this framework, an increase in water content due to wetting is said to trigger a reduction in the interparticle bonding and the corresponding degradation of strength and deformation properties at the macroscale. At the stage when the water phase becomes continuous, the behaviour can then be defined in mechanical terms alone; for example, by employing an averaging procedure in which the compressibility of the mixture is expressed as a function of properties of constituents (free water and air) and the microstructure of saturation ([11,12]). Note such an approach incorporates the average ‘pore size’ as an independent characteristic dimension. Alternatively, the problem may be phrased using the classical notions of unsaturated soil mechanics [13-15].

In the next section, the formulation of the problem is discussed including the development of implicit (backward Euler) integration scheme. Later, the governing equations describing the transient hydro-mechanical coupling are reviewed and the framework is applied to examine the stability of a slope in cohesive soil, subjected to a period of intense rainfall. In solving the problem, the evolution of the phreatic surface is monitored and is coupled with mechanical analysis incorporating the chemical interaction.

2. FORMULATION OF THE PROBLEM

2.1 Constitutive relation

The general approach for describing the evolution of properties of clays in the presence of the interparticle bonding is based on the framework of chemo-plasticity, similar to that of ref. [10]. Within this approach, the progress in chemo-mechanical interaction is monitored by a scalar parameter $\zeta$. Here, this parameter may be interpreted as the change in the initial suction pressure $u_s^0$, at the irreducible wetting fluid saturation, in REV; i.e., $\zeta \propto (u_s^0 - u_s) / u_s^0$, so that $\zeta \subset [0,1]$.

The evolution law can be taken in a simple linear form
\[ \frac{\partial \zeta}{\partial t'} = B(1 - \zeta); \quad dt' = gdt \]  

(1)

where \( g \in [0,1] \) depends on the chemical composition of the clay minerals and water, and \( B \) is a material constant. In the elastic range, the constitutive relation takes the form

\[ \varepsilon^e = \mathbb{D}^{-1} : \sigma \rightarrow \dot{\varepsilon}^e = \mathbb{D}^{-1} : \dot{\sigma} + \mathbb{D}^{-1} : \sigma = \mathbb{D}^{-1} : \dot{\sigma} + \zeta \dot{\sigma} \mathbb{D}^{-1} : \sigma \]  

(2)

where \( \sigma \) is the effective stress and \( \mathbb{D}^{-1} \) is the elastic compliance operator. Note that the differential form of eq. (2) may be expressed as

\[ \dot{\sigma} = \mathbb{D} : \dot{\varepsilon}^e - \zeta \left( \mathbb{D} : \dot{\varepsilon} \right) : \sigma \]  

(3)

Invoking now the additivity postulate, total strain rate can be written as

\[ \dot{\varepsilon} = \varepsilon^e + \varepsilon^p + \dot{\varepsilon} \]  

(4)

where \( \dot{\varepsilon} \) is the volumetric strain rate due to wetting. The latter may be taken as \( \dot{\varepsilon} = \epsilon \dot{\zeta} \mathbb{I} \), where \( \epsilon \) is the maximum expansion/contraction in the stress-free state. The plastic strain rates \( \varepsilon^p \) are defined following standard plasticity formalism, i.e.

\[ f = f(\sigma, \kappa, \zeta) \leq 0; \quad \dot{\varepsilon}^p = \dot{\lambda} \frac{\partial \psi}{\partial \sigma} \]  

(5)

where \( f = f(\sigma, \kappa, \zeta) \) is the yield function, \( \kappa = \kappa(\varepsilon^p) \) is the hardening parameter and \( \psi = \psi(\sigma, \zeta) \) is the plastic potential function.

Using the decomposition (4), the constitutive relation defining the stress rate may be expressed as

\[ \dot{\sigma} = \mathbb{D} : (\dot{\varepsilon} - \dot{\varepsilon}) - \mathbb{D} : \varepsilon^p - \zeta \left( \mathbb{D} : \dot{\varepsilon} \right) : \sigma \]  

(6)

2.2 Implicit integration-scheme

The constitutive relation defined by eq. (6) is subjected to the following constraints

\[ f = f(\sigma, \kappa, \zeta) \leq 0 \quad \dot{\lambda} \geq 0 \rightarrow f \dot{\lambda} = 0 \]  

(7)

During an active loading process, there is \( \dot{\lambda} > 0 \) and \( f(\sigma, \kappa, \zeta) = 0 \), so that \( \dot{f}(\sigma, \kappa, \zeta) = 0 \). The latter represents the consistency condition and takes the form

\[ \dot{f} = \frac{\partial f}{\partial \sigma} : \dot{\sigma} + \frac{\partial f}{\partial \kappa} \dot{\kappa} + \frac{\partial f}{\partial \zeta} \dot{\zeta} = 0 \]  

(8)

Following now the general return-mapping scheme [16,17], the stress and plastic strain at time \( t + \Delta t \) can be expressed as
\[
\begin{align*}
\mathbf{e}_{t+\Delta t}^p &= \mathbf{e}_t^p + \dot{\mathbf{e}}_{t+\Delta t}^p \Delta t \\
&= \mathbf{e}_t^p + \Delta \lambda_{t+\Delta t} \partial_\sigma \psi \left( \mathbf{\sigma}_{t+\Delta t}, \mathbf{\zeta}_{t+\Delta t} \right) \\
\mathbf{\sigma}_{t+\Delta t} &= \mathbf{\sigma}_t + \dot{\mathbf{\sigma}}_{t+\Delta t} \Delta t \\
&= \mathbb{D}_{t+\Delta t} : (\Delta \mathbf{\epsilon} - \Delta \epsilon)_{t+\Delta t} - \mathbb{D}_{t+\Delta t} : \Delta \mathbf{e}_{t+\Delta t}^p - \Delta \mathbf{\zeta}_{t+\Delta t} \left( \mathbb{D} : \partial_\xi \mathbb{D}^{-1} \right)_{t+\Delta t} : \mathbf{\sigma}_{t+\Delta t} 
\end{align*}
\] (9)

Dropping the subscript \( t + \Delta t \) and solving the second equation for \( \mathbf{\sigma}_{t+\Delta t} \), one obtains
\[
\begin{align*}
\mathbf{e}^p &= \mathbf{e}_t^p + \Delta \lambda \partial_\sigma \psi \\
\mathbf{\sigma} &= \mathbb{A}^{-1} \left( \mathbf{\sigma}_t + \mathbb{D} : (\Delta \mathbf{\epsilon} - \Delta \epsilon) - \mathbb{D} : \Delta \mathbf{e}^p \right) 
\end{align*}
\] (10)

where \( \mathbb{A} = \mathbb{I} + \Delta \mathbf{\zeta}_{t+\Delta t} \left( \mathbb{D} : \partial_\xi \mathbb{D}^{-1} \right)_{t+\Delta t} = \mathbb{I} + \Delta \mathbf{\zeta} \left( \mathbb{D} : \partial_\xi \mathbb{D}^{-1} \right) \). Note that the primary unknowns here are \( \mathbf{\sigma} = \mathbf{\sigma}_{t+\Delta t} \) and \( \Delta \lambda = \Delta \lambda_{t+\Delta t} \), while the parameter \( \kappa \) is a scalar valued function of plastic deformation, so that it is a dependent variable.

In order to solve the above set of equations, the general Newton-Raphson procedure is implemented. Following this scheme, the residuals can be defined as,
\[
\begin{align*}
\mathbf{r}_k &= \mathbf{\sigma}_k - \mathbb{A}^{-1} \left( \mathbf{\sigma}_k + \mathbb{D} : (\Delta \mathbf{\epsilon} - \Delta \epsilon) - \mathbb{D} : \Delta \mathbf{e}^p_k \right) \\
&= \mathbf{\sigma}_k - \mathbb{A}^{-1} \left( \mathbf{\sigma}_k + \mathbb{D} : (\Delta \mathbf{\epsilon} - \Delta \epsilon) - \Delta \lambda_k \mathbb{D} : \partial_\sigma \psi_k \right) \\
f_k &= f \left( \mathbf{\sigma}_k, \kappa_k, \Delta \lambda_k \right) 
\end{align*}
\] (11)

Expanding these residuals, using Taylor expansion, yields
\[
\begin{align*}
\mathbf{r}_k + \partial_\sigma \mathbf{r}_k : \mathbf{\delta} \mathbf{\sigma}_k + \partial_{\Delta \lambda} \mathbf{r}_k : \mathbf{\delta} \lambda_k &= 0 \\
f_k + \partial_\sigma f_k : \mathbf{\delta} \mathbf{\sigma}_k + \partial_{\Delta \lambda} f_k : \mathbf{\delta} \lambda_k &= 0 
\end{align*}
\] (12)

where \( \partial_\sigma \mathbf{r}_k = \mathbb{Q}_k \left( \mathbb{I} + \Delta \lambda \left( \mathbb{A}^{-1} : \mathbb{D} \right) : \partial_\sigma \psi \right)_k \) and \( \partial_{\Delta \lambda} \mathbf{r}_k = \left( \left( \mathbb{A}^{-1} : \mathbb{D} \right) : \partial_\sigma \psi \right)_k \).

Solving now the above set of equation, one has
\[
\mathbf{\delta} \mathbf{\sigma}_k = -\mathbb{Q}_k^{-1} \left( \mathbf{r}_k + \partial_{\Delta \lambda} \mathbf{r}_k : \mathbf{\delta} \lambda_k \right) 
\] (13)

and
\[
\mathbf{\delta} \lambda_k = \frac{f_k - \partial_\sigma f_k : \mathbb{Q}_k^{-1} \mathbf{r}_k}{\partial_\sigma f_k : \mathbb{Q}_k^{-1} \mathbb{C} : \partial_\sigma \psi_k - \partial_{\Delta \lambda} f_k} 
\] (14)

which fully defines the stress and plastic strain corrections during the Newton-Raphson iterations.

In order to specify the tangential stiffness operator, which is required for the global Newton-Raphson solution algorithm, the stress increment can be expressed as
\[
\Delta \mathbf{\sigma} = \mathbb{Q}^{-1} : \mathbb{A}^{-1} : \mathbb{D} : (\Delta \mathbf{\epsilon} - \Delta \epsilon) - \mathbb{Q}^{-1} : \mathbb{A}^{-1} : \mathbb{D} : \partial_\sigma \psi \Delta \lambda 
\] (15)

Defining now an operator \( \mathbb{R} = \mathbb{Q}^{-1} : \mathbb{A}^{-1} : \mathbb{D} \), and using the consistency condition, one obtains
\[ \Delta f = \partial_\alpha f : \Delta \sigma + \partial_{\Delta \lambda} f : \Delta \lambda = 0 \] 

so that

\[ \Delta \lambda = \frac{\partial_\alpha f : \mathbb{R} (\Delta \varepsilon - \Delta \epsilon)}{\partial_\alpha f : \mathbb{R} : \partial_\alpha \psi - \partial_{\Delta \lambda} f} \] 

Thus, the stress increment may be written as

\[ \Delta \sigma = \mathbb{D}_r : (\Delta \varepsilon - \Delta \epsilon) \] 

where \( \mathbb{D}_r \), i.e. the tangential stiffness operator, is defined as

\[ \mathbb{D}_r = \mathbb{R} - \frac{(\mathbb{R} : \partial_\alpha \psi) \otimes (\partial_\alpha f : \mathbb{R})}{\partial_\alpha f : \mathbb{R} : \partial_\alpha \psi - \partial_{\Delta \lambda} f} \] 

In the numerical examples provided later, the above backward Euler scheme is combined with subincrementation. This is primarily due to the fact that the chemical degradation is very fast and small time increments are required in order to obtain an accurate solution for the local stress trajectories.

3. APPLICATION OF CHEMO-PLASTICITY FRAMEWORK TO MODELING OF SOIL INFILTRATION

3.1 Description of unsaturated flow in porous media

In order to trace the evolution of phreatic surface during the rainfall infiltration, the problem is defined by invoking a coupled formulation for flow through unsaturated porous media[18]. Within this framework, the porous material is considered as a mixture of solid grains and voids; the latter filled with water and/or air.

Neglecting the inertia forces, the momentum balance equation for the solid-fluid mixture takes the form

\[ \nabla \cdot \hat{\mathbf{\sigma}} + \hat{\rho} \mathbf{g} = 0 \] 

subject to

\[ \mathbf{v} = \hat{\mathbf{v}} \quad \text{on} \quad \Gamma_d \]

\[ \mathbf{\sigma} \cdot \mathbf{n} = \hat{\mathbf{t}} \quad \text{on} \quad \Gamma_i \] 

Here, \( \hat{\mathbf{\sigma}} \) is the total stress, \( \mathbf{g} \) is the acceleration due to gravity, while \( \hat{\mathbf{v}} \) and \( \hat{\mathbf{t}} \) represent the velocity and traction prescribed on the boundaries \( \Gamma_d \) and \( \Gamma_i \), respectively. Furthermore, \( \hat{\rho} \) is the density of the mixture; the latter, neglecting the density of air, may be defined as

\[ \hat{\rho} = (M_s + M_w) / V = (1 - n) \rho_s + Sn \rho_w \] 

where \( n \) and \( S \) are the porosity and the degree of saturation, while the indexes \( s, w \) refer to solids and water, respectively.
For unsaturated soil, the stress transmitted by the skeleton, i.e. the effective stress \( \sigma \), is typically defined using Bishop’s relation
\[
\sigma = \hat{\sigma} - (\chi u_w + (1 - \chi) u_a) I \approx \hat{\sigma} - \chi u_w I \tag{22}
\]
where \( I \) is the identity tensor, \( u_w, u_a \) is water and air pressures, respectively, and \( \chi \) is the Bishop’s parameter. Apparently, if the air phase is continuous, the excess of air pressure is usually neglected, so that \( u_a \to 0 \) in eq. (22).

Note again that at the range of irreducible saturation, when the aqueous phase is present only in the vicinity of minerals, the material is conceptually considered as a continuum with an apparent cohesion. At this stage, an increase in water content due to wetting activates the chemomechanical interaction and leads to a microstructure of saturation in which the water phase becomes continuous. For the latter scenario, the simulations presented here were completed by identifying the parameter \( \chi \) with the degree of saturation \( S \), which is consistent with a similar assumption adopted by other investigators (e.g., [19,20]). It is noted, however, that the decomposition (22) is semi-empirical in nature and the problem may, in fact, be phrased by assuming \( \chi \to 1 \) (i.e. Terzaghi’s principle) and considering specific features of the geometry of microstructure of saturation. As shown in refs. [11,12], when the water phase is continuous, the evolution of suction pressure as well as the compressibility of the immiscible air-water mixture may be defined as an explicit function of the surface area of grains (or the air-water menisci) and the properties of constituents (i.e., free water/air).

Consider now the mass balance equation for the fluid phase, which may be expressed, after normalizing with respect to \( \rho_w^0 \), in the following form [18]
\[
\frac{1}{\rho_w^0} \left( \frac{d}{dt} \left( \rho_w S_n + \rho_w S_n I : \dot{\varepsilon} + \nabla \cdot \left( \rho_w S_n \nu_{w,v} \right) \right) \right) = 0 \tag{23}
\]
Assuming that solid grains are undeformable while the water is linearly compressible, the following relations may be established for a representative differential volume \( dV = dV_s + dV_v = dV_s + dV_w + dV_a \)
\[
\frac{\rho_s}{\rho_s^0} \frac{dV_s^0}{dV_s} = \frac{dV_s - \Delta dV_s}{dV_s} \approx 1 \\
\frac{\rho_w}{\rho_w^0} \frac{dV_w^0}{dV_w} = \frac{dV_w - \Delta dV_w}{dV_w} \approx 1 + \frac{u_w}{K_w} \tag{24}
\]
\[
n = 1 - \frac{dV_s}{dV} = 1 - \frac{dV_s}{dV_s} \frac{dV^0}{dV} = 1 - J_s J^{-1} \left( 1 - n^0 \right)
\]
where \( J = dV / dV^0 = \det F \) and \( F \) is the deformation gradient.
Substituting the above relations into eq. (23) and taking time derivatives (note that \( \dot{J} = J I : \dot{\varepsilon} \)), the following expression is obtained
\[ \frac{\rho_w}{\rho_0} S \left( n + \frac{1-n^0}{J} \right) \mathbf{i} \dot{\varepsilon} + \left\{ \frac{S n + \rho_w \rho \, dS}{K_w \, \rho_{w0} \, du_w} n \right\} \mathbf{i} \dot{u}_w + \nabla \cdot \left( \frac{\rho_w}{\rho_0} S \mathbf{n} \mathbf{v} \right) = 0 \] 

Introducing now the definitions

\[ \alpha = \frac{\rho_w}{\rho_0} \left( n + \frac{1-n^0}{J} \right) \]

\[ \frac{1}{Q} = \frac{S n + \rho_w \, dS}{K_w \, \rho_{w0} \, du_w} n \]

the mass balance relation can be expressed as

\[ S \alpha \mathbf{i} \dot{\varepsilon} + \frac{1}{Q} \mathbf{i} \dot{u}_w - \nabla \cdot \left( \frac{\rho_w}{\rho_0} S \mathbf{n} \mathbf{v} \right) = 0 \]

and is subjected to the following boundary conditions

\[ u_w = \bar{u}_w \quad \text{on} \quad \Gamma_w \]
\[ S \mathbf{n} \mathbf{v} = \bar{q} \quad \text{on} \quad \Gamma_g \]

The fluid flow in porous media is governed by Darcy’s law, which takes the form

\[ S \mathbf{n} \mathbf{v} = -\mathbf{k} \cdot \nabla \phi \]

In the equation above, \( \mathbf{v}_w \) is the relative velocity of water, \( \phi \) is the piezometric head and \( \hat{\mathbf{k}} = k \mathbf{l} \) is the permeability of the skeleton; with \( \mathbf{k} \) representing the permeability under fully saturated condition and \( k_s = k(S) \). Note that, if the soil is isotropic with respect to permeability, then \( \hat{\mathbf{k}} = k_s \mathbf{l} = \hat{k} \mathbf{l} \). The piezometric head can be expressed as \( \phi = \mathbf{x} \cdot \mathbf{g}/g + u_w/g \rho_w \), where the first term defines the elevation head and \( g \) is the magnitude of the gravitational acceleration. Given the above definitions, Darcy’s law may be written in an alternative form, as

\[ S \mathbf{n} \mathbf{v} = -\frac{\hat{k}}{\rho_w g} (\nabla u_w - \rho_w \mathbf{g}) \]

Now, using stress decomposition (22), the weak form of eq. (20) can be expressed as

\[ \int_\Omega \delta \dot{\varepsilon} : \mathbf{\sigma} \, dV - \int_\Gamma \delta \dot{\varepsilon} : \chi u_w \mathbf{l} \, dV = \int_\Gamma \delta \mathbf{v} \cdot \mathbf{\tilde{t}} \, dS + \int_\Omega \delta \mathbf{v} \cdot \hat{\mathbf{p}} \mathbf{g} \, dV \]

where \( \varepsilon = \nabla^s \mathbf{v} \). Also, using the Darcy’s law (30), the mass-balance may be expressed in a weak form as

\[ \int_\Omega \delta u_w \, S \alpha \mathbf{l} \dot{\varepsilon} \, dV + \int_\Omega \delta u_w \frac{1}{Q} \mathbf{l} \dot{u}_w \, dV - \int_\Omega \nabla \delta u_w \cdot \frac{\hat{k}}{\rho_w g} \nabla u_w \, dV \]

\[ = \int_{\Gamma_g} \delta u_w \frac{\rho_w}{\rho_0} \mathbf{\tilde{q}} \, dV - \int_\Omega \nabla \delta u_w \cdot \frac{\hat{k}}{\rho_w g} \rho_w \mathbf{g} \, dV \]
Here, the velocity $v$ and pressure $u_w$ are both smooth and continuous functions that satisfy the boundary conditions, i.e.

$$v \in \mathcal{U}, \quad \mathcal{U} = \{ v | v \in C^0, \ v = \tilde{v} \text{ on } \Gamma_d \}$$

$$u_w \in \mathcal{V}, \quad \mathcal{V} = \{ u_w | u_w \in C^0, \ u_w = \tilde{u}_w \text{ on } \Gamma_w \}$$

(33)

where $\mathcal{U}$ and $\mathcal{V}$ are the set of kinematically admissible velocity and pressure spaces. Note that $\delta u$ and $\delta u_w$ are also required to have similar properties as those in eq. (33), while both must vanish on the respective boundaries, i.e.

$$\delta v \in \mathcal{U}^0, \quad \mathcal{U}^0 = \{ \delta v | \delta v \in C^0, \ \delta v = 0 \text{ on } \Gamma_d \}$$

$$\delta u_w \in \mathcal{V}^0, \quad \mathcal{V}^0 = \{ \delta u_w | \delta u_w \in C^0, \ \delta u_w = 0 \text{ on } \Gamma_w \}$$

(34)

Finally, note that under the restrictions of small deformation theory, i.e. $J \approx 1$, $n^0 = n$, and $\rho_w = \rho_w$, the material parameters defined in eq. (26) become identical to those defined in ref.[18], i.e.,

$$\alpha \approx 1; \quad \frac{1}{Q} \approx n \frac{dS}{du_w} + \frac{S_n}{K_w}$$

3.2 Finite element discretization

In order to derive the set of discretized FE equations, a proper approximation for both velocity and pressure fields is required. Assuming the following approximations

$$v(x,t) = \hat{u}(x,t) \approx N_d(x)\hat{\bar{u}}(t) \rightarrow \nabla \hat{u}(x,t) \approx B_d(x)\hat{\bar{u}}(t)$$

$$u_w(x,t) \approx N_w(x)\bar{u}_w(t) \rightarrow \nabla u_w(x,t) \approx B_w(x)\bar{u}_w(t)$$

(35)

the space-discretized form of equations (31) and (32) can be derived as,

$$\int_{\Omega} B_d^T \sigma dV - Q \hat{u}_w - f^{(1)} = 0$$

$$\tilde{Q} \hat{\bar{u}} + S\hat{\bar{u}}_w - H\bar{u}_w - f^{(2)} = 0$$

(36)

where,
\[ Q = \int_{\Omega} B_d^T \chi m_N d\Omega \]
\[ \dot{Q} = \int_{\Omega} N^T \alpha m \dot{B}_d d\Omega \]
\[ S = \int_{\Omega} N^T \frac{1}{Q} N_w d\Omega \]
\[ H = \int_{\Omega} B_w^T \frac{k}{\rho_w^0} B_w d\Omega \]
\[ f^{(1)} = \int_{\Gamma_d} N_d \tilde{t} dS + \int_{\Omega} N_d \dot{\rho} g d\Omega \]
\[ f^{(2)} = \int_{\Gamma_e} N_e \frac{\rho_w}{\rho_w^0} \tilde{q} d\Omega - \int_{\Omega} B_e^T \frac{k}{\rho_w^0} \rho_w g d\Omega \]

and \( m \) is the matrix form of the identity tensor \( I \). The set of equations (36) must be discretized in time as well. Using a conventional Euler-backward integration scheme, the following relations are obtained

\[ r_{t+\Delta t}^{(1)} = \left( \int_{\Omega} B_d^T \sigma d\Omega \right)_{t+\Delta t} - Q_{t+\Delta t} \bar{u}_{w}^{t+\Delta t} - f_{t+\Delta t}^{(1)} \]
\[ r_{t+\Delta t}^{(2)} = \bar{Q}_{t+\Delta t} \bar{u}_{w}^{t+\Delta t} + (S_{t+\Delta t} - \Delta t H_{t+\Delta t}) \bar{u}_{w}^{t+\Delta t} - \Delta t f_{t+\Delta t}^{(2)} \]

The above equations are nonlinear and a general Newton-Raphson scheme is required. Using an iterative algorithm, leads to

\[
\begin{bmatrix}
K_{t+\Delta t} & -Q_{t+\Delta t} \\
\bar{Q}_{t+\Delta t} & S_{t+\Delta t} - \Delta t H_{t+\Delta t}
\end{bmatrix}
\begin{bmatrix}
\delta \bar{u}_{w}^{t+\Delta t} \\
\end{bmatrix}_i =
\begin{bmatrix}
r_{t+\Delta t}^{(1)} \\
r_{t+\Delta t}^{(2)}
\end{bmatrix}_i
\]  

(39)

where,

\[
\begin{align*}
(u_{w}^{t+\Delta t})_{i+1} &= (u_{w}^{t+\Delta t})_i + (\delta u_{w}^{t+\Delta t})_i \\
(u_{w}^{t+\Delta t})_{i+1} &= (u_{w}^{t+\Delta t})_i + (\delta u_{w}^{t+\Delta t})_i
\end{align*}
\]  

(40)

and

\[ K = \int_{\Omega} B_d^T D_T B_d d\Omega \]

(41)

where \( D_T \) is the tangential stiffness operator which has been defined in the previous section.

4. NUMERICAL SIMULATIONS

4.1 Deviatoric hardening model

The simulations presented here employ the framework of deviatoric hardening (cf. [21]). Within this approach, the loading surface \( f = f(\sigma, \kappa, \zeta) \) is defined as
\[ f = \sqrt{3} \bar{\sigma} - \eta \varphi (\theta) (\sigma_m + c \cot \phi) = 0 \]  

(42)

Here, \( \sigma_m = -\sigma : I / 3 \), \( \bar{\sigma} = \sqrt{J_2} = \sqrt{1/2s:s} \), and \( \theta = \sin^{-1}(-3\sqrt{J_3}/2\bar{\sigma}^3) / 3 \); where \( s \) is the stress deviator and \( J_3 = \sqrt{s \cdot s} \). The parameter \( \theta \) represents Lode’s angle and is defined within the interval \(-\pi / 6 \leq \theta \leq \pi / 6\), while \( g(\theta) \) satisfies \( g(\pi / 6) = 1 \) and \( g(-\pi / 6) = K \), where \( K \) is a constant. In equation (42), \( \phi \) is the friction angle and \( c \) is the cohesion. The specific mathematical expression for \( g(\theta) \) implemented here is that proposed by Willam-Warnke [22]. The hardening parameter \( \eta = \eta(\kappa) \) is defined using the following hyperbolic form

\[ \eta = \eta_f \frac{\kappa}{A + \kappa} \]  

(43)

where \( A \) is a material constant and \( \eta_f \) defines the value of \( \eta \) at failure, i.e. \( \eta \rightarrow \eta_f \) for \( \kappa \rightarrow \infty \). Assuming that the condition at failure are consistent with Mohr-Coulomb criterion, we have \( \eta_f = 6 \sin \phi / (3 - \sin \phi) \). Furthermore, the flow rule is assumed to be non-associated and the potential function is taken in the form

\[ \psi = \sqrt{3} \bar{\sigma} + \eta_c (\sigma_m + c \cot \phi) \ln \frac{\sigma_m + c \cot \phi}{\sigma_m^0} = 0 \]  

(44)

where, \( \eta_c = \text{const.} \) is a material constant.

In order to incorporate the deviatoric-hardening model in the chemo-plasticity framework, the strength parameters \( \eta_f \) and \( c \), as well as the Young’s modulus \( E \), are assumed to undergo a progressive degradation in the course of chemical interaction. The evolution laws are taken in a simple linear form

\[ \eta_f = \eta_f^0 (1 - G_\zeta \zeta) \]
\[ c = c^0 (1 - G_\zeta \zeta) \]
\[ E = E^0 (1 - G_\zeta \zeta) \]  

(45)

where \( G \)'s are material constants and the kinetics of the interaction process, viz. evolution of \( \zeta \), is governed by eq.(1). Note that, given the last equation in (45), the elastic operator \( D \) satisfies

\[ D = D^0 \left(1 - G_\zeta \zeta\right) \]
\[ D^{-1} = D^{0-1} / \left(1 - G_\zeta \zeta\right) \quad \rightarrow \quad D^{0} : D^{0-1} = I \]  

(46)

so that

\[ D : D^{-1} = g(\zeta) I; \quad g(\zeta) = \frac{G_\zeta}{(1 - G_\zeta \zeta)} \]  

(47)

Hence, the fourth-order tensor \( A \), defined in the previous sections takes the form,

\[ A = I + \Delta \zeta \left(D : D^{-1}\right) \rightarrow A^{-1} = \frac{1}{1 + \Delta \zeta g(\zeta)} I \]  

(48)
In what follows, some numerical examples are provided. The first one, which deals with the point integration algorithm, is focused on examining the effect of water injection in a sample subjected to a sustained deviatoric load of a prescribed intensity. The second example deals with an initial boundary-value problem, which involves assessment of slope stability under conditions of an intense rainfall.

4.2 Example # 1

The first example involves sample of a cohesive soil that is tested in triaxial compression under some initial confining pressure. The sample, in its natural state of compaction, is subjected to an axial load of a prescribed magnitude, which is subsequently kept constant while the water is said to be injected. The latter results in time-dependent degradation of mechanical properties, which stems from chemical interaction taking place in the neighborhood of interparticle contacts.

The mechanical properties of the material, in its initial state, are taken as

\[ K = 100\text{MPa}; \quad G = 45\text{MPa}; \quad c = 50\text{kPa}; \quad \eta_f = 1.4; \quad \eta_e = 1.2; \quad A = 0.0005; \]

Note that \( c \) represents here the apparent cohesion, which results from interparticle bonding and it’s subsequently lost upon wetting. The degradation parameters, related to chemical interaction, are assumed as

\[ G_1 = 20\%; \quad G_2 = 100\%; \quad G_3 = 50\%; \quad B = 0.92; \]

The constant \( B \) is chosen in such a way that at \( t = 5\text{sec} \), the parameter \( \zeta \), eq. (1), reaches the value of 0.99, i.e. 99% of the reaction is said to be completed. The simulations correspond to initial confining pressure of \( p = -500\text{kPa} \). The water injection is assumed to be instantaneous, so that the problem is solved by employing the point integration scheme, as discussed earlier.

The key results are presented in Figs. 1-2. Fig.1 shows the time-dependent history of axial strain corresponding to different deviatoric stress intensities \( q = \sigma_3 - \sigma_1 \), ranging from 800 kPa to 1000 kPa. Note that for the first stage of loading, i.e. application of deviatoric stress \( q \), the response is time-independent as it is governed by standard plasticity framework. Fig.2 shows the time history of \( \eta / \eta_f \). The value of the parameter \( \eta \) is evaluated here from eq. (42), so that

\[ \eta = \frac{\sqrt{3\sigma}}{g(\theta)(\sigma_m + c \cot \phi)} \quad (49) \]

while at failure, there is \( \eta = \eta_f \). Thus, the ratio \( \eta / \eta_f \in [0,1] \) is indicative of the extent of damage within the material.

It is evident from Figs.1-2 that if the wetting commences at low values of deviatoric stress intensities, i.e. \( \eta / \eta_f < 0.7 \), the stationary conditions are reached. At higher intensities, the degradation of strength properties upon wetting triggers a spontaneous failure of the sample.
Figure 1- Displacement history versus time

Figure 2- Value of $\eta/\eta_f$ versus time
4.3 Example # 2

The numerical analysis presented here, involves a slope in a cohesive soil (clay) subjected to a period of an intense rainfall. The slope examined in this study has dimensions typical of engineered slopes in Singapore; it is also representative of shallow slopes in the province of Manitoba (Canada) that underwent a translational failure in the late 1990’s. A major rainfall event of a prescribed intensity is considered. Note that the actual amount of rainfall that can infiltrate the ground at a given time ranges from zero to infiltration capacity, which depends on moisture content and porosity of the specific soil. Apparently, if the precipitation rate exceeds the infiltration rate, the runoff will usually occur. In the simulations presented here, no antecedent rainfall is applied prior to the major event.

The numerical analysis incorporates the transient coupled formulation for unsaturated flow, as described in Section 3. As indicated earlier, the primary purpose of employing this framework lies in its ability of tracing the evolution of the phreatic surface. In the simulations, the progress of the wetting front is monitored and the framework of chemo-plasticity (Section 2.1) is used to model the evolution of mechanical characteristics of clay. The overall stability of the slope is assessed by examining the time history of the parameter $\eta / \eta_f$, eq. (49), which defines the extent of damage.

The simulations were carried out assuming the following material parameters

$$E = 100 \text{MPa}; \quad \nu = 0.35; \quad \eta_f = 0.98; \quad \eta_c = 0.77; \quad c = 20 \text{kPa}; \quad A = 1.0 \times 10^{-5};$$

The kinetics of the chemical interaction and the degradation constants were selected as

$$G_1 = 10\%; \quad G_2 = 75\%; \quad G_3 = 10\%; \quad B = 460.5;$$

while the parameters governing the fluid flow were taken as

$$k = 0.864 \text{m/day}; \quad k_s \approx 1.0; \quad e = 1.0;$$

Note that while the choice of these parameters is somewhat arbitrary, their values are typical for lightly-overconsolidated clays. It needs to be emphasized that the example given here serves primarily as an illustration of the proposed methodology, so that the quantitative aspects are rather secondary.

The loading process incorporated two stages. The first one involved the solution due to own weight of the material, while the second one was the simulation of the infiltration process and its coupling with the mechanical response. Fig.3 shows the geometry of the problem and the boundary conditions corresponding to the first stage. The total height of the slope was taken as $H = 10 \text{m}$. The gravity load was applied incrementally in five layers, in order to reflect the construction sequence. The key results are shown in Figs.4-5. Fig.4 shows the distribution of $\eta / \eta_f$, while Fig.5 gives the corresponding distribution of equivalent plastic strains at the end of construction stage. Here, the maximum value of $\eta / \eta_f$ is 0.8 which clearly indicates that the slope is stable.
Fig. 6 presents the boundary conditions for the second stage of the analysis, i.e. infiltration process. In this phase, the slope is said to be exposed to a heavy rainfall (i.e., precipitation in excess of 0.75 cm per hour). Along the ground surface, the water pressure is assumed to increase linearly from an initial value of $-5kPa$, which corresponds to $S = 5\%$, to zero in a period of 4 hr and then is maintained constant. Such boundary conditions are analogous to those in ref.[20] and imply that the horizontal surfaces can absorb water at the rate which depends on the permeability, while the water cannot congregate along the slope. In addition, a negative pressure $u^0_w = -5kPa$ is applied at the bottom. This ensures that water can flow out of the domain which, in turn, implies that the groundwater level (which was initially far below the ground surface) cannot be affected by this rainfall.

The infiltration analysis was performed for a period of 30 days. Fig. 7 shows the distribution of the degree of saturation at the end of rainfall, while Fig. 8 presents the corresponding contours of $\eta / \eta_f$. It is evident now that, in a large area around the slope, there is $\eta / \eta_f \rightarrow 1$. The latter is indicative of a failure of the slope in this region.
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**Figure 6** - Geometry and boundary conditions in infiltration analysis followed by dry analysis

**Figure 7** - Saturation at the end of rainfall (30 days)

**Figure 8** - Value of $\eta / \eta_f$ at the end of rainfall (30 days)

**Figure 9** - Equivalent plastic strain at the end of rainfall (30 days)
5. FINAL REMARKS

In this paper, a methodology for modeling a coupled hydro-mechanical response of clayey soils has been presented. Within this framework, as long as the water phase is discontinuous, the material is treated as a single phase medium undergoing evolution of mechanical properties as a result of chemo-mechanical interactions. At this level of saturation, the approach does not require a specification of suction-saturation relationship as the suction pressure is said to be the product of interaction of a complex system of mineralogical and chemical factors.

A return-mapping algorithm has been developed for the proposed chemo-plasticity framework. In analyzing the problem of slope infiltration, the backward Euler scheme has been combined with subincrementation. This was primarily due to the fact that the chemical degradation is very fast and small increments are required in order to obtain an accurate solution for the local stress trajectories. This algorithm significantly improves the convergence of the global solution for unsaturated flow in porous media.

The governing equations for the fluid flow in unsaturated media have been derived here using a continuum framework that incorporates the notion of a deformable control volume. The final set of equations for the discretized system is the same as that obtained using a classical approach, viz. ref. [18].

The primary application given here involved a coupled hydro-mechanical analysis of a slope exposed to an intense rainfall. It was demonstrated that the water infiltration may trigger a loss of stability resulting from degradation of strength properties. The assessment of stability itself was based on examining the distribution of the ratio \( \eta / \eta_f \) that is indicative of the extent of damage. For quantitative purposes, such an assessment is rather restrictive and a more accurate representation is required. Therefore, the future work will focus on development and implementation of numerical procedures that account for modeling of localized failure. These will involve the use of Extended Finite Element Method [23] and/or the procedures incorporating the volume averaging in the neighborhood of the shear zone [24].
REFERENCES


Discrete modeling of cohesive crack propagation via an enhanced continuum approach

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SUMMARY

In this paper, a methodology for modeling of discrete crack propagation in brittle materials is outlined. Within the proposed approach, the discontinuity is explicitly embedded in the constitutive relation that governs the discontinuous motion within a representative elementary volume. This methodology, which was originally developed for smeared modeling of localized deformation, is enhanced here to deal with the discrete crack propagation problems. In particular, the approach is coupled with the level-set method in order to explicitly trace the crack path trajectory. In addition, a new implicit scheme is developed for accurately imposing the continuity condition along the interface. Some numerical examples are provided incorporating the proposed approach. The simulations include a simple tension test, a three-point bending test as well as a mixed mode cracking test in which a specimen is subjected to both shear and tension. It is demonstrated that the framework incorporating an enhanced constitutive relation with embedded discontinuity gives results that are very close to those obtained using Extended FEM, while the former requires significantly less computational effort. A comparison with a standard smeared approach is also provided in order to highlight the nature of the contribution.

KEYWORDS: discrete crack propagation, embedded discontinuity, extended FEM, constitutive modeling

1. INTRODUCTION

This study focuses on the development and implementation of a methodology for describing the discrete crack propagation within the context of a constitutive law with embedded discontinuity (CLED) that has been previously used for smeared modeling of localized deformation [1,2]. Here, a rigorous analytical derivation of the governing equations is provided first, which is based on averaging the discontinuous motion in the neighborhood of the macrocrack. The approach is then coupled with the Level-set method for capturing the trajectory of crack propagation and to enable an accurate assessment of the characteristic length parameter that appears in the formulation. An implicit integration scheme is developed for imposing the continuity condition along the interface and a simple, yet efficient algorithm is introduced for finding the direction of crack propagation. The framework is applied to numerical analysis of problems involving cohesive crack propagation and the results are compared with those obtained from Extended Finite Element simulations. A comparison of the proposed methodology with a standard smeared approach is also provided in order to highlight the nature of the contribution.

Modeling of damage initiation and propagation has been one the most intensely researched topics over the last few decades. The existing analytical solutions are restricted to an elastic material and involve simple

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geometries and boundary conditions. Therefore, they are not directly relevant to practical engineering problems. The latter require, in general, a numerical simulation that typically involves the use of the Finite Element Method (FEM). The early methodologies for capturing the progressive damage were based on tracing the crack propagation on the element boundaries [3]. In addition, some smeared techniques have also been proposed that incorporated plasticity-based strain-softening relations [4-6]. Later, in order to avoid remeshing in the context of FEM, mesh-free Galerkin method was introduced [7,8]. More recently, after introduction of the partition of unity approach [9], the Extended Finite Element Method (XFEM) has been developed [9], which enables incorporation of discontinuous displacement fields as well as the tip enrichments into the approximation space.

XFEM was initially formulated for mesh-independent modeling of tensile crack propagation [10,11]. The first extension of the original framework incorporated the crack tip enrichment and the contact condition [12,13]. Later, the framework was combined with the Level-set method for tracking the propagating crack in the solution domain [14]. Modeling of cohesive crack within XFEM framework was first introduced in ref.[15,16]. The XFEM was also used in the context of dynamic problems [17,18], localization problems [19,20], and modeling of multiphase media [21,22]. The primary difficulty in implementing XFEM is the need to deal with additional degrees of freedom. In particular, a special treatment for activating enriched DOFs is required that generally increases the computational effort compared with the standard FEM. The main advantage of this method is the ability to incorporate any asymptotic function in the discretized model.

Along with the development of the X-FEM procedures, a level-set method was introduced [14,23] for tracing the crack propagation path. The latter representation is particularly suitable for problems involving frictional interfaces (e.g., a shear band localization), however serious numerical complexities may arise in problems involving multiple-cracking/branching, which require the use of multiple level-sets. In order to overcome these problems, an efficient approximation was introduced in ref. [24], whereby instead of dealing with a continuous level-set, the crack growth was represented discretely by activation of crack surfaces at individual particles (or nodes), so that no explicit representation of the crack's topology was required. A similar approximation has also been employed within the mesh-free approach [25,26], where the crack has been represented as a set of adjacent particles (nodes). The above methodologies proved to be quite robust for static/dynamic problems involving multiple cohesive cracks; their efficiency, however, has not yet been verified for problems involving shear band localization.

In parallel with advances in finite element techniques, methodologies have also been developed to describe discontinuous/localized deformation by enhancing the standard phenomenological constitutive laws. The first such approach [1] advocated the use of volume averaging to estimate the properties of an initially homogeneous medium intercepted by a shear band/interface. The proposed constitutive relation incorporated the properties of constituents (viz. intact material and interface) as well as a characteristic dimension associated with the structural arrangement. This approach was later revised [27] and applied to a broad range of practical engineering problems (e.g., [28-30]). In addition, other continuum frameworks have been developed employing various regularizations techniques that included the use of micro-polar continua [31,32] non-local theories [33], as well as gradient-dependent formulations [34-36]. It needs to be mentioned that the latter approach was recently employed to eliminate stress/strain singularities at the crack tips ([37,38]). These results are of significance in the context of using tip enrichments within the XFEM. In general, all methodologies mentioned above are primarily intended for smeared modeling of evolution of damage in cohesive-frictional materials.

In this paper, the problem of cohesive crack propagation in a class of brittle materials, like concrete, is investigated. The main focus here is on the extension of the methodology employing a constitutive law with embedded discontinuity (CLED) to model the discrete nature of the process. This is achieved by enhancing this approach, which was formerly used in a ‘smeared’ sense, with the level-set approximation. The results presented here are compared with those obtained using XFEM approach. In addition, a comparison with the standard smeared approach is also provided. In section 2.1, the analytical representation of a discontinuous motion is reviewed, along with the space discretization employed in XFEM. The approach incorporating a constitutive model with embedded discontinuity is presented in section 2.2., followed by
the formulation of an implicit integration scheme for imposing the continuity condition along the interface. In section 3, the constitutive model for the interfacial material is described and the strategy for modeling the crack propagation is outlined. In the subsequent section, the field equations of the problem are briefly reviewed, for completeness. In section 5, a number of numerical examples are provided that involve simulations of a simple extension test, a three-point bending test as well as a mixed mode cracking test in which a specimen is subjected to both shear and tension. It is demonstrated that both frameworks, i.e. XFEM and FEM incorporating an enhanced constitutive law with embedded discontinuity (CLED), yield virtually identical response, thus giving advantage to the latter one as it does not require the incorporation of any additional degrees of freedom. The conclusions emerging from this study are presented in section 6. All simulations conducted here are based on FEM/CLED and XFEM programs that are developed by authors.

## 2. DESCRIPTION OF A DISCONTINUOUS MOTION

A discontinuous motion \( \mathbf{v}(x,t) \) in the domain \( \Omega \) that contains a discontinuity surface \( \Gamma_d \) can be defined as [39]

\[
\mathbf{v}(x,t) = \hat{\mathbf{v}}(x,t) + \mathcal{H}_{\Gamma_d} \mathbf{\bar{v}}(x,t)
\]

where, \( \hat{\mathbf{v}}(x,t) \) and \( \mathbf{\bar{v}}(x,t) \) are continuous functions in the solution domain \( \Omega \) and \( \mathcal{H}_{\Gamma_d} = \mathcal{H}(\phi) \) is the Heaviside step function that can be expressed in its symmetric form as

\[
\mathcal{H}(\phi) = 2\int_{-\infty}^{\phi} \delta(\varphi) d\varphi - 1 = \begin{cases} +1 & \phi > 0 \\ -1 & \phi \leq 0 \end{cases}
\]

Here, \( \phi = \phi(x) \) is the signed distance from the discontinuity interface \( \Gamma_d \), and \( \delta(\varphi) \) is the Dirac delta function which is defined as being singular at \( \phi = 0 \) and equal to zero elsewhere. Denoting a jump of a function on the discontinuity interface by \( [\bullet] = \bullet^+ - \bullet^- \), the rate of separation between the opposite crack faces, i.e. \( \dot{g} \), can be defined as

\[
\dot{g} = [\dot{\mathbf{v}}] = \left( \dot{\hat{\mathbf{v}}} + \mathcal{H}_{\Gamma_d} \dot{\mathbf{\bar{v}}} \right)^+ - \left( \dot{\hat{\mathbf{v}}} + \mathcal{H}_{\Gamma_d} \dot{\mathbf{\bar{v}}} \right)^- = \dot{h} \mathbf{\bar{v}}
\]

where \( \dot{h} = [\mathcal{H}] = \mathcal{H}^+ - \mathcal{H}^- \)

where, based on the representation (2), the jump in the step function is \( \dot{h} = 2 \). Considering that \( \nabla \mathcal{H}(\phi) = \mathcal{H}' \nabla \phi \) and \( \mathcal{H}'(\phi) = \dot{h} \delta(\phi) = \dot{h} \delta_{\Gamma_d} \), the velocity gradient of the discontinuous motion (1) can be expressed as

\[
\nabla^s \mathbf{v} = \nabla^s \dot{\bar{v}} + \mathcal{H}_{\Gamma_d} \nabla^s \dot{\mathbf{\bar{v}}} + \delta_{\Gamma_d} (\dot{h} \nabla \phi \otimes \mathbf{n})^s
\]

where \( \mathbf{n} = \nabla \phi \) is the normal to the interface, and the superscript \( s \) refers to the symmetric part of the gradient operator.

### 2.1. Space discretization for XFEM strategy

Within the XFEM strategy, a discontinuous field can be incorporated into the approximation space by introducing enrichment functions and additional degrees of freedoms. Thus, the discontinuous motion (1) can be approximated by

\[
\mathbf{v}^h(x,t) = \hat{\mathbf{v}}^h(x,t) + \mathcal{H}_{\Gamma_d} \mathbf{\bar{v}}^h(x,t) = \hat{\mathbf{N}}(x) \dot{\mathbf{d}}(t) + \mathcal{H}_{\Gamma_d} \tilde{\mathbf{N}}(x) \dot{\mathbf{d}}(t) = \mathbf{N}(x) \dot{\mathbf{d}}(t)
\]

where, \( \hat{\mathbf{N}}(x) \) and \( \tilde{\mathbf{N}}(x) \) are the enrichment functions.
where, \( \hat{N} \) and \( \tilde{N} \) are standard finite element shape functions that may have different orders of approximation \([40]\) and \( \hat{d} \) and \( \tilde{d} \) are standard and enriched degrees of freedom, respectively. In order to achieve a better representation of the enriched approximation and to avoid the use of blending elements, the shifted form of approximation \((5)\) can be employed \([40]\), viz.

\[
v^h(x, t) = \hat{N}(x) \dot{d}(t) + \tilde{N}(x) \Psi(x) \dot{d}(t) = N(x) \dot{d}(t)
\]

Here, \( \Psi(x) \) is the shifted form of the step function defined as

\[
\Psi(x) = \begin{bmatrix}
\mathcal{H}(\phi) - \mathcal{H}(\phi_1) & 0 & \ldots & 0 \\
0 & \mathcal{H}(\phi) - \mathcal{H}(\phi_2) & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & \mathcal{H}(\phi) - \mathcal{H}(\phi_n)
\end{bmatrix}
\]

and \( n \) is the number of interpolation functions. Note that since \( \mathcal{H}^+ - \mathcal{H}^- = I \), where \( I \) is the identity matrix, the crack opening \( g^h(x, t) \) can be expressed as

\[
g^h(x, t) = \left[ \hat{N}(x) \right] \dot{d}(t) + \left[ \tilde{N}(x) \Psi(x) \right] \dot{d}(t) = h \tilde{N}(x) \dot{d}(t)
\]

### 2.2. The approach incorporating a constitutive law with embedded discontinuity (CLED)

Averaging the velocity gradient \((4)\) over a Representative Elementary Volume (REV), which includes the discontinuity interface, one obtains

\[
\frac{1}{\Delta v} \int_{\Delta v} \nabla^s v \, dv = \frac{1}{\Delta v} \left( \int_{\Delta v} \nabla^s \hat{v} \, dv + \int_{\Delta v} \mathcal{H}_{rs} \nabla^s \tilde{v} \, dv + \int_{\Delta v} \delta_{rs} \left( h \tilde{v} \circ n \right)^s \, dv \right)
\]

\[
= \frac{1}{\Delta v} \left( \int_{\Delta v} \nabla^s \hat{v} \, dv + \int_{\Delta v} \mathcal{H}_{rs} \nabla^s \tilde{v} \, dv + \int_{\Delta a} \left( h \tilde{v} \circ n \right)^s \, da \right)
\]

where, \( \Delta v \) is the volume of REV and \( \Delta a \) is the area of the discontinuity inside the REV. Assuming that the variations of the integrands in \((9)\) are small, one has

\[
\nabla^s v = \nabla^s \hat{v} + \frac{\Delta v^+ - \Delta v^-}{\Delta v} \nabla^s \tilde{v} + \frac{\Delta a}{\Delta v} \left( h \tilde{v} \circ n \right)^s
\]

Defining now \( \chi = \Delta a / \Delta v \) and \( \kappa = (\Delta v^+ - \Delta v^-) / (h \Delta v) \), and using \( \dot{g} = h \tilde{v} \) one obtains

\[
\dot{\varepsilon} = \nabla^s \varepsilon
\]

\[
\dot{\varepsilon} = \dot{\varepsilon} + \ddot{\varepsilon} \quad \text{where} \quad \dot{\varepsilon} = \nabla^s (\hat{v} + \kappa \dot{g})
\]

\[
\ddot{\varepsilon} = \chi \left( \dot{g} \circ n \right)^s
\]

In eq. \((11)\), \( \dot{\varepsilon} \) represents the deformation in the intact material while \( \ddot{\varepsilon} \) is the strain rate due to discontinuous motion along the interface averaged over REV. In general, \( \ddot{\varepsilon} \) may include both elastic and plastic deformations in the intact material. Note that the representation \((11)\) may be simplified by assuming that the discontinuity divides the element into two approximately equal volumes, in which case \( \kappa \) approaches zero, i.e. \( \kappa \rightarrow 0 \).
Using now the additivity postulate and following the standard plasticity procedure, the stress rate in the intact material $\mathbf{\sigma}_I$ can be defined as,

$$
\dot{\mathbf{\sigma}}_I = \mathbb{D} : \mathbf{\ddot{e}} = \mathbb{D} : (\mathbf{\dot{e}} - \mathbf{\ddot{e}})
$$

(12)

where $\mathbb{D}$ is the fourth order stiffness operator. The traction vector across the interface must remain continuous, i.e. $\mathbf{n} \cdot \mathbf{\sigma}_I = \mathbf{n} \cdot \mathbf{\sigma}_r$. Thus, imposing this constraint and writing the constitutive relation for the interfacial material in the rate form as $\mathbf{\dot{\sigma}}_r \cdot \mathbf{n} = \mathbf{1} = \mathbf{K} \cdot \mathbf{\dot{g}}$, one obtains,

$$
\mathbf{n} \cdot \mathbb{D} : \mathbf{\ddot{e}} = \mathbf{K} \cdot \mathbf{\dot{g}} \quad \text{where} \quad \mathbf{K} = \mathbf{R} \cdot \mathbf{K}^* \cdot \mathbf{R}^T
$$

(13)

In equation (13), $\mathbf{K}$ is the tangential stiffness operator for the interfacial material in the global coordinate system while $\mathbf{K}^*$ defines the same operator related to the local coordinate system along the interface. Using eq. (13), together with eq. (11) and eq. (12), one obtains

$$
\mathbf{\dot{\sigma}}_I = \mathbb{D}_r : \mathbf{\dot{e}} \quad \text{where} \quad \mathbb{D}_r = \mathbb{D} - \mathbb{E} : \mathbb{D}
$$

(15)

Note that using matrix notation, relations (11), (14) and (15) can be expressed as

$$
\{\mathbf{\dot{e}}\} = \{\mathbf{\ddot{e}}\} + \{\mathbf{\dot{e}}\} \quad \text{where} \quad \{\mathbf{\ddot{e}}\} = \mathbf{L} \{\mathbf{v}\}
$$

$$
\{\mathbf{\dot{e}}\} = \mathbf{\chi} \{\mathbf{n}\} \{\mathbf{\dot{g}}\}
$$

$$
\{\mathbf{\dot{e}}\} = \mathbf{[E] [D]} \{\mathbf{\ddot{e}}\} \quad \text{where} \quad \mathbf{[E]} = \mathbf{\chi} \{\mathbf{n}\} \mathbf{[-K]}^{-1}\{\mathbf{n}\}^T
$$

$$
\mathbf{[-K]} = \mathbf{[K]} + \mathbf{\chi} \{\mathbf{n}\}^T \mathbf{[D]} \{\mathbf{n}\}
$$

(16)

$$
\{\mathbf{\dot{\sigma}}_I\} = \mathbb{D}_r \{\mathbf{\dot{e}}\} \quad \text{where} \quad \mathbb{D}_r = \mathbb{D} - \mathbb{E} : \mathbb{D}
$$

(17)

where, $\{\mathbf{\nabla} \mathbf{\cdot} \} = \mathbf{L} \{\mathbf{\bullet}\}$ and

$$
\{\mathbf{n}\} = \begin{bmatrix}
n_1 & 0 & 0 \\
0 & n_2 & 0 \\
0 & 0 & n_3 \\
n_2 & n_1 & 0 \\
n_3 & 0 & n_1 \\
0 & n_3 & n_2
\end{bmatrix}; \quad \{\mathbf{L}\} = \begin{bmatrix}
\frac{\partial}{\partial x} & 0 & 0 \\
0 & \frac{\partial}{\partial y} & 0 \\
0 & 0 & \frac{\partial}{\partial z}
\end{bmatrix}
$$

The above defined relations are identical to those given in refs.[27], while the starting point in this representation is the analytical expression for the discontinuous motion (1).

Examining the formulation of the problem, it can be seen that the primary difference between the XFEM and the CLED approach is the way in which the discontinuity is perceived. In XFEM, the discontinuity is defined using an enriched approximation space that includes the discontinuous motion, while in
FEM/CLED, it is defined as an internal variable embedded within a plasticity based approach through a volume averaging. Thus, no enrichments and/or additional DOFs are required, so that it can be easily implemented as a user-defined material subroutine within any commercial FEM package.

2.3. Implicit integration of the constitutive relation

In order to calculate the increment $\Delta g$, the continuity condition $n \cdot \sigma = t$ must be imposed. For this purpose, an implicit scheme is developed here. Based on eq.(12), the state of stress at $t + \Delta t$ can be expressed as

$$\sigma = \sigma' + \mathbb{D} : \Delta \varepsilon - \mathbb{D} : \Delta \tilde{\varepsilon} \quad \text{where} \quad \Delta \tilde{\varepsilon} = \chi (\Delta g \otimes n)$$

(18)

Note that if the intact material is assumed to be elastic, which is the case here, the primary unknown in the expression (18) is $\Delta g$. This implies that for a prescribed motion along the interface, the stress state is known. Thus, the discontinuous motion along the interface can be defined by imposing the continuity condition. The latter can be expressed in the residual form as

$$r^k = n \cdot \sigma^k_n - t^k$$

(19)

Using a standard Newton-Raphson method, one can write

$$r^{k+1} \approx r^k + \frac{\partial r^k}{\partial g} \cdot \delta g^k = 0 \quad \Rightarrow \quad \delta g^{k+1} = -\left(\frac{\partial r^k}{\partial g}\right)^{-1} \cdot r^k$$

(20)

where

$$\frac{\partial r^k}{\partial g} = n \cdot \frac{\partial \sigma^k_n}{\partial g} - \frac{\partial t^k}{\partial g} = -\left(\chi n \cdot \mathbb{D} \cdot n + K^k\right)$$

(21)

Thus, the stress correction can be expressed as

$$\delta \sigma^k_n = \chi : \mathbb{D} (\delta g^k \otimes n) = -\mathbb{D} : \delta \tilde{\varepsilon}$$

(22)

while the key variables can be updated as

$$\Delta g^{k+1} = \Delta g^k + \delta g^{k+1}$$

$$\Delta \tilde{\varepsilon}^{k+1} = \Delta \tilde{\varepsilon}^k + \delta \tilde{\varepsilon}^{k+1}$$

(23)

$$\Delta \sigma^{k+1}_n = \Delta \sigma^k_n + \delta \sigma^{k+1}_n$$

Finally, using the stress increment $\Delta \sigma = \mathbb{D} : (\Delta \varepsilon - \Delta \tilde{\varepsilon})$ and imposing the continuity condition in its incremental form, i.e. $n \cdot \Delta \sigma = \Delta t$, the tangential stiffness operator can be defined as

$$\Delta \sigma = \mathbb{D}_T : \Delta \varepsilon \quad \text{where} \quad \mathbb{D}_T = \mathbb{D} - \mathbb{D} : \mathbb{E} : \mathbb{D}$$

(24)

which completes the implicit integration scheme for the considered constitutive relation.
3. DESCRIPTION OF INTERFACIAL MATERIAL AND THE CRACK PROPAGATION PROCESS

For the crack initiation, the simple maximum tensile stress criterion is used and the subsequent behavior is described using the framework of strain-softening. The propagating crack is traced by the Level-set method for both XFEM and FEM/CLED techniques.

3.1. Constitutive model for the cohesive zone

In order to describe the mechanical characteristics of the interfacial material, a simple damage model, similar to that proposed in ref.[15], is employed. Within this framework, an exponential relation for the evolution of cohesive forces acting on the crack faces is assumed, i.e.

\[ F_i(g_n) = \begin{cases} 
F_i & g_n \leq \delta_c \\
F_i e^{-\frac{E_i (g_n - \delta_c)}{G_f}} & g_n > \delta_c
\end{cases} \]  \hspace{1cm} (25)

where, \( \delta_c \) is the critical separation for imposing the contact condition in a penalty approach, \( F_i \) is the initial tensile strength of the material, and \( F_i(g_n) \) is the tensile strength at separation \( g_n \). The failure criterion is written as

\[ f(t_n, g_n) = t_n - F_i(g_n) \]  \hspace{1cm} (26)

During an active loading process, there is \( f(t_n, g_n) = 0 \), so that the normal traction \( t_n \) can be expressed as

\[ t_n = F_i \exp\left(-\frac{E_i}{G_f}(g_n - \delta_c)\right) \]  \hspace{1cm} (27)

The shear traction \( t_i \) can be defined in terms of discontinuity in the tangential component of displacement \( g_i \),

\[ t_i = d K_i g_i = \frac{F_i}{F_i} K_i g_i \]  \hspace{1cm} (28)

where \( d = F_i / F_i \) is the damage parameter and \( K_i \) is the shear stiffness of the interfacial material. Referring the problem to the local coordinate system along the crack, the incremental form of eqs. (27) and (28) can be expressed as

\[ \dot{i}_n = k_{11} \ddot{g}_n + \left\{-\frac{E_i}{G_f} \exp\left(-\frac{E_i}{G_f}(g_n - \delta_c)\right)\right\} \dot{g}_n \]

\[ \dot{i}_i = k_{12} \ddot{g}_n + \left\{-\frac{E_i}{G_f} \exp\left(-\frac{E_i}{G_f}(g_n - \delta_c)\right) K_i g_i \right\} \dot{g}_n + \{d K_i\} \dot{g}_i, \quad i = 1, 2 \]  \hspace{1cm} (29)

where the indexes 1, 2 define the in-plane orientations. Thus, the constitutive relation for the interfacial material can be expressed in the rate form,
\[
t' = K^* \cdot \mathbf{g}^* \quad \text{where} \quad K^* = \begin{bmatrix} k_{11} & 0 & 0 \\ k_{21} & k_{22} & 0 \\ k_{31} & 0 & k_{33} \end{bmatrix}
\]

where \( K^* \) is the tangential stiffness operator.

3.2. The strategy for tracing the crack propagation within XFEM and FEM/CLED

As shown in several previous studies [14,23], the geometry of crack propagation can be traced by the level-set method that is introduced within XFEM. Based on this approach, a moving/propagating interface \( \Gamma_d(t) \) can be defined as the zero level set of a function \( \phi(x,t) \), i.e., \( \Gamma_d(t) = \{ x | \phi(x,t) = 0 \} \). The function \( \phi(x) \) itself can be expressed as the signed distance function

\[
\phi(x) = \text{sign}(n_r \cdot (x - x_r)) \min \|x - x_r\|
\]

where \( n_r \) is a normal to the direction of propagation, \( x \) is an arbitrary point in \( \Omega \), and \( x_r \) is the point located on the interface at the minimum distance from \( x \).

For two dimensional XFEM simulations, as performed in this study, the interface is defined as a polygon of line segments passing through elements in which a crack has formed. Hence, for a node that is common for two adjacent enriched elements, the level set function can be defined as the minimum distance from this node to the respective line segments associated with these elements. For each element, the values of the level-set function at Gauss points can be determined from nodal values using FEM interpolation functions, i.e. \( \phi = \sum N_j \phi_j \).

In the case of FEM/CLED, i.e. the framework incorporating a constitutive law with embedded discontinuity, the same approach is used for tracing the propagating crack. Thus, by analogy to XFEM, the crack is introduced at the element level and the characteristic dimension \( \chi \) is evaluated based on the volume of the element and the geometry of the propagating crack. Consequently, at all Gauss points associated with this element the constitutive relation employing the volume averaging is used. Given the similarity of this procedure to the general methodology for tracing the interface adopted in XFEM, the results obtained from these two approaches are very similar. Also, the strain-softening response is numerically very stable.

(i) Determination of the direction of propagation

The problems involving the crack propagation in brittle materials are typically dealt with using the framework of fracture mechanics. The approach involves evaluation of an integral, known as J-integral, which is a measure of the rate of fracture energy. For a linearly elastic material, the J-integral is in fact the strain energy release rate and it can be related to the stress intensity factors [41] which, in turn, can be used for specifying the direction of crack propagation. In this case, the assessment of the crack orientation involves the stress state in the neighborhood of the crack tip and, as a result, an accurate/smooth crack path can be captured. However, the main limitation of this approach is that the relation between the direction of propagation/J-integral and the stress intensity factors is valid only for an elastic material subjected to tension. Thus, for inelastic materials and/or in the compressive stress regime, this approach is not applicable.

A more general strategy, which is employed here, is to define the onset of cracking as well as the direction of propagation based on a failure criterion that is embedded in the constitutive relation. For failure in the tensile regime, for example, the orientation of crack is commonly assumed to be orthogonal to the
direction of the major principal stress and the onset of cracking is defined based on the critical value of this stress component. This critical value is defined as \( \zeta = \sigma_{ij} / F_i \), so that for \( \zeta \to 1 \) the interface (crack) is assumed to be formed. The main problem associated within this strategy is that the stress state at the crack tip is not, in general, as accurate as required. Although this may not affect the global accuracy of the solution, it can be important in terms of predicting the crack paths propagation. A simple enhancement that can make this criterion more accurate is to adopt a procedure that is conceptually similar to that employed in assessment of the J-integral. Thus, the crack orientation can be established at each integration point in a region around the tip element and then averaged to assess the actual direction of propagation. This procedure can be used for modeling of damage in both tensile and compressive regime; it can also be used for evaluating the onset of cracking. As shown later in the numerical examples given, such a strategy results in a smooth pattern of the crack propagation, similar to the one obtained based on the J-Integral calculations. Fig. 1 illustrates the algorithm employed for these simulations. Here, the candidate elements are the same as those embedded within the contour of the J-integral, except the ones in which the crack has already formed. At the same time, the candidate integration points are the ones for which \( \zeta = \sigma_{ij} / F_i \to 1 \). The computational procedure is briefly summarized in Table 1.

![Fig.1 Strategy for tracing the crack propagation used within XFEM and FEM/CLED](image)

**Table 1. The flow chart for analysis and identification of cracked elements**

1. **Apply the load increment**
2. **Form the stiffness and internal load operators and solve the nonlinear system**
   - For intact elements, the constitutive relation describing the homogeneous deformation mode is used at each Gauss point. For cracked elements, the XFEM or CLED approach is employed
3. **Check the failure criterion and form the new cracked elements**
   a. **Find the average value of** \( \zeta = \sigma_{ij} / F_i \) **for tip and standard elements**
   b. **Define the new elements that must be enriched**
   c. **For the crack, update the level-set or define new level-set**
(ii) On computational effort associated with both methodologies

In standard FEM packages, all data structures (i.e. number of DOFs, nodal connectivity, etc.) are allocated prior to the analysis. However, for the crack propagation problems remeshing is required and, as a result, the size of the data structures is progressively changing. In addition, the transfer of data is required form the old mesh to the new one, which significantly impacts the efficiency of this approach.

For the XFEM simulations, the mesh remains fixed and the data transfer is not required; however, the total number of DOFs is changing as the crack propagates. Thus, within this approach the size of the problem is progressively increasing. Perhaps the simplest strategy to resolve this issue is to introduce the required enrichments at all nodes or just within an estimated domain where the crack may potentially propagate. Such a scheme will ensure that the size of data structures remains constant during the crack propagation. At the same time, however, the total number of equations and the size of required data structures are likely to be significantly larger than those for the same mesh without enrichment. This will increase the computational effort significantly as compared to standard FEM.

Another problem that will impact the computational cost of the XFEM, is the modified integration scheme associated with the enriched elements and one time data transfer that is required at the transition stage. The best scheme that results in an accurate integration within these elements is the triangulation technique that divides the element into two different regions, one with $\phi < 0$ and the other with $\phi > 0$. Thus, the shape functions are continuous in both these domains and the standard Gauss quadrature can be used for the integration process. The modified scheme will increase the computational effort, as more integration points are involved; however, in most cases the number of enriched elements is much less than total number of elements, so that the impact is not overly significant.

In the XFEM code developed for the purpose of this study, the following strategies are used. First, additional enriched DOFs are assigned a priori to nodes that are located in the region where the crack is likely to form. Second, all these additional DOFs are treated as boundary conditions at the stage when they are not yet activated. This is done by setting all terms associated with these DOFs to zero in the stiffness matrix and in the force vector. Third, the routine that is used for solving the global system of equations is modified so that the zero rows/columns can be removed from the global system. These remedies help to improve the numerical efficiency; however the computational effort is still significantly higher than that associated with the standard FEM.

It should be stressed that for the FEM incorporating the constitutive model with embedded discontinuity, none of above mentioned difficulties arise. The data structures and the solution strategy are the same as those for standard FEM and a continuous body. The discontinuity is taken into account at the level of constitutive relation. There are no additional DOFs involved and no special integration scheme is required. Thus, the main advantage of FEM/CLED over the XFEM is that the former maintains the efficiency of the standard FEM, while, the initiation/propagation routine is the same for both methodologies. As demonstrated through the simulations provided in section 5, the results based on both these frameworks are very close.

4. THE GOVERNING EQUATIONS OF THE PROBLEM

Consider a body $\Omega$ that includes a discontinuity surface $\Gamma_d$. The body is subjected to the traction $\mathbf{t}$ on $\Gamma_t$, velocity $\mathbf{v}$ on $\Gamma_v$, and the gravity force $\rho \mathbf{g}$ on $\Omega$, as shown in Fig.2. Along the discontinuity surface $\Gamma_d$, the interfacial forces are present within the part $\Gamma_I$. 
Fig. 2 A schematic representation of the boundary value problem

The equations of equilibrium can be written as

$$\nabla \cdot \sigma + \rho \mathbf{b} = 0$$  \hspace{1cm} (32)

and are subjected to the following boundary conditions

$$\mathbf{v} = \mathbf{v} \quad \text{on} \quad \Gamma = \Gamma_v$$
$$\mathbf{n} \cdot \sigma = \mathbf{t} \quad \text{on} \quad \Gamma = \Gamma_t$$
$$\mathbf{n} \cdot \sigma = \mathbf{t} \quad \text{on} \quad \Gamma = \Gamma_t$$
$$\mathbf{n} \cdot \sigma = \mathbf{0} \quad \text{on} \quad \Gamma = \Gamma_d$$ \hspace{1cm} (33)

where \( \mathbf{n} \) is a unit vector normal to \( \Gamma_\alpha \) with \( \alpha = (t, I, d) \).

In order to formulate the weak form of eq. (32) satisfying the boundary conditions (33), the integral of the inner product of the test function \( \mathbf{w} \) and the equilibrium function (32) must vanish over the solution domain \( \Omega \), i.e.

$$\int_\Omega \mathbf{w} \cdot (\nabla \cdot \sigma + \rho \mathbf{b}) \, d\Omega = 0$$  \hspace{1cm} (34)

Based on the minimum continuity condition for the trial and test functions \( \mathbf{v} \) and \( \mathbf{w} \), and also the kinematic boundary conditions, both these functions must lie in \( \mathcal{U} \) and \( \mathcal{V} \) spaces, known as kinematically admissible trial and test spaces, i.e.

$$\mathbf{v} \in \mathcal{U}, \quad \mathcal{U} = \left\{ \mathbf{v} \left| \mathbf{v} \in C^0, \quad \mathbf{v} = \mathbf{v} \quad \text{on} \quad \Gamma = \Gamma_v \right. \right\}$$
$$\mathbf{w} \in \mathcal{V}, \quad \mathcal{V} = \left\{ \mathbf{w} \left| \mathbf{w} \in C^0, \quad \mathbf{w} = \mathbf{0} \quad \text{on} \quad \Gamma = \Gamma_v \right. \right\}$$ \hspace{1cm} (35)

Expanding eq. (34) using the discontinuous divergence theorem (see eq. (39) in Appendix) and imposing the boundary conditions (33), one obtains

$$a) \quad \int_\Omega \nabla \mathbf{w}^h : \sigma (\mathbf{v}^h) \, d\Omega = \int_{\Gamma_1} \mathbf{w}^h \cdot \mathbf{t} \, d\Gamma + \int_{\Omega} \mathbf{w}^h \cdot \rho \mathbf{b} \, d\Omega$$
$$b) \quad \int_\Omega \nabla \mathbf{w}^h : \sigma (\mathbf{v}^h) \, d\Omega + \int_{\Gamma_1} \| \mathbf{w}^h \| \cdot \mathbf{t} \, d\Gamma = \int_{\Gamma_1} \mathbf{w}^h \cdot \mathbf{t} \, d\Gamma + \int_{\Omega} \mathbf{w}^h \cdot \rho \mathbf{b} \, d\Omega$$ \hspace{1cm} (36)

Here, the first equation (36a) is the weak form that is used in FEM/CLED approach while the second one, eq. (36b), applies to the case that the domain is discontinuous, i.e. for XFEM. The discretized form and an
implicit solution method for equations (36) are discussed in the Appendix. This completes the formulation of the problem that is employed in the numerical simulations provided in following section.

5. NUMERICAL SIMULATIONS

In this section, some numerical examples are provided that are solved using the two different methodologies, i.e. XFEM and FEM incorporating a constitutive law with embedded discontinuity. As explained earlier, in both cases, the Level-set method is used for tracing the crack propagation. The first problem involves a direct tension test. The second simulation presented here is the three-point bending test; the problem has the geometry analogous to that employed in ref. [16]. The third problem is based on an experimental study performed by Nooru-Mohamed, as described in ref. [42], and involves a sample subjected to a combination of shear and tension. All simulations are carried out under two-dimensional plane-strain conditions.

5.1. Simple tension test

The first simple illustrative example involves a direct tension test conducted on a plate with dimensions of $100 \times 100 \times 50$ (in mm), discretized into 9 quadrilateral elements ($3 \times 3$). The plate is fixed in the horizontal direction along the left edge and in the vertical direction from the left-bottom corner. A horizontal displacement is applied along the right boundary, see Fig.3. Mechanical properties of the material are assumed as follows,

$$ E = 29 \times 10^3 \text{ MPa}; \quad v = 0.25; \quad F_t = 3.0 \text{ MPa}; \quad G_f = 0.1 \text{ N/mm}; \quad \delta_c = 0.001 \text{ mm} $$

where, $E$ is the elasticity modulus, $v$ is the Poisson’s ratio, $F_t$ is the tensile strength, $G_f$ is the fracture energy appearing in the cohesive law, eq. (25), and $\delta_c$ is the critical displacement at the onset of cracking. Note that for the given boundary conditions, the stress state is uniform, while the crack is assumed to form in the middle of the sample, in the direction normal to the imposed displacement.

![Fig. 3 Direct tension test](image1)

![Fig. 4 Load-displacement response of the structure](image2)

The load-deflection response using both XFEM and FEM/CLED techniques is plotted in Fig.4. It is evident from this figure that the result corresponding to both methodologies are the same.

5.2. Three point bending problem

The second example given here involves a simply supported concrete beam subjected to an increasing vertical displacement applied in the middle of the span, Fig.5. The geometry is taken from the ref.[16]. The
beam has dimensions $l = 600\, \text{mm}$ and $b = t = 150\, \text{mm}$, where $t$ is the out of plane thickness, and the material properties are as follows

$$E = 36.5 \times 10^3\, \text{MPa};\quad v = 0.1;\quad F_t = 3.19\, \text{MPa};\quad G_f = 0.05\, \text{N/mm};\quad \delta_c = 1 \times 10^{-4}\, \text{mm}$$

The key results of the analysis are presented in Figs.6-8. Figs.6 shows the damage pattern. The failure process involves development of tensile cracks near the middle of the span and subsequent propagation of a dominant vertical crack in the center of the beam. These results are now compared in Fig.7 with the solution using the original smeared cracking approach, i.e. CLED without the enhancement for discrete representation of crack path. The load-displacement ($\delta$) response is shown in Fig.8. The behaviour becomes unstable after reaching the peak (see the figure on the left-hand side). It is evident that the solution based on the enhanced FEM/CLED is virtually identical to that obtained using XFEM methodology, while there is a markable difference in the results of CLED approach corresponding to discrete and smeared cracking.
5.3. Nooru-Mohamed mixed mode cracking test

The third problem that is studied here is based on the experimental test performed by Nooru-Mohamed [42] and involves a mixed mode cracking. The geometry of the problem is shown in Fig. 9. The specimen has the dimensions of $l = b = 200$ mm, $c = 25$ mm, and out of plane thickness $t = 50$ mm. Material properties, are as reported in [42], i.e.

$$E = 29 \times 10^3 \text{ MPa}; \quad \nu = 0.15; \quad F_i = 3.67 \text{ MPa}; \quad G_f = 0.05 \text{ N/mm}; \quad \delta_c = 1 \times 10^{-3} \text{ mm}$$

The loading process consists of two different stages. First, a horizontal displacement of $\delta_x = 0.005$ mm is applied along the vertical faces under $\delta_y = 0$. At this stage, referred to as the shearing stage, no cracks are formed. Then, a vertical displacement $\delta_y$ is imposed along the horizontal faces, while the $\delta_x$ remains constant. This stage results in onset and propagation of tensile cracks. The response of the structure is shown Figs. 10-13.

Fig. 10 shows the cracking pattern superimposed on the contours of horizontal and vertical displacements, while Fig. 11 gives a similar representation in terms of displacement vectors. In this case, two macrocracks form, at the notches, and propagate towards the center of the specimen. The fracture
pattern is consistent with the experimental evidence [42] and it’s identical for both XFEM and FEM/CLED approaches.

Figs 12-13 present the evolution of the components of the reaction force against imposed boundary displacements as well as the crack tip opening. Again, as the vertical displacement is imposed, the response becomes unstable. The global characteristics are very similar for both methodologies, i.e. XFEM and FEM/CLED. This is particularly evident both prior to as well as at the early stages of the onset of global instability, which is of primary interest for practical engineering purposes. At very advanced stages of deformation, the enhanced volume averaging method predicts less crack opening than the XFEM.

Fig. 9 Mixed mode cracking test (\( l = b = 200 \& c = 25 \text{ mm} \))

Fig.10 Cracking pattern superimposed on the contours of horizontal (u) and vertical (v) displacements (mm)
Fig. 11 Left: Cracking pattern and the displacement vector plotted on the deformed shape (scale factor=100); Right: Experimental results [42]

Fig. 12 Reaction components (RX and RY) vs. vertical displacement (DY)

Fig. 13 Reaction force vs. CMOD (crack mouth opening displacement)
CONCLUDING REMARKS

In this work, the problem of cohesive crack propagation has been addressed using two conceptually different methodologies. The main approach involved incorporation of a constitutive law with embedded discontinuity. Such a methodology is conceptually similar to that introduced earlier for smeared modeling of strain localization. Here, an enhancement to this approach has been proposed that allows for modeling of the discrete nature of crack propagation.

A smeared representation of damage results, in general, in a less accurate assessment of the ultimate load of the structure. Furthermore, the crack is said to form at each Gauss point and, as a result, it may propagate within the equilibrium iterations. The latter leads to numerical instabilities developing near the peak load, which present difficulties in advancing the analysis past this stage. Nevertheless, the simplicity of this framework makes it still very attractive in terms of application to practical engineering problems.

The main focus in this study is on incorporation of discrete representation of crack within the CLED methodology. For this purpose, the level-set method has been implemented to trace the topology of damage. The latter is defined at the level of an element, which improves the numerical stability and allows advancing the analysis into the range of the globally unstable (softening) response without major convergence issues. The original CLED approach has been also enhanced by developing an implicit scheme for imposing the continuity condition along the interface.

The second methodology employed here, which has been primarily used as a verification tool for the CLED simulations, was the Extended Finite Element method. Within this framework, the approximation space is enhanced by incorporating a discontinuous displacement field. The methodology is attractive, but computationally more costly compared to standard FEM. The primary advantage of the XFEM is its ability to incorporate any type of enrichment into the discretized system based on the analytical solution of the problem, while the major gain from CLED is the computational efficiency and simplicity of implementation, which are both important in the context of practical engineering applications.

In order to properly compare these two approaches, a series of numerical simulations have been conducted. Those included a direct tension test, a three point bending test and a numerical analysis of the Nooru-Mohamed mixed mode cracking test. It was demonstrated that the discrete representation of CLED yields very similar results to the ones obtained from XFEM in terms of the evolution of damage propagation and the assessment of the ultimate load. At the same time, as mentioned earlier, the approach based on standard FEM incorporating a constitutive model with embedded discontinuity (FEM/CLED) is numerically more efficient than XFEM approach as it does not require any additional DOF.

REFERENCES


APPENDIX

(i) Discontinuous divergence theorem

Consider a body $\Omega$ that includes a discontinuity $\Gamma_d$, as shown in the figure below.

Fig. 14 Region $\Omega$ that includes the discontinuity $\Gamma_d$

The integral over the domain $\Omega$ can now be decomposed into two separate integrals, one over $\Omega^+$ and the other over $\Omega^-$, i.e.

$$
\int_{\Omega} \nabla \cdot f \, d\Omega = \int_{\Omega^+} \nabla \cdot f \, d\Omega + \int_{\Omega^-} \nabla \cdot f \, d\Omega
$$

(37)

Based on the divergence theorem, the integrals over the domains $\Omega^+$ and $\Omega^-$ can be converted to the surface integrals over $\Gamma^+$ and $\Gamma^-$. Thus, the discontinuous form of the divergence theorem can be expressed as

$$
\int_{\Omega} \nabla \cdot f \, d\Omega = \int_{\Gamma^+} f^+ \cdot n^+ \, d\Gamma + \int_{\Gamma^-} f^- \cdot n^- \, d\Gamma
$$

$$
= \int_{\Gamma} f \cdot n \, d\Gamma - \int_{\Gamma_d} [f] \cdot n \, d\Gamma
$$

(38)

where $[f] = (f^+ - f^-)_{\text{on } \Gamma_d}$.

Thus, using the above discontinuous divergence theorem and the chain rule, the first term in eq. (34) can be expressed as

$$
\int_{\Omega} w \cdot \text{div } \sigma \, d\Omega = \int_{\Omega} \text{div}(w \cdot \sigma) \, d\Omega - \int_{\Omega} \nabla w : \sigma \, d\Omega
$$

$$
= \int_{\Gamma} w \cdot \sigma n \, d\Gamma - \int_{\Gamma_d} [w \cdot \sigma n_d] \, d\Gamma - \int_{\Omega} \nabla w : \sigma \, d\Omega
$$

(39)

Substituting (39) into eq. (34), one obtains

$$
\int_{\Omega} \nabla w : \sigma \, d\Omega + \int_{\Gamma_d} [w \cdot \sigma n_d] \, d\Gamma = \int_{\Gamma} w \cdot \sigma n \, d\Gamma + \int_{\Omega} w \cdot \rho b \, d\Omega
$$

(40)

(ii) Space discretization and the solution methodology

For both the XFEM and FEM/CLED, the approximation functions can be introduced based on classical FEM approach as
where, \( N \) is the set of all shape functions, i.e. standard FEM interpolations as well as enrichments, and \( \vec{d} \), \( \vec{w} \) are the sets of nodal degrees freedom associated with these shape functions. Substituting the approximation (41) into weak form (36), dropping \( \vec{w} \), the residual force vector \( \mathbf{R} \) can be written as

\[
\begin{align*}
\mathbf{R} &= \mathbf{U} - \mathbf{W} = \left( \int_{\Omega} \mathbf{B}^T \mathbf{\sigma} d\Omega + \int_{\Gamma_{v}} \left[ \mathbf{N} \right]^T \mathbf{t}_{\text{coh}} d\Gamma \right) - \left( \int_{\Gamma_{v}} \mathbf{N}^T \mathbf{\bar{e}} d\Gamma + \int_{\Omega} \mathbf{N}^T \mathbf{\rho} \mathbf{b} d\Omega \right) \\
&= \int_{\Omega} \mathbf{B}^T \mathbf{\sigma} d\Omega + \int_{\Gamma_{v}} \left[ \mathbf{N} \right]^T \mathbf{t}_{\text{coh}} d\Gamma - \left( \int_{\Gamma_{v}} \mathbf{N}^T \mathbf{\bar{e}} d\Gamma + \int_{\Omega} \mathbf{N}^T \mathbf{\rho} \mathbf{b} d\Omega \right)
\end{align*}
\]

(42)

This relation is, in general, nonlinear due to nonlinearity in the material response. Thus, in order to find the solution, Newton-Raphson procedure is typically used. Following a standard Newton-Raphson scheme, the residual (42) at time step \( t + \Delta t \) at \( k \)th iteration can be expressed as

\[
\mathbf{R}_{t+\Delta t}^k = \mathbf{U}_{t+\Delta t}^k - \mathbf{W}_{t+\Delta t}^k
\]

(43)

Using the Taylor expansion, one can write

\[
\begin{align*}
\mathbf{R}_{t+\Delta t}^{k+1} &\approx \mathbf{R}_{t+\Delta t}^k + \frac{\partial \mathbf{R}_{t+\Delta t}^k}{\partial \vec{d}} \delta \vec{d}^{k+1} = 0 \\
&\Rightarrow \delta \vec{d}^{k+1} = -\left( \frac{\partial \mathbf{R}_{t+\Delta t}^k}{\partial \vec{d}} \right)^{-1} \mathbf{R}_{t+\Delta t}^k
\end{align*}
\]

(44)

where the global tangential stiffness matrix is defined as

\[
\frac{\partial \mathbf{R}_{t+\Delta t}^k}{\partial \vec{d}} = \int_{\Omega} \mathbf{B}^T \mathbf{B} d\Omega + \int_{\Gamma_{v}} \left[ \mathbf{N} \right]^T \mathbf{K} \left[ \mathbf{N} \right] d\Gamma
\]

(45)

and the relation for updating nodal unknowns are

\[
\Delta \vec{d}_{t+\Delta t}^{k+1} = \Delta \vec{d}_{t+\Delta t}^k + \delta \vec{d}^{k+1}
\]

\[
\vec{d}_{t+\Delta t} = \vec{d}_i + \Delta \vec{d}_{t+\Delta t}
\]

(46)

Note that the integration scheme for the constitutive relation and the interfacial forces is discussed in the main body of the paper.
On modeling of discrete propagation of localized damage in cohesive-frictional materials

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SUMMARY

In this paper, the problem of propagation of localized deformation associated with formation of macrocracks/shear bands is studied in both tensile and compressive regimes. The main focus here is on enhancement of the constitutive law with embedded discontinuity to provide a discrete representation of the localization phenomenon. This has been accomplished by revising the formulation and coupling it with the level set method for tracing the propagation path. Extensive numerical studies are conducted involving various fracture modes, ranging from brittle to frictional, and the results are compared with the experimental data as well as those obtained using XFEM methodology.

KEY WORDS: Embedded discontinuity model, XFEM, Constitutive modeling, Level set method, Localized deformation

1. INTRODUCTION

The research reported here is focused primarily on the problem of damage propagation in frictional materials. The approach incorporates a constitutive law with embedded discontinuity (CLED). This methodology, developed in refs. [1,2], has been previously used within the context of smeared modeling of localization problems. The primary novelty here is an extension of this framework to describe the discrete nature of the frictional damage process associated with elasto-plastic deformation. This has been achieved by revising the original approach and coupling it with the level-set representation to capture the path of the macrocrack/shear band propagation. Within the proposed framework the discontinuity is defined at the element level rather than at an integration point, which is in contrast to the classical smeared approach. Thus, in the presence of a discontinuous motion, the volume of a finite element itself is perceived as a representative elementary volume (REV). In what follows, an analytical derivation of the governing equations is provided first based on averaging the motion characteristics in the vicinity of discontinuity. An implicit return mapping algorithm is then developed for integration of the governing elasto-plastic constitutive relation. A simple numerical strategy is also introduced for specifying the direction of propagating macrocrack based on orientation-averaging in the domain adjacent to the tip. The framework is subsequently applied to numerical analysis of problems involving a cohesive/mixed...
mode fracture as well as strain localization associated with formation of a shear band, and the results are compared with those obtained from XFEM simulations.

Since the rise of computational era in the 1960’s, an intensive amount of research has been conducted on modeling of the evolution of damage. The focus was initially on brittle materials and one of the first attempts, within the finite element framework, was based on separating the element edges during the crack formation process ([3,4]). In order to improve the accuracy, this approach was later combined with adaptive re-meshing ([5-7]); however, it proved to be computationally inefficient. The other methodology that was pursued was the smeared cracking approach. This approach was initiated in late 1960’s in a work by Rashid ([8]). Because of its simplicity and suitability in FEM formulation, it has been widely used in 1970’s and 1980’s for modeling of damage ([9-12]). The approach is well suited for simulating the evolution of cracking in brittle materials, like concrete, at early stages of the loading process, as the damage is then associated with formation of multiple micro-cracks within the considered domain. However, the marco-cracking and its discrete nature cannot be properly modeled within this approach. Furthermore, the formulation suffers from mesh-size dependency. An alternative approach to address the issues related to discrete crack propagation involves the boundary integral formulation [13]. The framework is consistent with that of the linear fracture mechanics; it can provide very accurate results in relation to the analytical solutions, however, its extension to deal with material nonlinearity is complex. The next approach that was developed was the one presented in ref. [1]. The methodology was based on a smeared representation, incorporating volume averaging, and the focus was on resolving the issue related to the mesh-size dependency. This was accomplished by incorporating a characteristic dimension that was explicitly related to geometry of the discretized domain. An attempt conceptually similar to this work was later presented in ref. [14] following a different mathematical format.

Another ways to incorporate the strong discontinuities within the FEM approximation space was the use of elements with embedded discontinuities [15] and/or regularized discontinuous finite elements [16]. In addition, element free Galerkin methods have also been employed for simulating the damage evolution as they show higher accuracy compared to standard FEM interpolations ([17]). Introduction of reproducing kernel and partition of unity concepts [18-20] has opened a new door in numerical modeling of crack propagation and led to the introduction of the Extended Finite Element Method or XFEM [21-23]. This approach is well suited for describing the discrete nature of the crack propagation process and an extensive research has been conducted on this topic over the last few decades. The approach has been coupled with the level-set method for tracing the propagating crack [24,25] and later used in modeling the discontinuities in a wide range of applications including dynamic problems [26], hydro-mechanical problems [27-29], thermoelasticity [30-32], contact problems [33,34], and shear band formation [35,36]. The approach has also been used for discontinuous modeling within the newly developed isogeometric method [37].

In this article, the problem of damage propagation associated with shear band localization is investigated. As mentioned earlier, the main focus here is on employing an enhanced approach incorporating a constitutive law with embedded discontinuity (CLED). The enhancement deals with proposing a strategy to capture the path of damage propagation in a discrete way and coupling of this methodology with the level-set representation. The results are compared with experimental evidence and/or those obtained using XFEM approach. In section 2.1, the analytical representation of a discontinuous motion along with its implementation in the XFEM is reviewed. Section 2.2 focuses on the formulation of a constitutive law incorporating a strong discontinuity, which is then followed, in section 3, by the formulation of a new return mapping scheme. The enhanced crack
propagation strategy that is used within this framework is outlined in section 4. In section 5, the results of extensive numerical studies are discussed. First, some illustrative examples dealing with cohesive crack propagation are provided, which include a double cantilever problem investigated in [38] and the simulation of an mixed-mode cracking test performed in [39]. Later, the problems involving a shear band localization are examined including the simulation of a plane strain biaxial compression test [40], as well an assessment of a slope stability. It is demonstrated that both frameworks, i.e. FEM incorporating the enhanced constitutive law with embedded discontinuity (CLED) and XFEM, yield virtually identical response, thus giving advantage to the former one as it does not require the incorporation of any additional degrees of freedom. The conclusions emerging from this study are presented in section 6. All simulations conducted here are based on FEM/CLED and XFEM programs that were developed by the authors.

2. DISCONTINUOUS MOTION: XFEM VS. CONSTITUTIVE LAW WITH EMBEDDED DISCONTINUITY

Consider a body \( \Omega \), as shown in Fig. 1, that includes a discontinuous surface \( \Gamma_d \). The discontinuity can be described as \( \Gamma_d = \{ x_\alpha \mid x_\alpha \in \Omega \land \phi(x_\alpha) = 0 \} \) where \( \phi(x_\alpha) \) is the signed distance function that can be expressed as \( \phi(x_\alpha) = \text{sign} \left( n_\alpha (x_\alpha - \tilde{x}_\alpha) \right) \min \| x_\alpha - \tilde{x}_\alpha \| \), while \( \tilde{x}_\alpha = \{ x_\alpha \mid x_\alpha \in \Gamma_\alpha \} \) and \( \alpha \) is the coordinate indicator. The normal vector \( \vec{n}_i \) to the interface \( \Gamma_d \) can be defined as \( \vec{n}_i = \phi_i / \| \phi_i \| \). The latter is directed from \( \Omega^- \) to \( \Omega^+ \) and thus, the tangential vector \( \vec{m}_i \) may be expressed as a result of counterclockwise 90° rotation of \( \vec{n}_i \), as shown in Fig. 1.

![Fig. 1. A body \( \Omega \) with a discontinuity \( \Gamma_d \).](image)

Within this body, a discontinuous motion \( v_i(x_\alpha, t) \) can be described as a sum of two continuous functions \( \hat{v}_i(x_\alpha, t) \) and \( \tilde{v}_i(x_\alpha, t) \) combined with a discontinuous step function \( \mathcal{H}_{\Gamma_d} \), i.e.

\[
v_i(x_\alpha, t) = \hat{v}_i(x_\alpha, t) + \mathcal{H}_{\Gamma_d} \tilde{v}_i(x_\alpha, t)
\]

(1)

Here \( \mathcal{H}_{\Gamma_d} = \mathcal{H}(\phi) \) is the Heaviside function that can be expressed in its symmetric form as
\( \mathcal{H}(\phi) = 2\int_{-\infty}^{\phi} \delta(\varphi) \, d\varphi - 1 = \begin{cases} \frac{1}{2} & \varphi \geq 0 \\ -1 & \varphi < 0 \end{cases} \)  

(2)

where \( \delta(\phi) \) is the Dirac delta function that is defined as singular at \( \phi = 0 \) and zero elsewhere. Denoting a jump of a function at the point \( x_a = \bar{x}_a \) located on discontinuity surface \( \Gamma_d \) as \( \llbracket \bullet \rrbracket = \bullet^+ - \bullet^- \), the discontinuous motion \( \mathbf{\dot{g}}_i \) can be defined as

\[
\mathbf{\dot{g}}_i = \llbracket \mathbf{v}_i \rrbracket = h \mathbf{\hat{n}}_i
\]

(3)

where, \( h \) is the jump of Heaviside function at \( x_a = \bar{x}_a \) and can be evaluated as \( h = \llbracket \mathcal{H} \rrbracket = \mathcal{H}^+ - \mathcal{H}^- \). Based on the representation (2), it can be shown that \( h = 2 \). Considering that \( \mathcal{H}_p(\phi) = \mathcal{H}^p \phi \) and \( \mathcal{H}_p'(\phi(x_a)) = h \delta(\phi(x_a)) = h \delta_{\Gamma_d} \), the velocity gradient of the discontinuous motion (1) can be expressed as

\[
\mathbf{\dot{v}}_{i,j}(x_a,t) = \mathbf{\dot{v}}_{i,j}(x_a,t) + \mathcal{H}_{\Gamma_d} \mathbf{\dot{v}}_{i,j}(x_a,t) + \delta_{\Gamma_d} \mathbf{\dot{g}}_i(t) \mathbf{\hat{n}}_j
\]

(4)

where \( \mathbf{\hat{n}}_j = \mathbf{\phi}_j \) is the normal to the interface, as defined earlier.

### 2.1. Incorporation of discontinuous motion into the FE approach: XFEM

Based on the partition of unity property of FEM interpolations, the enriched shape functions can be directly incorporated into the approximation space through the generalized FEM or Extended FEM. Thus, the discontinuous motion (1) can be approximated by

\[
\mathbf{v}^h_{i}(x_a,t) = \mathbf{\hat{v}}^h_{i}(x_a,t) + \mathcal{H}_{\Gamma_d} \mathbf{\hat{v}}_{i,j}(x_a,t)
\]

\[
= \sum_{I=1}^{\hat{I}} \hat{N}_I(x_a) \hat{\mathbf{\dot{d}}}_h(t) + \sum_{I=1}^{\tilde{I}} \mathcal{H}(\phi(x_a)) \tilde{N}_I(x_a) \tilde{\mathbf{\dot{d}}}_h(t)
\]

(5)

where, \( \hat{N}_I \) and \( \tilde{N}_I \) are standard finite element shape functions, \( \hat{I} \) and \( \tilde{I} \) are sets of standard and enriched nodes, and \( \hat{\mathbf{\dot{d}}}_h(t) \) and \( \tilde{\mathbf{\dot{d}}}_h(t) \) are standard and enriched degrees of freedom associated with node \( I \) and direction \( i \), respectively. In order to achieve a better representation of the enriched approximation and to avoid the use of blending elements, the shifted form of the enrichment function \( \mathcal{H} \) can be used, i.e. \( \psi^I(x_a) = \mathcal{H}(\phi(x_a)) - \mathcal{H}(\phi(x_a^I)) \), as introduced in [41]. Note that the crack opening \( \mathbf{\dot{g}}^h_{i}(x_a,t) = \llbracket \mathbf{v}^h_{i}(x_a,t) \rrbracket \) can be expressed as

\[
\mathbf{\dot{g}}^h_{i}(x_a,t) = \sum_{I=1}^{\hat{I}} \hat{N}_I(x_a) \hat{\mathbf{\dot{d}}}_h(t) + \sum_{I=1}^{\tilde{I}} \mathcal{H}(\phi(x_a)) \tilde{N}_I(x_a) \tilde{\mathbf{\dot{d}}}_h(t) = h \sum_{I=1}^{\hat{I}} \hat{N}_I(x_a) \hat{\mathbf{\dot{d}}}_h(t)
\]

(6)

where \( h \) is the jump in shifted enrichment function that is \( h = \mathcal{H}^+ - \mathcal{H}^- \).
2.2. Constitutive law with embedded discontinuity (CLED)

In order to incorporate a discontinuous motion into a constitutive model, one can invoke the additivity postulate, similar to that employed in plasticity. Thus, the total strain rate $\dot{\varepsilon}_{ij}$ can be decomposed into a continuous part $\ddot{\varepsilon}_{ij}$ and an additional part $\dot{\varepsilon}_{ij}$, that is due to discontinuous motion along the interface, i.e.

$$\dot{\varepsilon}_{ij} = \ddot{\varepsilon}_{ij} + \dot{\varepsilon}_{ij}$$  \hspace{1cm} (7)

The continuous strain rate itself can be decomposed into an elastic and a plastic part, viz. $\ddot{\varepsilon}_{ij} = \ddot{\varepsilon}_{ij}^e + \ddot{\varepsilon}_{ij}^p$. In order to define a proper measure for the discontinuous strain rate, the representation (4) can be employed which provides an analytical representation of a motion that includes a discontinuity. As can be seen from this equation, there are two parts associated with the motion; one is a continuous part that is defined through $\gamma_{ij} = \gamma_{ij}^0 + \gamma_{ij}^T$ and the other one is associated with the discontinuous motion along the interface, i.e. $\gamma_{ij} = \delta_{ij} \frac{\dot{\gamma}_{ij} (\delta_{ij}, n_j)}{\Delta a}$. It is clear that the continuous part of the motion will produce a strain rate in the continuous part of body, known as the intact material, while the discontinuous part will generate the strain rate due to deformation within the interfacial material. It is evident from the nature of the Dirac delta function that this component acts only along the interface and it can be distributed over the small enough REV through averaging procedure. Thus, taking the volume average of this term over the REV that includes the discontinuity $\Gamma_d$, the discontinuous strain $\dot{\varepsilon}_{ij}$ can be defined as

$$\dot{\varepsilon}_{ij} = \frac{1}{\Delta v} \int_{\Delta v} \delta_{ij} (\dot{\gamma}_{ij}, n_j)^T \, dv = \frac{1}{\Delta v} \int_{\Delta a} (\dot{\gamma}_{ij}, n_j)^T \, da$$  \hspace{1cm} (8)

where, $\Delta v$ is the volume of REV and $\Delta a$ is the area of the discontinuity inside the REV. Considering the last integral to represent an average value of the dyadic product $\dot{\gamma}_{ij} n_j$ over the differential area $\Delta a$ and defining $\chi = \Delta a / \Delta v$, one can approximate eq.(8) as

$$\dot{\varepsilon}_{ij} = \frac{\Delta a}{\Delta v} (\dot{\gamma}_{ij}, n_j)^T$$  \hspace{1cm} (9)

In conclusion, the strain decomposition including discontinuous motion can now be expressed as

$$\dot{\varepsilon}_{ij} = \ddot{\varepsilon}_{ij} + \dot{\varepsilon}_{ij} = \ddot{\varepsilon}_{ij}^e + \ddot{\varepsilon}_{ij}^p + \chi (\dot{\gamma}_{ij}, n_j)^T$$  \hspace{1cm} (10)

Note that the representation (10) is, in fact, identical to the strain decomposition introduced in ref. [2]. In eq. (10), one can interpret $\ddot{\varepsilon}_{ij}$ as the deformation in the intact material and $\ddot{\varepsilon}_{ij}$ as the discontinuous motion averaged over a REV. It should be noted that in contrast to XFEM, where additional DOFs are introduced as external variables, the current representation employs unknown rates of velocity discontinuities $\dot{\gamma}_{ij}$, which can be defined through a plasticity based approach by imposing the continuity condition along the interface.
The strain localization is typically associated with an elastic response of the intact material. Thus, in order to formulate the problem, we can invoke the elastic constitutive operator, so that

$$\dot{\epsilon}_{ij} = D_{ijkl}(\dot{\epsilon}_{kl} - \dot{\epsilon}_k^p) = D_{ijkl}^e \dot{\epsilon}_{kl} - D_{ijkl}^e (\chi \dot{g}_k n_i)$$  \hspace{1cm} (11)

Now, the interfacial constitutive model relates the rate of traction, which is a function of the discontinuous motion, to the velocity discontinuity $\dot{g}_i$. Thus, $i = K_{ij} \dot{g}_j$ where $K_{ij}$ is the tangential stiffness operator for the interface material. By imposing the continuity condition $n_i \sigma_{ij} = t_j = K_{ij} \dot{g}_i$ along the interface, it can be shown that

$$\dot{\epsilon}_{ij} = E_{ijpq} D_{pqkl}^e \dot{\epsilon}_{kl}^p; \quad E_{ijpq} = \chi n_i (K_{jp} + \chi n_i D_{ijpq}^e n_k)^{-1} n_q$$  \hspace{1cm} (12)

Therefore, the constitutive relation for the case of embedded discontinuity can be written as

$$\dot{\sigma}_{ij} = D_{ijkl} \dot{\epsilon}_{kl}; \quad \tilde{D}_{ijkl} = D_{ijkl}^e - D_{ijkl}^e E_{pqrs}^e D_{pqrs}$$  \hspace{1cm} (13)

It should be pointed out that the discontinuous motion involving the presence of localization is defined here via eq.(12). By combining eqs.(12) and (9), the velocity discontinuity can be expressed as an explicit function of a given macroscopic strain rate. Unlike in the original smeared representation, the discontinuity is defined here at element level, not at individual Gauss points, and it’s traced by the level-set method; thus, the location and orientation of the crack is known exactly, as in XFEM. In this way, the value of the characteristic dimension $\chi = \Delta a / \Delta v$ can be accurately assessed.

It is noted that if the intact material undergoes plastic deformation, the stress rate $\dot{\sigma}_{ij}$ should be defined as

$$\dot{\sigma}_{ij} = \tilde{D}_{ijkl} (\dot{\epsilon}_{kl} - \dot{\epsilon}_k^p)$$  \hspace{1cm} (14)

In this case, the yield function $f$ and the non-associated flow rule can be expressed as

$$f = f(\sigma_{ij}, \kappa) \leq 0; \quad \psi = \psi(\sigma_{ij}) = \text{const}; \quad \dot{\epsilon}_{ij}^p = \lambda \dot{\psi} \frac{\partial \psi}{\partial \sigma_{ij}}$$  \hspace{1cm} (15)

where $\kappa$ is a hardening parameter. For an active loading process, the consistency condition can be written as

$$\dot{f} = \frac{\partial f}{\partial \sigma_{ij}} \dot{\sigma}_{ij} + \frac{\partial f}{\partial \kappa} \dot{\kappa} + \lambda \frac{\partial \psi}{\partial \sigma_{ij}} = 0$$  \hspace{1cm} (16)

Substituting now the stress rate defined in equation (14) one obtains, after some algebraic manipulations

$$\dot{\lambda} = \frac{1}{H} \frac{\partial f}{\partial \sigma_{ij}} \tilde{D}_{ijkl} \dot{\epsilon}_{kl}; \quad \dot{H} = \frac{\partial f}{\partial \sigma_{ij}} \tilde{D}_{ijkl} \frac{\partial \psi}{\partial \sigma_{kl}} - \frac{\partial \psi}{\partial \kappa} \frac{\partial \kappa}{\partial \lambda}$$  \hspace{1cm} (17)
Thus, substituting relations (17) back into (14), the tangential stiffness operator can be defined as

\[ \dot{\sigma}_{ij} = D_{ijkl}\dot{e}_{kl} \quad \text{and} \quad D_{ijkl} = \tilde{D}_{ijkl} - \frac{1}{H} \tilde{D}_{ijkl} \frac{\partial \sigma_{kl}}{\partial \sigma_{rs}} \frac{\partial f}{\partial \sigma_{rs}} \tilde{D}_{rskl} \]  

(18)

In conclusion, for the elements that experience the localized deformation in the form of a macrocrack/shear band, the trial stress rate can be found using equation (13), i.e. assuming linear response of the intact material. If the trial stress does not violate the loading condition, no correction is required. If not, i.e. in the case of an active plastic process, the stress increment and the tangential operator must be updated based on relations (18).

3. IMPLICIT INTEGRATION SCHEME FOR CLED

For the completeness of the presentation, the numerical integration scheme is briefly discussed here. In case of XFEM analysis, the nonlinearity of the interfacial material is handled within the Newton-Raphson solver itself, as the discontinuous motion \( g_i \) is an external variable. At the same time, the nonlinearity of the intact material can be dealt with using a standard implicit integration scheme. The implementation of CLED requires, however, a development of an appropriate a return mapping algorithm which is presented below.

The procedure invokes the specification of trial stress that is assessed using the elastic stiffness operator. Thus, for an element with embedded discontinuity, the trial stress can be expressed as

\[ \sigma_{ij}^{\text{trial}} = \sigma_{ij} + \tilde{D}_{ijkl}\Delta \varepsilon_{kl} \]  

(19)

where \( \tilde{D}_{ijkl} \) is defined in eq. (13). Once the trial stress is determined, the value of the yield function must be evaluated. In the case when \( f^{\text{trial}}(\sigma_{ij}^{\text{trial}}, \kappa') < 0 \) or \( f^{\text{trial}}(\sigma_{ij}^{\text{trial}}, \kappa') = 0 \land (\partial f / \partial \sigma_{ij})\Delta \sigma_{ij} < 0 \), the material remains in the elastic range, so that the representation (13) results in correct response. For the case of an active loading process, i.e. \( f^{\text{trial}} = f(\sigma_{ij}^{\text{trial}}, \kappa') > 0 \), according to the return mapping scheme [42], the residuals at iteration \( \nu \) can be written in terms of stress and plastic strain increment at \( t + \Delta t \) as

\[ r_{ij}^{\nu} = \sigma_{ij}^{\nu} - \left( \sigma_{ij} + \tilde{D}_{ijkl}(\Delta \varepsilon_{kl} - \Delta \varepsilon_{kl}^{\nu}) \right) \]

\[ f^{\nu} = f(\sigma_{ij}^{\nu}, \kappa^{\nu}) \]  

(20)

Using Newton-Raphson algorithm, residuals (20) can be expressed as

\[ r_{ij}^{\nu+1} \approx r_{ij}^{\nu} + \frac{\partial r_{ij}^{\nu}}{\partial \sigma_{mn}} \delta \sigma_{mn}^{\nu} + \frac{\partial r_{ij}^{\nu}}{\partial \lambda} \delta \lambda^{\nu} = 0 \]

\[ f^{\nu+1} \approx f^{\nu} + \frac{\partial f^{\nu}}{\partial \sigma_{mn}} \delta \sigma_{mn}^{\nu} + \frac{\partial f^{\nu}}{\partial \lambda} \delta \lambda^{\nu} = 0 \]  

(21)
Solving now equation (21) for \((\delta \lambda, \delta \sigma^v)\), yields

\[
\delta \lambda^v = \frac{f^v - \frac{\partial f}{\partial \sigma_{ij}} Q_{ijkl}^{-1} r_{kl}^v}{\frac{\partial f}{\partial \sigma_{ij}} Q_{ijkl}^{-1} \tilde{D}_{klmn} \frac{\partial \psi}{\partial \sigma_{mn}} - \frac{\partial f}{\partial \kappa} \frac{\partial \delta \lambda}{\partial \kappa}} ; \quad \delta \sigma_{ij}^v = -D_{ijkl} \frac{\partial \psi}{\partial \sigma_{kl}} \delta \lambda^v
\]

(22)

where \(Q_{ijkl} = \delta_{ij} \delta_{kl} + \Delta \lambda (\frac{\partial^2 \psi}{\partial \sigma_{ij} \partial \sigma_{kl}})\). Note that if increments are small enough, \(\Delta \lambda \to 0\), one obtains \(Q_{ijkl} \approx \delta_{ij} \delta_{kl}\). Thus, stress updates can be expressed as

\[
\Delta \sigma_{ij}^{v+1} = \Delta \sigma_{ij}^v + \delta \sigma_{ij}^v
\]

\[
\Delta \lambda^{v+1} = \Delta \lambda^v + \delta \lambda^v
\]

(23)

This correction process must be continued until the convergence is achieved, i.e. \(f(\sigma_{ij}^{v+1}, \kappa^{v+1}) \leq 0\). Note that at the end of each iteration, \(\Delta g_i, \Delta \sigma_{ij}, D_{ijkl}\) must be updated as the discontinuous motion \(\Delta g_i\) is a function of the stress state.

4. CRACK PROPAGATION STRATEGY: INITIATION AND TRACING THE DIRECTION

The onset of cracking is typically assessed based on a failure criterion specific to the material. Thus, if the trajectory describing the averaged stress state, within a finite element, approaches the failure surface, one may assume that the deformation localizes into a macrocrack. For the simulations conducted here, the maximum tensile strength criterion (for the cohesive crack propagation) and the Mohr-Coulomb criterion (for the description of frictional shear band formation) were employed.

As proposed in a number of previous studies, e.g. [24], the level set method can be used for tracing the propagating crack. Based on this methodology, a moving/propagating interface \(\Gamma_d(t)\) can be defined as the zero level set of a function \(\phi(x, t)\), i.e., \(\Gamma_d(t) = \{x_a \mid \phi(x_a, t) = 0\}\). A function that can represent such a property is the signed distance function as proposed in [43]. For the numerical simulations conducted here, the level-set method has been coupled with both XFEM and FEM/CLED.

In most of the published works, the J-integral method is used to evaluate the stress intensity factors and to define the direction of the crack propagation. However, the main drawback associated with this method is that it is limited to elastic-brittle materials that undergo a tensile damage. A simple and effective way of defining the onset of fracture and the direction of the propagating crack is to invoke a specific form of the failure criterion. For failure in tension, for example, the maximum tensile stress criterion may be employed which stipulates that the direction of crack is perpendicular to that of major principal stress. In case of frictional materials, commonly described by Mohr-Coulomb criterion, the crack is also said to form at a prescribed orientation of \(45 \pm \phi / 2\) relative to the direction of minor principal stress. Note that for an elasto-plastic strain-hardening material, the direction of localization is often defined as a bifurcation problem [44].
should be pointed out that the integral approaches, such as the J-integral method, have an implicit averaging nature; i.e., they provide average measures defined over a domain of interest. Using a similar concept of average property, a simple algorithm is implemented here for assessing the direction of propagation of the discontinuity surface. In a typical scenario, the stress state at most integration points in the vicinity of the crack tip is close to the failure envelope. Therefore, the scheme used here for assessing the direction of propagation is based on checking the failure criterion at the integration points adjacent to the tip element. The average direction of propagation is then established based on the orientations associated with the neighboring integration points. This algorithm is illustrated schematically in Fig. 2. Note that by implementing this methodology, a stable crack pattern propagation is achieved for both XFEM and CLED, which is not the case without incorporation of the averaging scheme.

![Diagram showing crack propagation methodology used for both XFEM and FEM/CLED](image)

**5. NUMERICAL SIMULATIONS**

In this section, different boundary value problems are examined involving both FEM with a discontinuity embedded within the constitutive relation and XFEM. Note that XFEM is used here as a verification tool for assessing the accuracy of the results based on FEM/CLED formulation. The primary focus is on examining the damage propagation in frictional materials; however, for a more complete representation, some illustrative examples involving cohesive crack propagation are also provided. The key results are discussed in two separate sections; each section starting with a brief review of the interfacial model that is employed for the associated numerical study. For the case of crack propagation, the first example is based on the work reported in [38], while the second one incorporates the results of an experimental study conducted in [39]. For the strain localization involving a shear band formation, a plane strain biaxial test reported in ref. [40] is simulated first. This study also involves an examination of the issue of sensitivity of the solution to mesh size/alignment. Later, numerical simulations involving an assessment of stability of a slope excavated in a material with an apparent cohesion are provided. All simulations reported here involve two-dimensional configurations.
5.1. Cohesive crack propagation: interface model and the results of numerical simulations

For this study, a cohesive crack model with an exponential decay has been employed (after ref. [45]). Within this framework, the tensile strength of the material is defined as

\[ F_i(g_n) = F_i \exp\left(\frac{-F}{G} g_n\right) \]  

(24)

where, \( F_i \) is the initial strength at the onset of fracture, \( G \) is the fracture energy release rate, and \( F_i(g_n) \) is the tensile strength at separation \( g_n \). The failure function is defined as

\[ f(t_n, g_n) = t_n - F_i(g_n) \]  

(25)

For an active loading process, setting \( f(t_n, g_n) = 0 \) will clearly result in \( t_n = F_i(g_n) \). For the simulations conducted here, it was assumed that tangential component of cohesive force is negligible, i.e. \( t_m = 0 \). Therefore, the constitutive relation in the local coordinate system, along the crack, can be expressed as

\[ t_i^* = K_{ij}^* g_j^*; \quad K_{ij}^* = \begin{cases} -\frac{F^2}{G} \exp\left(\frac{-F}{G} g_n\right) & i = j = 1 \\ 0 & \text{otherwise} \end{cases} \]  

(26)

where \( K_{ij}^* \) is the tangential operator.

5.1.1. Double cantilever beam test

The first example involves the simulation of mode 1 crack propagation in a double cantilever beam. The geometry and the boundary conditions are shown in Fig. 3 and were chosen based on the information provided in ref. [38]. The beam has the dimensions of \( 400 \times 200 \text{mm} \) with a thickness of \( 1000 \text{mm} \); the notch is \( 120 \times 12.5 \text{mm} \). Due to the symmetry, only half of the domain was discretized. Following the original reference, a total number of 1005 structured quadrilateral elements were employed. The beam was analyzed under plane stress condition.
The load consisted of applying the vertical displacement at point $A$ of the beam and the material properties were taken as

$$
E = 36.5 \text{ GPa}, \quad f_t = 3 \text{ MPa}, \quad v = 0.18, \quad G_j = 3 \text{ N/m}
$$

(27)

Note that the value of $G_j$, assumed after ref. [38], is quite low which is indicative of a relatively high strain softening rate. The ref. [38] provides a detailed discussion on the influence of $G_j$ on the solution, in particular on the issue of convergence.

The resultant force vs displacement characteristics are depicted in Fig. 4 for FEM/CLED as well as XFEM simulations. It is noted that for both solutions the descending branch exhibits some oscillations, which are purely numerical. The problem may be rectified by incorporating more refined implicit/explicit integration schemes (cf. [38]). The cracking pattern superimposed on the vertical displacement field is shown in Fig. 5. It is evident here that virtually identical response is obtained from both methodologies, in terms of the cracking pattern as well as the mechanical characteristics.
5.1.2. Mixed mode cracking of concrete

The example given here involves the simulation of experimental tests conducted by Galvez and his co-workers [39] at Delft University. The geometry of the problem is shown in Fig. 6. The problem involves four-point bending of a notched concrete beam under the action of two independent actuators.

In the original experimental studies, the specimens were tested at different values of $D$ and $K$. The simulations conducted here correspond to $D = 300\,\text{mm}$ and involve two limiting cases of the value of $K$, viz. $K=0$ (no constraint) and $K \to \infty$ (point $A$ fixed). The problem was again considered as plane-stress and was analyzed as displacement-controlled (viz. $\delta$). The material properties were taken as follows,

$$E = 38\,\text{GPa}, \quad v = 0.2, \quad f_r = 3\,\text{MPa}, \quad G_f = 70\,\text{N/m}$$

while the thickness was assumed to be equal to 50mm.

The cracking pattern, for both cases considered in the analysis, is shown in Fig. 7 together with the relevant experimental data. Fig. 8, shows the scaled images of the deformed shape for FEM/CLED as well as XFEM simulations. The load vs. crack mouth opening displacement (CMOD) and the load-vertical displacement characteristics are plotted in Fig. 9 and Fig. 10 respectively. It is quite evident the predictions using both methodologies are virtually identical and are fairly consistent with the experimental data reported in ref.[34].
Fig. 7. Left: Cracking pattern from the FEM/CLED and XFEM analysis. Right: Experimental results [39]

Fig. 8. Deformed shape for both FEM/CLED and XFEM simulations; left: $K=0$ and right: $K \to \infty$

Fig. 9. Load vs CMOD and load vs vertical displacement response ($K=0$)

Fig. 10. Load vs CMOD and load vs vertical displacement response ($K \to \infty$)
5.2. Shear band localization: interface model and the results of numerical simulations

For the case involving localized deformation associated with the inception of a shear band, a frictional contact model is incorporated. The yield and the plastic potential surfaces are defined as
\[ f(t_n, t_m) = |t_m| + \mu(g)(t_n + c) = 0; \quad \psi(t_m) = |t_m| = \text{const}; \quad \gamma = |g_m| \] (29)

where \((t_n, t_m)\) are the normal and tangential components of the traction vector, \(g_m\) is the tangential displacement along the interface, and \(\gamma\) is the strain-softening parameter that is identified with \(g_m\). The softening function is assumed in an exponential form
\[ \mu = \mu_r + (\mu_0 - \mu_r) \exp(\alpha \gamma) \] (30)

where, \(\mu_r\) is the value of friction coefficient at failure, \(\mu_r\) is the residual value and the parameter \(\alpha\) controls the rate of rate of softening. The constitutive relation can be formulated by invoking the standard plasticity formalism.

5.2.1. Modeling of localized deformation in a biaxial test on dense sand

The numerical analysis carried out here involves the simulation of a biaxial (plane strain) test conducted on a dense Ottawa sand at the confinement of 100kPa [40]. The sample had the dimensions of \(83.3 \times 152.4 \times 80.8\) mm and the deformation was recorded by digital monitoring of nodal displacements of the grid that was imprinted on the membrane surface (see Fig. 11).

The simulations were carried out assuming that the material remains elastic prior to the onset of localization. The latter was defined as \(\eta \rightarrow \eta_f\) in the classical Mohr-Coulomb criterion. In the softening regime, the response was said to be associated with localized deformation mode, whereby the behaviour of the shear band material was defined through the interfacial constitutive model defined above. The key material properties, as reported in ref. [40], were as follows
\[ E = 23\ MPa, \quad \nu = 0.3, \quad \phi = 48.2^\circ \]

where \(\phi\) is the friction angle. For the interface, three different values of the residual friction coefficient were selected, viz. \(\mu_r = \mu_0\) (perfectly-plastic response), \(\mu_r = 0.8\mu_0\) (i.e., 20% degradation) and \(\mu_r = 0.3\mu_0\).

The boundary conditions involved no friction at the end platens while the localization was triggered by introducing an inhomogeneity in the center of the specimen (20% increase in the value of \(E\)). For the localized deformation mode, it was assumed that the shear band within an element forms at \(57^\circ\) with respect to the horizontal, which was the actual value measured in the experiment. Note that this value is lower than the usual estimate based on Mohr-Coulomb criterion, i.e. \(45^\circ + \phi / 2\), which is likely due to the fact that the material displayed some inherent anisotropy. It is noted again that the orientation of the localization plane can, in general, be determined through an independent criterion, such as that associated with the bifurcation properties of the constitutive relation (cf.[44,46]).

The main results of simulations are presented in Fig. 11. The figures on the left show the deformation mode, both the predicted and experimentally observed, while the figure on the right
gives the corresponding material characteristics. The results of simulations are, in general, fairly consistent with the experimental data.

![Fig. 11. Shear band formation in biaxial plane strain test: a) cracking pattern and post localization deformation mode; b) Load-axial displacement curve](image)

![Fig. 12. Post failure response of the sample; left: FEM/CLED and right: XFEM analysis](image)

It is noted that the analysis presented above employs a mesh that is oriented along the shear band in order to avoid potential numerical issues. In general, however, the results of simulations based on FEM/CLED are virtually independent of discretization, as the mathematical framework incorporates a characteristic dimension. In order to demonstrate this, a sensitivity analysis has been conducted employing, in addition to previous mesh, two structured grids of different size. The results, which are shown in Fig.13, clearly show that the predicted localization patterns as well as the global mechanical characteristics are almost the same for all three types of FE meshes.
5.2.2 Modeling of shear band initiation and propagation in a cohesive slope subjected to foundation loading

The last example given here involves an assessment of stability of a slope in cohesive soil (overconsolidated silty clay) subjected to a foundation loading. The geometry adopted is shown in Fig. 13. The soil was modeled using a plasticity based deviatoric hardening model [47,48], while the foundation was assumed to be rigid-elastic. The material properties for the soil were taken as

\[ E = 100 \text{MPa}; \quad \nu = 0.35; \quad \eta_f = 0.98; \quad \eta_c = 0.77; \quad C = 40 \text{kPa}; \quad A = 1.0 \times 10^{-5} \]

where \( \eta_f \) and \( \eta_c \) are slope of Mohr-Coulomb failure line and the dilation lines in \( p-q \) space, respectively, \( C \) is the cohesion, and \( A \) is the hardening parameter. For the interfacial properties, a cohesionless Mohr-Coulomb criterion was assumed, as described earlier. Here, the friction coefficient is measured as \( \tilde{\eta}_f = \tau / \sigma \), where \( \sigma \) and \( \tau \) are normal and tangential values of traction acting along the interface at the onset of localization. A degradation of 30% over a sliding of 0.1mm, along with \( k_n = k_m = 10^{-8} \text{N/m} \), was assumed for the interfacial model.

The boundary conditions are shown in Fig. 13. The first step involved the analysis due to own weight of soil. Later, the foundation load was imposed through 100 increments. The criterion for the onset of localization was set as \( \eta \rightarrow 0.9\eta_f \). The direction of the shear band was established as \( 45^\circ + \phi / 2 \), which corresponds to the orientation that maximizes the Coulomb failure function.

Fig. 15 shows the distribution of the failure ratio \( \eta / \eta_f \) at three different stages of the loading process. The shear band is initiated at the left corner of the foundation. Subsequently, the main localized zone forms at the right hand side and propagates until a complete failure of the slope. The load displacement response and the cracking pattern at the end of simulation are plotted in Fig. 15 and Fig. 16. Once again, it is evident that the value of the critical load triggering the loss of stability is virtually the same for both methodologies, i.e. FEM/CLED and XFEM.
Fig. 13. Geometry of the slope and the boundary conditions; H=10m

Fig. 14. Failure ratio at different stages of shear band propagation; top: FEM/CLED, bottom: XFEM simulations

Fig. 15. Force displacement response from both FEM/CLED and XFEM analysis

Fig. 16. Shear band pattern
6. CONCLUDING REMARKS

The present study was focused on simulation of cohesive crack propagation as well as modeling of the onset and propagation of localized deformation associated with a shear band formation. The primary methodology employed here involved a constitutive relation with embedded discontinuity. A new formulation was presented based on the description of discontinuous motion and an implicit integration scheme was derived incorporating nonlinear properties of the intact material. The approach was coupled with the level-set method for explicit modelling of the discrete crack propagation process. Four different sets of numerical simulations were conducted. The first example involved cohesive mode 1 crack propagation. Next, a mixed mode cracking was examined by simulating the experimental study of Galvez et al. [34]. Subsequently, the localized deformation associated with formation of a shear band was investigated. The analysis involved the simulation of a plane strain test on a granular material as well as the problem involving the assessment of slope stability. For all studied problems, a close correlation between the results from FEM/CLED and XFEM was achieved in terms of both the failure mechanism, i.e. the cracking/shear band pattern, as well as the global load-displacement response; in particular, the assessment of ultimate load.

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Modeling of deformation and localized failure in anisotropic rocks

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ABSTRACT
This paper deals with description of the deformation process in argillaceous rocks that display a strong inherent anisotropy. Both, the homogeneous and the localized deformation modes are considered. The effects of anisotropy are incorporated by invoking the microstructure tensor approach. The strain localization is assumed to be associated with formation of a macrocrack the orientation of which is defined using the critical plane approach. The propagation of damage is traced within the context of a boundary value problem by employing a constitutive law with embedded discontinuity. The crack path is monitored in a discrete manner by using the level-set method. The closest-point projection algorithm is developed for the integration of the constitutive relations at both stages of the anisotropic deformation process, i.e. the homogenous mode as well as that involving an embedded discontinuity. The problem of macrocrack formation in a biaxial plane strain compression test is studied. It is demonstrated that friction between loading platens can play an important role in the process of evolution of damage and may significantly affect the compressive strength.

Keywords: Constitutive modeling, anisotropy, localization, discrete crack propagation, embedded discontinuity

1. Introduction

Many geomaterials display a structural anisotropy which is closely related to their microstructure. The primary focus here is on the argillaceous rocks, which are sedimentary rocks formed from clay deposits. These rocks, which include shales and argillites, are characterized by the presence of closely spaced bedding planes and exhibit a strong directional dependence of strength as well as deformation properties. The understanding of the mechanical behaviour of argillaceous rocks is of a significant importance due to their widespread applications in many types of geotechnical projects, including petroleum extraction, carbon dioxide sequestration as well as a deep geological disposal of radioactive waste. The primary concern in this case is the onset and propagation of damage due to excavation, transport of pore fluids and/or the elevated temperature.

The description of the mechanical behaviour requires, first of all, the specification of conditions at failure under an arbitrary stress state. In addition, a general framework must be provided for the evaluation of the deformation field, which may include discontinuities such as macrocracks. Over the last few decades, an extensive research effort has been devoted to modeling of the mechanical behaviour of anisotropic rocks. A comprehensive review on this topic, examining different approaches, is provided in the articles by Duveau and Henry (1998) and Kwasniewski (1993). One

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of the first attempts to describe the conditions at failure in anisotropic rocks was the work reported by Pariseau (1968), which was an extension of Hill’s criterion (Hill, 1950). This was followed by more complex tensorial representations (Amadei, 1983; Boehler and Sawczuk, 1977; Nova, 1980). The application of the latter criteria to practical problems is generally difficult due to a large number of independent material functions/parameters that appear in the formulation. A simple and pragmatic approach, which incorporates a scalar anisotropy parameter that is a function of a mixed invariant of the stress and the structure orientation tensor, has been developed by Pietruszczak and Mroz (2001). This approach was later applied to modeling of sedimentary rocks (Lade, 2007; Pietruszczak et al., 2002).

Numerical approaches dealing with crack propagation in continuous isotropic media have been investigated for several decades. Many attempts have been made to accurately model both the smeared nature of the onset of cracking at initial stages of loading as well as the discrete nature of macrocrack propagation. The research started in early 1960’s when the node separation technique was introduced (Ngo and Scordelis, 1967). This was followed by the adaptive remeshing (Ingraffea, 1977) as well as introduction of the smeared damage models (Bažant and Cedolin, 1979; Nayak and Zienkiewicz, 1972; Rashid, 1968). The issue of mesh-size dependency was first addressed in the early 1980’s within the context of a constitutive law with embedded discontinuity (Pietruszczak and Mroz, 1981; see also Pietruszczak, 1999). Later, several attempts were made to incorporate the discontinuous motion into the interpolation functions (Belytschko et al., 1994; Fish and Belytschko, 1988; Simo et al., 1993). The concept of reproducing kernels (Liu et al., 1995) and partition of unity (Melenk and Babuška, 1996) resulted in development of a methodology for modeling crack propagation through the Extended Finite Element Method X-FEM (Belytschko and Black, 1999; Moës et al., 1999; Sukumar et al., 2000). This approach was then combined with the level-set method for tracing of the paths crack propagation (Chessa and Belytschko, 2003) and was applied to a broad class of problems providing stable, mesh independent results. The only concern in relation to this approach is the necessity of dealing with additional enrichment functions for the cracked elements. The latter requires updating mesh data structures throughout the analysis as well as the use of a special integration technique. In a recent study, the idea of tracing the propagating crack in a discrete way was combined with the embedded discontinuity approach (Haghighat and Pietruszczak, 2013) and applied to modeling of crack/shear band inception and propagation in brittle materials. The approach shows an accurate mesh-independent response without requiring any special techniques in terms of implementation.

This paper is an extension of the work reported earlier (Pietruszczak et al., 2002) and deals with description of the deformation process in argillaceous rocks. Both, the homogeneous and the localized modes are considered here while the effects of anisotropy are incorporated by invoking the microstructure tensor approach. The strain localization is assumed to be associated with formation of a macrocrack and a simple methodology is proposed for identifying the orientation of the crack based on the critical plane approach. In section two, the plasticity framework incorporating an anisotropic deviatoric hardening model is presented, followed by the formulation of a constitutive model with embedded discontinuity. The section is concluded by introducing a simple criterion for initiation of crack and specification of its orientation. In section three, the closest-point projection algorithm is developed for the integration of the constitutive relations at both stages of the anisotropic deformation process. Section four focuses on numerical modeling of shear band formation in Tournemire argillite. The crack path is monitored in a discrete manner by using the level-set method. The effects of boundary conditions, orientation of bedding planes, and mesh-sensitivity of the approach are studied. It is demonstrated that friction between loading
platens can play an important role in the process of evolution of damage and may significantly affect the strength characteristics that are commonly perceived as a material property.

2. Formulation of the problem

The deformation process in argillaceous rocks incorporates two main stages; the first one is associated with a homogeneous deformation and the second one involves a failure mode associated with inception of a macrocrack. Thus, in order to describe the mechanical behaviour, one has to formulate a constitutive relation dealing with an inherently anisotropic response prior to failure, an appropriate failure criterion, and a framework describing the post-failure response involving the localized deformation. These three key points are addressed below. First, an anisotropic deviatoric hardening model is presented describing the response prior to the onset of failure. Then, a failure criterion is introduced which incorporates the critical plane approach for identifying the direction of the macrocrack. Finally, a constitutive law with embedded discontinuity is introduced that is capable of describing the post localization response within a REV. In the last case, the dominant factor controlling the mechanical characteristics is the interfacial response.

2.1. Constitutive relation describing the homogeneous deformation mode

The elasto-plastic framework employed in this study incorporates the microstructure tensor approach (Pietruszczak and Mroz, 2001). In order to define the anisotropy parameter(s), the formulation employs a generalized loading vector that is defined as

\[ L = L_\alpha e^{(\alpha)}; \quad L_\alpha^2 = \epsilon^{(\alpha)} \cdot \epsilon^{(\alpha)} = (e^{(\alpha)} \cdot \sigma) \cdot (e^{(\alpha)} \cdot \sigma) \]  

(1)

where \( e^{(\alpha)} \), \( \alpha = 1, 2, 3 \), are the base vectors, which specify the preferred material axes. Thus, the components of \( L \) represent the traction moduli on planes normal to the principal material axes. Introduce now a microstructure tensor \( a \), which is a measure of material fabric. While different descriptors may be employed to quantify the fabric, the eigenvectors of this operator are said to be collinear with \( e^{(\alpha)} \). The projection of the microstructure tensor on the direction \( L \) becomes

\[ \mathcal{C} = \ell \cdot a \cdot \ell; \quad \ell = L / (L \cdot L)^{1/2} \]  

(2)

Here, the scalar variable \( \mathcal{C} \), referred to as anisotropy parameter, specifies the effect of load orientation relative to material axes and can be defined as the ratio of joint invariant of stress and microstructure tensor \( tr(\sigma \cdot A \cdot \sigma) \) to the stress invariant \( tr(\sigma \cdot \sigma) \). It is a homogeneous function of stress of the degree zero, so that the stress magnitude does not affect its value. Note that Eq.(2) can be expressed as

\[ \mathcal{C} = \delta^*(1 + \ell \cdot A \cdot \ell) = \delta^*_0 (1 + \zeta); \quad \zeta = \ell \cdot A \cdot \ell \]  

(3)

where \( A = dev(a) / \delta^*_0 \) is a symmetric traceless tensor with \( \delta^*_0 = tr(a) / 3 \). The representation (3) can be generalized by employing a polynomial expansion which incorporates higher order terms in dyadic products \( \zeta \), i.e.

\[ \mathcal{C} = \delta^*_0 (1 + \zeta + a_1 \zeta^2 + a_2 \zeta^3 + a_3 \zeta^4 + \cdots) \]  

(4)
where \(a_1, a_2, a_3, \ldots\) are the expansion coefficients. Using the notion of this scalar anisotropy parameter, as defined viz. eq.(4), any isotropic failure criterion can be extended to the case of anisotropy by assuming

\[
F(\mathbf{\sigma}) = F(I_1, I_2, I_3, \zeta)
\]  

(5)

where \(I_1, I_2, I_3\) are the basic stress invariants.

The parameter \(\vartheta\) is typically identified with a relevant strength descriptor, whose value is then assumed to depend on the orientation of the sample relative to the direction of loading. In this work a simple linear form of eq.(5) has been adopted, which corresponds to the well-known Mohr-Coulomb criterion, i.e.

\[
F(\mathbf{\sigma}) = F(\sigma_m, \bar{\sigma}, \theta, \zeta) = \sqrt{3\bar{\sigma}} - \eta_f(\zeta)g(\theta)(\sigma_m + C) = 0
\]  

(6)

Here, \(\sigma_m = -\text{tr}(\mathbf{\sigma})/3\), \(\bar{\sigma} = \sqrt{\text{tr}(\mathbf{s} \cdot \mathbf{s})/2}\), where \(\mathbf{s}\) is the deviatoric part of the stress tensor; while \(\theta\), which is defined as \(\theta = -\sin^{-1}(\sqrt{27/4} J_3/\bar{\sigma}^3)/3\) with \(J_3 = \text{tr}(\mathbf{s} \cdot \mathbf{s})/3\), denotes the Lode’s angle. Moreover,

\[
g(\theta) = \frac{3 - \sin \phi}{2\sqrt{3} \cos \theta - 2 \sin \theta \sin \phi}; \quad \eta_f = \frac{6 \sin \phi}{3 - \sin \phi}; \quad C = c \cot \phi
\]  

(7)

where \(\phi, c\) are the angles of friction and cohesion, respectively. Note that the strength descriptors, in this case \(\eta_f\) and \(C\), are assumed to be orientation-dependent and have the representation analogous to that of eq.(4). However, in the context of the failure criterion (6), the parameter \(C\) is associated with a hydrostatic stress state. The latter is, in fact, invariant with respect to orientation of the sample. Thus, the effects of anisotropy can be primarily attributed to variation in the strength parameter \(\eta_f\).

The general plasticity formulation can be derived by assuming the yield/loading surface in the form consistent with representation (6), i.e.

\[
f = \sqrt{3\bar{\sigma}} - \eta f g(\theta)(\sigma_m + C) = 0; \quad \eta = \eta(\kappa, \zeta) = \eta_f(\zeta) \frac{\xi \kappa}{A + \kappa}; \quad d \kappa = \left(\frac{2}{3} \dot{\mathbf{e}}^p : \dot{\mathbf{e}}^p\right)^{1/2}
\]  

(8)

where \(\dot{\mathbf{e}}^p\) is the deviatoric part of the plastic strain rate and \(A\) and \(\xi\) are material parameters. According to the hardening rule, for \(\kappa \to \infty\) there is \(\eta \to \xi \eta_f\), where \(\xi > 1\). The parameter \(\xi\) is introduced here in order to define the transition to localized deformation, which is assumed to occur at \(\eta = \eta_f\). Note that the latter equality implies that \(f = F\), so that the conditions at failure are consistent with Mohr-Coulomb criterion (6). The plastic potential can be chosen as

\[
\psi = \sqrt{3\bar{\sigma}} + \eta_c g(\theta)(\sigma_m + C) \ln \left(\frac{\sigma_m + C}{\sigma_m^0}\right) = 0
\]  

(9)

where, \(\eta_c\) is the dilatancy coefficient defined as \(\eta_c = \alpha \eta_f\) with \(\alpha\) assumed as a material constant.
Now, the constitutive relation can be expressed in the general form
\[
\sigma = D : \dot{\varepsilon} = D : (\dot{\varepsilon} - \dot{\varepsilon}^p), \quad \dot{\varepsilon}^p = \lambda \dot{\varepsilon} \partial_y
\] (10)
where the yield and potential functions are defined by eqs. (8) and (9). Here, \( D \) is the anisotropic elastic operator. For an elastic loading trajectory, \( \dot{\lambda} = 0 \), which implies \( \dot{\varepsilon}^p = 0 \). For an active (plastic) loading process, \( f(\sigma, \kappa) = 0 \) and \( \dot{\lambda} > 0 \). Imposing the consistency condition, the plastic multiplier can be expressed as
\[
\partial_a f : \dot{\varepsilon} + \partial_{\lambda} f \dot{\lambda} = 0 \to \dot{\lambda} = \frac{\partial_a f : D : \dot{\varepsilon}}{\partial_a f : D : \partial_y - \partial_{\lambda} f}
\] (11)
where
\[
\partial_a f = \frac{\partial f}{\partial \sigma_r} \dot{\varepsilon}_a + \frac{\partial f}{\partial \sigma} \dot{\varepsilon}_a \sigma_m + \frac{\partial f}{\partial \theta} \dot{\varepsilon}_a \theta + \frac{\partial f}{\partial \vartheta} \dot{\varepsilon}_a \vartheta
\]
\[
\partial_a y = \frac{\partial y_r}{\partial \sigma_r} \dot{\varepsilon}_a + \frac{\partial y_r}{\partial \sigma} \dot{\varepsilon}_a \sigma_m + \frac{\partial y_r}{\partial \theta} \dot{\varepsilon}_a \theta + \frac{\partial y_r}{\partial \vartheta} \dot{\varepsilon}_a \vartheta
\] (12)
Substituting eq.(11) back into eq.(10), the tangential elasto-plastic operator \( D_T \) can be defined as
\[
\sigma = D_T : \dot{\varepsilon}, \quad D_T = \frac{D : \partial_a y}{\partial_a f : D : \partial_y - \partial_{\lambda} f}
\] (13)
The integration scheme for the above constitutive relation is presented in section 3.

2.2. Description of localized deformation: a constitutive law with embedded discontinuity (CLED)

A discontinuous motion within a body can be expressed in the form
\[
v(x, t) = \tilde{v}(x, t) + \mathcal{H}(\phi) \tilde{v}(x, t)
\] (14)
where \( \tilde{v} \) and \( \tilde{v} \) are two continuous functions and \( \mathcal{H}(\phi) \) is the Heaviside step function. The latter depends on \( \phi = \phi(x, t) \), which is the level-set function that represents the geometry of the crack. The symmetric part of the gradient operator of (14) can be expressed as
\[
\nabla^s v(x, t) = \nabla^s \tilde{v}(x, t) + \mathcal{H}(\phi) \nabla^s \tilde{v}(x, t) + \delta(\phi) (n \otimes \tilde{v})^s
\] (15)
Note that \( \nabla^s \mathcal{H}(\phi) = \delta(\phi) \nabla \phi \), where \( \delta \) is the Dirac delta function defined as being singular at \( \phi = 0 \) and zero elsewhere. The gradient of a level-set function represents the normal to the surface, i.e. \( \nabla \phi = n \). The level-set that is employed here is the signed distance function, i.e. \( \phi(x) = \text{sign} \{ n_r \cdot (x - x_r) \} \min \| x - x_r \| \), as introduced in Sukumar et al. (2001). As mentioned in the introduction, different methodologies can be used to incorporate the discontinuous motion into the solution. In the approach pursued here the discontinuity is embedded in the constitutive law by averaging the localized deformation over the REV.
Examining eq. (15), it can be noted that the first two terms describe the motion in the intact part of the REV while the third term that involves the Dirac function is associated with the localized deformation along the crack. This term can be averaged over the differential volume \( \Delta v \)

\[
\frac{1}{\Delta v} \int_{\Delta v} \delta(\phi)(\mathbf{n} \otimes \mathbf{g})^T \, d\Omega = \frac{1}{\Delta v} \int_{\Delta a} (\mathbf{n} \otimes \mathbf{g})^T \, d\Gamma
\]

(16)

Here, \( \Delta a \) represents the surface area of the crack within the REV, while \( \mathbf{g} \) is the discontinuous motion along the interface, i.e. \( \mathbf{g} = \| \mathbf{v} \| = \| \mathbf{\gamma} \| \mathbf{\delta} \). Ignoring the variation of this discontinuous motion within a small-enough REV, one may express eq. (16) as

\[
\frac{1}{\Delta v} \int_{\Delta v} \delta(\phi)(\mathbf{n} \otimes \mathbf{g})^T \, d\Omega \approx \chi(\mathbf{n} \otimes \mathbf{g})^T \quad \text{with} \quad \chi = \frac{\Delta a}{\Delta v}
\]

(17)

Thus, the total strain rate can be divided into two elementary parts. The first one, denoted as \( \hat{\mathbf{\varepsilon}} \), is associated with the intact part of the REV, while and the other one, referred to as \( \mathbf{\varepsilon} \), represents the discontinuous motion along the crack averaged over the REV, i.e.

\[
\mathbf{\varepsilon} = \hat{\mathbf{\varepsilon}} + \mathbf{\varepsilon} \quad \text{where} \quad \hat{\mathbf{\varepsilon}} = \chi (\mathbf{n} \otimes \mathbf{g})^T
\]

(18)

Adopting the additivity of strain rates, the stress field within the REV can be defined as

\[
\mathbf{\sigma} = \mathbb{D} : \dot{\mathbf{\varepsilon}} = \mathbb{D} : (\hat{\mathbf{\varepsilon}} + \hat{\mathbf{\varepsilon}})
\]

(19)

In order to determine the velocity discontinuity \( \mathbf{g} \) that is embedded in the constitutive relation (19), the continuity of the rate of traction along the interface is imposed, i.e. \( \dot{\mathbf{t}} = \mathbf{n} \cdot \mathbf{\sigma} \). Thus,

\[
\{ \mathbf{n} \cdot \dot{\mathbf{\sigma}} \} = \{ \mathbf{n} \cdot \mathbb{D} : \dot{\mathbf{\varepsilon}} - \chi \mathbf{n} \cdot \mathbb{D} : (\mathbf{n} \otimes \mathbf{g}) \} = \{ \dot{\mathbf{t}} = \mathbf{K} : \mathbf{g} \}
\]

\[
\rightarrow \dot{\mathbf{\varepsilon}} = \mathbb{E} : \mathbb{D} : \dot{\mathbf{\varepsilon}} \quad ; \quad \mathbf{E} = \chi \mathbf{n} \otimes (\mathbf{K} + \chi \mathbf{n} \cdot \mathbb{D} \cdot \mathbf{n})^{-1} \otimes \mathbf{n}
\]

(20)

where \( \mathbf{K} \) is the tangential operator which defines the interfacial properties. Thus, the constitutive relation within the region experiencing the discontinuous motion may be finally expressed as

\[
\dot{\mathbf{\sigma}} = \mathbb{D} : \dot{\mathbf{\varepsilon}} \quad \text{where} \quad \mathbb{D} = \mathbb{D} - \mathbb{D} : \mathbb{E} : \mathbb{D}
\]

(21)

where \( \mathbb{D} \) is the tangential operator.

2.3. Specification of the orientation of macrocrack at its inception

The issue of the onset of localization may be perceived as a bifurcation problem (Rudnicki and Rice, 1975). Such an approach, although mathematically rigorous, strongly relies on the constitutive description of homogeneous deformation, including the type of hardening and/or flow rule, and the predictions are not always consistent with the experimental evidence. A simpler approach is to assume that the inception of localized damage occurs when the failure function reaches a critical value. For the analysis conducted in this work, the Mohr-Coulomb criterion (6) is checked at every Gauss point within the volume of a finite element that is considered as a REV. If the average value of \( F \) approaches zero, the element is said to undergo a discontinuous motion; the level-set is updated and the next load increment is applied. In order to carry out the integration of the constitutive law (21), the orientation of the macrocrack must be defined. This is accomplished by invoking the critical plane approach as explained below.
Within the context of the critical plane framework (Pietruszczak and Mroz, 2001), the failure function is defined as a function of the components of traction vector $\mathbf{t} = \mathbf{n} \cdot \mathbf{s}$ acting on a plane with unit normal $\mathbf{n}$. For reproducing the bias in the special distribution of strength parameters, say $h(\mathbf{n})$, a scalar descriptor $\phi$ is defined such that

$$F = F[\mathbf{t}, h(\mathbf{n})]; \quad h = \hat{h}(1 + \phi + b_1\phi^2 + b_2\phi^3 + b_3\phi^4 + \cdots), \quad \phi = \mathbf{n} \cdot \Omega \cdot \mathbf{n} \quad (22)$$

where, $b_1, b_2, b_3$ are constants and $\Omega$ is a symmetric traceless tensor whose eigenvectors coincide with the principle material axis.

Thus, the Coulomb failure function can be expressed here as

$$F = |\tau| - (\mu_f \sigma + c) \quad (23)$$

where $\tau, \sigma$ are tangential and normal components of traction $\mathbf{t}$, and the friction coefficient $\mu_f$ as well as cohesion $c$ are both assumed to be orientation dependent, i.e. $\mu_f = \mu_f(\mathbf{n})$ and $c = c(\mathbf{n})$, and their distribution is defined viz. representation (22). The problem of the specification of the direction of macrocrack can then be defined as a constrained optimization problem for failure function (22), i.e.

$$\max_{\mathbf{n}} F = \max_{\mathbf{n}} F[\mathbf{t}, h(\mathbf{n})] \quad | \quad F = 0 \land \mathbf{n} \cdot \mathbf{n} = 1 \quad (24)$$

The above equation may be solved by any known optimization technique, such as Lagrange multipliers, and the result would define the direction of the localization plane at any integration point.

It should be noted that the conditions at failure as stipulated by eqs. (23) and (24) are consistent with the Mohr-Coulomb representation (6) provided the strength parameters $h(\mathbf{n})$, eq. (22), are properly identified. This issue is addressed further in section 4, which deals with the numerical implementation. In general, the solution will provide two conjugate orientations. Here, the orientation that maximizes the product $\Delta \varepsilon : (\mathbf{n} \otimes \mathbf{m})$, where $\mathbf{m}$ is the direction of discontinuous motion $\mathbf{g}$, is selected to define the prevailing orientation of the localization plane, as suggested by Rabczuk and Belytschko (2007).

### 3. The numerical integration schemes

As indicated in the previous section, the deformation process involves two stages; one deals with a homogeneous deformation that is governed by the constitutive law (13) and the other one is associated with localized deformation, viz. eq. (21). In what follows, the implicit integration schemes for both these cases are derived.

#### 3.1. The integration scheme for elasto-plastic model governing the homogeneous deformation mode

In this case, in order to simplify the algebra, it is convenient to refer the problem to the coordinate system associated with the principal material axes. According to eq.(10), the constitutive relation takes the form
\[ \sigma = \sigma_i + \mathbb{D} : (\Delta \varepsilon - \Delta \varepsilon^p), \quad \Delta \varepsilon^p = \Delta \lambda \partial_\alpha \psi \]  

(25)

where \( \mathbb{D} \) is the elastic stiffness operator, \( \psi \) is the potential function defined in eq.(9) and \( \Delta \lambda \) is the plastic multiplier. Here, the variables without a subscript refer to time \( t + \Delta t \). Using the closest point projection approach (Simo, 1998), the plastic strain and the yield function residuals at time \( t + \Delta t \) can be expressed as

\[ R^{(k)} \equiv -\varepsilon^{p(k)} + \varepsilon_n^p + \Delta \lambda^{(k)} \partial_\alpha \psi^{(k)} \]

\[ f^{(k)} \equiv f(\sigma^{(k)}, \lambda^{(k)}) \]  

(26)

Linearizing the above equations, one can write

\[ R^{(k)} + \partial_\alpha R^{(k)} : \delta \sigma^{(k)} + \partial_\lambda R^{(k)} : \delta \lambda^{(k)} = 0 \]

\[ f^{(k)} + \partial_\alpha f^{(k)} : \delta \sigma^{(k)} + \partial_\lambda f^{(k)} : \delta \lambda^{(k)} = 0 \]  

(27)

with the derivatives expressed as \( \partial_\alpha R^{(k)} = \mathbb{C} + \Delta \lambda \partial_\alpha \psi \) and \( \partial_\lambda R^{(k)} = \partial_\alpha \psi \), where \( \mathbb{C} \) is the compliance operator. Denoting \( \mathbb{Q} = \partial_\alpha R^{-1} \), the plastic multiplier, stress and plastic strain corrections can be determined as

\[ \delta \lambda^{(k)} = \frac{f^{(k)} - \partial_\alpha f^{(k)} : \mathbb{Q}^{(k)} : R^{(k)}}{\partial_\alpha f^{(k)} : \mathbb{Q}^{(k)} : \partial_\alpha \psi^{(k)} - \partial_\lambda f^{(k)}} \]

\[ \delta \sigma^{(k)} = -\mathbb{Q}^{(k)} : [R^{(k)} + \partial_\alpha \psi^{(k)} \delta \lambda^{(k)}] \]

\[ \delta \varepsilon^{p(k)} = -\mathbb{C} : \delta \sigma^{(k)} \]  

(28)

and the updated variables can be specified as

\[ \Delta \lambda^{(k+1)} = \Delta \lambda^{(k)} + \delta \lambda^{(k)} \]

\[ \sigma^{(k+1)} = \sigma^{(k)} + \delta \sigma^{(k)} \]

\[ \varepsilon^{p(k+1)} = \varepsilon^{p(k)} + \delta \varepsilon^{p(k)} \]  

(29)

Note that the anisotropy parameter \( \vartheta \) is embedded in the gradient operators \( \partial_\alpha f, \partial_\alpha \psi \) as indicated in eq.(12)

3.2. The integration scheme for constitutive model with embedded discontinuity

Considering eq.(19), one can express the stress state in the intact material at \( t + \Delta t \) as

\[ \sigma = \sigma_i + \mathbb{D} : (\Delta \varepsilon - \Delta \varepsilon^p) \quad \text{where} \quad \Delta \varepsilon = \chi (\mathbf{n} \otimes \Delta \mathbf{g})^p \]  

(30)

The interfacial constitutive model can be defined as

\[ \mathbf{t} = \mathbf{t}_i + \mathbf{K} : (\Delta \mathbf{g} - \Delta \mathbf{g}^p), \quad \Delta \mathbf{g}^p = \Delta \gamma \partial_\gamma \psi \]  

(31)

In the examples provided in section 4, the yield and plastic potential functions for the interface material are taken in a simple linear form
where \( g \) is the tangential component of plastic part of velocity discontinuity and \( \mu \) is the friction coefficient. The latter is assumed to be monotonically decreasing according to an exponential relation (32), in which \( \mu_0, \mu_r \) are the initial and residual values of \( \mu \) and the rate of degradation is governed by the parameter \( \omega \).

Imposing the consistency condition \( \Delta f = 0 \) along the interface, one obtains

\[
\Delta t = K^{op} \cdot \Delta g \quad \text{where} \quad K^{op} = K - \frac{(\nabla f) \otimes (\nabla f)}{\nabla f \cdot \nabla f - \nabla f} \quad (33)
\]

In order to formulate the return mapping scheme, the following residuals are introduced

\[
R^{(k)}_1 \equiv \tilde{\varepsilon}^{(k)} + \varepsilon^{(k)} + \chi (n \otimes \Delta g^{(k)})' \\
R^{(k)}_2 \equiv n \cdot \sigma^{(k)} - t^{(k)} \quad (34)
\]

Linearizing these residuals

\[
R^{(k)}_1 + \partial \cdot R^{(k)}_1 : \delta \sigma^{(k)} + \partial \cdot R^{(k)}_1 : \delta g^{(k)} = 0 \\
R^{(k)}_2 + \partial \cdot R^{(k)}_2 : \delta \sigma^{(k)} + \partial \cdot R^{(k)}_2 : \delta g^{(k)} = 0 \quad (35)
\]

and substituting for the derivatives, one has

\[
R^{(k)}_1 + \partial \cdot \delta \sigma^{(k)} + \chi (n \otimes \Delta g^{(k)})' = 0 \\
R^{(k)}_2 + n \cdot \delta \sigma^{(k)} - K : \delta g^{(k)} = 0 \quad (36)
\]

Solving now eqs.(36) for stress and strain corrections, one obtains

\[
\delta g^{(k)} = [\chi (n \cdot \mathbb{D} \cdot n) + K^{(k)}]^{-1} \left( R^{(k)}_2 - n \cdot \mathbb{D} : R^{(k)}_1 \right) \\
\delta \sigma^{(k)} = -\mathbb{D} : (R^{(k)}_1 + \chi (n \otimes \delta g^{(k)})') \\
\delta \varepsilon^{(k)} = C : \delta g^{(k)} \quad (37)
\]

with

\[
g^{(k+1)} = g^{(k)} + \delta g^{(k)} \\
\sigma^{(k+1)} = \sigma^{(k)} + \delta \sigma^{(k)} \\
\varepsilon^{(k+1)} = \varepsilon^{(k)} + \delta \varepsilon^{(k)} \quad (38)
\]

Note that the tangential operator is defined here viz eq.(21).

4. Numerical study: bi-axial plane strain tests on Tournemire argillite

The numerical study presented here deals with the description of localized damage in Tournemire argillite rock subjected to plane strain biaxial compression. The focus is on examining
the influence of boundary conditions, as well as the orientation of the bedding planes, on the failure mechanism and the resulting assessment of compressive strength. The study makes use of the results of triaxial tests that have been reported by Abdi and Evgin (2013). Those results were employed to identify the material parameters/functions that enter the formulation, as discussed in section 2. The details on the identification procedure, which is based on a comprehensive examination of a series of tests conducted at different orientation of the sample relative to the direction of loading and different confining pressures, are provided in the forthcoming proceedings of the ISRM Congress (Haghighat and Pietruszczak, 2015). Based on that study, the following material parameters were identified for the anisotropic deviatoric hardening model describing the homogeneous deformation mode, viz. section 2.1

\[ E_n = 12.5 \text{ GPa}, \quad E_t = 21 \text{ GPa}, \quad G_{nt} = 4.57 \text{ GPa}, \quad \nu_{nt} = 0.16, \quad \nu_t = 0.08 \]

\[ \hat{\eta}_f = 1.07252, \quad A_i = 0.170336, \quad a_i = 5.49565 \]

\[ \alpha = 0.99, \quad \xi = 1.25, \quad C = 10.61 \text{ MPa}, \quad A = 0.0012 \]

where \( n, t \) define the normal and tangential direction, respectively, in the coordinate system attached to a bedding plane. As an illustration, the spatial variation of the strength parameter \( \eta_f \), eq.(6), is depicted in Fig.1 below.

---

Fig. 1- Variation of strength parameter \( \eta_f \) vs left) microstructure parameter \( \xi \) and right) loading angle

---

Given the distribution of \( \eta_f \) as a function of the loading angle, the corresponding values of the friction angle \( \phi \) and the cohesion \( c \) can be calculated from \( \phi = \sin^{-1}(3\eta_f/(6+\eta_f)) \) and \( c = C\eta_f(3 - \sin \phi)/(2\sqrt{3} \cos \phi) \), respectively. The latter values are required for identification of the critical plane framework, which is employed to define the orientation of the localization plane. The best-fit approximation, which retains the second-order terms, i.e.

\[ \mu = \hat{\mu}(1 + \Omega_y n_i n_j + A_i(\Omega_y n_i n_j)^2), \quad c = \hat{c}(1 + \Omega_y n_i n_j + A_i(\Omega_y n_i n_j)^2) \]

and \( \mu = \tan \phi \), results in the following set of coefficients

\[ \hat{\mu} = 0.51063, \quad \hat{c} = 5.41646, \quad \Omega_y = 0.19448, \quad A_i = 4.79833 \]
The corresponding spatial variation of strength parameters is plotted in Fig. 2. It should be noted that since $C$ is defined as orientation independent, the distribution of both descriptors displays a similar bias.

![Fig. 2- Distribution of friction angle $\phi$ and cohesion $c$ with respect to the orientation of the bedding planes $\beta$](image)

For the interfacial material, once the localization occurs the parameter $\mu_f^0$, eq. (32), is determined based on the ratio of the components of the traction vector, i.e. $\mu_f^0 = -|\tau|/\sigma$. The simulations presented here were conducted assuming the following set of elastic moduli and the degradation coefficients, eq. (32)

$$K_n = K_t = 1 \times 10^5 \text{MPa/mm}, \quad \mu_f^0 = 0.7 \mu_f^0, \quad \omega = 5.45 \text{mm}^{-1} \quad (41)$$

These values were selected on a rather intuitive basis as no explicit experimental evidence is available.

The set up for the biaxial test and the corresponding boundary conditions are shown in Fig. 3. The sample has in plane dimensions of $100 \times 50$ mm and out of plane thickness of $50$ mm. The load was applied incrementally in two stages. The first one involved subjecting the sample to a confining pressure $P_0$. After this, the displacement field was set to zero and the vertical displacement $\delta$ was applied.

![Fig. 3- Biaxial test configuration and boundary conditions](image)
In order to simulate the actual test conditions, a simple elastic spring model was used to incorporate the effect of friction between the loading platens and the sample. Five different stiffness coefficients were employed ranging from \( K =1\times10^{-4} \) to \(1\times10^{10} \) N/mm which are representative of frictionless and fully constrained (sticking friction) conditions, respectively. Fig.4 shows the evolution of the interfacial displacement in an inclined sample, \( \beta = 45^\circ \), for different values of coefficients \( K \).

![Figure 4](image)

Fig. 4- Average horizontal sliding between plate and sample for the case of \( \beta = 45^\circ \)

Fig. 5 shows the distribution of the damage ratio \( \eta / \eta_f \), which is defined according to eqs.(8) and (6). Note that \( 0 \leq \eta / \eta_f \leq 1 \), with \( \eta / \eta_f = 1 \) signifying the onset of macrocrack formation. The distribution corresponds to the instant just before the onset of localization and refers to a sample tested at \( \beta = 45^\circ \). The results shown in Fig.5 correspond again to different frictional constraints at the end platens (viz. the coefficients \( K \)). It is evident from this figure that for low values of \( K \), i.e. \( K \leq 1\times10^1 \) N/mm, the stress and deformation fields remain homogeneous. On the other hand, for \( K \geq 1\times10^3 \) N/mm, i.e. when the friction is more significant, the deformation is localized into a shear band/macrocrack that forms at the corners and/or at the center of the sample.

![Figure 5](image)

Fig. 5- Damage ratio \( \eta / \eta_f \) for different values of friction at the end platens; \( \beta = 45^\circ \)
Fig. 6 shows the corresponding load-displacement characteristics. As can be seen here, the value of the coefficient $K$ significantly affects the ultimate (peak) load. This implies that the friction between loading platens and the sample plays an important role in the assessment of both the load capacity and the actual failure mode of the sample.

![Load displacement curves for different values of friction at the end platens; $\beta = 45^\circ$](image)

Fig. 6- Load displacement curves for different values of friction at the end platens; $\beta = 45^\circ$

Fig. 7 shows the evolution of the damage ratio $\eta / \eta_f$ just before the onset of localization for tests conducted at different orientations of the bedding planes. The results correspond to $K \geq 1 \times 10^5$ N/mm. It is evident here that in case of horizontal and vertical bedding planes, the failure mode is largely diffused while for the inclined samples, there is an indication of a shear band/macrocrack formation. The actual failure mechanism, as obtained from numerical simulations, is depicted in Fig. 8 for various bedding planes orientations.

![Damage ratio evolution](image)
Fig. 7- Damage ratio $\eta / \eta_j$ at the crack initiation for different orientations of bedding planes $\beta$; $K \geq 1 \times 10^5$

Fig. 8-The predicted failure pattern in samples tested at different orientation of bedding planes $\beta$

The last study conducted here deals with the issue of the mesh dependency of the solution based on the approach followed in this work. The key results are shown in Figs. 9 and 10. The simulations involved three different discretizations. The basic mesh, i.e. mesh 1, is identical to the one employed in all simulations presented earlier. Mesh 2 is a refined structured mesh while mesh 3 is an unstructured mesh that is oriented along the direction of the shear band corresponding to the localization pattern predicted from the previous meshes. The load- displacement cures are provided in Fig. 9, whereas Fig. 10 shows the deformed shape with the scale factor of 10. It is quite evident here that the solution is mesh-independent, i.e. the ultimate load as well as deformation pattern are virtually the same.
5. Concluding remarks

In this study, the problem of description of deformation and progressive damage in anisotropic rock formations was examined. The primary focus was on modeling of the discrete propagation pattern associated with strain localization. The deformation prior to failure was described using an elasto-plastic formulation incorporating the microstructure tensor approach. The onset of failure was defined by employing a simple stress criterion formulated within the context of a deviatoric
hardening model. The orientation of the localization plane was then established based on the critical plane approach by converting the strength parameters used in the elasto-plastic model. The constitutive law with embedded discontinuity was used to model the post failure response associated with localized failure mode. The discrete propagation of damage was monitored through the level-set method. The closest-point projection integration scheme was derived for both the anisotropic deviatoric hardening model and the constitutive law with embedded discontinuity.

The mechanical characteristics of Tournemire shale were examined and the effect of boundary condition on the shear band formation was investigated for a series of biaxial plane strain compression tests. It was shown that in the case of a frictionless interface between loading platens and the sample, the deformation field remains homogeneous and the failure mode is diffused. With a presence of friction, however, the stress state is significantly perturbed which results in formation of a shear band/macrocrack. In this case, the ultimate strength of the sample is noticeably less than the one attained under frictionless conditions. A series of simulations for samples with different orientations of bedding planes was also conducted. It was shown that in samples with horizontal and vertical bedding planes, the failure mode is diffused for both frictionless and fully constrained cases; however the peak strength is still noticeably different for both these cases.

In summary, the results of simulations clearly demonstrated that friction between loading platens can play an important role in the process of evolution of damage and may significantly affect the strength characteristics that are commonly perceived as a material property. This is particularly the case for inclined samples.

Finally, the mesh-dependency of the solution was examined using three different discretizations. Two structured meshes of different size and one mesh oriented along the direction of shear band were employed. It was concluded that by invoking the constitutive law with embedded discontinuity, which incorporates a characteristic dimension, the solution is virtually mesh independent.

References


MODELING OF DELAYED FAILURE OF EMBANKMENTS DUE TO WATER INFILTRATION

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Abstract

The primary focus here is on modeling of fracture propagation in soils with apparent cohesion subjected to a period of intense rainfall. In this case, a micromechanically-based description represents an overwhelming task due to a very complex system of mineralogical and chemical factors. This is particularly evident at the range of irreducible saturation. Recognizing this limitation, the approach followed here is based on the framework of chemo-plasticity. The formulation incorporates an assumption that the injection of water triggers a volume change (swelling/collapse) that is coupled with a reduction in suction pressures which, in turn, results in degradation of the strength and deformation properties. The modeling of localized failure mode is based on a constitutive law formulated through volume averaging in the neighborhood of the embedded discontinuity. The latter is enhanced by employing the level set method. The governing equations are applied to examine the stability of a slope in cohesive soils, subjected to a period of intense rainfall.

Keywords: Chemo-plasticity; Slope-stability; Shear band modeling.

1. INTRODUCTION

Increased precipitation often leads to a loss of stability of geotechnical structures. Examples include here the natural slopes and embankments constructed in cohesive soils. In recent years, several case histories have been documented, both in Canada as well as in other parts of the world (e.g., in China, Korea, Malaysia, South America), whereby the failure of engineered and/or natural slopes was related to the loss of apparent cohesion triggered by the local weather conditions [1-3]. The primary difficulty in modeling the loss of stability due to a heavy rainfall lies in assessing the in-situ conditions and in describing the coupling between the time-dependent process of water infiltration and the evolution of the stress/pore pressure field. The problem is typically analyzed by integrated software in which the transient seepage is coupled with traditional limit equilibrium slope stability analysis [4-6]. Alternatively, the frameworks for unsaturated soil are implemented in which the suction pressure is considered as a state parameter and an optimization technique is used to search for a critical slip surface (e.g., [4]). In general, the conventional methods for assessing the stability of unsaturated soils, based on the limit equilibrium approach, significantly underestimate the safety factors. Therefore, more accurate techniques are required.

The specification of properties of unsaturated clayey soils is difficult. This is particularly the case when dealing with low degrees of saturation, i.e. within the range of irreducible saturation, as the latter involves a very complex system of mineralogical and chemical factors. In clays, the
bond strength increases rapidly with decreasing water content. The water in the vicinity of minerals, however, has quite different properties which cannot, in fact, be quantified due to complex chemical interactions. Therefore, the assessment of suction pressures and their evolution is difficult, which is the main reason why the developments in the area of mechanics of unsaturated soils have not found their utility in a parallel development of design methodologies. Recognizing the above limitations, a different approach is pursued here. In particular, at the range of irreducible saturation (cf. [7]), when the water phase is discontinuous, the behavior of the material is described based on a phenomenological framework of chemo-plasticity (cf. [8-10]). Within this framework, an increase in water content due to wetting is said to trigger a reduction in the interparticle bonding and the corresponding degradation of strength and deformation properties at the macroscale. At the stage when the water phase becomes continuous, the behaviour can then be defined in mechanical terms alone; for example, by employing an averaging procedure in which the compressibility of the pore space is expressed as a function of properties of constituents (free water and air) and the microstructure of saturation ([11,12]).

The research presented here is an extension of the work recently reported by [13], and it is focused on the development of a general methodology that includes modeling of the onset and propagation of failure in geotechnical structures subjected to water infiltration. In the next section, a brief overview is given pertaining to the evolution of microstructure of saturation during the infiltration process. In the subsequent section, the formulation of the problem is discussed, viz. chemo-plasticity, including the notion of modeling of localized deformation. Two numerical examples are given. The first one, aimed at illustrating the proposed methodology, deals with simulation of a biaxial test on dense sand. The second one involves a transient hydro-mechanical analysis investigating the stability of a slope in cohesive soils subjected to a period of intense rainfall. In solving the problem, the evolution of the phreatic surface is monitored and coupled with mechanical analysis incorporating the propagation of localized damage triggered by the chemical interaction.

2. ON MICROSTRUCTURE OF SATURATION IN GRANULAR SOILS

During the infiltration process the microstructure of saturation undergoes a progressive evolution, which should be accounted for in the course of specification of hydraulic/mechanical properties of the material. In general, referring to Fig.1, four different types of microstructure can be distinguished in partially saturated soils [14]:

(A) At very low degrees of saturation, the gas phase is continuous while the liquid phase is discontinuous (i.e., the liquid phase is present only within the interparticle contact areas)

(B) At higher degrees of saturation, both the gas and the liquid phase remain continuous

(C) As the degree of saturation is further increased, the gas phase becomes discontinuous (e.g., bubbles embedded in the liquid phase)

(D) Large bubbles may be entrapped in saturated matrix (‘gassy’ soil).

The common types are (A) to (C) and during the infiltration process the microstructure will abruptly change from one type to another. The last structure (D) is formed when the gas (produced by decomposition of organic matter) pushes against the soil skeleton creating gas voids of a size that is much larger than the average particle size.

It should be noted that for soil types B, C and D the liquid (water) phase is continuous and has known mechanical properties. In this case, for each specific geometric arrangement of the
microstructure of saturation, the mechanical properties can be defined in terms of properties of the skeleton, air and the free water. In this case, the formulation incorporates the degree of saturation as well as the ‘average pore size’ which is considered to be an independent characteristic dimension (c.f. [11,12]). Alternatively, the problem has also been phrased using the notions of unsaturated soil mechanics [15] whereby the suction pressure is introduced as an independent state variable. Note, however, that the latter approach does not make any explicit reference to the type of microstructure.

At the range of irreducible saturation, which is of main focus here, the water phase is discontinuous and the soil microstructure is of the type A. In this case, the specification of properties, particularly in clayey soils, is difficult as the problem involves complex physical-chemical interactions and the properties of water in the vicinity of minerals cannot be easily quantified. Thus, the control/measurement of suction pressures is rather problematic and the problem cannot be approached as purely mechanical one. In view of these difficulties, the approach adopted here for the type A soil is based on the phenomenological framework of chemo-plasticity which is preferred to the classical notions of unsaturated soil mechanics.

![Figure 1. Microstructure of partially saturated soils: Soil types A through D](image)

### 3. FORMULATION OF THE PROBLEM

#### 3.1. Chemo-plasticity framework

The general approach for modeling the evolution of properties of clays in the presence of the interparticle bonding is based on the framework of chemo-plasticity. The particular formulation outlined here is analogous to that described in the recent article by [13]. Within this approach, the progress in chemo-mechanical interaction is monitored by a scalar parameter $\zeta$, which may be interpreted as the change in the initial suction pressure $u_s^0$, at the irreducible wetting fluid saturation, in REV; i.e. $\zeta \propto (u_s^0 - u_s^0) / u_s^0$, so that $\zeta \in [0,1]$.

The evolution law can be taken in a simple linear form

$$\frac{\partial \zeta}{\partial t'} = B(1 - \zeta); \quad dt' = gdt$$

where $g \in [0,1]$ depends on the chemical composition of the clay minerals and water, and $B$ is a material constant. In the elastic range, the constitutive relation takes the form

$$\varepsilon^e_{ij} = C^e_{ijkl} \sigma_{kl} + \epsilon \zeta \delta_{ij}$$

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Here, $\sigma_{ij}$ is the effective stress, $C_{ijkl}^e$ is the elastic compliance operator and the last term represents the volumetric strain due to wetting, with $\epsilon$ being the maximum expansion/contraction in the stress-free state. Note that the differential form of eq. (2) may be expressed as

$$\dot{\epsilon}_{ij} = C_{ijkl}^e \delta_{kl} + \left( \partial_{\zeta} C_{ijkl}^e \sigma_{kl} + \epsilon \delta_{ij} \right) \dot{\zeta}$$

(3)

In order to specify the plastic strain rates, the functional form of the yield criterion $f = 0$ is assumed to be affected by the chemical interaction, i.e.

$$f = f(\sigma_{ij}, \kappa, \zeta) = 0; \quad \kappa = \kappa(\varepsilon_{ij}^p); \quad \dot{\varepsilon}_{ij}^p = \lambda \frac{\partial \psi}{\partial \sigma_{ij}}$$

(4)

where $\kappa = \kappa(\varepsilon_{ij}^p)$ is the hardening parameter and $\psi = \psi(\sigma_{ij}, \zeta)$ is the plastic potential function.

Employing now the consistency condition, the plastic multiplier $\dot{\lambda}$ can be defined as

$$\dot{\lambda} = \frac{1}{H} \left( \frac{\partial f}{\partial \sigma_{ij}} \dot{\sigma}_{ij} + \frac{\partial f}{\partial \zeta} \dot{\zeta} \right); \quad H = - \frac{\partial f}{\partial \kappa} \frac{\partial \kappa}{\partial \varepsilon_{ij}^p} \frac{\partial \psi}{\partial \sigma_{ij}}$$

(5)

Thus, invoking the additivity postulate and using the equations (3)-(5), the constitutive relation may be expressed as

$$\dot{\epsilon}_{ij} = C_{ijkl} \sigma_{kl} + b_{ij} \dot{\zeta}; \quad b_{ij} = \partial_{\zeta} C_{ijkl} \sigma_{kl} + \frac{1}{H} \frac{\partial f}{\partial \zeta} \frac{\partial \psi}{\partial \sigma_{ij}} + \epsilon \delta_{ij}; \quad C_{ijkl} = C_{ijkl}^e + \frac{1}{H} \frac{\partial \psi}{\partial \sigma_{ij}} \frac{\partial f}{\partial \sigma_{kl}}$$

(6)

Note that the inverse form, defining the stress rates for given strain rates, can be expressed as

$$\dot{\sigma}_{ij} = D_{ijkl} \left( \dot{\epsilon}_{kl} - b_{ij} \dot{\zeta} \right); \quad D_{ijkl} = C_{ijkl}^{-1}$$

(7)

### 3.2. Description of localized deformation

In this work, the propagation of localized failure is modeled by employing the volume averaging to estimate the properties of an initially homogeneous medium intercepted by a shear band/interface [16,17]. The constitutive relation incorporates the properties of constituents (i.e., intact material and interface) as well as a characteristic dimension associated with the structural arrangement. This approach is later enhanced by incorporating the level set method, similar to that used in Extended Finite Element Method [18,19], in order to capture a discrete nature of the shear band propagation process.

A discontinuous motion within a representative volume $\Delta V$ which contains a discontinuity surface $\Gamma$, can be defined as

$$v_i(x_i,t) = \hat{v}_i(x_i,t) + \mathcal{H}_r \bar{v}_i(x_i,t)$$

(8)

where, $v_i(x_i,t)$ and $\hat{v}_i(x_i,t)$ are continuous functions and $\mathcal{H}_r$ is the Heaviside step function. Denoting the velocity discontinuities across the interface as $\bar{v}_i = \left[ \frac{1}{3} v_i \right]$, a symmetric part of the velocity gradient $v_{ij}^s$ can be expressed...
\begin{equation}
\mathbf{\dot{v}}_{i,j}^s = \mathbf{\hat{v}}_{i,j}^s + \mathbf{H}_t \mathbf{\tilde{v}}_{i,j}^s + \mathbf{\delta}_t (\mathbf{\dot{g}}_i, n_j)^s
\end{equation}

where, \( \mathbf{\delta}_t \) is the Dirac delta function. The procedure for assessing the equivalent properties within a representative volume \( \Delta V \) intercepted by a shear band is based on averaging scheme, viz.

\begin{equation}
\frac{1}{\Delta V} \left( \int_{\Delta V} \mathbf{v}_{i,j}^s \, dV \right) = \frac{1}{\Delta V} \left( \int_{\Delta V} \left( \mathbf{\hat{v}}_{i,j}^s + \mathbf{H}_t \mathbf{\tilde{v}}_{i,j}^s \right) \, dV + \int_{\Delta V} \mathbf{\delta}_t (\mathbf{\dot{g}}_i, n_j)^s \, dV \right)
\end{equation}

which implies

\begin{equation}
\mathbf{v}_{i,j}^s = \mathbf{\hat{v}}_{i,j}^s + k \mathbf{\tilde{v}}_{i,j}^s + \mathbf{\chi} (\mathbf{\dot{g}}_i, n_j)^s
\end{equation}

Here, \( \mathbf{v}_{i,j}^s \)'s and \( \mathbf{\dot{g}}_i \) are volume averages of the respective variables defined in eq.(10), \( \mathbf{\chi} = \Delta A / \Delta V \) and \( k = (\Delta V^+ - \Delta V^-) / \Delta V \), while \( \Delta A \) is the surface area of the interface/shear band within the representative volume. Note that the decomposition (11) may be simplified by assuming that the discontinuity divides the representative element into two approximately equal volumes, in which case there is \( k \to 0 \). Identifying now the symmetric parts of the displacement gradients with the corresponding strain rates, one can write

\begin{equation}
\mathbf{\dot{e}}_y = \mathbf{\hat{e}}_y + \mathbf{\tilde{e}}_y; \quad \mathbf{\tilde{e}}_y = \mathbf{\hat{v}}_{i,j}^s + k \mathbf{\tilde{v}}_{i,j}^s; \quad \mathbf{\hat{e}}_{i,j} = \mathbf{\chi} (\mathbf{\dot{g}}_i, n_j)^s
\end{equation}

In eq.(12), \( \mathbf{\hat{e}}_y \) defines the strain rate in the intact material, while \( \mathbf{\tilde{e}}_y \) is the strain rate due to discontinuous deformation along the interface averaged over the representative volume. In general, \( \mathbf{\hat{e}}_y \) may include both elastic and plastic components.

Within the context of the chemo-plasticity framework, as discussed in the previous section, the average stress rates in the intact material can now be defined as

\begin{equation}
\mathbf{\hat{\sigma}}_y = D_{ijkl} \left( \mathbf{\hat{e}}_kl - b_{kl} \mathbf{\tilde{\zeta}} \right) \quad \Rightarrow \quad \mathbf{\hat{\sigma}}_y = D_{ijkl} \left( \mathbf{\hat{e}}_kl - \mathbf{\hat{e}}_kl - b_{kl} \mathbf{\tilde{\zeta}} \right); \quad \mathbf{\tilde{\zeta}} = \mathbf{\chi} (\mathbf{\dot{g}}_i, n_j)^s
\end{equation}

The stress rate \( \mathbf{\hat{\sigma}}_y \) is subjected to the continuity condition that requires

\begin{equation}
\mathbf{\hat{\sigma}}_y n_j = i_j = K_y \mathbf{\dot{g}}_j
\end{equation}

where \( i_j \) is the traction along the interface and \( K_y \) defines the stiffness properties of the interfacial material. Note that the latter can be described using the plasticity formalism

\begin{equation}
i_j = K_y \mathbf{\dot{g}}_j; \quad f_t = f_t (t, \kappa); \quad \mathbf{\dot{g}}_i^p = \lambda \frac{\partial \psi_r}{\partial t}; \quad \kappa = \kappa (g_i^p)
\end{equation}

where, \( \mathbf{\dot{g}}_i^p \) is the plastic part of the velocity discontinuity, \( f_t, \psi_r \) are the yield and plastic potential functions, respectively, and \( \kappa \) is the softening parameter. Combining representations (13) and (14) leads, after some algebraic transformations, to the localization rule

\begin{equation}
\mathbf{\dot{g}}_i = n_p E_y D_{ijkl} \left( \mathbf{\hat{e}}_kl - b_{kl} \mathbf{\tilde{\zeta}} \right); \quad E_y = K_y + \chi D_{abg} n_a n_b
\end{equation}
which defines the local velocity discontinuities in terms of average macroscopic strain rates. Note that for a standard rate-independent plasticity there is $\dot{\zeta} \to 0$ and the representation given in [17] is recovered.

The strategy for monitoring the propagation of shear band within the context of finite element (FE) analysis is similar to that explained in the companion paper that deals with modeling of fracture process in brittle materials [13]. The interface is traced using the level set method, so that it is represented as a polygon of line segments passing through elements in which the shear band develops. The characteristic dimension $\chi$ is then evaluated based on the geometry of the element and that of the propagating localization zone.

4. APPLICATION OF CHEMO-PLASTICITY FRAMEWORK TO MODELING OF SOIL INFILTRATION

In order to trace the evolution of phreatic surface during the rainfall infiltration, the problem is defined by invoking a coupled formulation for flow through unsaturated porous media. Within this framework, the porous material is considered as a mixture of solid grains and voids; the latter filled with water and/or air. For the mathematical details pertaining to FE formulation of the initial boundary-value problem the reader is referred to the original article [13].

The numerical simulations presented here are based on the classical plasticity approach incorporating the notion of deviatoric hardening [20]. Within this approach, the loading surface $f = f(\sigma_{ij}, \kappa, \zeta)$ is defined as

$$ f = \sqrt{3} \bar{\sigma} - \eta h(\theta)(\sigma_m + c \cot \phi) = 0; \quad \eta = \eta_f \frac{\kappa}{A + \kappa} $$

(17)

Here, $\sigma_m = -\sigma_{ii}/3$, $\bar{\sigma} = (s_{ij}s_{ij})^{1/2}$ and $\theta = \sin^{-1}(-3\sqrt{3}J_3/2\bar{\sigma}^3)/3$; where $s_{ij}$ is the stress deviator and $J_3 = s_{ij}s_{jk}s_{ki}$. The parameter $\theta$ represents Lode’s angle and the function $h(\theta)$ implemented here is that proposed by [21]. Furthermore, in eq.(17), $\phi$ is the friction angle, $c$ is the cohesion and the hardening effects are attributed to accumulated plastic distortions, i.e. $\dot{\kappa} = (\dot{\varepsilon}_{ij}^p \dot{\varepsilon}_{ij}^p)^{1/2}$ where $\varepsilon_{ij}$ is the strain deviator. Note that in the hardening function given above, $A$ is a material constant and $\eta_f$ defines the value of $\eta$ at failure, i.e. $\eta \to \eta_f$ for $\kappa \to \infty$.

Assuming that the condition at failure are consistent with Mohr-Coulomb criterion, we have $\eta_f = 6\sin \phi / (3 - \sin \phi)$. Furthermore, the flow rule is assumed to be non-associated and the plastic potential function is taken in the form

$$ \psi = \sqrt{3} \bar{\sigma} + \eta_c (\sigma_m + c \cot \phi) \ln \frac{\sigma_m + \frac{c}{\sigma_m} \cot \phi}{\sigma_m^0} = 0 $$

(18)

where, $\eta_c = \text{const.}$ is a material constant.

In order to incorporate the deviatoric-hardening model within the chemo-plasticity framework, the strength parameters $\eta_f$ and $c$, as well as the Young’s modulus $E$, are assumed to undergo a progressive degradation in the course of chemical interaction. The evolution laws are taken in a simple linear form
\[ \eta_f = \eta_f^0 (1 - G_1 \zeta); \quad c = c^0 (1 - G_2 \zeta); \quad E = E^0 (1 - G_3 \zeta) \]  \hfill (19)

where \( G \)'s are material constants and the kinetics of the interaction process, viz. evolution of \( \zeta \), is governed by eq.(1).

In the localized regime, the interfacial constitutive relation is derived by invoking the classical Coulomb criterion and attributing the strain softening effects to irreversible sliding along the interface. Thus,

\[ f_t = \|t, \mathbf{m}_t\| - \mu(\gamma)(\|t, n_i + c\|) = 0; \quad \psi_t = \|t, \mathbf{m}_t\| = \text{const}. \]  \hfill (20)

where \( n_i \) is a unit vector normal to the shear band/interface, \( \mathbf{m}_i \) is an arbitrary vector normal to \( n_i \), \( c \) is the cohesion and \( \mu \) defines the frictional properties. The latter are assumed to degrade as a function of discontinuity in tangential component of velocity \( \dot{\gamma} = \dot{g}_t^p m_t \), i.e.

\[ \mu(\gamma) = (\mu_0 - \mu_r) + \mu_r \exp(-\alpha \gamma) \]  \hfill (21)

where \( \alpha \) is a constant and \( \mu_r \) defines the residual value of \( \mu \).

In what follows, two numerical examples are given. The first one is aimed at illustrating the proposed methodology and involves a numerical simulation of the onset and propagation of a shear band in a sample of dense sand subjected to axial compression under plane strain conditions. The second example deals with a coupled hydro-mechanical analysis, which involves assessment of slope stability under conditions of an intense rainfall.

### 4.1. Modeling of localized deformation in a biaxial test on dense sand

The numerical analysis carried out here involves the simulation of a biaxial (plane strain) test conducted on a dense Ottawa sand at the confinement of 100kPa [22]. The sample had the dimensions of \( 83.3 \times 152.4 \times 80.8 \) mm and the deformation was recorded by digital monitoring of nodal displacements of the grid that was imprinted on the membrane surface (see Fig.2).

The simulations were carried out assuming that the material remains elastic prior to the onset of localization. The latter was defined as \( \eta \to 0.99 \eta_f \) in the Mohr-Coulomb criterion (16). In the softening regime, the response was said to be associated with localized deformation mode, viz. eq.(15), whereby the behaviour of the shear band material was defined through eqs.(19) and (20). The key material properties, as reported by [22], were as follows

\[ E = 23 \text{ MPa}, \quad \nu = 0.3, \quad \phi = 48.2^\circ \]

while for the interface, the following material constants were employed

\[ k_N = k_T = 1000 \text{ N/mm}; \quad \mu_r = 0.6 \mu_0; \quad \alpha = 0.2 \text{ mm}^{-1} \]

where \( k_N, k_T \) are the elastic moduli.

Note that since prior to the onset of localization the material is said to be elastic, the value of \( E \) represents the secant Young’s modulus. For the localized deformation mode, the simulations were completed assuming that the shear band orientation was \( 57^\circ \) with respect to the horizontal, which was the actual value measured in the experiment. In general, however, this value should be determined through an independent criterion, such as that associated with the bifurcation properties of the constitutive relation (cf. [23]).
The boundary conditions involved no friction at the end platens while the localization was triggered by introducing an inhomogeneity in the center of the specimen (25% increase in the value of $E$). The main results of simulations are presented in Fig. 2. The figures on the left show the deformation mode, both the predicted and experimentally observed, while the figure on the right gives the corresponding material characteristics. The results of simulations are, in general, fairly consistent with the experimental data.

![Figure 2. Shear band formation in biaxial plane strain test: a) cracking pattern and post localization deformation mode; b) load-deflection curve](image)

### 4.2. Modeling of shear band initiation and propagation in clayey slopes subjected to a heavy precipitation

The analysis presented here is an extension of the recent work reported by [13]. The study involves a slope in a cohesive soil (silty clay) subjected to a period of an intense rainfall. The slope has the geometry typical of engineered slopes in Singapore; it is also representative of shallow slopes in the province of Manitoba (Canada) that underwent a translational failure in the late 1990’s.

In order to trace the evolution of the phreatic surface, a transient coupled analysis incorporating unsaturated flow was conducted. In the simulations, the history of infiltration was monitored and the framework of chemo-plasticity (Section 2.1) was used to model the degradation of mechanical properties of clay. The overall stability of the slope was assessed by examining the time history of the onset and propagation of localized damage. The simulations were carried out assuming the same material parameters as in the original reference, i.e.

\[
E = 100 \text{MPa}; \quad \nu = 0.35; \quad \eta_f = 0.98; \quad \eta_c = 0.77; \quad c = 20 \text{kPa}; \quad A = 1.0 \times 10^{-5}
\]

The constants governing the kinetics of the chemical interaction and the rate of degradation were taken as

\[
G_1 = 0.10; \quad G_2 = 0.75; \quad G_3 = 0.10; \quad B = 460.0 \text{sec}^{-1}
\]

while the parameters defining the shear band properties were selected as

\[
k_x = k_f = 1000.0 \text{MN/m}; \quad \mu_s = 0.6 \mu_f; \quad \alpha = 100.0 \text{ m}^{-1}
\]

The soil permeability was assumed as $1 \times 10^{-5} \text{m/sec}$. The transition to localized deformation was defined again in terms of the critical ratio of $\eta / \eta_f$ as $\eta \rightarrow 0.95 \eta_f$, while the local orientation
of the shear band was assumed to be at $45^\circ + \phi / 2$ with respect to the direction of the minor principal stress.

The loading process incorporated two stages. The first one involved the solution due to own weight of the material, while the second one dealt with the simulation of the infiltration process and its coupling with the mechanical response. The total height of the slope was taken as $H = 10 \text{m}$. The gravity load was applied incrementally in five layers, in order to reflect the construction sequence. By the end of first stage, the maximum value of $\eta / \eta_f$ was in the range of 0.8, indicating that no localized deformation developed (see [13]). Fig.6 presents the boundary conditions for the second stage of the analysis, i.e. the infiltration process. In this phase, the slope was said to be exposed to a heavy rainfall (i.e., precipitation in excess of 0.75 cm per hour). The boundary conditions for this stage of analysis are shown in Fig.3. Along the ground surface, the water pressure was assumed to increase linearly from an initial value of $-5 \text{kPa}$, which corresponds to $S = 5\%$, to zero in a period of $4 \text{hr}$ and then was maintained constant. Such boundary conditions are analogous to those assumed in the article by [24] and imply that the horizontal surfaces can absorb water at the rate which depends on the permeability, while the water cannot congregate along the slope.

The infiltration analysis was performed for a period of 30 days. Fig.4 shows the distribution of the degree of saturation at the end of rainfall, while Fig.5 presents the corresponding contours of $\eta / \eta_f$ and those of accumulated plastic distortions, respectively. It is evident here that, in the area around the toe of the slope, there is $\eta / \eta_f \to 1$. Finally, Fig.6 shows the predicted shear band formation. The latter is indicative of a failure mechanism forming in this region.

Figure 3. Geometry and boundary conditions for the infiltration analysis

Figure 4. Saturation at the end of rainfall (30 days)
5. FINAL REMARKS

In this paper, the problem of shear band propagation in cohesive-frictional materials has been investigated. The primary focus was on modeling of fracture process in soils with apparent cohesion subjected to a period of intense rainfall. The approach was based on employing (at very low degrees of saturation) the framework of chemo-plasticity, whereby the injection of water was assumed to trigger a reduction in initial suction pressures which, in turn, resulted in degradation of the strength and deformation properties. The modeling of fracture propagation at the macroscale incorporated a constitutive law formulated through volume averaging in the neighborhood of the embedded discontinuity. This methodology was enhanced by coupling with the level set method that has been previously used for the same class of problems within the context of the Extended Finite Element approach. A new analytical formulation has been presented for the decomposition of strain rates in the presence of a discontinuous motion.

Besides the coupled hydro-mechanical analysis dealing with environmental loads, another illustrative example has been provided that focused on the evolution of localized damage triggered by mechanical load. In particular, the propagation of fracture was examined within the context of a sample of dense sand subjected to biaxial compression under initial hydrostatic pressure. The results of simulations clearly demonstrate the ability of the volume averaging approach to describe the process of onset and propagation of localized deformation in geomaterials.

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