Computers & Geosciences 65 (2014) 13–23

Contents lists available at ScienceDirect

Computers & Geosciences

journal homepage: www.elsevier.com/locate/cageo

Hydro-mechanical model for wetting/drying and fracture development in geomaterials

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ARTICLE INFO

Article history:
Received 25 April 2013
Received in revised form
16 December 2013
Accepted 18 December 2013
Available online 28 December 2013

Keywords:
Coupled modeling
TOUGH2
Lattice models
Discrete fracture network
Desiccation cracking
Voronoi tessellation

ABSTRACT

This paper presents a modeling approach for studying hydro-mechanical coupled processes, including fracture development, within geological formations. This is accomplished through the novel linking of two codes: TOUGH2, which is a widely used simulator of subsurface multiphase flow based on the finite volume method; and an implementation of the Rigid-Body-Spring Network (RBSN) method, which provides a discrete (lattice) representation of material elasticity and fracture development. The modeling approach is facilitated by a Voronoi-based discretization technique, capable of representing discrete fracture networks. The TOUGH–RBSN simulator is intended to predict fracture evolution, as well as mass transport through permeable media, under dynamically changing hydrologic and mechanical conditions. Numerical results are compared with those of two independent studies involving hydro-mechanical coupling: (1) numerical modeling of swelling stress development in bentonite; and (2) experimental study of desiccation cracking in a mining waste. The comparisons show good agreement with respect to moisture content, stress development with changes in pore pressure, and time to crack initiation. The observed relationship between material thickness and crack patterns (*e.g.*, mean spacing of cracks) is captured by the proposed modeling approach.

1. Introduction

Geomechanical processes are known to play an important role in hydrogeological behavior (Neuzil, 2003; Rutqvist and Stephansson, 2003). Linkage between mechanics and hydrogeology occurs in two fundamental ways: (1) through interactions between rock strain, the geometry of pores and fractures, and their permeability and porosity; and (2) through interactions between fluid pressure and rock mechanical stress (Rutqvist and Stephansson, 2003). Although a number of numerical models have been developed using a continuum approach for the analysis of hydro-mechanical behavior under single phase flow conditions (*e.g.*, Noorishad et al., 1982) and multiphase flow conditions (*e.g.*, Rutqvist et al., 2002), the modeling of hydro-mechanical coupling with mechanistic representation of damage and fracture initiation/propagation remains a major difficulty (Tang et al., 2002). Such processes are of particular importance for mechanically weak geomaterials such as clays and shales. As a further complication, fractures can exhibit transient behavior as a result of self-sealing processes (Bastiaens et al., 2007). Such issues are important, *e.g.*, for geo-environmental issues related to nuclear waste disposal (Bossart et al., 2004), geologic carbon sequestration (Chiaramonte et al., 2008), and hydraulic fracturing (Kim and Moridis, 2013). Various numerical models have been developed to simulate the fracture behavior of geomaterials and structures. Such models can be broadly categorized, depending on whether the domain of interest is represented by continuum or discrete elements (Jing and Hudson, 2002). Discrete models are based on discontinuous approximations of the field variable over the computational domain, which facilitates the modeling of fracture and other discontinuous phenomena. This category includes lattice models, in which complex system behavior is represented by a collection of primitive two-node elements interconnected on a set of nodal points (Herrmann and Roux, 1990). Lattice models have been effective in studying the role of disorder in the fracture of a variety of materials, including concrete (van Mier, 1997). Particle-based methods, including the discrete element method (Cundall, 1971), are another means for studying the interactions of discrete features and their collective influence on the behavior of geological systems. Various alternative approaches are also available, such as cellular automata (Pan et al., 2012) or boundary element methods (Shen et al., 2004) to simulate fracture propagation in geomaterials. Although effective mechanical-damage models are available in the literature, the capabilities for simulating hydro-mechanical coupled processes, including fracture development, are still limited, especially for modeling fracture propagation in three dimensions.

Regarding fluid flow processes in the subsurface, discrete fracture network (DFN) models have been used for decades in situations where flow is dominated by a limited number of discrete pathways over the domain of interest, *e.g.*, in naturally fractured formations

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http://dx.doi.org/10.1016/j.cageo.2013.12.009

(Dershowitz et al., 2004). DFN models successfully addressed shortcomings of conventional continuum methods that do not capture observed preferential transport along highly localized channels. The directional dependence of flow on fracture network geometry is particularly strong in sparsely fractured rock (Painter and Cvetkovic, 2005). Discrete fractures are typically represented in 3-D numerical models as planar regions or parallel-plane 3-D objects with high aspect ratios. In 2-D numerical models, fractures take the form of line segments or 2-D objects with high aspect ratios. DFN models have often been restricted to the representation of fracture flow paths, whereas transport within the low-permeable rock matrix is either ignored or represented by approximate methods. When the matrix volume needs to be represented explicitly, such as when mechanical processes are considered, the complex geometry of discrete fractures and matrix blocks can lead to difficulties in mesh generation, particularly in the presence of fracture connections at small angles and fractures with small interceding gaps (Paluszny et al., 2007; Reichenberger et al., 2006). Simple and reliable methods are needed to introduce potential fracture planes into the computational domain. Furthermore, some problems require a dynamic representation of fracture development within the matrix and its coupling with fluid flow.

This paper presents a newly established linking of the finite volume method (*via* the TOUGH2 package (Pruess et al., 2011)) and a lattice model based on the Rigid-Body-Spring Network (RBSN) concept (Kawai, 1978; Asahina et al., 2011). TOUGH2 is used to simulate multiphase flow and transport through discrete fractures and within the matrix, whereas elasticity and fracture development are modeled by RBSN. The coupled analyses account for dynamically changing hydrologic-mechanical (HM) conditions that often exist in geological systems. Fractures are represented as discrete features that interact with a porous and permeable matrix. Existing or newly developed fracture configurations are mapped onto an unstructured, 3-D Voronoi tessellation of a spatially random set of points. One advantage of linking TOUGH2 and RBSN resides in their common utilization of a set of nodal points and properties of the corresponding Voronoi tessellation (*e.g.*, natural neighbor and volume rendering definitions). Shared use of the Voronoi tessellation facilitates every stage of the analyses, including model construction and results interpretation. Fractures propagate along Voronoi cell boundaries as HM-induced stresses evolve and exceed prescribed material strength values. After describing the methodology in Section 2, the basic capabilities of the modeling approach are demonstrated through two example applications: swelling stress development in bentonite (Section 3) and desiccation cracking in mining waste (Section 4).

2. Methodology

This section starts with brief reviews of the existing codes TOUGH2, for multi-phase flow and transport, and RBSN, for elasticity and fracture development of geomaterials (Sections 2.1 and 2.2). The linking between TOUGH and RSBN is described in Section 2.3. Several advantages of the coupled TOUGH–RBSN simulator stem from its use of Voronoi-based discretization techniques (Okabe et al., 2000), which allow discretization of dynamically changing DFNs with embedded matrix in a simple and straightforward manner. Although TOUGH2 has the capability to simulate temperature variations and some of their effects, the examples considered herein are limited to isothermal conditions.

2.1. Hydrological modeling: TOUGH2 simulator

TOUGH2 is a widely used general-purpose simulator for fluid and heat flows of multiphase and multicomponent mixtures in porous and fractured materials (Pruess et al., 2011). The numerical solution scheme is based on the integral finite difference (or finite volume) method and is compatible with both regular and unstructured numerical grids. Simulations presented here use TOUGH2 with the equations of state (EOS) Module 4 for the hydrological processes of water flow and vapor diffusion. EOS Module 4 accommodates the transport of liquid water, water vapor, and air as a noncondensible ideal gas, and accounts for vapor-pressure-lowering effects (Pruess et al., 2011). For investigations involving hydro-mechanical continuum behavior, Rutqvist et al. (2002, 2011) have coupled TOUGH2 to a commercial mechanics simulator, FLAC3D (Itasca, 2009), which has been extensively used in geo-environmental applications.

As an integrated finite difference method, TOUGH allows for flexible gridding that can accommodate representation of fractures or fracture networks embedded in a porous permeable geomaterial (*e.g.*, Zhang et al., 2004; Rutqvist et al., 2013). Fractures and their interconnections form in response to the hydro-mechanical properties and conditions, and are embedded within the matrix. By utilizing a discrete fracture approach, however, continuity of the fracture network is not assumed but rather explicitly modeled. Flow within fractures is generally assumed to follow Darcy's law. The intrinsic permeability assigned to individual fractures is often based on a parallel-plate model (Bear, 1972).

2.2. Mechanical-damage model: Rigid-Body-Spring Networks

2.2.1. Model formulation

Elasticity and fracturing of the permeable medium are modeled using the RBSN method (Kawai, 1978; Bolander and Saito, 1998), which can be viewed as a type of lattice model. Lattice topology is defined by the Delaunay tessellation of the nodal points within the computational domain. The basic unit of the RBSN is a 1-D lattice element (Fig. 1) that consists of: (1) a zero-size spring set located at the centroid of the Voronoi facet common to nodes i and j; and (2) rigid-arm constraints that link the spring set and the nodal degrees of freedom. Each node has six degrees of freedom for the 3-D case. The spring set is formed from three axial springs and three rotational springs (referenced to local coordinate axes n–s–t), as shown in Fig. 1, where the rotational springs have been omitted for clarity. The axial spring stiffnesses scale in proportion to A_{ij}/h_{ij}, where A_{ij} is the Voronoi facet area associated with nodes i and j, and h_{ij} is the distance between the same nodes. The spring stiffnesses are

$$k_s = k_t = \beta_1 k_n = \beta_1 \beta_2 E \frac{A_{ij}}{h_{ij}}, \quad k_{\phi n} = E \frac{J_p}{h_{ij}}, \quad k_{\phi s} = E \frac{I_{ss}}{h_{ij}}, \quad k_{\phi t} = E \frac{I_{tt}}{h_{ij}} \tag{1}$$

in which E is the Young's modulus, subscript ϕ signifies the rotational spring terms, J_p, I_{ss}, and I_{tt} are the polar and two

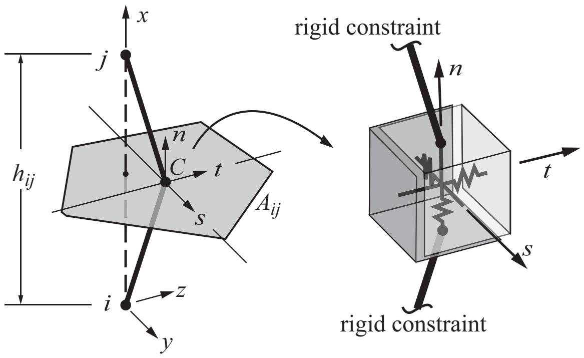

Fig. 1. Typical lattice element ij with a zero-size spring set located at centroid C of area A_{ij}, which is the area of the Voronoi facet common to neighboring Voronoi cells associated with matrix nodes i and j.