Supplemental Materials

Models for solid deformation and fluid flow

Understanding the mechanics of hydraulic fracturing requires more than an understanding of the behavior of the materials involved, considered separately. It is also necessary to consider models developed for describing and predicting the behavior of shale and of fluids in relation to one another, both how rock deforms and fractures in response to fluids, and how fluids flow in response to the structure of rock.

Hydro-mechanical models, which deal with both the fluid and solid bodies, are needed to account for shale deformation and changes in crack patterns. Analytical penny-shaped crack models were proposed to describe idealized fracture propagation, but hydraulic fracturing can be modeled more realistically with Finite Element Methods (FEM) at the reservoir scale (e.g., Adachi et al., 2007). FEM are numerical techniques that find approximate solutions to problems of this type. Extended Finite Element Methods (XFEM) use complex mathematical equations to update the position of the fracture tip (e.g., Mohammadi, 2008). In contrast, cohesive surface models assume a predefined fracture propagation path, and elasto-plastic models represent discrete fractures by irreversible deformation induced by differential stress (e.g., Schrefler et al., 2006). Current models fail at predicting the feedback effects between hydraulic fracture propagation and dissipative phenomena (i.e., irreversible deformation and micro-crack propagation) ahead of the fracture tip.

Note that micromechanics and upscaling were successfully used to determine the mechanical properties of porous solids subject to deformation and damage (Deudé et al., 2002; Lu and Elsworth, 2012; Lubarda and Krajcinovic, 1993). In those models, damage represents micro-cracks, considered as inclusions, with postulated shape and space distributions. Governing equations depend on the scale of observation: micromechanical models are formulated at the scale of pores and micro-cracks, which makes the approach questionable for attempting to capture the growth of micro-cracks into larger-scale fractures (Lacy et al., 1999). Moving to larger scales, the equations that govern the deformability of rock may still be valid, while those that govern regimes of fluid flow may not (Schubnel et al., 2006).

One way to account for crack connectivity is to introduce percolation thresholds (i.e., the transition from no- or low-flow to higher flow), which was done in a few upscaling schemes (Kondo and Dormieux, 2004). However, these upscaling schemes do not capture the three dimensional effects of micro-crack connectivity and pore shape on flow path. Moreover, micro-crack coalescence requires increasing the scale of observation, or modeling the transition from a distribution of micro-cracks (represented as continuum damage) to a discrete fracture. Transition between smeared micro-crack propagation and discrete fracture propagation was modeled based on the assumption that the characteristic dimension of the microstructure was known (Mazars and Pijaudier-Cabot, 1996), which is impractical for the prediction of damage and fractures in rocks that have discontinuities at multiple scales (such as shale).

Some other models were proposed, but were limited to periodic microstructures (e.g., Pruess et al., 1990; Zimmermann et al., 1996) or flat debonded micro-cracks (Suzuki, 2012).

In contrast with micromechanics models just discussed, continuum mechanics approaches capture the average geometrical changes (e.g., size, aspect ratio, orientation) undergone by elements of the microstructure (e.g. pores, cracks, capillaries) under variable far field boundary conditions (e.g. stress, pore pressure, temperature, chemical concentrations). Biot's theory of poromechanics couples macroscopic deformation to porosity changes. Thermodynamic models of in-pore crystallization relate variations of macroscopic stress to changes of pore orientation (Lecampion, 2010; Scherer, 2004).

However, nanometer-scale pores can contain only a few molecules of carbon dioxide or hydrocarbon,

which cannot be represented as a fluid continuum in a classical fluid flow model. Adsorption, adhesion of atoms, ions, or molecules from a gas, liquid, or dissolved solid to a surface, at this scale is controlled by chemical potentials; and the energy dissipated by the resulting fabric changes cannot be expressed by means of porosity changes and pore pressures, which are the variables used in continuum poromechanics. In meso-pores (less than a micron in size), adsorption is controlled by the energy of interfaces, which can be expressed in function of a surface stress. Stress/strain relationships are similar to the ones obtained in Biot's theory of elasticity, but encompass an adsorption stress and an adsorption strain (Vandamme et al., 2010). In micro-pores and micro-cracks (a micron in size and larger), porosity controls rock poromechanical behavior. Therefore, in nano-porous rocks, constitutive laws at different scales are governed by independent thermodynamic variables, which cannot be related by space averaging techniques employed in classical up-scaling schemes and poromechanics.

Turning from models of rock deformation to models of fluid flow in relation to rock structure, a large number of rock permeability models are based on the Kozeny-Carman relation (Carman, 1937; Kozeny, 1925), which assumes that fluid flows in a bundle of parallel pipes contained in a representative volume of rock. The mental picture of parallel pipes has some appeal; not only does it make the structure of shale easy to visualize, but it is mathematically tractable. However, it is an inadequate model of shale behavior.

Several approaches have been proposed to relate permeability to microstructure in a way that is less tidy but more adequate than the image of parallel pipes. These include: (1) modified Kozeny-Carman permeability formulas (Berryman and Blair, 1986; Brace et al., 1968; Mavko and Nur, 1997) that relate flow properties to other physical properties that indirectly account for tortuosity (e.g., electrical conductivity); (2) statistical flow networks models (Arson and Pereira, 2013; Dienes, 1982; Schubnel et al., 2006), characterized by the probability density functions of the dimensions, aspect ratios and orientations of geometric elements of the network (e.g., tubes, penny-shaped cracks, ellipsoids); (3) fractal network models (e.g., Tyler and Wheatcraft, 1990); and (4) mechanical homogenization schemes adapted to fluid flow (Kondo and Dormieux, 2004).

Fluid flow does not only depend on microstructure, but also on other coupled processes that include suction, diffusion (molecular intermingling) and dissolution. Most models that relate capillary pressure to pore size (e.g., Van Genuchten, 1980) assume that the pore network is a bundle of pipes of constant cross section, which are entirely filled with the same fluid (e.g., liquid or gas). Infiltration models capture the positive feedback effect of the dissolution front propagation on reactive fluid flow (e.g., Chadam et al., 1988). The dissolution front is assumed to be planar (e.g., Zhao et al., 2008), which is insufficient to model reactive flow in two or three dimensions.

By contrast, the percolation theory (Stauffer and Aharony, 1994) can be used to predict the space organization of connected fluid segments in a network with a pre-defined topology. The probability law of network site occupancy is assumed to be known for each invading fluid. When used for fractal flow networks, this binary modeling approach explains why population dynamics obey power laws. However, because the probability of site occupancy is assumed *a priori*, the percolation theory does not link the evolution of fluid fronts to macroscopic flow constraints.

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