

## Review Article

# Recent Developments in Multiscale and Multiphase Modelling of the Hydraulic Fracturing Process

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Recently hydraulic fracturing of rocks has received much attention not only for its economic importance but also for its potential environmental impact. The hydraulically fracturing technique has been widely used in the oil (EOR) and gas (EGR) industries, especially in the USA, to extract more oil/gas through the deep rock formations. Also there have been increasing interests in utilising the hydraulic fracturing technique in geological storage of CO<sub>2</sub> in recent years. In all cases, the design and implementation of the hydraulic fracturing process play a central role, highlighting the significance of research and development of this technique. However, the uncertainty behind the fracking mechanism has triggered public debates regarding the possible effect of this technique on human health and the environment. This has presented new challenges in the study of the hydraulic fracturing process. This paper describes the hydraulic fracturing mechanism and provides an overview of past and recent developments of the research performed towards better understandings of the hydraulic fracturing and its potential impacts, with particular emphasis on the development of modelling techniques and their implementation on the hydraulic fracturing.

## 1. Introduction

Hydraulic fracturing, or fracking, is a technique used in the mining industry and involves the controlled cracking of the rock formation with the use of high pressure liquid fluids [1]. The technique of hydraulically fracturing the rocks has been well known since it has been widely used for Enhanced Oil Recovery (EOR) and Enhanced Gas Recovery (EGR) in the oil and gas industries, especially in the USA, to extract more oil/gas through the deep rock formations [2, 3]. Hydraulic fracturing is a combination of processes, such as the deformation of the formation due to an external mechanical load (i.e., fluid pressure), the fluid flow through preexisting cracks of the formation, and the propagation of cracks [4, 5]. While the technology behind these processes has been used for more than 30 years in the name of energy exploitation, underground formations constitute a complex system of variables (both rock and well properties) that are not fully understood and thus are still under investigation [6, 7].

Scientists over the years have concluded that there is a clear relationship between the increase of CO<sub>2</sub> and human activities [8–10]. Overpopulation and therefore extensive industrial activities contribute greatly to the increase of greenhouse gas emissions and countries have agreed to a common mitigation plan in order to reduce the CO<sub>2</sub> emissions to acceptable levels and achieve a low carbon energy future [9, 11–14]. Carbon Capture and Storage (CCS) is a promising method that plays a central role as part of the mitigation plan [10, 15–18]. CCS is a five-step procedure which embraces all stages of industrial production [19]. Specifically, it involves the capture of high amounts of CO<sub>2</sub> produced from industrial facilities before they are released into the atmosphere, its liquefaction and pipeline transport into the site (oil and gas reservoirs, saline formations), injection under high pressure, and storage in deep underground formations [20]. Figure 1 illustrates all stages of the CCS technology from capture until storage. The hydraulic fracturing technique on porous media has become part of the injection and storage stage of CCS [1, 21] and therefore it is essential to

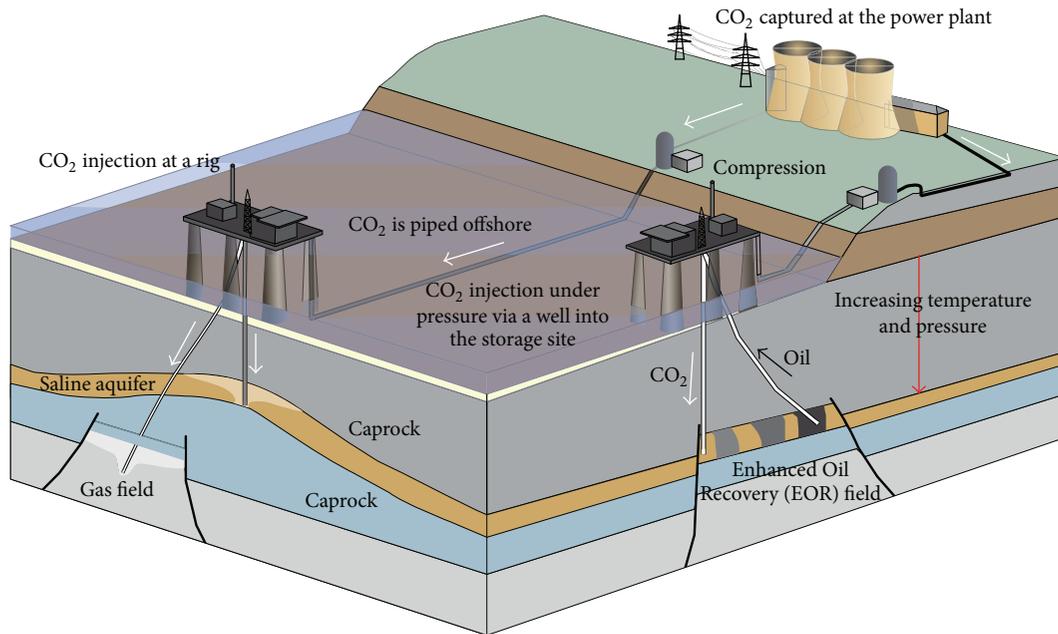


FIGURE 1: Schematic of CCS infrastructure showing the five steps of the technology and the geological media of storage [137].

understand the mechanisms that involve permanent storage and reduction of CO<sub>2</sub>.

The economic benefits from energy exploitation and especially the extraction of natural gas from shale gas formations through hydraulic fracturing methods are estimated to be considerable. The USA has already moved towards extensive shale gas exploitation, making Europe the next one to follow in the search of energy production and economy growth. Specifically, in the UK there are some promising estimations of the amount of shale gas from numerous formations throughout the nation. According to the British Geological Survey (BGS) and the Department of Energy and Climate Change (DECC), the Bowland Shale formation is estimated to contain about 1300 trillion cubic feet of shale gas, with about 10 per cent recoverable [22]. The scenario for UK shale gas production looks to be more encouraging, according to the Institute of Directors (IoD), suggesting high investments and numerous jobs [23], while suggesting considerable reductions of imported gas (around 37 per cent) in terms of consumption until 2030, which may lead to further reductions of the import costs, assisting towards a more balanced economy and energy security [24]. However, it is important to add that the economic implications are under speculation since they are based mostly on estimations, inferred from the US experience, and not on actual production.

## 2. Enhanced Oil and Gas Recovery

Enhanced Oil Recovery (EOR) and/or Enhanced Gas Recovery (EGR) is regarded as the most effective schemes for a low carbon energy future, since CO<sub>2</sub> injection and oil/gas extraction from hydrocarbon reservoirs can be performed concurrently [25]. During this process, fluids are injected

under high pressure into porous formations, with the aim of storing the liquefied CO<sub>2</sub> under an impermeable caprock, and cause controlled cracking to improve reservoir productivity [7]. Figure 2 illustrates a hydraulic fracturing technique in a shale gas formation, where the fracturing fluid is injected within the shale under high injection pressure to reactivate or open new fractures into the formation. The fractures stay open with the use of shale proppants (sand or ceramics) so that the shale gas can travel towards the well [26].

Between the two methods, EGR is relatively new and is still under investigation. The main reason is the concerns for degrading gas production due to the mixture between the initial gas in place and the injected CO<sub>2</sub> [27]. Furthermore, ongoing research aims to provide further insight into such matters, focusing on investigating the factors that affect the process of EGR and storage. Such an example is the work by Khan et al. [28], who replicated a 3-dimensional reservoir sandstone model using actual experimental data and simulated an EGR process, while sequestering CO<sub>2</sub>. Their findings refer to that one specific reservoir and can confirm that the CO<sub>2</sub> injection is applicable in increasing natural gas recovery and storing high amounts of CO<sub>2</sub> at the same time. The conventional procedure of oil extraction involves the injection of water; however, a large amount of oil stays trapped within the pores of the formation (about 50 per cent) after the primary production, and further recovery can be achieved by injecting liquefied carbon dioxide [29]. The latter exists in a supercritical state (dense phase fluid), with reduced viscosity (0.04–0.08 Cp) and surface tension, which means that the vapour and liquid forms of the CO<sub>2</sub> coexist. The component acts like a gas and a compressible fluid at the same time and can take the shape of its vessel, while having a density (about 600–800 kg/m<sup>3</sup>) like a fluid [27]. This supercritical state is achieved at depths above 800–850 m,

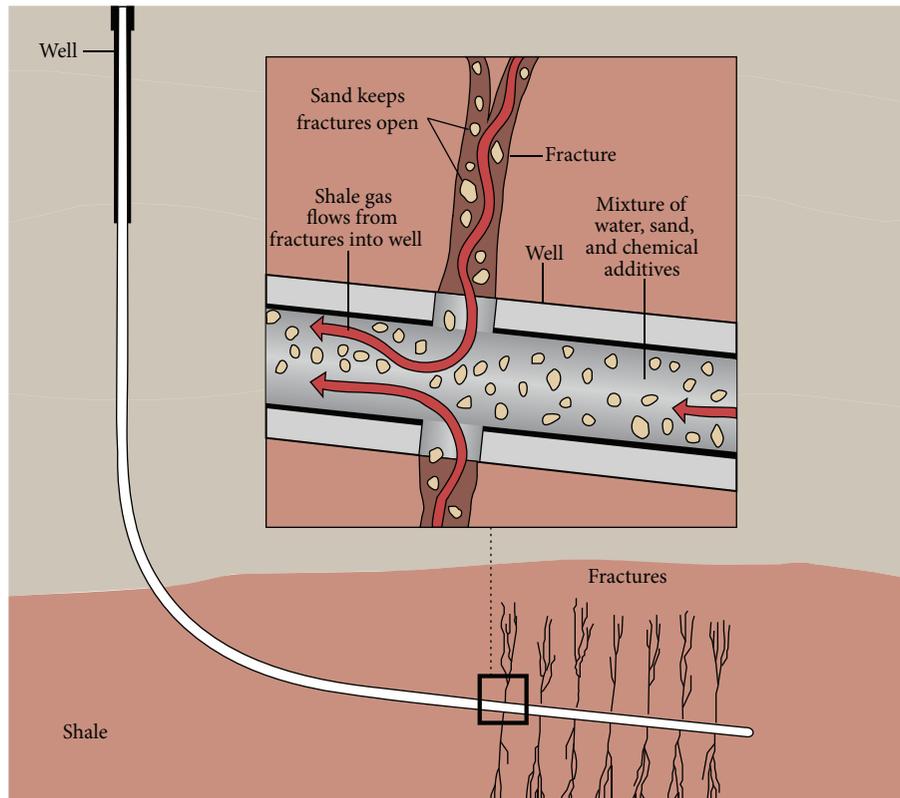


FIGURE 2: Schematic of the hydraulic fracturing technique in a shale gas formation [138].

pressures beyond 7.38 MPa, and temperatures higher than 31°C, respectively [25]. Due to the dense phase and the fact that it is easily miscible with other oils, it gives the CO<sub>2</sub> great potential to dissolve and relocate the oil in the reservoir. This technique is a key technology to reduce the anthropogenic emissions produced from overpopulated regions, such as China, while satisfying the extensive demands on electricity [30]. Although hydraulic fracturing is part of the technology used for gas/oil extraction, and thus widely used, it is still lacking the development of appropriate regulations for environmental safety and sustainability.

### 3. Hazards in Hydraulic Fracturing

Regardless of the choice of liquid (water or liquefied CO<sub>2</sub>), the hydraulic fracturing process requires the use of a considerable fluid pressure in order to introduce the liquid into the rock formation, until it exceeds the overall strength of the rock (both compressive and tensile) [31]. Therefore, valid estimates of the mechanical behaviour of the rock material under intense injection conditions are crucial to the efficient planning and operation of hydrocarbon reservoirs. This constant increase in the fluid pressure during injection causes redistribution of the in situ effective stresses within the reservoir. Although in this process the controlled fracturing of the reservoir is desirable, such stress changes may induce irreversible effects into the rock strata, thus causing possible reactivation of the existing faults. Moreover, the effects of

active faults on the process of leakage are an area where more research has to be performed; scientists generally suggest that the existence of seismogenic faults affects the permeability structure of the zone enhancing fluid transport [32]. In the process of hydraulic fracturing, the latter may lead to possible leakage of liquefied CO<sub>2</sub> [33] or flowback water, thus resulting in potential hazards. Moving towards a bigger picture, the major effects are the possible contamination of shallow groundwater layers by the migration of the toxic components of the flowback fluids as well as the leakage of methane, which acts as a greenhouse gas, into the atmosphere [34].

**3.1. Flowback Fluid.** Flowback fluid is the recovered fracturing fluid after the pressure release and the extraction phase and it mainly consists of a formation fluid and hydraulic fracturing fluid (fluid, proppants, and chemical additives). The key point is that the flowback fluid differs from the initial fracking fluid that was used during injection, with respect of composition. The majority of the volume of sand and proppants stays trapped within the pores of the formation, while the chemical additives react due to intense injection conditions, such as high temperature, resulting in reaction products. Therefore there is a potential risk of contamination of freshwater resources if flowback fluid is allowed to flow uninhibitedly. The exposure of the chemicals of the fracking fluid and the risk to groundwater reserves are linked to factors including underground or aboveground accidents

during transport and the concentration/handling of the possible hazardous substances [35]. Currently, the issue of potential implications on the quality of water is a matter of debate. This is due to lack of available information on the composition of the chemicals used in hydraulic fracturing procedures, and therefore scientists focus on this part of research aiming to shed more light. Recent studies are dealing with the ecotoxicological assessment of undiluted fracturing fluids, which indicate a hazardous effect on aquatic life. These studies are based on component-based prognostic models rather than measuring the ecotoxicological effect of a fracturing fluid as a whole [36]. This provides better accuracy of the overall results, allowing the prognosis of the effect of the mixture components individually. Generally, flowback fluids contain a mixture of hydraulic fracturing fluid and formation water. The potency of flowback fluid depends on the mix ratio of the formation water and fracturing fluid and although a high proportion of the fracturing fluid may be retained in the formation there is a high tendency for flowback to take place as a result of imposed fracturing operations [37]. At present, very limited studies have dealt with the chemical composition of flowback or its potential pollutants, and there are no studies investigating the difference in fracturing fluid from formation water that contains no fracturing fluid in flowback. The work performed by Olsson et al. [37] aims to bridge the knowledge gap by analysing the composition and volumes of flowback from different sites in Germany. This research has revealed that no single technology can meet the criteria for the overall treatment of flowback; thus they categorized the flowback fluid into groups and suggested some treatment methods. Furthermore, the accidental penetration of the fracturing and flowback fluids into the water aquifers and their impact on the human-health becomes critical and has been addressed recently. Such an example is the work by Gordalla et al. [35] who focused on the assessment of the ingredients of the fracturing fluids on the human-toxicological point of view, the influence of the flowback, and the possible hazards of freshwater reserves and suggested methods for minimising the environmental impact. Moreover, apart from the importance of extending the available information on the chemical composition of fracturing fluids or the environmental impact of the flowback and its proposed treating methods, it is of equal importance to investigate the underground formations and their interaction with the potential migrating fracturing fluids or methane. Such an example is the work by Lange et al. [38] who aimed to identify fault zones as preferential pathways that facilitate the movement of fracturing fluids/methane in unconventional gas reservoirs and analysed the effectiveness of the different layers of overburden.

**3.2. Risk of Contaminated Aquifers.** The extensive use of unconventional fracking (horizontal drilling and high volume hydraulic fracturing), especially in the USA, has triggered a public debate regarding possible health issues related to drinking water. Although industry claims that shale gas fracking is safe with minimum environmental impacts, the European Commission states that the extraction of unconventional hydrocarbons (shale gas) generally imposes a larger

environmental footprint than conventional gas extraction [39]. Risks from ongoing operations may include surface and groundwater contamination, water resource depletion, air and noise emissions, land take, disturbance to biodiversity, and impacts related to traffic. People's concern, especially in European countries where groundwater is their main resource of drinking water, has forced countries to seek expert opinion. A typical example is Germany and the ExxonMobil initiative [40]. The latter has formed a multidisciplinary working group in order to identify the possible environmental risks for the Lower Saxony Basin. Their main task is to assess the available technology (drilling and technical processes) and develop a strategy that fits the requirements for safe hydraulic fracturing operations. Part of this assessment is the "*information and dialogue process on hydraulic fracturing*," focusing on the characterization of the hydrogeological system, the chemical reactions under which leakage may occur, the possible leakage pathways, and the development of suitable models and their results [34, 38].

#### **4. Modelling of Rock Fragmentation and Fluid Flow Problems**

Moreover, the rapid growth in computer power and modelling has resulted in the development of a large number of software packages used for the numerical analysis of complex engineering problems, such as the identification of problematic (low bond strength) material parameters in masonry structures [41]. The reason for this is that it is very difficult for the analytical modelling to measure and describe accurately the complicated problems associated with fracturing. In subsurface investigations in particular, where heterogeneity and a wide range of complex inner mechanisms coexist, numerical modelling is necessary to represent real life scenarios. Numerous mathematical solutions have been applied to look, for example, into the critical mechanical parameters, such as the stress envelope, the porosity and permeability of the material and the effect of layering within the rock, or the way that these are influenced by the external mechanical load [42]. However, studies that employ modelling and simulation of rocks at the microscale [43–45] are fewer and their focus on the complex interplay between the microproperties and their corresponding effect on the material's behaviour during the calibration procedure provides at best a general guidance. Therefore, a review on the micro-meso-level modelling using Discrete Element Method is first provided in this section to highlight the research progress in recent years in this area, followed by the broader overview of multiscale and multiphase coupling models.

**4.1. Discrete Element Methodology.** The DEM is an alternative approach, to the Finite Element Method (FEM), which aims to describe the macroscopic mechanical behaviour of materials as a result of the interaction of its constitutive individual elements. Specifically, in DEM the material is described as a discontinuum, consisting of numerous distinct particles which represents the inhomogeneities within the material (joints and/or fractures) in the particle scale [45, 46]. Initially particle scale models were developed in order to simulate the

behaviour of soils and sands (noncohesive materials) [47]. The transition from the aforementioned modelling to the one that simulates the micromechanical behaviour of solid rocks is commonly known as the bonded particle model (BPM) for rock [45]. In a BPM, the breakage of interparticle bonds simulates the nucleation of a microcrack, while microcracking is achieved by coalescence of multiple bond breakages. The DEM methodology and the particle-based models have been employed in several computer packages in the field of rock mechanics, such as the particle flow code (PFC), the YADE, the universal distinct element code (UDEC), and the discontinuous deformation analysis (DDA).

The advantages of the DEM methods over other traditional techniques, such as the Finite Element Method (FEM), are the simpler representation of the geometries of real rocks, which contain discontinuities, the easier simulation of complex engineering problems without the use of complicated constitutive equations, and thus provide statistically more accurate results. Conversely, the increased simplification requires extensive experimental validation to verify the numerical results of the method and proves that the microscopic models can produce equivalent macroscopic behaviour of real rocks. Finally, the increased computational time due to the nature of the DEM approach (solving the governing equations for a large volume of particles) is another limitation that researchers have to tackle.

*4.1.1. Particle Flow Code (PFC).* Each of these approaches is based on the DEMs governing formulations, which include the calculation of the relative motion of the discrete elements, such as slip, rotation, or even complete detachment. More specifically in PFC each particle's motion is calculated by the equation of motion, given by

$$F_i + F_i^d = \begin{cases} m\ddot{x}_i, & \text{for } i = 1, 2, 3, \\ I\dot{\omega}_{(i-3)}, & \text{for } i = 4, 5, 6, \end{cases} \quad (1)$$

where  $F_i$  is the generalized force which includes the gravitational force,  $F_i^d$  is the damping force,  $m$  is the particle's mass,  $\ddot{x}_i$  is the particle's translational acceleration,  $I$  is the moment of inertia, and  $\dot{\omega}$  is the angular acceleration.

For the cases where the virtual particles are connected with bonds (reproducing the cementation between grains in real rocks), the updated body forces and moments, due to the presence of bonds, are calculated via the force displacement law:

$$\begin{aligned} F_i^T &= F_i^n + F_i^s, \\ M_i^T &= M_i^n + M_i^s, \end{aligned} \quad (2)$$

where  $F_i^T$ ,  $M_i^T$  are the total force and moment vectors and  $F_i^n$ ,  $F_i^s$ ,  $M_i^n$ , and  $M_i^s$  are the axial and shear components with respect to the contact plane, respectively. Details on the PFC calculation cycle based on the DEM can be found in Sousani et al. [48]. However each approach has its own limitations. The PFC utilises the BPM model, since the parallel bond rock modelling has been widely used

to simulate the fracturing mechanism in brittle rocks, but previous versions had the disadvantage of unrealistic ratios between the obtained tensile and unconfined compressive strength, to low nonlinear failure envelopes in terms of triaxial tests, or the problematic modelling of the interfaces due to the inherent roughness of the interface surfaces [49]. To tackle these limitations of PFC, a number of enhancement measures have been developed with the aim of providing a more accurate nonlinear mechanical behaviour, strength ratios, and friction coefficients. The basic concepts include the "cluster logic" (bonded particles packed together to form angular shapes or blocks that resemble natural grain structures, Figure 3(a)), performed by Potyondy and Cundall [45], the "clump logic" (bonded particles that behave collectively as a single unbreakable rigid body, Figure 3(b)) from Cho et al. [50], the flat-joint contact model (a more efficient contact formulation, where disk-shaped particle contacts simulate a finite-length interface that has relative rotation, even upon bond breakage, Figure 3(c)) from Potyondy [51], and finally the smooth-joint contact model (SJM) and the synthetic rock mass approach (SRM), respectively, from Mas Ivars [52, 53].

The SJM model simulates the behaviour of an interface disregarding the particle contact orientations locally alongside the interface, while the SRM model is a combination between the BPM and the SJM models that describes the mechanical behaviour of jointed rock masses, including anisotropy, brittleness, and scaling effects which cannot be achieved by empirical methods.

*4.1.2. Open-Source Software YADE.* Recently, another particle-based code has been developed, called YADE, as an alternative approach to the well-known commercial PFC code as previously described [54, 55]. YADE aims to be more flexible by adding new modelling capabilities, several simulation methods (e.g., DEM, FEM, and Lattice Geometrical Model (LGM)) can be coupled within the same framework and also the scientific community can provide direct feedback for improvement of the code with the use of an open-source platform. The fundamental principles of YADE are similar to those of PFC with respect to small deformations and fracturing (linear elastic interparticle forces and bond breakage, resp.) but new features, simulating rock discontinuities and ensuring frictional behaviour regardless of the inherent roughness, have been implemented as an alternative approach to the SJM and SRM models [56]. In addition, the use of YADE in studying the failure of brittle rocks has led to the creation of additional features, such as the interaction range coefficient, which helps to accurately simulate high ratios of compressive to tensile strengths as well as nonlinear failure envelopes [57]. However, YADE as well as many of the open-source software packages appear to be inefficient when compared to commercial software such as PFC, mainly due to the complexity of the user's interface and the lack of user defined functions. Moreover, open-source software solutions tend to develop mainly in line with specific purposes and also rely on the pool of open resources to help to discover errors and bugs. Some applications of the YADE code include three-dimensional simulations of the progressive damage in fractured rock masses [56], or the

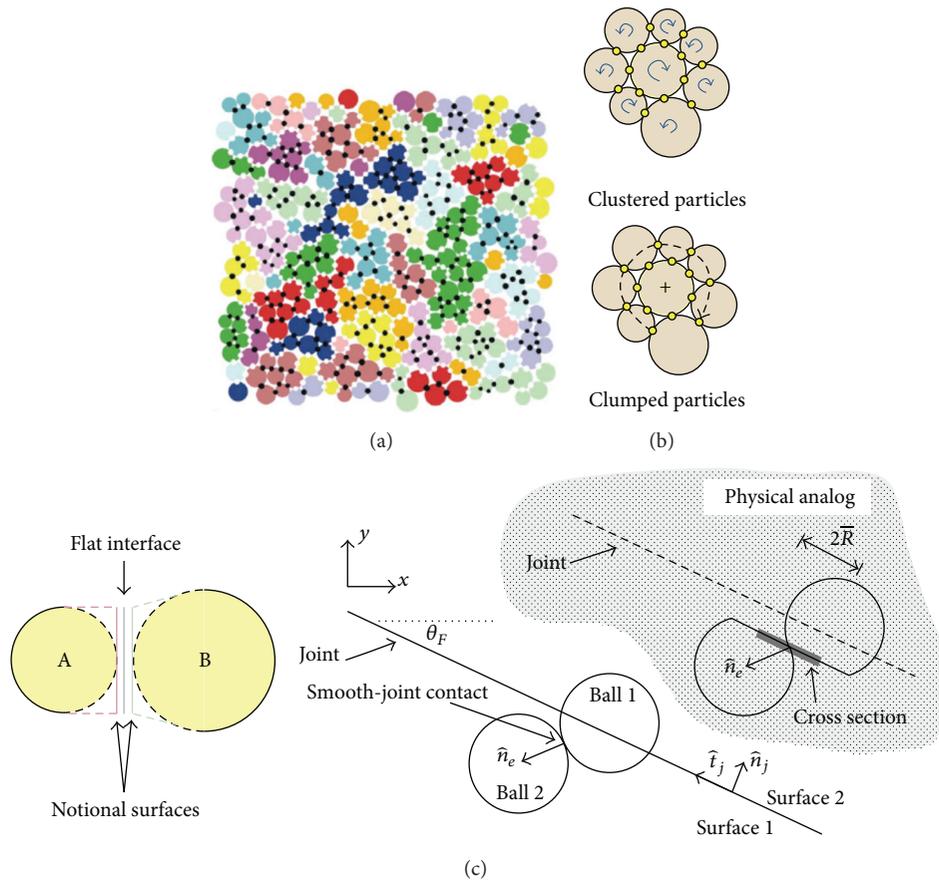


FIGURE 3: Developments on the BPM model for better representation of the nonlinear behaviour of hard rock and more realistic values of the ratio between tensile and unconfined compressive strengths. (a) The “cluster” logic [45], (b) the “clump” logic versus the “cluster” logic [50], (c) the flat-joint contact model [51], and smooth-joint contact model (SJM) [139].

effect of preexisting fractures of the brittle materials, under triaxial loading, on their mechanical behaviour [58, 59]. In the aforementioned simulations the open-source code YADE has been collaborated with the Discrete Fracture Network (DFN) in order to model the three-dimensional structure of the discrete features.

**4.1.3. Universal Distinct Element Code (UDEC).** Another type of modelling, which is based on the DEM equations, is the UDEC, employed to study rock masses that contain numerous fractures [60, 61]. The computational domain in UDEC is quantized into blocks using a finite number of intersecting discontinuities and each block is discretized with the use of a finite difference scheme in order to calculate stresses, strains, and deformation. The basic limitation of this technique was the fact that the failure mechanism in rocks was described either through plastic yielding or through deformation of preexisting fractures. Therefore new fractures could not be modelled and hence fracturing of intact rocks was impossible. This limitation was addressed by Lorig and Cundall [62] who introduced a polygonal block pattern into the modelling and enhanced UDEC’s simulation capability. UDEC is a relatively new approach to rock failure and thus verifications and improvements of the code are some of the

required tasks of experts in the field. Applications of the code can be found on modelling of the triaxial tests of the lithophysal rock samples, where the laboratory triaxial testing is considered almost impossible [63]. Extended results of this study on the same rock material, with the use of the UDEC, are presented by Damjanac et al. [64] who focused on the mechanical degradation of the behaviour of the material. An upscaled version of the developed model was employed to investigate the stability of the drifts from the region (Yucca Mountain) considering the in situ thermal and seismic loading as well as the time-dependent degradation.

**4.1.4. Discontinuous Deformation Analysis (DDA).** Finally, the DDA is a method also based on DEM but with similarities with the Finite Element Method (FEM) and was originally introduced by Shi and Goodman [65]. DDA is employed to simulate the stress, strain, sliding, and detachment/rejoining of systems containing rock blocks. Similarly to the FEM, the basic structure of the method, in terms of formulations, contains linear equations which results from differentiating and minimizing each energy contribution to the system. Improvements of the method have been employed over the years with the latest work being performed by Tang and Lu [66]. They combined the DDA method with the Rock Failure

Process Analysis (RFPA) software, the latter based on continuum mechanics [67], to investigate large scale deformations of discontinuous rock systems using the capability of RFPA to capture small deformation, crack initiation/propagation, and coalescence in intact rocks.

#### 4.2. Combined FEM/DEM and Other Hybrid Techniques.

The FEM and its improved approaches are considered a standard technique that can be successfully applied to numerous problems, such as the modelling and evaluation of rock materials or rock failure with internal discontinuities [68–70]. An example of a FEM is the two-dimensional finite difference programme FLAC [71]. This programme is employed to investigate the behaviour of materials such as soil and rocks and more specifically it simulates soil and rock structures that may undergo plastic deformation once their maximum yield limits have been reached. FLAC users create a grid, which consists of elements and zones, which fits the shape of the sample to be modelled. However, due to its geometric limitations, more discretization methods have been developed to address its difficulties, such as the extended Finite Element Method (XFEM) [72] for computing the three-dimensional crack propagation [73, 74], specifically focusing on the improvement of meshing sensitivity employed to compute the fragmentation problems [75]. A number of hybrid techniques have been developed based on the FEM with DEM implementations. This combination is called the hybrid continuum-discontinuum method or the combined FDEM and includes models such as the ELFEN (Finite Element/Discrete Element System) [76] or the Y-Geo software [77, 78] which are based on the Finite Element Method to describe the solid part of interest but also adopt the theory of the Discrete Element Method. The concept in FDEM is the transfer from continuum to discontinuum through fragmentation. Specifically, the sample's matrix is modelled with the use of continuum mechanics and as the test progresses the equations of motion are integrated. Then the initiation of cracks/fragmentations is such that it satisfies suitable fracture criteria, which therefore leads to the formation of new individual discrete bodies. Comparing the FDEM with the FEM and the DEM, respectively, we can claim that it is more capable of capturing the behaviour of postrock fragmentation and also it is more flexible in modelling deformable and unique-shaped particles. Furthermore, between the two modelling techniques, the Y-Geo approach resembles more a discrete method. Specifically, the representation of a sample with the use of Y-Geo is closer to a particle-based model, where the particles and their bonds are replaced by deformable triangle elements and four-noded cohesive elements [77], whereas in ELFEN a transfer between a continuous elastoplastic sample and a sample with discrete fractures is achieved by importing cracks into the sample [79].

4.3. *Modelling of Fluid Flow in Hydraulic Fracturing.* A wide range of engineering problems could utilise the DEM approach coupled with fluid models to analyse the fracking process within the rock specimen [21] or the influence of the significant parameters, such as the injection pressure, to a successful injection/storage application [80]. Also it is used

to simulate the behaviour of materials such as sandstone and limestone and the fluid-solid interactions among them [45, 81]. Initially, the fluid-solid interactions were described by the lattice Boltzmann method, which computes the fluid flow and solves the discretised form of the Boltzmann equation, based on the Navier-Stokes equation [82]. Other methods for computing the fluid flow include Direct Numerical Simulation (DNS) [83, 84], where the flow variables (e.g., pressure and velocity) exist as a function of space and time and can be obtained from the numerical solutions of the Navier-Stokes formulations, and Computational Fluid Dynamics (CFD). However, the need to provide linkages between the coexisting fluid and the solid phases necessitates a coupling of these techniques with the modelling of the solid phase, such as the DEM. The lattice Boltzmann and the DEM coupling have been described in detail by Boutt et al. [85], while approaches that incorporate CFD with the DEM have been presented in the work by Tsuji et al. [86] and Xu and Yu [87]. In their work, the interaction between the solid and gas phases in a fluidized bed has been modelled by solving Newton's second law of motion, with respect to the motion of particles, and the Navier-Stokes equation with respect to the motion of the gas. Most of these coupling schemes are applied to granular or uncohesive materials and in cases where the domain is dominated by fluid phases. Therefore, phenomena such as the deformation of the solid material and fracturing are not captured due to either the limitations in the coupling technique or the delineation of the study.

## 5. Developments on Modelling of Hydraulic Fracturing and Engineering Applications

Understanding the behaviour of the underground rock formations is itself a complex subject and it has been investigated by several researchers in the past [88–90]. The complexity of the hydraulic fracturing technique has resulted in more challenges in this area. There was extended ongoing research, both theoretical and experimental, in an attempt to understand the phenomena involved [45, 85, 89, 91–94]. Several models have been developed focusing on rock mechanics and the modelling of fractures; such an example can be seen in Zhuang et al. [95, 96], where 2D and 3D modelling of a fracture using a meshless method have been developed in order to provide stress analysis and describe the crack evolution or the study of cohesive crack models [97]. The motivation behind the extended modelling researches is that they can be applied to solve some large scale engineering problems; such an example is the investigation of rock stability and rock failure (joints in rock masses) near hydropower stations [98].

Recent developments also focused on the behaviour of hydraulically pressurized intact rocks in the micro or mesoscale [44, 99–101]. Such an example is the work by Marina et al. [43], who replicated a hydraulic fracturing test in a laboratory, and was performed on a thick-walled hollow cylinder limestone rock sample. The work studied the mechanical behaviour of the limestone sample under fluid pressure differential and the comparison between the fracturing pattern of the virtual model and the laboratory rock sample. The modelling of the rock and the analysis

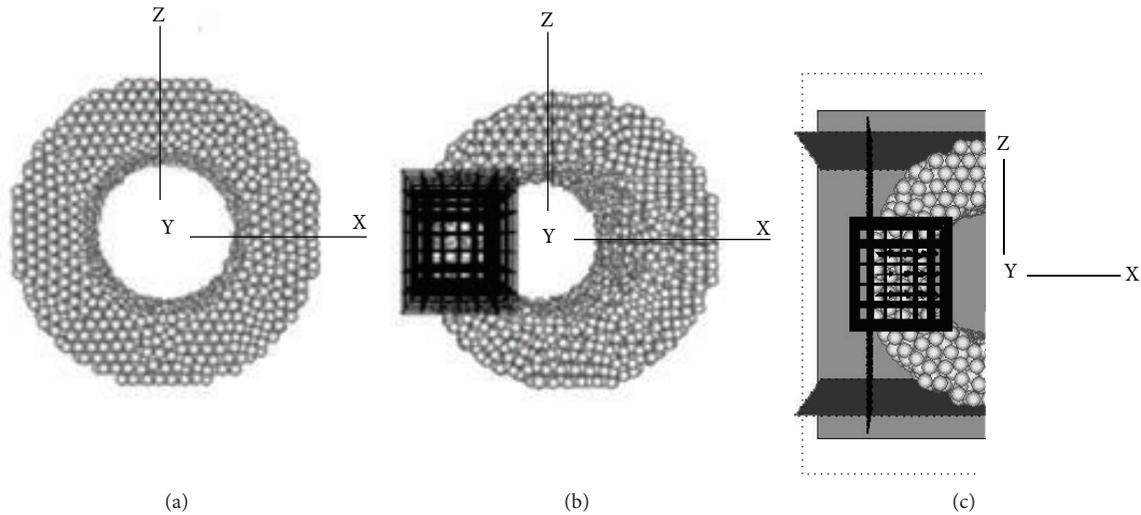


FIGURE 4: (a) Schematic of the virtual limestone model with the use of the DEM approach, (b) application of the fluid cell grid around a slice of the sample, and (c) fluid velocity vectors indicating the horizontal fluid movement from the outside surface towards the hollow core [43].

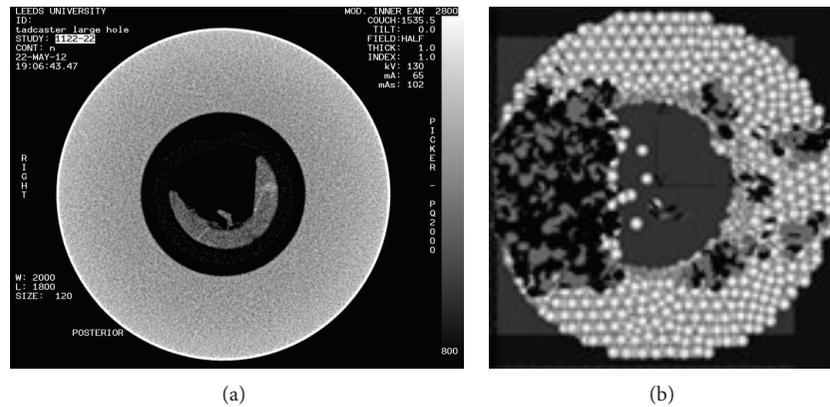


FIGURE 5: (a) Scan image of the limestone specimen inside the test tube at the moment of collapse (35 MPa) of the cavity wall and (b) microcracking of the virtual assembly at the moment of collapse (32.3 MPa) [43].

of the fracturing mechanism were performed with the use of the DEM approach (Figure 4(a)). The particles were bonded together with parallel bonds (adopting a spring-like behaviour), where each contact point has a maximum tensile strength in the normal direction and maximum shear contact-force strength due to the contact bond. Therefore, every time either the calculated maximum tensile or shear force exceeds the tensile or shear strength ( $\sigma_{\max} \geq \bar{\sigma}$ ,  $\tau_{\max} \geq \bar{\tau}$ ) of the spring (bond), the parallel bond breaks and this results in a microcrack. Furthermore, the simulation of the fluid flow was performed with the use of fluid cells that encapsulate the region of interest and provide measurements, as shown in Figures 4(b) and 4(c).

The numerical results were validated by Lamé's theory and were also found to be in very good agreement with the experimental results. They also captured the fracturing pattern within the rock samples induced by the hydraulic pressure (Figure 5).

A similar study in the particle scale has been conducted by Al-Busaidi et al. [102], who investigated the initiation and propagation of hydrofractures as well as the resulting seismic

output and compared these results with experimental data produced from other scientists. Generally, their approach can replicate most of the observations from the hydrofracturing experiments. More specifically, the numerical modelling was two-dimensional and part of the study used a number of homogeneous samples. The numerical results demonstrated some consistencies with the experimental results, showing a damage pattern along the potential macrocrack track. Another example is the work by Wang et al. [103], who simulated a hydraulic fracturing process of a coal seam and analysed the relation between the macroscopic and the mesoscopic mechanical parameters of the material. They focused on the influence of the mechanical properties in the macroscale to the initiation and the size of cracks, the empirical calculation of the breakdown pressure, and the analysis of the crack propagation due to the injection conditions. They compared their results with data derived from field observations.

The basic intention of the fracturing process is to maximise the reservoir's permeability, but the permeability of a fractured formation is highly affected by the openings of

the fractures. However, the fractures tend to close after a hydraulic fracturing operation and thus suitable proppants have to be selected, blend in a certain ratio with the fracturing fluid, fill the fractures, and keep them open after fluid injection [2]. Therefore estimation of the residual openings [46, 104, 105] or the permeability of the fracture openings [106], which are filled with proppants, as well as the optimisation of the used proppants [107] is of great significance for EGR/EOR applications. A number of studies have focused on the transport of suspended proppant particles within the fracture and the interaction between the formation and the proppant. Specifically Deng et al. [26] investigated the shale-proppant interactions and evaluated the fracture aperture under the influence of different pressure levels, proppant sizes, and Young's modulus of the shale. According to their findings, the softer is the shale particle; then the larger is the pressure and the proppant suggesting a smaller crack opening and larger plastic zone for other given conditions.

*5.1. Direct Applications of Hydraulic Fracturing Studies.* Other studies have focused on large scale numerical modelling and the observation of the behaviour of substantial formations. The work by Mas Ivars et al. [53] is an example of a large scale 3D modelling approach (10 up to 100 m), obtaining a qualitative and quantitative understanding of the mechanical behaviour of the rock formation both before peak and after peak. They used the synthetic rock mass (SRM) approach which is based on the bonded particle model (BPM) for rock and the smooth-joint contact model (SJIM) in order to replicate the intact rock and the in situ joint network, respectively. However, due to the nature of their study, factors that affect the behaviour of the formation in the particle scale, such as the grain size, the porosity, and the pore structure, were not considered. Other studies have dealt with the simulation of seismic events, produced from fluid pressure distributions, on large scale reservoirs ( $2 \times 2$  km) with the use of discrete particle joints models [108]. Furthermore, many rock engineering projects, such as mining or exploitation of geothermal energy resources, are directly related to drilling and thus fracturing, which drives research towards the investigation of the wellbore instability for hard and low porosity sedimentary rocks [109]. Fundamental and numerical analysis, such as the work performed by Zhang et al. [110] and Marina et al. [43], were developed to deal with the effect of rock geometry and various pressure differentials on the wellbore instability. Comparisons of the numerical results towards analytical solutions and experimental data provide a better understanding of the behaviour of the material and the propagation of cracks in both mesoscopic and large scale rocks. Furthermore, factors such as measurements of the minimum in situ stress and permeability are significant for the design of hydraulic fractures, which affect several engineering applications, and therefore extended research has been conducted relating the changes in the rock permeability with in situ stresses [111–115] as well as the influence of the in situ stresses to the fracturing pattern (propagation and closure) on pressure sensitive materials [104]. It is significant to observe how individual studies, such as the aforementioned or others related to the influence of stress and deformation

on the propagation of hydraulic fractures [116–118], become part of the bigger picture of hydraulic fracturing and can be connected with more recent studies focusing on the use and stability of the proppants in the fractures (as previously discussed). Recently more engineering applications have emerged where the fracking procedure is the dominant part. Examples of such projects are the waste disposal by the injection of slurries, in depths between 600 and 830 m, into appropriate sandstone and shale formations [119] and the production of heat from the hot dry rocks within geothermal reservoirs [120]. Therefore understanding the mechanisms involved in fracking, in order to control and ameliorate the process and maximise its benefits, is essential.

Furthermore, the investigation of groundwater flow under high water pressures and possible groundwater inrush incidents is of high significance especially for the ongoing operations on hydropower stations [121] and in coal mining [122]. The effect of high external water mechanical load and pore pressure is a key issue to the overall stability of the groundwater cavities and thus numerical analysis is essential in order to prevent possible leakage and help assist towards efficient design. The selection of an appropriate method to investigate groundwater flow and simulate pore pressure in fractured masses depends on several parameters, such as the boundary conditions, the scale of the reservoir, and the geological conditions of the area. However, the most popular methods for such analysis include the continuum medium approach [123], the Discrete Fracture Network (DFN), and methods coupling both continuum and discrete media [121, 124]. However, each individual approach has its own limitations. The continuum medium approach has proven to be inadequate in describing large scale regions since it has to oversimplify the fractured formation as a homogeneous zone [125]. The DFN approach cannot produce the detailed set of the geometrical parameters for individual fractures, while requiring extensive computational time for large scale simulations [126, 127]. The third approach can be considered more efficient since it combines the advantages of both continuum and discrete methods.

*5.2. Critical Parameters Which Affect the Hydraulic Fracturing Mechanism.* The complexity of analysing the hydraulic fracturing further increased by a large number of variables in the process, such as varying material properties (compressive/tensile strength, elastic constants, properties of particles and bonds, etc.), stress boundary conditions, the viscosity of the fracturing fluid, the grain size and permeability of the rock, and the preexisting fractures within the rock's matrix. The majority of the aforementioned variables are currently under investigation; such an example is the work by Sousani and Ingham [48, 128] who investigated the effect of the orientation and the number of the samples' preexisting fractures to the cracking mechanism. Some of the observations indicate that in samples containing fractures below  $45^\circ$  horizontal expansion of the microcracks is gaining ground (along the max compressive stress), whereas for fractures above  $45^\circ$  microcracking is observed to extend perpendicular to the max compressive stress. It was also observed that the effect of the confining stress combined with the heterogeneity of

the material, due to fracture, affects the orientation of the microcracking; finally, it was validated that extensive cracking is directly related to energy release, resulting in an increase of the kinetic energy within the sample.

Another example is the work performed by Martinez [129] who investigated the influence of varying material properties and boundary conditions in the microscale on the fracturing mechanism of poorly consolidated rock formation. Based on his overall results, he suggests that conventional theory ignores the mechanisms, such as shear cracking, which control the propagation of fractures with respect to poorly consolidated rocks and that the assumption of linear elastic behaviour of the material is not always dominant in Discrete Element Method (DEM) simulations. More examples are the work by Shimizu et al. [130–132], who dealt with the effect of the fluid viscosity and the grain size, to the behaviour of the hard rock. They observed that in the case of a homogeneous material and the use of a high viscous fluid the breakdown pressure was much higher than in the case of heterogeneous material. Their findings can be attributed to the defects between grains, due to differences of grain size, which therefore trigger the initiation of fracking. Their results were in agreement with laboratory results [93, 133, 134] which show a decrease of breakdown pressure with increasing grain size. Also they concluded that when low fluid viscosity was used, the fracture propagated along the direction of maximum compressive stress and the fluid penetrated directly into the fracture. The opposite occurred in the case of high viscosity, where the fluid cannot penetrate into the fracture unless the latter propagates first.

Other researchers have produced similar studies, such as Ishida et al. [135, 136], who performed a set of similar hydraulic experiments (the same in situ stress and flow rate) in the laboratory, using low and high viscous fluids (water/oil and supercritical/liquid CO<sub>2</sub>, resp.). The aim of their study was to investigate the effect of fluid viscosity to the breakdown pressure and compare the results from both studies. According to their findings they suggest that the supercritical CO<sub>2</sub> (sc-CO<sub>2</sub>) tends to initiate cracks which extend more three-dimensionally compared to the liquid CO<sub>2</sub> (l-CO<sub>2</sub>) which generates cracks that extend in a fat plane. The comparison between the aforementioned results and the acoustic emissions from the use of water and oil were observed to be distributed in a narrower region. Furthermore, they concluded that the breakdown pressures were lower for the sc-CO<sub>2</sub> than for the l-CO<sub>2</sub>, while the breakdown pressures produced from water and oil were significantly higher in comparison. Furthermore, Bruno [114] investigated the damage and the stress-induced permeability anisotropy in weakly cemented geological materials in the microscopic level. His results are well compared with the acoustic emissions of experimental data, with the reduction scale of the stress-induced permeability being dependent on the relationship between the amount of intergranular bonds and the stress levels. Specifically, the fluid permeability is reduced for both low and near hydrostatic stress levels, whereas for high deviatoric stress levels the flow channels increase affecting the induced permeability reduction. An

overall anisotropy of the permeability is observed in the macroscopic level.

## 6. Conclusions

This paper provides a synopsis and an overview of the past and recent developments of hydraulic fracturing, its applications, its possible hazards, and the available computational methods for analysing this technique. Even though hydraulic fracturing has been extensively used for several decades as a method of exploiting energy sources, there is still requirement for further research developments due to the difficulty of understanding the complex underground mechanisms and the limitations of the available mathematical models.

A number of studies have focused on the possible hazardous behaviour of the fracking mechanism, both experimentally and numerically, with some of the topics including the contamination of shallow aquifers from flowback fluids, poor well integrity, the effect of active faults and leakage pathways, and induced seismicity. The outcome of these works has resulted in the development of advanced mathematical models that can be successfully applied in real world operations. The FEM has been widely used for numerous engineering problems. However, its limitations have led to other improved techniques, such as the DEM. The latter is an alternative approach that has become well recognized in this field since it is free from mesh sensitivity compared to the FEM and can provide more accurate reproductions of materials in terms of inhomogeneities and discontinuities.

Modelling the failure mechanism of hard rocks is a challenging task and the presence of preexisting discontinuities (fractures, faults) makes the problem even more complex. This paper presents a review on the available mathematical and computational models for simulating the mechanical behaviour of rock formations and fluid flow, as well as some critical studies and their fundamental outcome. Following the references provided in this paper, the readers can access the detailed discussion and formulation of a specific modelling approach. Even though scientists have developed advanced modelling techniques, such as the DEM, the XFEM, or the FDEM approaches, more research is required to fully understand the fracking mechanism. Areas such as the modelling of rocks with preexisting fractures under injection conditions in the microscale and the effect of fracture orientation and different injection and reservoir conditions, the transition between the models in different scales to improve the accuracy of modelling the field scale hydraulic fracturing process with the considerations and benefits of the microscopic mechanisms, and the influences of the chemical composition of the fracturing fluids are some of the topics that need to be addressed in the future.

## Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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