1 Title: Image-based Stokes flow modeling in bulk proppant packs and propped fractures under
2 highloading stresses.

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23 Abstract

24
25 Rock fracturing, followed by proppant injection, has been used for years to improve oil and gas
26 production rates in low permeability reservoirs and is now a routine part of producing from low-
27 permeability resources such as a shales and tight sands. While field data makes clear the
28 effectiveness of this technique, there is still much room to improve on the science, including how
29 the proppant-filled fracture system responds to changes in loading stress and the corresponding
30 impact on the proppant structure and fracture width, which affect permeability and conductivity.
31 Here, we use high-resolution x-ray computed tomography (XCT) to image two unsaturated
32 rock/fracture/proppant systems: one with shale, one with Berea sandstone. Both systems were
33 imaged under a series of stress levels typical of producing reservoirs. The resulting XCT images
34 were segmented, analyzed for structural and porosity changes, and then used for image-based
35 flow modeling of Stokes flow using both finite element (FEM) and LatticeBoltzmann (LBM)
36 methods. The images and quantitative grain analysis showed expected changes as stress
37 increased: rearrangement of the packing structure, corresponding reduction in porosity, and some
38 embedding at rock walls to a depth of less than 0.5 times the proppant diameter. The shale

1 system exhibited more embedding than the Berea system. At the highest stress in the Berea
2 system (20kpsi or 1380MPa), individual proppant particles failed and the broken particles caused
3 significant loss of permeability. For the shale system, the embedding had a significant effect on
4 the simulated permeability/fracture conductivity. Simulation results for each of the loadings
5 showed that permeability is less sensitive to loading than experimental (vendor-reported)
6 permeability values, but also show reasonable agreement at 8kpsi (55MPa) for both systems.
7 Another somewhat surprising result is that fracture permeability for the single-layer proppants
8 confined between shale is similar to what would be predicted from bulk proppant results, despite
9 the significantly different flow geometry in the monolayer fracture.

Keywords

Propped fracture conductivity, bulk proppant permeability, loading stress, Darcy flow, finite
element method, Lattice Boltzmann method.

1 Introduction

Hydraulic fracturing with proppants has been used for many years to enhance extraction of oil
and gas (Cooke, 1973; Graham & Kiel, 1968). In the past decade, advances in hydraulic
fracturing and horizontal well techniques have enabled dramatic expansion of commercial shale
gas production in North America (Hart, Sayers, & Jackson, 2011; Sondergeld, Newsham,
Comisky, Rice, & Rai, 2010). This new source of natural gas will play an important role in
energy resources worldwide due to reduced greenhouse gas emissions and its availability in the

1 United States, as well as in China, Canada, Poland, etc. (Hart et al., 2011). Hydraulic fracturing
2 and horizontal well techniques have also revived gas and oil recovery from existing vertical
3 wells that were becoming commercially non-viable (Castro, Bass, Pirogov, & Maxwell, 2013;
4 Gutierrez et al., 2014; Ramurthy, Magill, Sanchez, & Parker, 2013; Wornstaff, Hagen, Ignacz,
5 Chorney, & Pedersen, 2014).

6
7 Hydraulic fracturing is the process of injecting fluids at high pressure to fracture the producing
8 rock and create high-conductivity flow paths from the source rock or reservoir to the well
9 (Cipolla, 2009). Proppants are added to the fracturing fluid to prop the fracture open after the
10 fracturing pressure is reduced. For the proppants to be effective, it is essential that they maintain
11 paths of high conductivity (Brannon, Wood, & Wheeler, 2006; Kaufman, Penny, & Paktinat,
12 2008; Warpinski, Mayerhofer, Vincent, Cipolla, & Lolon, 2008).

13
14 Despite its widespread use, many aspects of the hydraulic fracturing process remain poorly
15 understood. For example, a field study showed that of more than 100 Barnett shale gas wells,
16 almost half did not produce, and most of the production came from a small number of wells
17 (Maxwell, 2011). Among many factors that can affect the productivity of a well, formation
18 permeability and fracture conductivity are certainly two of the dominant factors. The network of
19 fractures dominates early flow, whereas matrix permeability becomes important on the gas
20 decline and ultimate recovery (King, 2010; Luffel, Hopkins, & Schettler Jr., 1993; Warpinski et
21 al., 2008).

22
23 While the permeability of bulk proppant can be considered an intrinsic property (a function of
24 grain/pore size distribution, shape of the grains, tortuosity, specific surface, porosity), fracture
25 conductivity, which combines proppant permeability with fracture width, depends on proppant
26 interactions with the fracture walls. Thus, it is important to be able to evaluate bulk proppant
27 permeability as well as relate this measurement to fracture conductivity. Different proppants can
28 have different permeabilities due to factors such as material, size, roundness, sphericity, etc.
29 Mechanical properties of a material also affect conductivity due to compression or failure during
30 loading. Other stress-related factors expected to impact fracture conductivity include
31 rearrangement of the proppant packing structure and embedment into the fracture walls.

Work from as early as 1973, found a two-order-of-magnitude reduction in proppant conductivity when the loading stress was increased from 1000 to 10000 psi (6.895 to 68.95 MPa)(Cooke, 1973). A conductivity cell was developed to measure permeability of bulk proppants for different combinations of stress, temperature, fluids (oil, brine, and gas) and a variety of sizes and types of proppants. A load was applied to the piston of the stainless steel cell that contained the proppants, and permeability was determined by flow experiments. The author measured a reduction in permeability up to two orders of magnitude for sand proppants as the pressure was increased from 1000 to 10000 psi (6.895 to 68.95 MPa) at 150 °F (65.6 °C). Much and Penny (1987) used a similar setup to test the conductivity of sand and intermediate strength ceramic proppants (ISP) but used both steel pistons and sandstone cores as column walls. They found that as the loading stress increased, there was a large decrease (>50%) in Jordan sand conductivity, whereas ceramic proppants decreased ~30%. In addition, ceramic proppants presented at least 50% higher conductivity than Jordan sand. Much and Penny (1987) attributed the differences to the observation that sand crushes at lower loading stresses than ceramic proppants. They concluded that “ceramic ISP proppants can provide conductivities over 1000% greater than sand proppants at equal concentrations and conditions.” Fredd, McConnell, Boney, and England (2001) observed similar behavior in a conductivity cell when they tested Jordan sand and bauxite proppants between two sandstones cores from the Texas Cotton Valley formation. Jordan sand started to crush after a loading stress of 2000 psi (13.79 MPa) whereas sintered bauxite did not crush below 5000 psi (34.47 MPa). Pre-experiment sieve analysis revealed that both proppants had less than 5% of the particles smaller than 300 µm. Post-experiment sieve analysis, however, showed that 65% of the Jordan sand particles were lower than 300 µm while bauxite had only 35%. The bauxite conductivity decreased from 2000 mD·ft to 10 mD·ft ($6.48 \times 10^{-6} \text{ m}^2 \cdot \text{m}$ to $3.24 \times 10^{-8} \text{ m}^2 \cdot \text{m}$) and Jordan sand from 400 mD·ft to 0.35 mD·ft ($1.30 \times 10^{-6} \text{ m}^2 \cdot \text{m}$ to $1.13 \times 10^{-9} \text{ m}^2 \cdot \text{m}$), when the stress increased from 1000 to 7000 psi (6.895 to 48.26 MPa). Dusterhoft, Nguyen, and Conway (2004) used a conductivity cell in which the proppant pack was sandwiched between two Ohio sandstones. They tested bauxite, ISP, and economical lightweight proppants (ELW). All of the proppant systems exhibited a trend of decreasing conductivity as the loading stress increased from 2000 to 12000 psi (13.79 to 82.74 MPa) (bauxite: 7050 to 2016 mD·ft or 2.283×10^{-5} to $6.528 \times 10^{-6} \text{ m}^2 \cdot \text{m}$; ISP: 7874 to 946 mD·ft or 2.250×10^{-5} to $3.063 \times 10^{-6} \text{ m}^2 \cdot \text{m}$; ELW:

6779 to 393 mD·ft or 2.195×10^{-5} to $1.273 \times 10^{-6} \text{ m}^2 \cdot \text{m}$). However, each type of proppant had a different range in which the proppants crushed (bauxite: 8000-10000 psi (55.16-68.95 MPa); ISP: 6000-8000 psi (41.37-55.16 MPa); ELW: 4000-6000 psi (27.58-41.37 MPa)), showing that the material strength is an important factor affecting conductivity. This behavior was especially evident for coated proppants (coating was added to increase conductivity) because they had higher initial porosity but also exhibited crushing at higher stresses because of higher point-load stresses. The uncoated proppants, on the other hand, crushed less, which the authors attribute to the lower porosity. They also observed intrusion of formation fines due to significant failure at the interface. Ye, Tonmukayakul, Weaver, and Morris (2012) developed a dynamic compression device and investigated permeability changes for 20-40 high-strength ceramic proppant. Similar to other results, they measured a decrease in permeability from 680 D at 120 psi ($6.71 \times 10^{-10} \text{ m}^2$ at 827 kPa) to 420 D at 7100 psi ($4.15 \times 10^{-10} \text{ m}^2$ at 48.95 MPa), showing the high-strength ceramic proppants are not as susceptible to crushing as other materials. It is clear that the proppant material is an important factor in conductivity and that its failure point needs to be taken into account when comparing conductivity reductions.

Another important factor highlighted by these experiments is the type of column wall used for the flow experiments. Steel pistons are commonly used (Cooke, 1973; Ye et al., 2012). However, this arrangement has a number of distinct differences from a real system, including the inability of the proppant to embed into the wall and the smoothness of the container wall (which influences local packing structure). Experiments reported by Much and Penny (1987) showed different conductivities for steel pistons and sandstone cores. At lower loading stresses (< 2000 psi or 13.79 MP), when there is neither crushing nor embedding, conductivities are higher with steel pistons (except for Jordan sand at 225°F or 107 °C), which the authors attribute to wall effects introduced by the pistons. In addition, they found that embedding becomes an important factor for loading stresses of 8000 psi (55.16 MPa) or higher for sandstone cores, a situation that is clearly not seen for steel pistons.

X-ray computed tomography (XCT), a technique that allows for the nondestructive imaging of the internal features of the system, is a valuable tool to visualize grains and pore space in 3D. Cheremisin et al. (2011) modified the standard conductivity cell to accommodate a large-scale

XCT scanner and compared the performance of rod-shaped proppants with average diameter equal to 12-18 sieve of spherical proppants against 12-18 sieve ISP at different loading stresses. Experimental results showed a decrease in conductivity for both proppants from 2000 to 6000 psi (13.79 to 41.37 MPa): 7250 to 3250 mD·ft (2.348×10^{-5} to $1.052 \times 10^{-5} \text{ m}^2 \cdot \text{m}$) for rod shaped and 2750 to 2000 mD·ft (8.904×10^{-6} to $6.476 \times 10^{-6} \text{ m}^2 \cdot \text{m}$) for spherical. X-ray images at 100- μm voxel resolution were obtained for both proppants at 4000 psi (27.58 MPa). Cheremisin et al. (2011) then used pore network modeling to show differences between the pore structures of the two types of proppants and to simulate flow in the porous media. Finite element method was also used to simulate and visualize flow in the porous media. However, permeability or conductivity values were not reported.

Few groups have studied the effect of axial/vertical stress in conjunction with XCT. Raynaud, Ngan-Tillard, Desrues, and Mazerolle (2008) used XCT, scanning electronic microscopy (SEM), quantitative image analysis of thin sections, and mercury porosimetry to analyze Plaisancian marl and classify the different strain regimes (brittle-ductile transition, axial stress up to 1 MPa or 154 psi). Bésuelle, Viggiani, Lenoir, Desrues, and Bornert (2010) obtained XCT images (14 μm resolution) of a Callovo-Oxfordian argillite sample under axial load up to 10 MPa (1450 psi) to define localized deformation classifications from brittle (at 1 MPa) to ductile (at 10 MPa).

Petunin, Yin, and Tutuncu (2011) studied the relationship between stress and permeability using a CMS-300 permeameter. Four types of rock were used and exposed to loadings from 5-35 MPa (725-5000 psi). One carbonate sample (1.5 mm in diameter, 3.0 mm in length) was imaged using XCT at 2.8- μm voxel resolution in order to check experimental results. However, XCT was only used for initial validation (no loading) and XCT images after loading were not obtained.

Compared to experimental studies, relatively few numerical studies of proppant/fracture systems have been reported. Zhao, Cui, Yue, Wang, and Wu (2008) developed a two-fluid model to simulate the particle migration process in the fracture with various proppant concentrations and flow velocities. Koyama, Neretnieks, and Jing (2008) performed fluid and particle flow simulations in the 2D geometry of a single rock fracture using measured topographical data of the fracture surface obtained from laser scanning profilometer. In the work of Khanna, Kotousov,

Sobey, and Weller (2012), a fracture filled with a monolayer of proppant particles was modeled as an array of rigid spheres squeezed between two semi-infinite elastic bodies to evaluate the opening length of the fracture according to Hertz contact theory. Computational fluid dynamics (CFD) simulations were used to obtain conductivity at different loading stresses.

In this work, our approach is to use image-based pore-scale modeling, an increasingly popular method to predict flow and transport properties in porous media. The approach can help provide a fundamental understanding of transport in porous media and the topologic and geometric factors that affect it. Two main approaches for image-based pore-scale modeling have evolved since the use of XCT became widespread. One is network modeling, which discretizes the pore space into pores and throats and imposes mass conservation in this system (Bhattad, Willson, & Thompson, 2011; Lindquist, Lee, Coker, Jones, & Spanne, 1996; Øren & Bakke, 2003; K. Thompson et al., 2008). The second approach uses direct approximation of the equations of motion applied to the digitized image of the pore space. The Lattice Boltzmann method (LBM) is the most widely used of the latter approaches (Auzerais et al., 1996; Bosl, Dvorkin, & Nur, 1998; Guodong, Patzek, & Silin, 2004; Schure, Maier, Kroll, & Ted Davis, 2004). The alternatives to LBM are one of the more traditional computational fluid dynamics modeling methods such as finite element method (FEM) or finite volume method (FVM). Both structured grids (Arns, Knackstedt, Pinczewski, & Garboczi, 2002; Zhan, Schwartz, Toksöz, Smith, & Morgan, 2010) and unstructured meshes (Lane, 2011) have been used with CFD techniques for pore-scale modeling.

In this paper we report on nondestructive imaging of dry fracture/proppant systems under different loading stresses, followed by direct numerical simulation of flow in the digitized pore space to determine proppant permeability and fracture conductivity. Two rock/fracture/proppant systems were imaged using a high-pressure synchrotron-based XCT apparatus. The first system consisted of a bulk packing of 20-40 CarboHSP® high-strength sintered bauxite proppants placed between two Berea sandstone cores; the second was a monolayer of 30-60 CarboHSP® high-strength sintered bauxite proppants loaded between two shale cores. Both systems were imaged approximately at loads of 0, 4, 8, 12kpsi (0, 28, 55, 83 MPa) and the Berea system was also imaged at 20kpsi (138MPa). The image datasets were segmented (void/solid) and packing

parameters and pore structure were quantified. Two different image-based simulation techniques were used to compute permeability: finite element method approximation of the Stokes equation using unstructured meshes and the Lattice Boltzmann method operating directly on the voxel grid. For the proppant monolayer between shales, fracture conductivity was also calculated based on the average fracture width as determined from the images. From these results, we are able to better interpret the causes of permeability loss due to mechanical loading than has been possible from past experiments.

2 Materials and methods

2.1 Experimental setup

Two different rocks were used for this study: Berea sandstone and Pierre shale. Two Berea sandstone cores, 6.1 mm in diameter and 2 mm in height, were extracted from a 1 in (2.54 cm) core using a diamond-tipped hollow drill bit. The same approach was used for the Pierre shale, except that we were unable to extract single 6mm-long cores; hence, four cores were cut and stacked in pairs. The proppants, from CARBO Ceramics, were CarboHSP® high-strength sintered bauxite proppants. The proppants used in the Berea test were 20-40 (sieve) with a median particle diameter of 697 μm , and the proppants in the shale test were 30-60 (sieve) with a mean particle diameter of 430 μm .

The sample holder consists of an outer cylindrical plastic sleeve that is transparent to x-rays and strong enough to support the stresses with little deformation ($< 2\%$ for the Berea system and $< 1\%$ for the Shale system) (Figure 1). For the Berea system (Figure 1a), only one sleeve (inner diameter: 6 mm, outer diameter: 10 mm) was used. Steel anvils, used to apply the load to the rock-proppant-rock sample, were 6 mm in diameter and 2 mm in height. For the shale system (Figure 1b), two sleeves were used (inner diameters: 6, 10 mm; outer diameter: 10, 20 mm, respectively) to allow more stability for the stepped anvils. The rocks and proppants were packed by first placing a layer of rock on the lower anvil, then placing proppants while using a microscope to ensure they remained in a monolayer, and finally inserting another layer of rock on top.

Figure 1: Schematic of experimental setup for a.) Berea and b.) Shale.

2.2 Data acquisition

Once assembled, the samples were placed in the Advanced Photon Source GSECARS high pressure tomography module (Wang et al., 2005) in the 13-BMD hutch. The imaging at all loadings was performed using a total of 720 projection images as the specimen was rotated from 0° to 180° by 0.25° increments exposed to monochromatic x-ray beam at 37.00 and 35.00 keV (Berea and shale, respectively) while the incident x-ray flux was stabilized to within a few percent by monitoring the incident beam intensity using an ion chamber. The Berea sample was imaged in two overlapping volumes covering most of the Berea cores and all of the proppants. The entire shale sample (top steel anvil down through bottom steel anvil) was imaged in 3 overlapping regions. Imaging details are summarized in Table 1. After the entire sample was imaged at zero stress, a load was applied, and once stabilized at the desired stress level, the sample was imaged again using the same procedure. The Berea system was imaged at 0, 0.09, 0.18, 0.27, 0.45 tons (1 ton = 2000 lbs), corresponding to loading stresses 0, 4.0, 7.9, 11.9, and

19.9kpsi(0, 28, 54, 82, and 138MPa) respectively. The shale was imaged at 0, 0.09, 0.18, and 0.26tons, corresponding to loadingstresses 0, 4.1, 8.2, and 11.9 kpsi (0, 28, 57, and 82 MPa).The loading stresses were calculated by dividing the load applied at each step by the corresponding sample (Berea or shale) cross-sectional area. Henceforth, the loading stresses are denominated 0, 2, 4, 8, 12, and 20 kpsi for simplicity.

Table 1: Imaging details.

Imaging Details	Berea	Shale
Voxel Dimensions (μm)	11.8	12.0
Energy (keV)	37.00	35.00
Exposure (s)	0.3	0.2
Rotations	720	720
Subvolumes scanned per load	2	3

2.3 Image processing

Image reconstruction, the process of converting 2D projection images into a 3D volumetric file, was performed using a filtered back-projection algorithm developed by GSECARS (Rivers, <http://cars9.uchicago.edu/gsecars/index.html>). Each voxel in the 3D volumetric data file (695×695×520 voxels) contains a linear attenuation value that depends on the composition of the phases within the voxel and the x-ray energy. The voxel sizes of the reconstructed images were 11.8 μm for the Berea system and 12.0 μm for the shale system.

The resulting 3D datasets were first converted to 8 bit data and then smoothed by an anisotropic diffusion (AD) filter (Bhattad, 2010). They were segmented using an indicator kriging (IK) algorithm based on the technique first developed by Oh and Lindquist (1999)and then modified as described inBhattad, Willson, and Thompson (2010).Each segmentation trial was evaluated both quantitatively (e.g., porosity) and qualitatively (i.e., comparison of segmented image to the original grayscale) to select the final segmented image to be used for further analysis. Finally, “islands-and-holes”removal was performed to remove physical voids from the proppant particles

(for computational reasons) and to clean up additional speckled noise. The image-processing steps are illustrated for the Berea system at 0-kpsi loading in Figure 2.

Figure 2: Image processing steps for the Berea-proppant system. Top to bottom: xy slice in the Berea; xy slice in the proppant-filled region; and xz slice showing the proppant-filled region with Berea above and below. Left to right: original 16-bit grayscale; after anisotropic diffusion; and after solid/void segmentation.

2.4 Image analysis

2.4.1 Porosity and surface area

For a given volume of interest, porosity is the ratio of void voxels to total voxels and specific surface area is the ratio of solid surface area to total volume. The solid surface area is calculated using the algorithm described by K. E. Thompson (2007). For the Berea/proppant sample, two

porosities are defined for the proppants. *Bulk porosity* is computed from a cube cut out from the interior of the packing, 3.54 mm (300 voxels) on a side. *Total porosity* is the porosity of the cylindrical sample, 6 mm in diameter and 3.54 mm in height, excluding the Berea cores; hence it includes wall effects caused by the cylindrical container. See Figure 3 for a 3D representation of both cutouts.

Figure 3: Berea-proppant system: 300^3 voxels cubic cutout (colored) used for permeability computation and volume used for bulk porosity and bulk permeability.

For the shale/proppant sample, a 4.80×3.60 mm (400×300 voxels) rectangle inscribed by the cylinder was selected in the xy -cross section. A vertical section 0.84 mm (70 voxels) high was extracted, which included portions of the top and bottom shale. Figure SI. 1 shows the shale/proppant computational domain. The porosity of this selected single fracture was calculated and defined as the *fracture porosity*. It is important to note that porosity value for the shale sample is an arbitrary number because it depends on the cutout selected and the volume of shale that is included in the cutout. However, a true fracture porosity was difficult to obtain accurately because of the non-uniform geometry of the shale face relative to the Cartesian image grid, and this approach provides a consistent and quantitative way to present porosity differences from one load to another.

2.4.2 Embedding

The amount of proppant embedding was estimated by visual inspection followed by direct measurement of embedded length using the gray-scale images. More embedding was observed near the container walls because the rock cores are not cut at a perfect 90° angle, which creates some weakness and/or space for the proppants to move into as stress is applied. Therefore, when measuring embedment in the Berea sample, a 300×300 *xy*-centered cutout with axial length remaining from top to bottom of the Berea was used. For the shale sample, the entire *xy*-cross section was observed, but proppants on the boundary were not included in this estimation.

2.5 Grain Analysis

Grain analysis of the 300³-voxel bulk proppant pack was performed using the methods described in K. E. Thompson, Willson, and Zhang (2006). This algorithm finds the maximal inscribed sphere for each grain by using a combination of erosion and nonlinear optimization. The grain centers are located and adjacent voxels belonging to that grain are collected by using a type of watershed algorithm. With this method, each grain is identified and labeled, which allows characterization of the grains to be performed by computing grain surface area, number of grain-to-grain contacts, contact areas, grain volume, grain position, grain orientation, and grain aspect ratio. The grain effective diameter was calculated as the average of the major and minor diameters; in other words, the average of the inscribed diameter and the particle length (K. E. Thompson et al., 2006; Willson, Ning, & Likos, 2012). Only grains that were fully contained in the cutout were included in the analysis to ensure that the grain-characterization parameters are representative.

2.6 Simulation

2.6.1 Numerical techniques: Finite element method

The finite element method was used to simulate fluid flow in the pore space. Unstructured meshes of the void space were created by importing segmented XCT images into the commercial software package AVIZO. While FEM simulations can be performed directly on the uniform

grid structures from XCT images by using voxels as elements, unstructured meshes allow the mesh resolution to be decoupled from the number of voxels in the image dataset and also allow local mesh refinement to be performed. Therefore, mesh resolution can be tailored to the numerical problems independently of the original image resolution, while still preserving the image structure. In this work, approximately 0.15 elements per voxel were generated for the bulk proppant packing at each loading stress. This value was determined based on numerical convergence as the mesh was continually refined. Figure SI. 2 shows the bulk proppant mesh refinement used at 0 psi for a smaller section of the domain (~1.2 mm or 100 voxels).

An in-house FEM algorithm (Lane, 2011) was used to determine permeability. In this algorithm, the Stokes equation is solved using P2P1 or Taylor-Hood tetrahedral elements (which employ quadratic approximations for velocity and linear shape functions for pressure). The boundary conditions at the inlet and outlet surfaces of the domain were assigned normal tractions equal to the desired applied pressure. No-slip boundary conditions were applied at the interior solid-void interfaces as well as the four sides of the simulation domain (not inlet or outlet). More details can be found in Lane (2011).

2.6.2 Numerical techniques: Lattice Boltzmann method

The Lattice Boltzmann method is a simplification of the Boltzmann equation that solves for particle distribution functions in a discrete phase space. For more details on the LBM equation and solution method, refer to Supplementary Information, Section 7.3.

LBM simulations in this study are done using the Parallel Lattice Boltzmann Solver (PALABOS, 2012) on Louisiana Optical Network Initiative (LONI) resources. The bounce-back boundary scheme is one of the no-flow boundary conditions commonly implemented in LBM simulations. The no-flow boundary is assumed to be at a halfway distance between the fluid and solid nodes for simple geometries. For more complex geometries this scheme puts the no-flow boundary somewhere between the fluid and solid nodes. The exact position of the no-flow boundary varies with the relaxation time used and the geometry (numerical resolution) of the numerical domain. The body force approach is used to replicate a pressure gradient at the inlet and outlet. More

1 details can be found in Takkiri Borujeni (2013), Takkiri Borujeni, Lane, Thompson, and Tyagi
2 (2013), and Chukwudozie (2011).

3
4 Ideally, the porous media domain used for simulations should be periodic representative
5 elementary volumes (REV) or unit cells. The domains used herefor the LBM simulations were
6 changed to periodic by adding ten layers of void voxels to each side. A body force approach,
7 which is an alternative to specifying pressure values at the inlet and outlet of the domain, was
8 used. Periodic boundary conditions were applied on all the external faces. A body force was not
9 applied on these added layers.

10
11 Applying high-pressure gradients (large body forces) in LBM simulations may cause continuity
12 errors that can grow at each time-step and break down the simulation. In order to increase
13 numerical resolution and avoid errors, the original domain (300^3 voxels) was sub-divided on
14 each side of the voxels by 2, i.e., increasing the total number of the voxels by a factor of 8.

15 **2.6.3 Permeability computations (total, bulk and monolayer)**

16
17 Permeability is a continuum-scale porous-media property that quantifies how easily a fluid can
18 flow through the pore space. Permeability is generally related to porosity, tortuosity and the
19 characteristic length in the pore space (the latter is often defined as hydraulic radius in
20 unconsolidated packings). It is defined by Darcy's law, which describes the linear relationship
21 between superficial (Darcy) velocity and pressure gradient:

$$22 \quad v = \frac{k}{\mu} \nabla P \quad (1)$$

23 where k is the permeability and μ is the dynamic viscosity of the fluid. To determine
24 permeability from the FEM or LBM flow simulations, we calculated the inlet/outlet flow rate

25 $Q = \iint \mathbf{v} \cdot \mathbf{dA}$, and then computed the superficial velocity Q/A based on the known inlet area.

26
27 Compared to permeability, conductivity is more widely used to describe transport in fractures.
28 The conductivity of a fracture is calculated as

$$29 \quad C = kw \quad (2)$$

where k is the permeability of the fracture and W is the opening width of the fracture.

We denote the permeability obtained from the 300^3 -voxel interior section of the proppant pack as the *bulk permeability* and the permeability obtained from multilayer proppants confined by cylindrical walls as the *total permeability*. For the shale fracture sample, both permeability and conductivity were calculated and defined as the *fracture permeability* and *conductivity* respectively. The cross sectional area of the fracture is the xz -plane perpendicular to the flow direction (y). The opening width is not uniform along the cross-sectional area. Therefore it was approximated as the average opening width and was estimated by visual inspection of the segmented image at each loading stress. The width was measured manually three times at each cross section for 40 different xz -cross sections. The average of these 120 measurements was used as the fracture width for a given loading stress in both cross-sectional-area and conductivity calculations.

2.6.4 Tortuosity

Tortuosity value quantifies the flow pattern of the fluid in the pore space of proppant packing. It can be defined as the ratio of the length of actual path of fluid to the shortest path length in the direction of the mean flow. Koponen et al. proposed that the tortuosity can be calculated based on velocity values on grid points (Koponen, Kataja, & Timonen, 1996):

$$\tau = \frac{\sum_{i,j,k} u_{mag}(i,j,k)}{\sum_{i,j,k} |u_z(i,j,k)|} \quad (3)$$

where u_{mag} is the magnitude of velocity, u_z is the z direction (flow direction) velocity and i, j, k is the location of lattice used to perform the computation.

3 Results and Discussion

XCT images of both the Berea and shale systems were analyzed to quantify the effects of loading stress on the proppant structure. For the Berea system, a detailed proppant grain analysis was

performed for all loadings. The bulk permeability in the Berea system was predicted and the structural changes including particle rearrangement and breakage caused by stress on the predicted permeability were characterized. The wall effects were quantified by comparing the porosity and permeability values in the interior versus the complete packings. Permeability and conductivity values for the shale fracture with a monolayer of proppants were calculated to quantify the effect of proppant embedment and/or rearrangement on transport properties for this system.

For the Berea system, the design consisted of bulk proppants instead of a monolayer – which would be a more realistic configuration – because the characteristics and behavior of bulk proppants under high loading stress needed to be determined for direct comparison to previous studies of bulk proppants. In addition, embedment at the rock-proppant interface was captured and analyzed. For the second system, a proppant monolayer was placed between shale cores. In a complementary study (Sanematsu, Willson, & Thompson, 2013), we studied the effect of embedding and crushing of the rock matrix interface on the flow.

In this work, we were mostly interested in the effect of loading stress on the flow through the proppants rather than the effect of fracture geometry and proppant distribution. For this reason, as well as ease of imaging, the fracture was created by stacking small rock cores instead of artificially or hydraulically fracturing the rocks.

3.1 Berea-proppant system

3.1.1 General observations

As loading stress increased, proppants rearranged, embedded into the rock and eventually crushed at the highest stresses (Figure 4). The rearrangement of proppant particles caused changes in the pore space, which in turn modified flow pathways and increased the number of grain-grain contacts and the tortuosity. As Figure 4 shows, crushing occurred at 12 and 20 kpsi (83 to 138 MPa), thus increasing the number of particles, creating more surface area, and reducing porosity. Embedment of proppants into the rock was relevant because it reduced the impact of near-wall packing structures that occur in rigid-wall systems. This embedment was first observed

at 8 kpsi (55MPa) (to an extent approximately 5% of d_{50}), similar to the trend found by Much and Penny (1987). At 20kpsi (138MPa), we observed single-particle embedment up to approximately 35% of the d_{50} . Overall movement of the Berea faces due to the applied stress was smaller: approximately 5-10% of d_{50} .

Figure 4: Horizontal (top row) and vertical (bottom row) cross-sections at each loading stress. Blue squares indicates FEM and LBM computational domains. Triangles and stars “follow” two different proppants at each loading stress.

3.1.2 Detailed grain analysis on 300³ cutout

A detailed analysis on a 300³ cutout (the same cutout used for flow simulations) was performed to quantify factors that could affect flow. Fractions of grains located at the faces and edges of the cutout were not used when computing average parameters on a per-grain basis (see Section 2.5 for details).

For the first 3 loadings (0, 4, 8 kpsi or 0, 28, 55MPa respectively), similar values were found for porosity, tortuosity, permeability and the number of grains, as well as for average grain characteristics such as specific surface area, effective diameter, aspect ratio, number of grain-to-grain contacts (Table 2). As seen in the XCT images, these results support the finding that

proppants did not crush from 0 to 8kpsi (0 to 55MPa), which agrees with Fredd et al. (2001), who found that a similar proppant did not crush up to 5 kpsi (34 MPa). At 12kpsi (83MPa), few grains were crushed (which agrees with Dusterhoft et al. (2004) who found that the crushing range for sintered bauxite was from 8 to 10 kpsi or 55 to 69 MPa). We also detected small changes in packing characteristics; i.e., the number of grains, number of grain-grain contacts, and aspect ratio, all increased (the latter indicating a departure away from spherical shape). The average grain volume, surface area and effective grain diameter decreased, supporting the visual observation that proppants were crushed. Changes were more apparent at 20kpsi (138MPa), where significant changes occurred in all of these characteristics, especially the number of grains, average grain effective diameter, average number of grain to grain contacts and average aspect ratio.

Table 2: Detailed grain analysis ($d_{50} = 697 \mu\text{m}$; *not performed in the 300^3 cutout. Anxy- centered cutout including the Berea-proppant interfaces was used).

Loading (kpsi)	0	4	8	12	20
(MPa)	0	28	55	83	138
Porosity (%)	32.92	31.69	32.75	32.14	28.46
Number of Grains	65	66	68	82	251
Inscribed Radius (μm)	319	313	304	251	131
Specific Surface Area ($\times 10^{-3} 1/\mu\text{m}$)	5.37	5.29	5.47	5.30	6.44
Effective Diameter (μm)	743	741	730	638	393
Aspect Ratio	1.34	1.36	1.47	1.83	2.70
Number of Grain-Grain Contacts	7.52	7.83	7.96	8.77	11.61
Tortuosity	1.27	1.27	1.26	1.28	1.36
Permeability (Darcy)	230.4	205.4	235.7	197.1	79.7
Single-Particle Embedment* ($\times 10 \mu\text{m}$)	4.7	5.9	15	32	50

3.1.3 Bulk permeability

Figure 5 shows predicted bulk permeability values using both FEM and LBM at all loading stresses. From 0 to 8kpsi (0 to 55MPa), bulk permeability remained essentially constant at approximately 225 Darcy. A small decline (12%) occurred at 12kpsi (83MPa), when crushing

1 began to occur. From 12 to 20kpsi (83 to 138MPa), the permeability was reduced by around 60%
2 which is due to substantial crushing of particles. Crushing was clearly the dominant factor
3 causing permeability reduction, which is consistent with conclusions of Fredd et al. (2001) based
4 on conductivity measurements and sieve analysis of the pre- and post-loaded proppants.

Figure 5: Berea-proppant system comparison of image porosity and bulk permeability predicted from FEM, LBM, CARBO Ceramics (proppant manufacturer) experimental results, Carman-Kozeny equation (4), Carman-Kozeny with tortuosity equation (5) at each loading stress.

From 0 to 8kpsi (55MPa), structural parameters such as porosity, average grain surface area and inscribed radius, remained relatively constant, as did the tortuosity, all of which caused permeability to remain essentially constant at these lower stresses. At 12kpsi (83MPa), however, proppant crushing began to alter the pore space, increasing tortuosity and thus reducing

permeability. At 20kpsi (138MPa), the major structural changes led to increased tortuosity by approximately 6% and decreased permeability by 60% (Figure 5 and Table 2).

In Figure 5, bulk permeability values obtained from simulations are compared with Modified API RP-61 (ISO 13503-3) experimental results published by CARBO Ceramics, the manufacturers of the 20-40 proppant used in the proppant/Berea imaging experiments (Palisch, Duenckel, Bazan, Heidt, & Turk, 2007). The experimental permeability results show a very smooth declining trend as loading stress was increased from 0 to 14kpsi (0 to 97MPa), in contrast to the image-based flow simulations which show a more sudden onset of permeability loss at the point where major structural changes occurred.

Additional insight is gained by computing the expected permeability using the Carman-Kozeny equation, an empirical equation widely used to predict the permeability of random sphere packs. Here it is expressed in two different forms (Bear, 2013). The first is

$$k = \frac{d_p^2 \phi^3}{180(1-\phi)^2} \quad (4)$$

where $d_p = 697 \mu\text{m}$ is the median particle diameter reported by the manufacturer and ϕ is the porosity (from Table 2).

The second form incorporates tortuosity (Wyllie & Spangler, 1952):

$$k = \frac{R_H^2 \phi}{k_0 \tau^2} \quad (5)$$

where R_H is the hydraulic radius, the ratio of void volume and surface area, k_0 is the shape factor of 2.5 and τ is the tortuosity (from Table 2).

Figure 5 shows that as loading stress increased from 0 to 12kpsi (0 to 83MPa), the discrepancy of permeability predicted from pore-scale simulations (FEM and LBM) and equation (4) was only $\pm 8\%$. At 20 kpsi (138MPa), equation (4) and equation (5) predicted permeability values 37% and 25%, respectively, higher than FEM simulations. The larger discrepancy of equation (4)– an

equation used specifically for sphere packs – is likely because the significant crushing caused the proppant pack to no longer resemble a uniform sphere packing.

Velocity fields in the pore space provide a definitive link between the explanations offered above for permeability loss and the pore-scale physics that ultimately govern fluid flow. Figure 6 shows, for each loading stress, the normalized magnitude of velocity in cross sections from the middle of the domains obtained from 3D FEM simulation. At lower loadings, there were wide-open pore spaces where particles were not packed tightly and contain high velocities. As loading increased, pore spaces became more compact, resulting in lower and more uniform velocities in the pore space.

Figure 6: Berea-proppant system cross sections showing normalized magnitude velocity field at each loading stress.

3.1.4 Wall effects

In order to investigate wall effects (which are expected to be relevant in a fracture geometry), the total porosity and total permeability were compared with bulk porosity and bulk permeability (where *bulk* refers to the internal cutout whereas *total* includes the full cross section including the area in contact with the container walls). It is important to note that the cylindrical plastic used as column walls did not deform considerably and proppants did not embed into the column walls. Thus, changes in porosity and permeability are not tied to wall deformation.

Figure 7 shows that both porosity and permeability follow the same declining trend as loading stress increases. The average total porosity (for all loadings) is around 6% higher than the average bulk porosity. The wall of the cylindrical container forces a more structured arrangement of proppants near the wall with sphere centers located a minimum of one radius away from the wall, which in turn corresponds to a larger local void fraction (Cohen & Metzner, 2004; Sodré & Parise, 1998). From 0 to 12kpsi (0 to 83MPa), the total permeability is approximately 31% higher than the bulk permeability, however, at 20kpsi (138MPa), the total permeability is 58% higher than the bulk permeability. This result shows that wall effects became especially important at 20kpsi (138MPa) when proppants were crushed and the internal pore space became more tortuous and tightly packed. It also means that flow channels close to the wall remained important contributors to the total flow at all loadings, and suggests that the internal structure was more affected by crushing and/or rearrangement than the near-wall region.

Figure 7: Comparison of bulk and total porosities and bulk and total permeabilities at each loading stress for the Berea-proppant system.

3.2 Shale-proppant monolayer system

3.2.1 Observations: embedment, fracture width, porosity and surface area

Visual inspection shows that the rock walls changed little from 0 to 4kpsi (0 to 28MPa). However, from 4 to 12kpsi (28 to 83MPa), there was considerable embedment of proppants reaching, at the highest loading, single-particle embedment up to approximately 40% of d_{50} (see Table 3 for details). From the XCT images (Figure 8), one can see that pathways between proppants and the wall narrowed or closed after the other proppants embedded. Another important consequence of embedding for a monolayer system is the reduction of the fracture width, which decreases the fracture conductivity.

Table 3: Structural changes in the shale fracture system ($d_{50} = 430 \mu\text{m}$).

Loading (kpsi)	0	4	8	12
(MPa)	0	28	55	83
Porosity	0.2	0.19	0.15	0.16
Specific Surface Area ($\times 10^{-3} 1/\mu\text{m}$)	5.05	4.26	4.07	5.49
Fracture Width ($\times 10 \mu\text{m}$)	46	46	36	31
Single-Particle Embedding ($\times 10 \mu\text{m}$)	34	37	49	66

Figure 8: xz slice through the Shale-proppant system at 0 kpsi (left) and at 12 kpsi (right).

Fracture porosity decreased as the loading stress increased (Figure 9), which was a consequence mainly of the narrowing of the fracture width (allowed by particle embedment). Specific surface area of the fracture (i.e. the specific surface area of the proppants plus the shale wall) decreased significantly as the stress increased from 0 to 8kpsi (55MPa) (Figure 9), which could be attributed to the embedment of proppants into the shale. Although there was further embedment from 8 to 12kpsi (55 to 83MPa), specific surface area increased, reaching a value even higher than at 0 kpsi. The XCT images in Fig. 7 indicate that some additional fissures in the shale became connected to the proppant-filled fracture at 12kpsi (83MPa), contributing to the large increase in total surface area. However, for the FEM simulation, these additional fissures were removed from the images such that permeability and conductivity values would be comparable to other loadings.

Figure 9: Porosity and surface area of the shale fracture as a function of the loading stress.

3.2.2 Permeability and conductivity

Conductivity is more relevant to well production than bulk proppant permeability because it takes into account both the width of the fracture and the material permeability between the fracture walls. In the shale system (Figure 10), permeability decreased by approximately 25% and another 15% when loading stress increased from 4 to 8 kpsi (28 to 55 MPa) and from 8 to 12 kpsi (55 to 83 MPa), respectively. The corresponding changes in conductivity were 40% and 25%, respectively. It can be seen from velocity fields (Figure 11) and the XCT images (Figure 8) that permeability reduction is mainly caused by two factors: particle rearrangement (which in turn causes a narrowing of the larger pores and pore throats) and embedment (which causes

closure of flow channels at some locations). Conductivity is reduced by these two factors, but also decreases due to the narrowing of the overall fracture width (Table 3).

Figure 10: Conductivity and permeability of the shale fracture as a function of the loading stress.

Figure 11: Shale-proppant system cross sections showing normalized magnitude velocity field at each loading stress.

3.3 Permeability comparison: Berea versus shale results

In Figure 12, bulk permeability values are presented for both the 20-40 proppant used in the Berea experiment and the 30-60 proppants used in the shale experiment. Results show lower permeability for the 30-60 proppant, as expected because of its smaller size. The 20-40 Berea results exhibit stress-independent permeability up to larger loadings, which is likely caused by the use of Berea versus shale at the walls and also the bulk versus monolayer packing geometry. All permeability results from our work are less dependent on applied stress than what is reported by earlier experimental work from the manufacturer (Palisch et al., 2007), until reaching stresses at which proppant particles start to crush.

Figure 12: Comparison of permeability predicted from FEM simulations and experimental results from vendor of both bulk proppants and monolayer of proppants at each loading stress.

4 Summary and conclusions

We have presented results from XCT imaging and image-based modeling that allow quantitative analysis of the impacts of loading on the proppant packing structure, pore space morphology, and flow properties.

For the bulk proppant contained between Berea sandstone faces, the XCT images captured structural changes (e.g. arrangement, embedding) for different loading stresses and failure of proppants at the highest loadings stresses. These results are consistent with other studies that

1 indirectly measured these changes. Flow simulations showed that the reduction of high velocity
2 was due to elimination of the largest flow channels, which in turn led to a more uniform velocity
3 field.

4
5 For the monolayer proppant placed between shale samples, proppant embedment was much more
6 pronounced at high loading stress. This caused a reduction of the fracture width and a
7 corresponding loss of fracture conductivity. As loading stress increased, narrowing of the main
8 flow channels led to a more uniform velocity field.

9
10 The two image-based simulation approaches used here, FEM and LBM, predicted very similar
11 permeabilities within the applied loading stresses. Finally, it is noteworthy that the permeability
12 was essentially independent of loading at the lower stresses (below 12kpsi or 83MPa). This
13 result differs from the manufacturer's data, which shows a correlation between loading and
14 permeability over the entire range.

15
16 The images used in this study can be further used to simulate flow from the matrix into the
17 fracture to understand skin effects, compaction of matrix pores, and effects of heterogeneity in
18 the proppant pack. In addition to the environment studied in this paper, it would be valuable to
19 understand how various fluids (e.g. oil, brine) affect the proppant arrangement and permeability
20 reduction under increasing loading stress.

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22
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7 Supplementary Information

7.1 Shale-proppant computational domain

Figure SI. 1: Computational domain of shale-proppant system: proppant monolayer between two shale cores.

7.2 Berea-proppant mesh

Figure SI. 2: Unstructured tetrahedral mesh generated from bulk proppant segmented 3D image at 0 psi. Note: only a small section of the domain (~1.2mm or 100 voxels) is shown here. Approximately 0.15 elements per voxel were generated at each loading stress. The commercial software Avizo was used to create unstructured mesh.

7.3 Lattice Boltzman method

The LBM equation with streaming and single velocity relaxation operator (LBGK) collision is

$$f_{\alpha}(x + e_{\alpha}\Delta t, t + \Delta t) = f_{\alpha}(x, t) - \frac{f_{\alpha}(x, t) - f_{\alpha}^{eq}(x, t)}{\tau} \quad (6)$$

where e_{α} are directions of particle and equilibrium distribution functions, f_{α}^{eq} , is

$$f_{\alpha}^{eq}(x, t) = w_{\alpha} \rho(x, t) \left[1 + \frac{e_{\alpha} \cdot u}{c_s^2} + \frac{(e_{\alpha} \cdot u)^2}{2c_s^4} - \frac{u^2}{2c_s^2} \right] \quad (7)$$

where w_{α} are weight factors specific to different directions, $c_s = 1/\sqrt{3}$ is the sound speed in the fluid, u is the velocity of the fluid, and ρ is the density of the fluid.

In LBM, positions of particles are limited to nodes of a lattice with equal spacing. In this work, the D3Q19 model is used. Velocity directions of a particle on a typical 3D lattice node is shown in Figure SI. 3.

Figure SI. 3: Velocity directions of a particle on a typical 3D lattice node.

Velocity vectors for this model are described below,

$$e_{\alpha} = \begin{cases} (0,0,0) & \alpha = 0 \\ (\pm 1, 0, 0), (0, \pm 1, 0), (0, 0, \pm 1) & \alpha = 1, 2, 3, 4, 5, 6 \\ (\pm 1, \pm 1, 0), (\pm 1, 0, \pm 1), (0, \pm 1, \pm 1) & \alpha = 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18 \end{cases} \quad (8)$$