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Key Points:

- We study hydromechanical coupling mechanisms in granular fault gouge undergoing particle rearrangements and fluid flow during failure
- Fluid flow and the spatiotemporal distribution of effective pressure affect particle arrangement
- Comparison of dry versus fluid-saturated cases shows that fluids tend to stabilize shear and increase the recurrence time of slip events

Supporting Information:

- Supporting Information S1

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On the micromechanics of slip events in sheared, fluid-saturated fault gouge

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Abstract We used a three-dimensional discrete element method coupled with computational fluid dynamics to study the poromechanical properties of dry and fluid-saturated granular fault gouge. The granular layer was sheared under dry conditions to establish a steady state condition of stick-slip dynamic failure, and then fluid was introduced to study its effect on subsequent failure events. The fluid-saturated case showed increased stick-slip recurrence time and larger slip events compared to the dry case. Particle motion induces fluid flow with local pressure variation, which in turn leads to high particle kinetic energy during slip due to increased drag forces from fluid on particles. The presence of fluid during the stick phase of loading promotes a more stable configuration evidenced by higher particle coordination number. Our coupled fluid-particle simulations provide grain-scale information that improves understanding of slip instabilities and illuminates details of phenomenological, macroscale observations.

1. Introduction

Fault gouge is produced by wear and accumulates within the fault offset. The gouge zone evolves via brecciation of the wall rock and comminution of the constituent materials. Earthquakes occur within fault gouge and at the boundaries between gouge and wall rock; hence, it is important to understand stick-slip dynamics and the processes by which elastic energy accumulates, during the interseismic period, followed by sudden release [Brace and Byerlee, 1966; Johnson *et al.*, 1973; Marone *et al.*, 1990]. The dynamics of such stick-slip instabilities have been studied in laboratory experiments and in numerical simulations for dry fault gouge [Scholz *et al.*, 1972; Marone *et al.*, 1990; Marone, 1998a, 1998b; Mair *et al.*, 2002; Anthony and Marone, 2005; Johnson and Jia, 2005; Mair and Hazzard, 2007; Johnson *et al.*, 2008, 2012; Ferdowsi *et al.*, 2013; Johnson *et al.*, 2013; Ferdowsi, 2014; Ferdowsi *et al.*, 2014a, 2014b, 2015].

Fluids play a significant role in altering the characteristics of stick-slip cycles; however, its role is poorly understood, and there are only a few studies in this regard [Scuderi *et al.*, 2014, 2015a; Scuderi and Collettini, 2016]. Contact strengthening and evolution of friction are thought as the most important influences of fluids on the stick-slip dynamics of granular fault gouge. In a fully saturated granular fault gouge, researchers have studied the change of permeability [Okazaki *et al.*, 2013; Candela *et al.*, 2014; Scuderi *et al.*, 2015b; Kaproth *et al.*, 2016; Leclère *et al.*, 2016], lubrication effect [Verberne *et al.*, 2014], and change of fluid pore pressure and its effects [Scuderi *et al.*, 2015a]. It is shown in experiments that the fluid pore pressure can cause triggered seismicity [Scuderi and Collettini, 2016]. Under low confining pressure, a strengthening behavior of fluid has been observed in recent experiments in submerged granular flows [Koivisto and Durian, 2017]. Progress in numerical modeling allows us to better understand the physics of granular media in grain scale [e.g., Dorostkar and Mirghasemi, 2016] and, specifically, the mechanisms at play in fluid-saturated granular fault gouge [e.g., Dorostkar *et al.*, 2017]. Numerical modeling allows us to study the same samples in dry and saturated conditions. Moreover, we can identify the effect of granular arrangements on the stick-slip behavior and extract microscale information before and during slip event and perform parametric studies of the most important parameters. In the simulations, we can also explicitly study the mechanical (e.g., change of fluid pore pressure and fluid-particle interaction) or chemical (e.g., pressure solution and frictional healing) effects of fluids on the stick-slip behavior. An important phenomenon during stick slip of granular porous media is the occurrence of

a 3-D fluid flow that is not well understood in experiments and previous numerical studies for spontaneous (not triggered) slip events [e.g., *Goren et al.*, 2010, 2011]. The use of numerical modeling provides a better understanding of the effect of fluid flow on macroscopic and grain-scale stick-slip behavior. The particle motion, their interaction forces, the details of fluid flow affecting particles, and their influence on the macroscopic behavior can be quantified in numerical simulations, as is applied for studding the fluid injection in a frictional layer and consequent induced seismicity [*Miller et al.*, 1996; *Rozhko*, 2010; *Aochi et al.*, 2014].

In this paper, we report results of stick-slip dynamics in a fluid-saturated fault gouge and compare it with dry condition. We use 3-D discrete element method simulations coupled with computational fluid dynamics (CFD-DEM) and extract grain-scale information in order to better understand the hydromechanical effects of fluid flow on the characteristics of a slip event. We present microscale information of a representative stick-slip cycle, selected based on our previous statistical analysis of a large number of slip events [*Dorostkar et al.*, 2017].

2. Methods

We used the discrete element method (DEM) coupled with computational fluid dynamics (CFD) and 3-D granular particles to investigate dry and fluid-saturated fault gouge [*Dorostkar et al.*, 2017]. In the DEM, the trajectory of Lagrangian solid particles is tracked by solving the equations of motion. Particle-particle interactions in the normal direction obey nonlinear Hertzian contact via the soft sphere method, which allows overlap between particles [*Hertz*, 1882; *Di Renzo and Di Maio*, 2004]. The tangential force is limited by Coulomb friction.

A two-way CFD-DEM simulation procedure is applied to describe the particle-fluid interactions. We use unresolved CFD-DEM, where each CFD cell contains several particles and an interstitial fluid between grains is not considered [*Goniva et al.*, 2012; *Kloss et al.*, 2012]. The coupling is considered by the modified Navier-Stokes equations taking into account the volume fraction occupied by particles as well as momentum exchange between particles and fluid. In addition, drag forces, pressure gradient forces, and viscous forces are summed with particle-particle interaction forces (in DEM) to incorporate the effect of the surrounding fluid on particle motion [*Zhou et al.*, 2010]. The momentum exchange includes drag forces between fluid and granular particles. We remark that we do not use lubrication forces in our CFD-DEM approach and keep the particle friction coefficient in dry and wet conditions constant. We use the Koch-Hill drag correlation appropriate for intermediate porosities as is the case in our study [*Koch and Hill*, 2001].

The granular layer (Figure 1) is confined in the z direction with two corrugated plates, which enhance shear within the gouge layer similar to laboratory experiments and tectonic fault zones [*Marone*, 1998a]. For gouge particles, periodic boundaries are applied in the x direction and frictionless walls are used in y direction. The sample size is $11 \times 1.5 \times 0.8 \text{ mm}^3$, sufficiently large to have proper 3-D particle interactions [*Ferdowsi et al.*, 2013; *Ferdowsi*, 2014]. Gouge particles have a polydispersed size distribution from 45 to 75 μm , consistent with laboratory experiments that exhibit stick-slip failure [*Scuderi et al.*, 2015a]. We conducted a series of trial runs to identify the confining stress and shear velocity that result in stick-slip dynamics. Normal load condition of 10 MPa (effective stress, supported by solid particles), close to that employed in the experimental studies we are interested in simulating [*Scuderi et al.*, 2014; *Scuderi et al.*, 2015a], and shear velocity of 0.6 mm/s are chosen.

The description of material properties and simulation setup is given in Table 1. Gouge layers are generated by randomly adding particles of the chosen size distribution. The granular layer is then confined, and the bottom plate is moved in the x direction to impose shear while holding the normal load constant.

After shearing sufficiently to develop steady state stick-slip dynamics, we introduce fluid at the onset of a stick-slip cycle everywhere in the sample at the same time with a fixed homogeneous density. The addition of fluid is a numerical procedure, and no change in position or additional force is imposed on particles. Pressure inlet/outlet boundary conditions (fixed value pressure equal to zero, nonperiodic) are considered for the left and right sides of the layer (x direction). Impermeable no-slip boundary conditions are applied to the other four surfaces (top, bottom, front, and back). We use the open source software LIGGGHTS [*Kloss et al.*, 2012] for the DEM solver, OpenFOAM [*Weller et al.*, 1998] for the CFD calculations, and CFDEMcoupling [*Goniva et al.*, 2012] to couple the two models. Details of the CFD cell size, coupling interval, and stability criteria are given in the supporting information.

Figure 1. The granular fault zone consists of 7996 spherical particles with a polydispersed size distribution ranging between 45 and 75 μm . The upper and lower boundaries of the layer are driven by corrugated plates that impose normal and shear load. Frictionless walls are located at the front and back of the layer. Periodic boundaries are applied in the x direction.

3. Results

Figure 2 shows representative data for the friction coefficient (Figure 2a), particle kinetic energy (Figure 2b), and relative thickness change (Figure 2d) for gouge layer sheared under dry and saturated cases. The macroscopic friction coefficient is the ratio of shear force divided by the normal force. The particle kinetic energy consists of both translational ($\frac{1}{2}m_p v_p^2$ where m_p and v_p are the particle mass and velocity) and rotational ($\frac{1}{2}I_p \omega_p^2$, where I_p and ω_p are moment of inertia and angular velocity of particle) components summed over all particles. The relative thickness change is computed as the difference of instantaneous and average thickness (over the entire simulation time) normalized by the average thickness. Figure 2c shows the fluid kinetic energy for the saturated case (computed as $\frac{1}{2}m_f u_f^2$ where m_f and u_f are the fluid mass and velocity). The fluid is added at $t=0$, indicated by arrows in Figure 2.

Our simulations of stick-slip failure under dry and saturated conditions (Figure 2) show that frictional strength increases nonlinearly, reaching a maximum and then dropping suddenly during failure. During the stick phase, elastic energy is stored in the granular layer, and a portion is released as particle kinetic energy during slip, as manifested by the sharp spike in Figure 2b. During the stick phase, the granular layer dilates, whereas during failure the gouge layer compacts, i.e., a decrease in layer thickness.

The friction coefficient during the stick phase of saturated and dry cases follows a similar curve until slip. However, for saturated conditions slip event (SE_{sat}) happens later and the stress drop is larger compared to dry conditions (SE_{dry}). We also observe an increase in recurrence time of particle kinetic energy release and drop in layer thickness. The released particle kinetic energy and drop in layer thickness are larger for saturated compared to dry conditions.

From Figure 2c, we see that the occurrence of SE_{sat} is associated with an increase in fluid kinetic energy. The red inset in Figure 2c shows the fluid kinetic energy fluctuations during the stick phase due to particles

Table 1. Simulation Properties

Property	Value	Property	Value
Particle density	2900 kg/m ³	Particle radius	45–75 μm
Number of particles	7996	Fluid density	1000 kg/m ³
Particle Poisson ratio	0.25	Fluid viscosity	1e ^{−3} Pa s
Particle Young's modulus	65 GPa	CFD time step	10 ^{−7} s
Particle friction coefficient	0.1	DEM time step	10 ^{−9} s
Particle restitution coefficient	0.87	Coupling interval	10 ^{−6} s
Sample size	11 × 1.5 × 0.8 mm ³	Number of CFD cell	1760

Figure 2. Characteristic behavior of a stick-slip cycle with constant shear velocity of 0.6 mm/s and normal load of 10 MPa for dry and saturated models. SE_{dry} and SE_{sat} mark the major slip events (SE) in dry and saturated cases, respectively. In horizontal axis, zero denotes the moment that fluid is introduced to the system for saturated model (marked by arrows). (a) Time series of friction coefficient, (b) particle kinetic energy, and (c) fluid kinetic energy for saturated model. The red inset shows fluid kinetic energy during the stick phase and has the same units as main panel axis. (d) Relative thickness change and (e) the average coordination number.

rearrangement or microslips. This inset shows that the fluid kinetic energy increases 6 to 8 orders of magnitude during the slip event. In Figure 2e, the average coordination number is shown. The coordination number is calculated in the same way for dry and saturated systems and represents number of contacts per particle (two particles are in contact if the distance between their centers is smaller than the sum of particle radii). This panel shows that introducing fluid, the coordination number increases and stays higher on average. The fluctuations in the coordination number are associated with fluid motion and particle rearrangement.

In Figure 3a and 3b, we present the distribution of particle kinetic energy over the middle portion of the specimen. This portion is found to be representative of the granular layer. The distribution shows domains with high particles kinetic energy (KE patches), both for SE_{dry} and SE_{sat} . We observe that the KE patches for SE_{dry}

Figure 3. (a and b) Distribution of kinetic energy of particles for the major slip event from Figure 2: (a) dry and (b) fluid-saturated cases. (c) Normalized particle-fluid interaction forces from fluid on particles. The value of particle-fluid interaction forces is normalized by the average value calculated for all particles (2.17×10^{-7} N). (d) Fluid velocity field, (e) particle velocity field, and (f) porosity change in fluid-saturated model.

are more localized in the center of the specimen, while the KE patches for SE_{sat} are extended over large parts of the specimen, meaning that in the saturated case more particles are mobilized during slip. Figure 3c shows that the normalized particle-fluid interaction forces (normalized by the average value over all particles) are spread over larger zones, which are approximately coincident with the domains of high KE. Figures 3d and 3e show the fluid and particle velocity field for SE_{sat}, where the color bar represents the magnitude of velocity and the arrows show the direction of velocity vector. We observe that fluid flow during slip is characterized by high fluid velocities, which are found to be more than 2 orders of magnitude higher than the fluid velocity during the stick phase. The fluid velocity during the stick phase is around 0.06 cm/s, which is close to driving plate velocity. We remark that the average particle Reynolds number (calculated for fluid velocity with respect to particles) during the stick phase is around 0.004 and for slip events ranges between 1 and 2.

Figure 4. (a) Average drag force and (b) average pressure gradient force. These values are averaged over the height and depth of the sample (y and z directions in Figure 1) for the major slip event in the fluid-saturated model marked in Figure 2.

A qualitative comparison of the zones with high KE, high fluid-interaction force, and high fluid flow (Figure 3) shows that these domains are approximately coincident. This means that there is a strong correlation between the occurrence of particle movement, fluid flow, and particle-fluid interactions. We also observe in Figure 3f that the regions of high fluid flow show small changes in porosity, whereas regions of porosity increase are juxtaposed with zones of consolidation.

To better understand the origin of the particle-fluid interaction forces, we determine the drag force and pressure gradient force along the domain length averaged over the depth and height of the sample. Figure 4 shows that drag force is several orders of magnitude higher than the pressure gradient force. These high values of drag force on particles are caused by the high fluid velocities during slip as observed in Figure 3d.

4. Discussion

We observed that the presence of fluid in a granular fault gouge increases stick-slip recurrence time and results in an increase of macroscopic friction drop, particle kinetic energy, and layer compaction during stick-slip failure (Figure 2). Given that the shear velocity and the shear stress are the same in the dry and saturated cases, a longer stick phase will lead to more storage of energy, followed by a larger release of energy during slip in the saturated case. This finding is in line with our previous statistical study on a large number of slip events, where we showed that the presence of fluid increases, on average, the recurrence time between events [Dorostkar *et al.*, 2017]. In this study, we showed that the presence of fluid in the granular layer allows rearrangement of particles reaching a more stable configuration with higher coordination number. The correlation between fluctuations in coordination number and fluid kinetic energy in fluid-saturated case witnesses this fact. Experimental observations also support our results that the fluid can stabilize the granular fault gouge and increase the recurrence time [Higashi and Sumita, 2009; Yamashita, 1999].

Another key finding is the striking increase of fluid kinetic energy and fluid velocities at slip, as seen in Figures 2c and 3d, respectively. These high fluid velocities are explained by the fact that the granular system undergoes rapid particle rearrangements at slip time, causing the fluid to move due to momentum exchange between particles and fluid. This momentum exchange is driven by drag forces between fluid and particles, as shown in Figure 4a. The high velocity of fluid flow in turn increases particle motions and their kinetic energy by drag forces, as seen in Figure 3b. The connection between these observations explains the high spatial correlation of patches of high KE, zones of high particle-fluid interactions, and fluid velocity, as shown in Figures 3b–3d, respectively. These mechanisms lead to growth of the size of the KE patches showing that a larger portion of granular layer is involved in the failure process. We note that as a result of these coupled mechanisms, also, the local porosity will change, although these changes are found to be rather small. We also mention that in our previous statistical analysis of a large number of slip events [Dorostkar *et al.*, 2017], it was found that the drag forces between fluid and particles are the primary driving forces leading to an increase of particle kinetic energy. This was demonstrated by showing that when we turn off the drag forces, the statistical distributions of particle kinetic energy for dry and saturated cases become identical. All

these observations show the important impact of fluid flow on the characteristics of a slip event. Our findings are in agreement with experimental observations, where the role of fluid pressure was also analyzed [Scuderi *et al.*, 2015a; Scuderi and Collettini, 2016]. In the laboratory experiments, total fluid pressure composed of both static and dynamic pressures, measured by pressure gauges, was found to increase during slip [Scuderi *et al.*, 2015a]. Although these experiments and our simulations are not completely similar, especially regarding boundary conditions, we might hypothesize that the increase in total pressure can be attributed to the increase in dynamic pressure. We showed indeed that the dynamic pressure, also called velocity pressure, which is defined as the fluid kinetic energy per volume, will increase during slip. In our simulations, the average pore pressure is very small (50–100 Pa) during the stick phase, whereas the local dynamic pressure can reach to 5–15 kPa depending on the event size close to that of experiments with the same confining stress [Scuderi *et al.*, 2015a].

5. Conclusions

We conducted 3-D CFD-DEM simulations for fluid-saturated granular fault gouge. We report grain-scale results of a characteristic stick-slip cycle for dry and fluid-saturated cases. Our grain-scale observations for a representative stick-slip cycle complement our macroscale observations and also are consistent with our previous statistical analysis using large number of slip events. The main findings of this research are summarized as follows:

1. The presence of fluid allows particle rearrangement reaching to a more stable configuration evidenced by higher coordination number in fluid-saturated case compared to dry case.
2. The release of particle kinetic energy during slip is higher in the saturated system, in contrast to the dry system, which is seen by more of the granular volume participating in failure process in saturated case.
3. The spatial correlation of regions with high fluid velocity, particle-fluid interaction, and particle kinetic energy during slip provides grain-scale evidence that the mechanisms of particle rearrangements, fluid velocity, and particle-fluid interaction force are strongly coupled phenomena.
4. The high velocity of flowing fluid during slip event, caused by particles rearrangement, results in an increase of drag force on particles leading in turn to a high particle kinetic energy as well as an increase in fluid dynamic pressure.

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