ABSTRACT

A fundamental property for porous media is the relationship between macroscopic physical and petrophysical properties and the morphology or shape of individual grains. Although it is widely accepted that grain anisotropy can affect physical and petrophysical properties of porous media, the exact relationship is not well understood because of the difficulty of separating grain shape effects from those due to other textural properties of clastic rocks, such as grain size, sorting, roundness, and packing. We develop and successfully test a new synthetic pore-scale model to represent clastic rocks with variable grain-size distributions and ellipsoidal grain shapes. The model also includes the structural effects of compaction and cementation.

Numerical simulations consider four grain packs with equal grain size but different grain aspect ratios. Results indicate that the calculated permeability depends on grain shape. Grain interaction and rearrangement during sedimentation and compaction cause the long axes of ellipsoidal grains to preferentially align with the horizontal plane perpendicular to the applied overburden stress. Important observed effects on permeability include: (1) after grain sedimentation, ellipsoidal grain packs exhibit a lower permeability in the vertical direction than in the horizontal directions, while permeability of spherical grain packs shows the opposite behavior, and (2) during compaction, permeability anisotropy remains in sphere packs, but disappears in ellipsoid packs due to the combined effects of compaction and preferential grain orientation. At equal porosity, the grain pack with the highest grain aspect ratio exhibits the highest permeability, which is consistent with experimental observations (Fraser, 1935).

Because of limitations of the algorithm used to calculate electrical conductivity, we did not observe significant anisotropy effects on formation factor due to grain shape. It was also found that increasing the aspect ratio of grains decreases the time of magnetic relaxation due to fewer grains and, therefore, smaller surface area in equal-porosity grain packs.

INTRODUCTION

Microstructure of sedimentary rocks has a substantial influence on macroscopic physical properties such as electrical conductivity, elastic moduli, relaxation times, permeability, and heat capacitance. The relationship between rock geometric microstructure and physical/petrophysical properties is an open fundamental problem whose solution is important to many applications ranging from oil and gas production to polymer physics and material science (Jin et al., 2006).

Petrophysical properties of porous media containing solid and fluid components with varying physical properties depend not only on the volumetric fractions of the constituents, but are also sensitive to the geometry of boundary surfaces between them (Sen et al., 1981). Boundary-surface effects are usually not considered when formulating macroscopic empirical laws or effective-medium responses. For example, the widely used Kozeny-Carman relationship and its modifications are derived from Poiseuille's equation, which is valid for laminar viscous flow in straight, non-communicating uniform tubes (Xu and Yu, 2008). Archie's equation (Archie, 1942) relates electrical resistivity of reservoir rock to its porosity and water saturation with no specific textural information about grain surfaces and topology of immiscible-fluid boundaries. Surface morphology also plays a crucial role in magnetization relaxation processes that govern NMR measurements (Jin et al., 2009).

Surface morphology of natural clastic sediments is largely dependent on its five textural properties: grain sizes, sorting, shape, roundness, and packing (method of deposition) (Fraser, 1935; Beard and Weyl, 1973). For example, poorly sorted grains generally have closer packing and lower porosity across a wide range of grain
sizes, as fine grains tend to fill the void space between large grains. Well-rounded grains with high sphericity should pack with a minimum of pore space. Likewise, as angularity increases and the shape of clastic grains departs from that of a perfect sphere, pore space should increase depending, of course, on grain fabric and/or orientation (Beard and Weyl, 1973). Packing is difficult to isolate from other textural parameters, and is, therefore, most difficult to measure and study with respect to its influence on petrophysical properties of natural sandstones. Using the ideal spherical shape of grains, Jin et al. (2008) numerically investigated the effect of packing on the pore space geometry and absolute permeability of granular porous media.

The effect of grain shape on the petrophysical properties of clastic rocks is not well understood because of paucity of laboratory data. Only a few attempts have been made to account for the influence of grain anisotropy on the macroscopic properties of porous media (Sen, 1981, 1984, Mendelson and Cohen, 1982, Kenyon, 1984, Coelho, et al., 1997). Wyllie and Gregory (1953) measured the formation factor and porosity for grains of various shapes separately. They found that the formation factor of an unconsolidated aggregate of grains is a function of the average shape of grains constituting the aggregate (Sen, et al., 1981). Atkins and Smith (1961) showed in their laboratory tests that the magnitude of $m$ in Archie’s law $F = \phi^m$ depends on the shape of individual grains in the system; it increases as grains become less spherical. This behavior was confirmed by Jackson et al. (1978) in their laboratory investigation. They further showed that variations in grain size and grain size distribution appeared to have little effect on the Archie’s cementation exponent.

For natural sands it would be difficult to separate the effects of grain shape from those due to grain size, sorting and roundness. This is particularly true for grains of low sphericity because of the difficulty of obtaining irregularly shaped grains of the same size. It is also extremely difficult, if not impossible, to study experimentally the packing structure of granular media consisting of different grain shapes and to quantify directly the effect of interactions among individual grains on the bulk behavior of the system (Cundall and Strack, 1979, Yang et al., 2002). Therefore, numerical simulations have become an attractive alternative for elucidating underlying mechanisms of granular systems from the grain scale.

Previous works linking grain geometry with physical/petrophysical properties other than for spherical grain packs are scarce. Almost all pore-level studies to date have focused on or based on spherical grains (Roberts and Schwartz, 1985; Bryant, et al., 1993; Bakke and Øren, 1997; Jin, et al., 2003; Gladkikh, et al., 2008). The effect of grain anisotropy on physical/petrophysical properties remains largely unexplored. Rock grains are typically far from perfectly spherical and are often elongated. Adequate grain-shape modeling is important to quantify effective-medium and petrophysical properties of granular porous media.

The present study is concerned with the way in which grain shape affects the petrophysical properties of porous media. As a first step in the attempt to analyze the effect of grain shape on rock petrophysical properties, we introduce a new approach based on the distinct-element method to represent sands with variable grain-size distributions and ellipsoidal grain shapes. Ellipsoids are used because their geometric shapes are close to those of sand grains. Furthermore, ellipsoids have the degrees of freedom necessary to simulate different grain shapes. They are relatively easy to handle mathematically, and do not exhibit the geometrical singularities of polyhedra. Ellipsoids also provide an opportunity to investigate the effect of grain shape, anisotropic fabric and their potential effects on the petrophysical properties of sands.

The paper is organized as follows: We first introduce the grain contact model used to approximate the mechanical behavior in the contact region of two ellipsoidal grains. The scheme of finding the grain contact is briefly detailed. We then describe our simulations of geological processes of grain sedimentation and compaction. Finally, we numerically generate four grain packs with the same grain size but different grain aspect ratios in a way which allows the grain shape to be investigated in isolation. Immediately after sedimentation, we simulate the compaction process in stages to reduce the porosity of grain packs. Absolute permeability, formation factor and NMR response of the constructed grain packs are assessed at discrete stages during the compaction process.

**GRAIN CONTACT MODEL AND DETECTION**

Granular media are composed of a large set of distinct grains that move relatively from one another and interact only at contact points. The bulk behavior of the system is determined by grain-grain interactions. Motion of an individual grain in the multi-grain system is determined by the resultant force and moment acting upon it. Grain motion can be described by the following Newton’s equations of motion (Jin et al., 2003; Jin, 2006):
Here, $x_i$ and $\theta_i$ ($i=1, 2, 3$) are the Cartesian coordinates of the grain's centroid and the angles of rotation about the centroid, respectively; $t$ is time; $m$ and $I$ are the mass and moment of inertia, respectively; and $F_i$ and $M_i$ are the components of the resultant force and moment, respectively, acting upon the grain. For a spheroidal grain (three principal semi-axes $R_a \neq R_b = R_c$), its rotational kinematic equations are decoupled and are amply described in the open technical literature (Lin and Ng, 1997).

When two grains collide, the resulting deformation causes the contact force $F_c$ (Fig. 1a). We model the grain contact region as a dash-pot, spring and slider system (Fig. 1b). To find the existence of overlap (or deformation) between ellipsoidal grains and determine its magnitude and location (including the position, normal and tangential directions of the contact plane), we use the geometric potential concept described in the literature (see, for instance, Perram and Wertheim, 1985, Ting, 1992, and Lin and Ng, 1997).

$F_i = m \frac{d^2x_i}{dt^2}$
$M_i = I \frac{d^2\theta_i}{dt^2}$

$U^p$, which is used to calculate the magnitude of the normal contact force between grains.

The net force acting on a grain is the vector sum of the following components: (1) body forces, from gravity and other external forces acting on the grain; (2) contact forces at contact points among grains or between a grain and the pack boundary; and (3) damping forces, resulting from the movement of a grain in a viscous fluid, or its non-ideal collisions with other grains or pack boundaries. Details about the method used to calculate the above forces can be found in the literature (see, for instance, Cundall and Strack, 1979, Lin and Ng, 1997, Jin et al., 2003, and Jin, 2006).

**SIMULATION OF GRAIN SEDIMENTATION AND COMPACTION**

In general, sedimentary rocks form by deposition of grains followed by compaction and cementation. The last two processes determine the final pore space geometry and connectivity. In this study, we focus our attention to both grain sedimentation and compaction processes. We simulate these two dynamic processes with the distinct element method (DEM) proposed by Cundall and Strack (1979). The method simulates the dynamic interactions of discrete grains honoring Newtonian mechanics. Most of the concepts described below are similar to the method proposed by Jin, et al. (Jin et al., 2003, and Jin, 2006), the difference being that our implementation is based on ellipsoidal grains.

**Sedimentation**

The sedimentation process is modeled using a “generate-settle” algorithm (Jin, et al., 2003, Jin, 2006). We first generate a predetermined number of grains according to a given grain-size distribution function. To mimic the stochastic nature of grain deposition, the generated grains are randomly placed one-by-one at randomly selected positions in the packing space according to some probability distribution function (Fig. 2a). No grain is allowed to contact with any other grains or boundaries during the placement of grains. Moreover, grains stay at their original positions before all grains settle in their own positions.

Once all grains are placed, they begin to settle down under gravity and other external forces (Fig. 2b). Grains can translate and rotate. They may collide with neighboring grains or boundaries, and bounce in arbitrary directions. This dynamic process comes to an end when all grains reach their stable positions with an essentially zero velocity as a result of the damping effect of energy dissipation (Fig. 2c).
Compaction
Diagenesis is the process that turns an unconsolidated grain (sediment) packing into a solid rock. The first stage of the process is compaction. Compaction occurs as the weight of the overlying layers increases. It forces the grains to move closer together, thereby reducing pore space and pressing out some of the contained air and water.

We simulate the compaction process by applying a simulated overburden pressure, and by moving the wall at the top of a grain packing downward at a constant strain rate (Fig. 2d). This strategy simulates the effect of the overburden layers that apply stress on the reservoir. In compaction modeling, grains may interpenetrate, similarly to pressure dissolution of grain contacts in natural rocks (Fig. 1a). We assume that the volume of grain interpenetration is dissolved under pressure, and transported out of the system by the fluid. In addition, compaction may result in the decrease of grain size due to the interpenetration. However, the change of the grain size is small and can be ignored in the simulation.

NUMERICAL RESULTS AND ANALYSIS
In this section, we apply our numerical simulation methods to construct four ‘simple’ models of grain packs. The four grain packs have the same grain size but different aspect ratios. The grain size is defined as the length of the shortest axis of a grain, while the aspect ratio is defined as the ratio of the length of longest axis of a grain to that of its shortest axis. In such a way, we can isolate grain shape from other texture properties and investigate its effect on rock petrophysical properties. Immediately after grain generation, we simulate the processes of grain sedimentation and compaction. The four numerical samples are compacted in stages at which we calculate porosity, permeability, formation factor, and NMR transverse relaxation.

Models of Porous Media
Fig. 3 shows four computer-generated random grain packs with the same grain size $R_b=0.1\,\text{mm}$ (note $R_c=R_b$) but different aspect ratios $R_c/R_b=1.0, 1.5, 2.0, 2.5$, respectively. Uniform grains are randomly placed within the physical domain with the dimension of $6\,\text{mm} \times 6\,\text{mm} \times 12\,\text{mm}$. No grain in the pack is allowed to make contact with other grains or physical boundaries. Orientation of each grain is also generated randomly. The generation process runs until no more grains can be placed into the domain. The total number of generated grains is (a) 19990, (b) 16406, (c) 13981, and (d) 11052, respectively. Fewer grains are generated with a larger aspect ratio.

After grain generation, we simulate grain sedimentation under gravity. Our approach simulates a dynamic process of grain sedimentation, in which grains are allowed to translate, rotate, and rebound. Fig. 4 shows the grain packs after the sedimentation process. We halt the deposition process when either the ratio of the mean unbalanced force on grains in the packing to the mean contact at the grain contacts, or the ratio of the maximum unbalanced force to the maximum contact force meet an a priori criterion (0.01 in this study). This latter condition means that some grains in the pack may not finally reach their physical stable positions.

One observes that in the sedimentation process grains do rearrange themselves to align their long principal axes more or less along the horizontal plane (Figs. 4c and 4d). If a periodic boundary condition were used in the horizontal direction, this preferential orientation would become more obvious, similar to what occurs in nature with elongated grains. Development of the
sedimentation algorithm with periodic boundary conditions is subject of future work.

Fig. 3: Graphical description of four grain packs with the same grain size \( R_a = 0.1 \text{ mm} \) but different aspect ratios: (a) \( R_a/R_b = 1.0 \), (b) \( R_a/R_b = 1.5 \), (c) \( R_a/R_b = 2.0 \), and (d) \( R_a/R_b = 2.5 \), respectively. Mono-size grains are randomly placed without contacts in the confining box with dimension of 6 mm x 6 mm x 12 mm. The number of grains in the packs is (a) 19990, (b) 16406, (c) 13981, and (d) 11052, respectively.

Fig. 5 shows the effect of cubic sample size on the porosity of the four model grain packs shown in Fig. 4. The cubic sample is located at the center of the pack. One observes that the spherical grain pack (Fig. 4a) does not exhibit a lower porosity compared to ellipsoidal grain packs (Fig. 4c-d). It is contradictory to the finding by Fraser (1935) that sand grains of high sphericity should tend to pack with a minimum of pore space and that, as the shape of clastic particles departs from that of a perfect sphere, porosity should increase. Fraser (1935) further indicated that the porosity of the sand pack depends on the fabric or orientation of grains. Similar to our simulations, Man et al. (2005) found in their simulations that ellipsoids can pack randomly more densely than spheres (Donev, et al., 2004).

Fig. 4: Grain packs obtained after simulation of gravity sedimentation for the four grain packs shown in Fig. 3. All grains are located in the low part of the confining box.

Fig. 5 Variation of porosity with cubic sample size for the four grain packs shown in Fig. 4.
In Fig. 5, one observes that porosity fluctuates rapidly when the size of the cubic sample is small, but approaches a constant value with increasing sample size. The porosity of the four grain packs is approximately 41.0%, 39.3%, 39.2%, and 38.8%, respectively. For the mono-sized sphere pack, our porosity is in consistent with the experimental porosity of 40.2% (Wyllie and Gregory, 1955) and the numerical porosity range of 40.0±2.0% (Berryman, 1983, Coelho, et al., 1997). However, it is higher, compared with the porosity value of 36.0% found by Finney in his experiment (Finney, 1968). The difference is due to the fact that we used the force equilibrium in the simulation to determine the final positions of grains in the pack. This force condition means that some grains may not finally reach their physical stable positions. We confirm this by observing that lots of grains in the pack have contacts of less than 4 (See, Fig. 6).

One also observes that the size-related fluctuation in porosity becomes negligible once the length of the cubic sample side exceeds 1 mm. However, in the remaining computation of petrophysical properties, we choose a larger fixed cubic volume with size equal to 2 mm x 2 mm x 2 mm in the center of grain packs. The selection of this size can reduce computational time; however, the simulation result is still representative for the corresponding grain pack (Jin, 2006).

**Coordination Number**

We also calculated the coordination number of grains for the four grain packs immediately after sedimentation and after compaction, respectively. The coordination number of grains is defined as the number of grain contacts that each grain makes in the pack. Fig. 6 displays the coordination number of grains for the four grain packs immediately after sedimentation (shown in Fig. 4). Fig. 7 describes the result after the four packs are compacted in the vertical direction to reduce their porosity from approximately 40.0% to 29.0%. Percentage of grains is the fraction of grains that have a given number of contact points with other grains in the pack.

For grain packs immediately after sedimentation, most of grains have between 3 and 8 contact points (Fig. 6). The average number of contact points is about 5.30, 5.10, 5.31, and 5.32, respectively. They are nearly the same. For a spherical grain pack, its mean value of grain contacts is less than the experimental or simulated limiting value of ~ 6.0 for random close packing of uniform spheres (Jodrey and Tory, 1985; Nolan and Kavanagh, 1992; Yang, et al. 1996). However, it is worth noting that our calculation of mean coordination number also includes grain-boundary contacts. It is expected that grains in the region close to the boundary exhibit fewer contact points. In addition, after sedimentation the packs may not reach complete stable equilibrium.

Compaction reduces sand bulk volume in response to applied stress. Compaction causes grains to be closer to each other, and increases the number of grain contacts. Fig. 7 shows that nearly all grains in the pack have at least five contact points. The average number of grain contacts is approximately 7.55, 7.41, 8.12, and 8.02, respectively.

**Absolute Permeability**

We use a D3Q19 lattice-Boltzmann algorithm (Jin, et al., 2004, 2007b) to simulate viscous flow of the single-phase fluid in the pore space of grain packs. To assess
possible anisotropy of the grain packs, simulations were performed individually for each of the \(x\)-, \(y\)-, and \(z\)-directions. Absolute permeability of grain packs was calculated from the simulated fluid velocity field using Darcy’s equation.

![Diagram](image1)

**Fig. 8:** Effect of compaction on the permeability of the spherical grain pack shown in Fig. 4a. Calculated permeability values in the \(x\)-, \(y\)-, and \(z\)-directions are labeled \(x\), \(y\), and \(z\), respectively.

Fig. 8 shows the calculated absolute permeability at different degrees of compaction for the spherical grain pack (Fig. 4a). Compaction causes anisotropy in the permeability of the grain pack. In Fig. 8, one observes that the calculated permeability is consistently higher in the \(z\)-direction than in the \(x\)- and \(y\)-directions, while it remains approximately the same in the \(x\)- and \(y\)-directions. This behavior is expected because compaction constrains flow channels in the \(x\)- and \(y\)-directions more than in the \(z\)-direction. Permeability anisotropy caused by compaction was also reported in other pore-scale modeling studies (Bryant et al., 1993; Jin et al., 2004).

We note that over larger distances, such as field scales, rock permeability is usually lower in the vertical (bedding-perpendicular) \(z\)-direction than in the horizontal (bedding) \(x\)- and \(y\)-directions. At a scale of a single rock layer, the opposite may be true if the rock grains are close to spherical (Jin et al., 2004). Grains of other shapes (for example, ellipsoid), on the other hand, tend to settle in such a way that the single-layer permeability in the \(z\)-direction is lower than in the bedding directions. This opposite permeability anisotropy, \(i.e\), the permeability in the \(z\)-direction is lower than that in the \(x\)- and \(y\)-directions, is also inferred from our study, as described below.

![Diagram](image2)

**Fig. 9:** Effect of compaction on the permeability of the ellipsoidal grain pack with aspect ratio equal to 1.5 (Fig. 4b). Calculated permeability values in the \(x\)-, \(y\)-, and \(z\)-directions are labeled \(x\), \(y\), and \(z\).

![Diagram](image3)

**Fig. 10:** Effect of compaction on the permeability of the ellipsoidal grain pack with aspect ratio equal to 2.0 (Fig. 4c). Calculated permeability values in the \(x\)-, \(y\)-, and \(z\)-directions are labeled \(x\), \(y\), and \(z\), respectively.

Permeability anisotropy caused by sedimentation and compaction is reduced when ellipsoidal, not spherical, grain shape is used to construct the grain pack. Figs. 9-11 describe the variations of calculated permeability at different degrees of compaction for the three ellipsoidal grain packs (Fig 4b-d). One observes that permeability anisotropy decreases during compaction as the aspect ratio of grains increases. However, this reduction in permeability anisotropy is caused by a more complicated mechanism than that of a spherical grain pack.
After sedimentation, the calculated permeability of the three ellipsoidal grain packs (Fig 4b-d) is smaller in the z-direction than in the x- and y-directions, and no longer equal in the x- and y-directions which, of course, depends on aspect ratio. However, permeability anisotropy of the spherical grain pack exhibits the opposite behavior: nearly equal in the two horizontal directions and slightly higher in the vertical direction (Fig. 8).

The difference in permeability anisotropy due to grain shape can be explained because the grain packing resulting from sedimentation under gravity is anisotropic. Overweight in the vertical direction results in grain interpenetration and reduces the size of flow channels along the horizontal direction, while flow paths along the vertical direction are mostly affected by grain rearrangement during sedimentation. On the other hand, ellipsoidal grains are more likely to rearrange so that their long semi-axes preferentially aligns with the horizontal direction, which makes the flow paths in the vertical direction more tortuous than those in the horizontal direction (Fig. 12a). Therefore, permeability in the vertical direction decreases with respect to that of horizontal directions.

The spatial orientation of grains in the pack can be investigated by visually inspecting cross-sections along the vertical direction through the centers of the grain pack. Fig. 12 shows such cross-sections (Fig. 4d) both immediately after sedimentation and after compaction. In Fig. 12, a circle implies that the long principal axis of the grain aligns along the horizontal direction. For an ellipse in the plot, if its major axis is along or inclined with respect to the horizontal direction, its corresponding grain is also more or less aligned with the horizontal direction. One observes that the interaction between grains during sedimentation and compaction does cause grains to preferentially align along the horizontal direction; compaction makes this preferential orientation more obvious (Fig. 12b).

For grain packs with higher grain aspect ratio, grain interactions and rearrangement play an important role in permeability changes during compaction. On one hand, compaction reduces the permeability in the x- and y-directions faster than in the z-direction. On the other hand, interaction between grains causes grains to preferentially orient along the horizontal directions, thereby causing the permeability to decrease faster in the z-direction than in the other two directions. The combination of these two mechanisms causes the permeability anisotropy to disappear in the first compaction stages for grain packs with aspect ratio of 2.0 and 2.5, shown in Figs. 10 and 11, respectively. However, one can expect compaction to play a more important role in the later compaction stages, whereby permeability anisotropy may once again appear.

Fig. 13 compares the variation of average permeability of four grain packs during compaction. Average permeability is defined as the arithmetic average of the calculated permeability in the x-, y- and z-directions. One observes that for the same value of porosity, the grain pack with the highest aspect ratio of grains exhibits the highest permeability. This result is inconsistent with Fraser’s (1935) finding that as the shape of clastic particles departs from that of a perfect sphere, porosity and permeability in most cases should increase depending, of course, on fabric and/or orientation of grains. Such a behavior is due mainly to
the bridging of pores by grains of lowest sphericity and, hence, looser original packing.

![Graph of Permeability vs. Porosity](image1)

**Fig. 13:** Variation of average permeability with porosity of the four grain packs shown in Fig. 4 during the compaction process. Average permeability is defined as the arithmetic average of the permeabilities calculated in the x, y, and z directions.

**Formation Factor**

We calculate the electrical conductivity of the four grain packs from the simulation of Brownian motion of diffusive particles (called walkers or random walkers) in the porous medium using a random-walk simulation algorithm (Jin, et al., 2007a). This algorithm allows one to model arbitrary media boundaries.

**Fig. 14** shows the variation of the calculated formation factor with different degrees of compaction for the four grain packs. The effect of grain shape on formation factor is negligible. However, such a conclusion should be further confirmed with alternative numerical simulation methods. The random walk simulation technique does not implicitly take into account the effect of medium anisotropy on electrical conductivity because walkers are not required to start at specific points in the pore space (e.g. on specific facets of the grain pack) or to follow preferential directions. In addition, the effective displacement length of walkers is measured without distinction of direction. Because of these latter conditions, the calculated electrical conductivity becomes the effective average of the electrical conductivities along orthogonal directions. It is likely that the preferred orientation of ellipsoidal grains during sedimentation and compaction will cause the porous medium to become electrically anisotropic, thereby causing the formation factor to be direction dependent.

![Graph of Formation Factor vs. Porosity](image2)

**Fig. 14:** Variation of the calculated formation factor with porosity of the four grain packs shown in Fig. 4 during the compaction process.

**NMR Response**

We performed numerical simulations of NMR transverse relaxation in digitized models of grain packs with the random-walk technique (Toumelin, et al., 2007, Jin, et al., 2009), assuming that the porous medium is fully brine-saturated. Simulations assumed a Carr-Purcell-Meiboom-Gill (CPMG) pulse sequence for transverse relaxation measurements with an inter-echo spacing of 1 ms. The value of $T_{2B}$ and of the diffusion coefficient $D_B$ for the bulk brine are chosen as 2800 ms and 2 $\mu$m$^2$/ms, respectively. Relaxivity $\rho$ is arbitrarily selected as 0.005 $\mu$m/ms. Simulations stop if the transverse relaxation time is larger than 2000 ms.

**Fig. 15** compares the simulated magnetization $M(t)$ obtained from the digitized representations of the four grain packs shown in Fig. 4. One observes that transverse magnetization decays faster as the grain aspect ratio $R_a/R_b$ decreases. The difference in decay time is due to different surface areas in the spatially digitized models: surface area decreases with increasing aspect ratio. Surface areas are 196.866 mm$^2$, 180.896 mm$^2$, 172.598 mm$^2$, and 168.788 mm$^2$ for the four grain packs with aspect ratio $R_a/R_b = 1.0, 1.5, 2.0, 2.5$, respectively. Note that the four digitized models have the same bulk volume of 8 mm$^3$ and nearly the same porosity of 40.0%, respectively. The difference in surface area could be explained as follows: grain packs with higher aspect ratio should tend to form looser original grain packs (larger pore space) due to the bridging of grains. Fewer grains with higher aspect ratio are needed to construct grain packs with the same porosity.
Fig. 15: Transverse magnetization response, $M(t)$, of the four grain packs shown in Fig. 4 (immediately after sedimentation). The plot in the upper-right corner is part of the simulated curves and is magnified to show the effect of grain shape on the transverse magnetization response.

However, such a conclusion cannot be generalized without considering the effect of discretization on the surface area of the grain pack (Jin, et al., 2009). It is well known that the process of discretizing an analytically defined surface inevitably leads to errors because a continuous surface is truncated into a finite number of rectangular shapes. For spherical grain packs, spatial discretization of the pore space caused overestimation (about 3/2) of the interface surface area which does not decrease with further reduction of voxel size (Jin, et al., 2009). For ellipsoidal grain packs, the overestimation could be between 1.0 and 1.5, less than that of spherical grain packs. Intuitively, one expects surface relaxation rate of spin magnetism to increase with increasing surface area (due to spatial discretization) since it usually entails a higher probability for magnetic spins to make contact with the boundary in digitized models. Obviously, the different enhancements of surface area in the digitized images could also lead to the difference in decay times shown in Fig 15.

**DISCUSSION AND CONCLUSIONS**

We developed a new synthetic pore-scale model with the distinct-element method to represent clastic rocks with variable grain-size distributions and ellipsoidal grain shapes. This approach simulates the dynamic processes of grain sedimentation and compaction by solving Newton’s equations of motion for each grain in the grain pack. Grains are assumed to be rigid with deformable contacts. Overlap between rigid grains is conceptually interpreted as the approach distance (local deformation) of the contacted grains. Mechanical behavior at the contact region between grains is modeled as a dash-pot, spring and slider system.

The intricate pore space geometry of clastic rocks is the result of a number of factors, which include grain size, sorting, shape, method of deposition, and compaction following deposition. It is very difficult to separate and determine experimentally the influence of these factors on final rock microstructure and associated petrophysical properties. Our ellipsoid-based DEM approach enables one to consider each of these factors separately and evaluate their relative influence and importance on petrophysical properties.

We investigated the effect of grain shape on the micro-geometry and property of sands. Four model grain packs were numerically generated with the same grain size but different grain aspect ratios. Simulations indicate that grains with higher aspect ratio are more likely to rearrange themselves to align their long axes along the horizontal plane (perpendicular to the direction of the applied stress or overburden pressure). This preferred orientation resulted in anisotropy of the microstructure of grain packs, and therefore on anisotropy of macroscopic properties.

Permeability anisotropy (i.e., variation of permeability with direction used in the calculations) was observed in our simulations. After grain sedimentation, the calculated permeability of the spherical grain pack becomes anisotropic: it is approximately equal in the $x$- and $y$-directions, and slightly higher in the $z$-direction. However, for ellipsoidal grain packs, the behavior of permeability anisotropy is different: permeability is smallest in the $z$-direction, while different in the remaining two directions. Permeability anisotropy remains during compaction for the spherical grain pack, but it decreases or disappears completely for ellipsoid grain packs, depending on grain aspect ratio. The reason for this different behavior is that, for spherical grain packs only overburden pressure plays a major role in reducing the size of flow channels in the horizontal directions, while the effect of grain rearrangement is negligible. On the other hand, for ellipsoidal grain packs, grain rearrangement plays a major role in the development of permeability anisotropy during both sedimentation and first stages of compaction, while subsequently overburden pressure becomes more important. Grain rotation, in response to applied stress, results in the preferred orientation of ellipsoidal grains along the horizontal plane. This behavior increases the tortuosity of flow paths in the vertical direction, and therefore causes permeability to decrease in that direction.
The formation factor of anisotropic porous media is direction dependent. However, the random-walk simulation algorithm used in our study to calculate formation factor did not explicitly account for the effect of anisotropy on electrical conductivity of porous media. Modifications are necessary to render the random-walk algorithm sensitive to direction. Our observation of negligible dependence of formation factor on grain shape is due to the fact that the random-walk algorithm implicitly yields an effective average of electrical conductivities along orthogonal directions. Further studies are necessary with random walks initialized at specific facets of the grain pack in order to calculate direction-dependent electrical conductivity. Alternatively, the electrical potential could be calculated by solving Laplace’s equation with separate boundary conditions, one at a time, on grain-pack facets perpendicular to a given orthogonal direction.

We found that transverse spin magnetization decays faster in grain pack with higher aspect ratio of grains, i.e., it decays faster in the spherical grain pack than in the ellipsoidal grain pack. The difference in decay times was found to relate to the larger surface area of the digitized sphere pack. However, this difference was small. It is known that discretizing grain packs into voxel representations increases the surface area of spheres and ellipsoids (Jin, et al., 2009), which may also explain the calculated difference in decay times. Therefore, such a conclusion cannot be generalized without considering the effect of spatial discretization on the surface area of grain packs.

Natural clastic rocks often have grains with very irregular and elongated shapes. It is very difficult to model exact grain shape with numerical simulations. As a first step, we used ellipsoidal grains in our simulation. Although ellipsoids still constitute ideal grain shapes, they provide the degrees of freedom necessary to simulate different grain shapes. Our study is but a first step toward improving the general understanding of the relation between geometric microstructure and petrophysical properties of hydrocarbon-bearing clastic rocks.

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